Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 8, 2023 – 10:29 am GMT

Deposition ID : D_1292128536

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

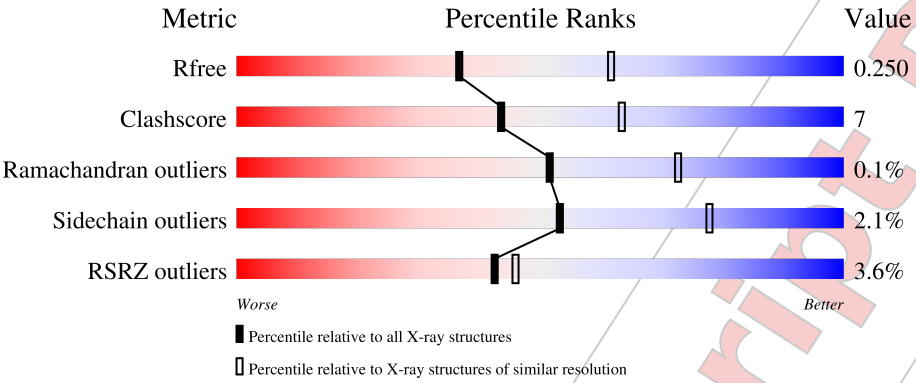
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	3% 82% 17%
2	B	431	6% 82% 17%
3	F	155	% 85% 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8117 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3396	2155	578	638	25	2	7	0

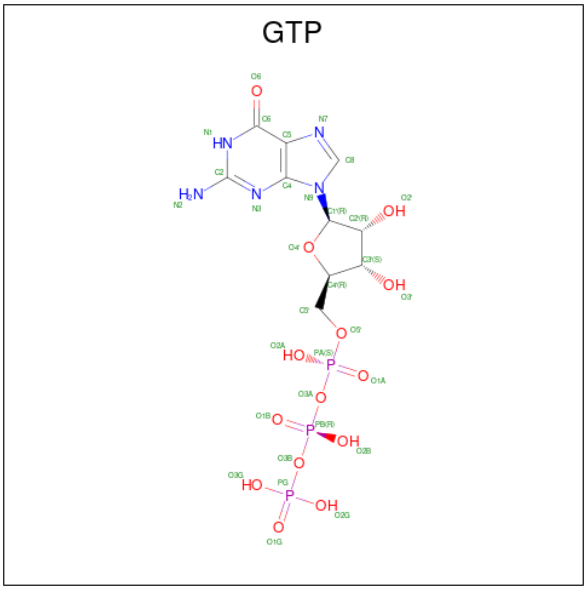
- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	3363	2112	570	654	27	0	2	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	155	1148	724	195	226	3	0	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	X	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	X	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

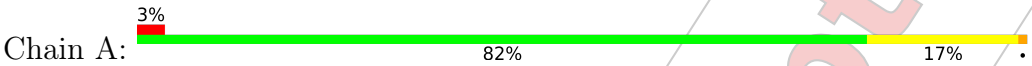
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	145	Total	O	0	0
			145	145		

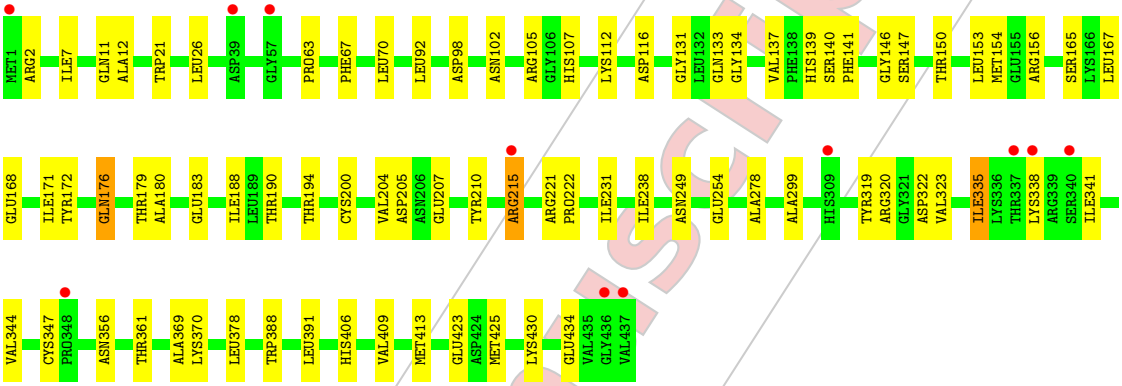
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1:

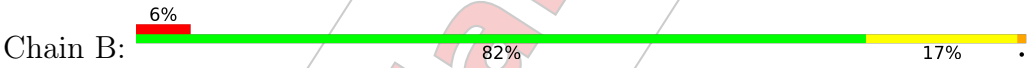
Chain A:

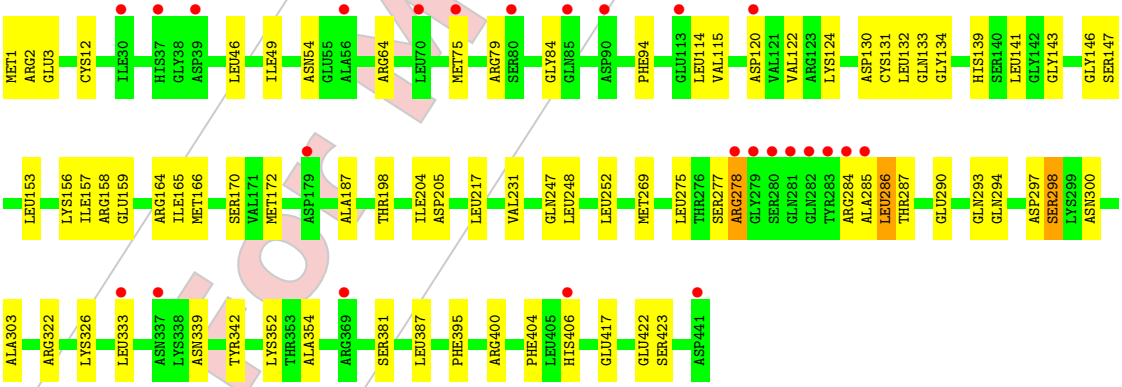




- Molecule 2:

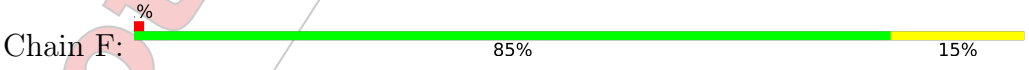
Chain B:





- Molecule 3:

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.47Å 91.19Å 82.70Å 90.00° 96.43° 90.00°	Depositor
Resolution (Å)	13.00 – 2.50 15.01 – 1.91	Depositor EDS
% Data completeness (in resolution range)	92.3 (13.00-2.50) 49.8 (15.01-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.89 (at 1.91Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.185 , 0.241 0.200 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8117	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/3491	0.48	0/4740
2	B	0.27	0/3440	0.48	1/4663 (0.0%)
3	F	0.24	0/1164	0.41	0/1583
All	All	0.27	0/8095	0.47	1/10986 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	114	LEU	CA-CB-CG	5.70	128.40	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	158	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3396	0	3309	44	0
2	B	3363	0	3213	53	0
3	F	1148	0	1145	13	0
4	X	64	0	24	1	0
5	X	1	0	0	0	0
6	S	145	0	0	1	0
All	All	8117	0	7691	105	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:O	1:A:112:LYS:NZ	2.07	0.88
3:F:27:ASP:OD1	3:F:62:ILE:HG13	1.76	0.85
1:A:176:GLN:HE22	1:A:207:GLU:HG3	1.42	0.82
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.54	0.72
2:B:46:LEU:HA	2:B:49:ILE:HB	1.73	0.70
2:B:1:MET:CE	2:B:133:GLN:CB	2.74	0.64
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.80	0.62
2:B:120:ASP:O	2:B:124:LYS:HG2	2.01	0.60
1:A:335:ILE:HG23	1:A:341:ILE:HD12	1.84	0.60
3:F:39:ASP:HB3	3:F:42:ALA:HB2	1.84	0.59
2:B:1:MET:CE	2:B:133:GLN:HB2	2.33	0.59
2:B:1:MET:HE1	2:B:133:GLN:HB2	1.84	0.59
2:B:79:ARG:HA	2:B:84:GLY:HA3	1.85	0.58
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.85	0.58
2:B:406:HIS:CD2	2:B:406:HIS:H	2.21	0.57
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.87	0.56
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.86	0.56
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.88	0.55
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.88	0.55
2:B:1:MET:CE	2:B:133:GLN:HB3	2.36	0.54
2:B:1:MET:HE1	2:B:133:GLN:CB	2.37	0.54
2:B:122:VAL:HG21	2:B:157:ILE:HD11	1.89	0.54
2:B:1:MET:HE3	2:B:133:GLN:HB3	1.90	0.54
2:B:1:MET:HE3	2:B:133:GLN:CB	2.39	0.53
1:A:11:GLN:OE1	2:B:247:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.90	0.53
3:F:133:LEU:HD11	3:F:165:LEU:HD23	1.90	0.53
1:A:2:ARG:HD3	1:A:133:GLN:HG2	1.90	0.53
2:B:54:ASN:OD1	2:B:64:ARG:NE	2.41	0.52
3:F:94:GLU:H	3:F:94:GLU:CD	2.14	0.51
2:B:143:GLY:O	2:B:147:SER:OG	2.25	0.51
1:A:406:HIS:HA	1:A:409:VAL:HG22	1.93	0.51
1:A:140:SER:HA	1:A:171:ILE:HB	1.93	0.51
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.12	0.50
1:A:26:LEU:HB3	1:A:361:THR:HG21	1.93	0.50
1:A:70:LEU:HB2	1:A:98:ASP:HA	1.94	0.49
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.93	0.49
2:B:12:CYS:HB2	4:X:503:GTP:C8	2.47	0.49
2:B:278:ARG:NH2	6:S:117:HOH:O	2.45	0.49
2:B:134:GLY:HA2	2:B:164:ARG:HB3	1.95	0.49
1:A:116:ASP:OD1	1:A:156:ARG:NH2	2.45	0.49
1:A:179:THR:HG21	2:B:247:GLN:HG2	1.95	0.49
2:B:156:LYS:O	2:B:159:GLU:HG2	2.13	0.49
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.94	0.49
2:B:287:THR:HG23	2:B:290:GLU:OE1	2.13	0.49
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.95	0.48
1:A:430:LYS:O	1:A:434:GLU:HG3	2.14	0.48
2:B:3:GLU:OE1	2:B:130:ASP:N	2.47	0.48
2:B:400:ARG:HD2	3:F:112:TRP:CE2	2.48	0.48
2:B:286:LEU:HD11	2:B:294:GLN:NE2	2.29	0.48
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.96	0.47
1:A:215:ARG:HH12	1:A:299:ALA:HB1	1.80	0.47
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.49	0.47
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.96	0.47
1:A:139:HIS:NE2	1:A:168:GLU:OE2	2.43	0.47
2:B:141:LEU:HB3	2:B:187:ALA:HA	1.97	0.47
2:B:2:ARG:O	2:B:133:GLN:NE2	2.38	0.46
1:A:102:ASN:HB3	1:A:105:ARG:HB2	1.98	0.46
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.77	0.46
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.52	0.45
3:F:79:MET:HE2	3:F:111:THR:HG21	1.99	0.45
1:A:249:ASN:HA	1:A:254:GLU:HB3	1.98	0.45
2:B:166:MET:HB3	2:B:198:THR:HA	1.98	0.45
1:A:139:HIS:ND1	1:A:146:GLY:O	2.50	0.45
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.52	0.45
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:ASP:OD1	2:B:298:SER:N	2.50	0.44
1:A:2:ARG:HA	1:A:131:GLY:O	2.17	0.44
2:B:286:LEU:HD22	2:B:286:LEU:HA	1.77	0.44
1:A:137:VAL:HG21	1:A:154:MET:SD	2.57	0.44
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.99	0.44
1:A:154:MET:HG3	1:A:194:THR:HG23	2.00	0.44
2:B:284:ARG:O	2:B:285:ALA:C	2.56	0.44
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.44
2:B:139:HIS:CE1	2:B:170:SER:OG	2.71	0.44
1:A:150:THR:O	1:A:154:MET:HG2	2.18	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.52	0.43
1:A:67:PHE:HB2	1:A:92:LEU:HD23	2.00	0.43
3:F:159:GLU:O	3:F:163:GLU:HG3	2.17	0.43
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.00	0.43
2:B:352:LYS:HD3	2:B:352:LYS:HA	1.87	0.43
2:B:322:ARG:HH11	2:B:322:ARG:HG2	1.83	0.43
3:F:76:ILE:HB	3:F:80:GLY:HA2	2.00	0.43
2:B:404:PHE:CE2	3:F:90:ILE:HD12	2.55	0.42
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.01	0.42
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.02	0.42
2:B:3:GLU:HB3	2:B:64:ARG:CZ	2.50	0.42
2:B:217:LEU:HD13	2:B:277:SER:HB3	2.01	0.42
3:F:121:ALA:HB1	3:F:161:LEU:HD21	2.02	0.42
2:B:115:VAL:HG23	2:B:153:LEU:HG	2.00	0.42
2:B:269:MET:HE3	2:B:381:SER:HB3	2.01	0.42
1:A:320:ARG:HA	1:A:356:ASN:O	2.20	0.41
1:A:434:GLU:HG3	1:A:434:GLU:H	1.68	0.41
3:F:62:ILE:HA	3:F:65:VAL:HG12	2.02	0.41
2:B:132:LEU:O	2:B:164:ARG:NH1	2.52	0.41
1:A:338:LYS:HB3	1:A:338:LYS:HE2	1.88	0.41
2:B:333:LEU:HD12	2:B:333:LEU:HA	1.84	0.41
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.94	0.41
2:B:75:MET:HG3	2:B:94:PHE:CG	2.55	0.41
2:B:139:HIS:HD2	2:B:146:GLY:O	2.04	0.41
2:B:1:MET:N	2:B:131:CYS:SG	2.80	0.40
1:A:134:GLY:HA3	1:A:165:SER:O	2.22	0.40
2:B:400:ARG:HD2	3:F:112:TRP:NE1	2.36	0.40
3:F:127:GLU:H	3:F:127:GLU:HG2	1.63	0.40
1:A:180:ALA:O	1:A:183:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	434/431 (101%)	419 (96%)	14 (3%)	1 (0%)	47 68
2	B	431/431 (100%)	414 (96%)	17 (4%)	0	100 100
3	F	153/155 (99%)	148 (97%)	5 (3%)	0	100 100
All	All	1018/1017 (100%)	981 (96%)	36 (4%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	365/365 (100%)	358 (98%)	7 (2%)	57 80
2	B	365/372 (98%)	358 (98%)	7 (2%)	57 80
3	F	119/120 (99%)	115 (97%)	4 (3%)	37 63
All	All	849/857 (99%)	831 (98%)	18 (2%)	53 78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	PHE
1	A	176	GLN

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Mol	Chain	Res	Type
1	A	215	ARG
1	A	221	ARG
1	A	335	ILE
1	A	370	LYS
1	A	423	GLU
2	B	278	ARG
2	B	286	LEU
2	B	293	GLN
2	B	298	SER
2	B	326	LYS
2	B	417	GLU
2	B	423	SER
3	F	46	SER
3	F	147	LYS
3	F	153	SER
3	F	167	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	91	GLN
1	A	176	GLN
1	A	256	GLN
1	A	301	GLN
2	B	139	HIS
2	B	197	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GTP	X	503	-	26,34,34	1.02	3 (11%)	32,54,54	0.69	1 (3%)
4	GTP	X	501	5	26,34,34	1.09	3 (11%)	32,54,54	0.72	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	X	503	-	-	5/18/38/38	0/3/3/3
4	GTP	X	501	5	-	5/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	501	GTP	C5-C6	-2.79	1.41	1.47
4	X	503	GTP	C5-C6	-2.69	1.41	1.47
4	X	503	GTP	C8-N7	-2.21	1.31	1.35
4	X	501	GTP	C8-N7	-2.17	1.31	1.35
4	X	501	GTP	C5-C4	-2.03	1.37	1.43
4	X	503	GTP	C5-C4	-2.01	1.38	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	501	GTP	O6-C6-C5	2.04	128.35	124.37
4	X	503	GTP	O6-C6-C5	2.02	128.33	124.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	501	GTP	C5'-O5'-PA-O1A
4	X	501	GTP	C5'-O5'-PA-O2A
4	X	503	GTP	PB-O3B-PG-O3G
4	X	503	GTP	C5'-O5'-PA-O1A
4	X	503	GTP	C5'-O5'-PA-O2A
4	X	501	GTP	PB-O3B-PG-O1G
4	X	501	GTP	PB-O3B-PG-O3G
4	X	501	GTP	C5'-O5'-PA-O3A
4	X	503	GTP	C5'-O5'-PA-O3A
4	X	503	GTP	C4'-C5'-O5'-PA

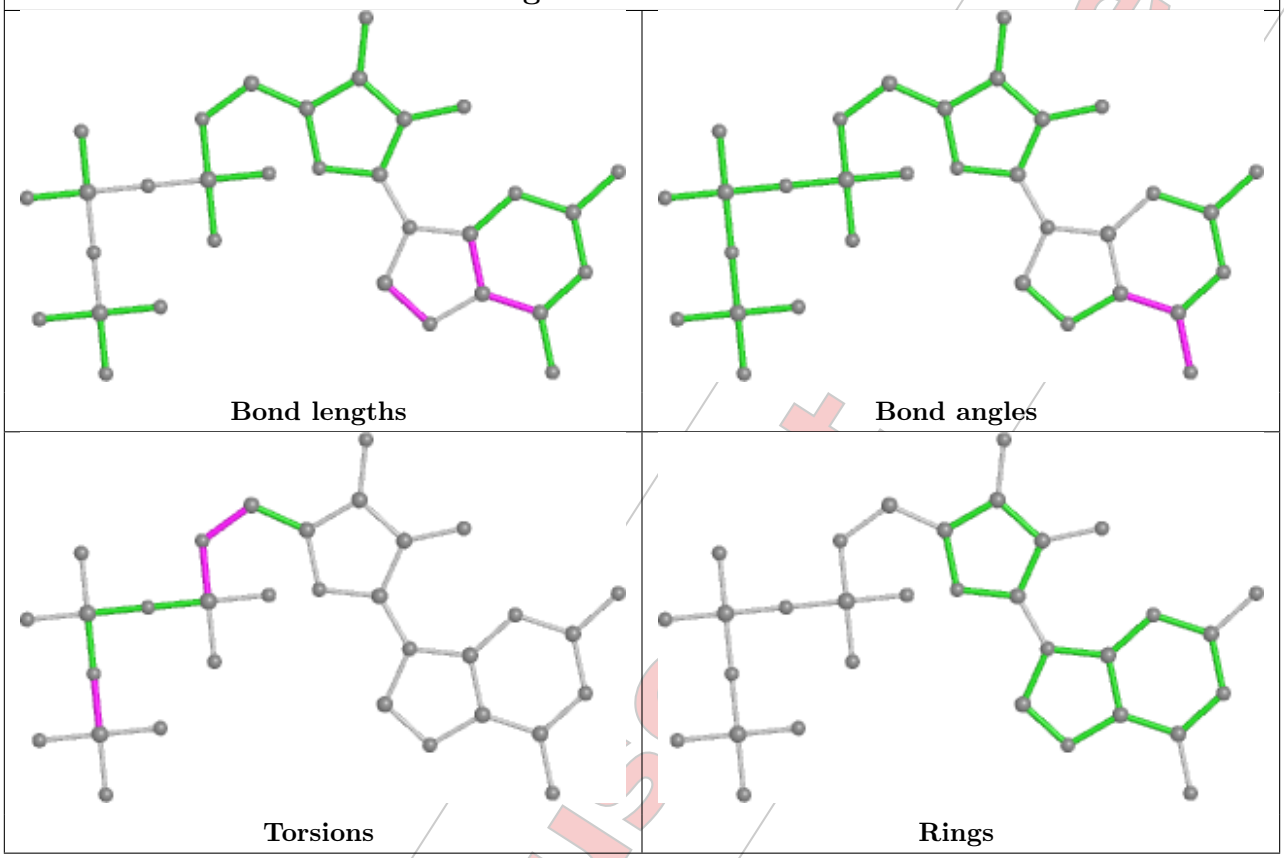
There are no ring outliers.

1 monomer is involved in 1 short contact:

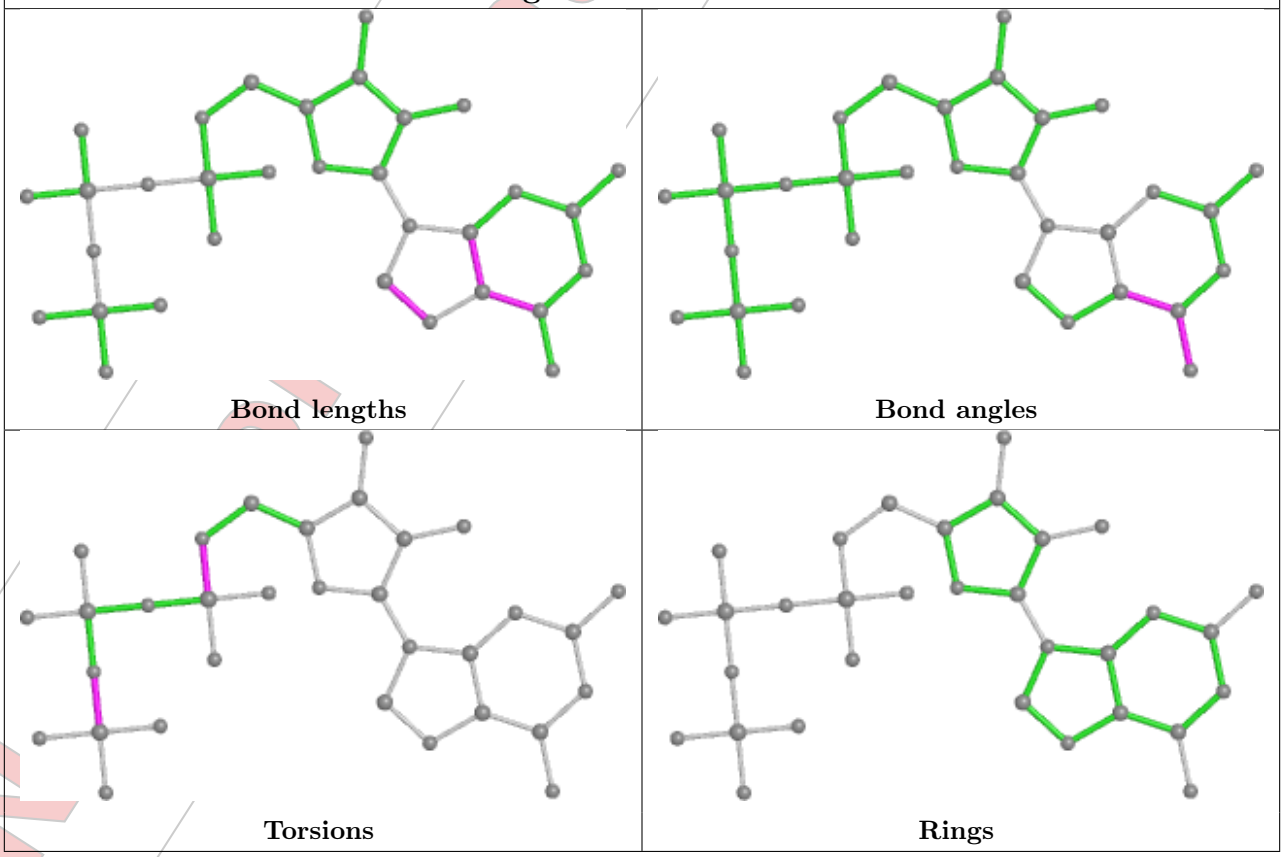
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	503	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP X 503



Ligand GTP X 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	40:LYS	C	47:ASP	N	4.92

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	431/431 (100%)	-0.51	11 (2%) 56 59	14, 29, 58, 109	2 (0%)
2	B	431/431 (100%)	-0.11	25 (5%) 23 24	18, 40, 75, 123	0
3	F	155/155 (100%)	-0.57	1 (0%) 89 90	19, 30, 53, 70	0
All	All	1017/1017 (100%)	-0.35	37 (3%) 42 46	14, 33, 68, 123	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	7.0
2	B	285	ALA	6.6
2	B	283	TYR	6.4
2	B	39	ASP	5.6
2	B	282	GLN	5.4
1	A	337	THR	5.3
2	B	37	HIS	5.2
2	B	279	GLY	4.7
2	B	281	GLN	4.5
2	B	284	ARG	4.5
2	B	280	SER	4.3
2	B	441	ASP	3.8
1	A	309	HIS	3.7
1	A	436	GLY	3.7
1	A	338	LYS	3.6
2	B	75	MET	3.3
1	A	348	PRO	3.1
1	A	1	MET	3.0
2	B	56	ALA	2.9
2	B	278	ARG	2.9
1	A	57	GLY	2.8
2	B	90	ASP	2.8
2	B	406	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	39	ASP	2.6
3	F	167	LYS	2.5
2	B	337	ASN	2.5
2	B	85	GLN	2.4
2	B	179[A]	ASP	2.4
2	B	113	GLU	2.4
2	B	30	ILE	2.3
2	B	369	ARG	2.3
2	B	333	LEU	2.2
2	B	80	SER	2.2
2	B	120	ASP	2.2
1	A	340	SER	2.2
1	A	215	ARG	2.1
2	B	70	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

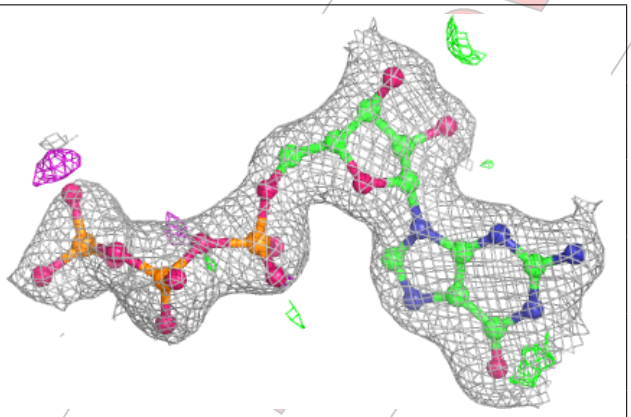
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

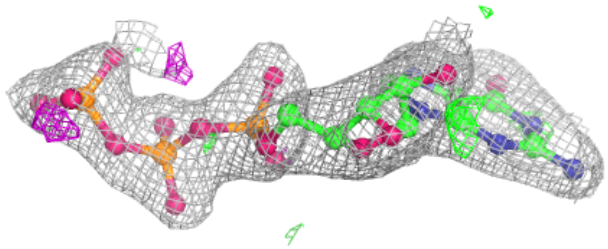
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GTP	X	503	32/?	0.93	0.12	32,36,48,72	0
4	GTP	X	501	32/?	0.97	0.09	10,18,29,32	0
5	MG	X	502	1/?	0.99	0.07	11,11,11,11	0

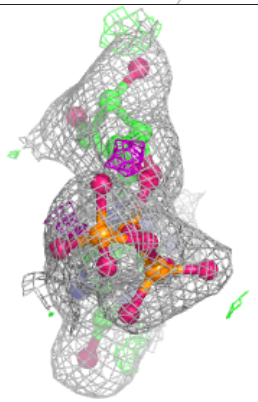
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP X 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

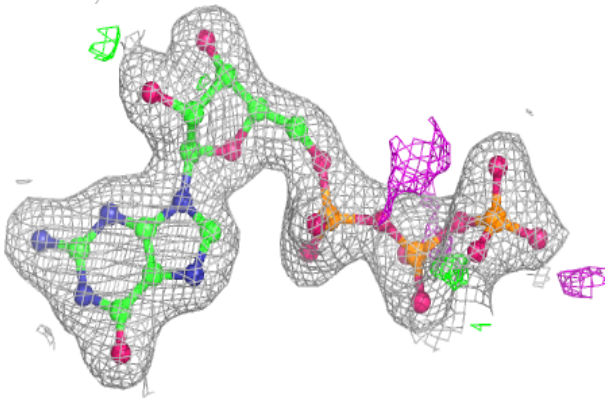


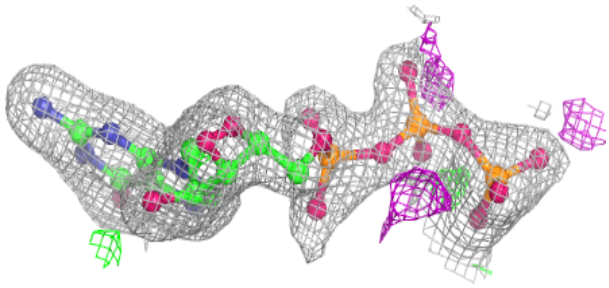


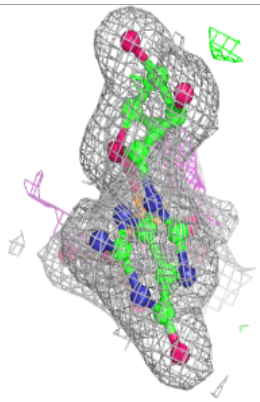


Electron density around GTP X 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2023 – 10:53 am GMT

Deposition ID : D_1292128504

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

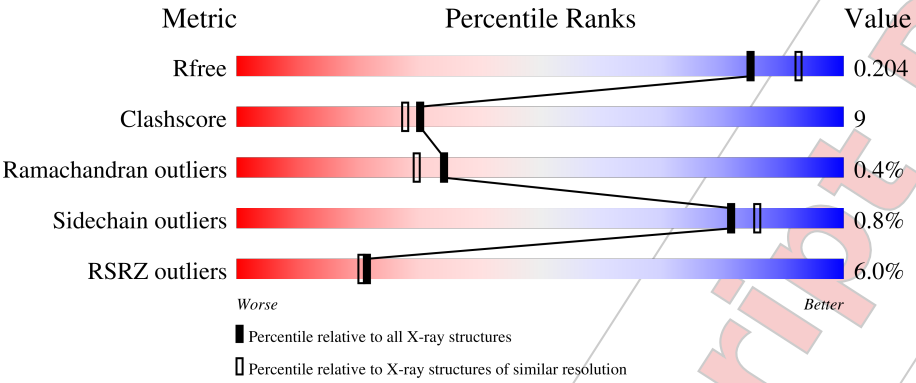
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	435	3% 82% 17%
2	B	430	10% 73% 26%
3	F	155	% 86% 14%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16106 atoms, of which 7693 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	435	6686	2150	3290	576	648	22	0	3	0

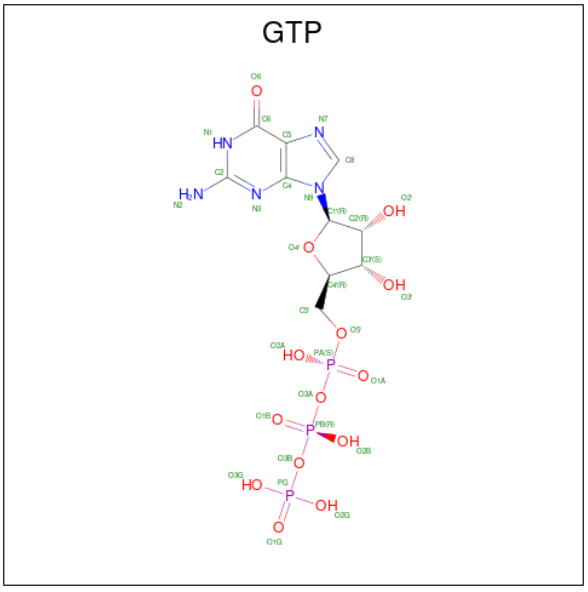
- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	430	6546	2103	3197	568	651	27	0	2	0

- Molecule 3 is a protein called Designed Ankyrin Repeat Protein (DARPIN) D1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	F	155	2322	730	1163	199	227	3	0	1	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

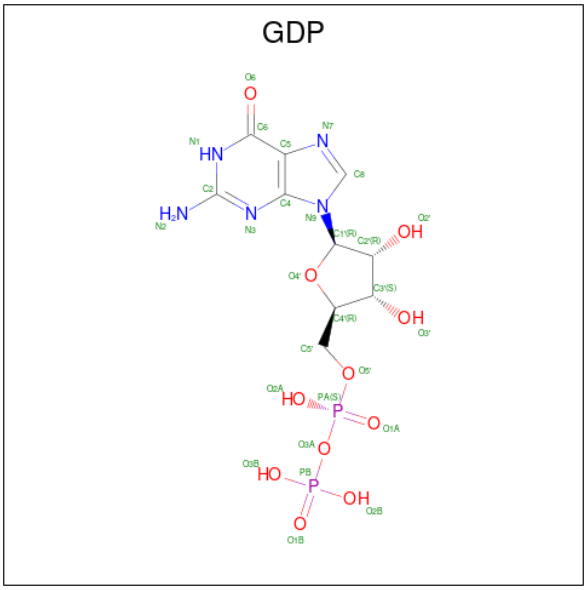


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	X	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	X	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 7 is a ligand with the chemical component id GAO but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for GAO. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	X	1	Total	C	H	N	O	S	0	0
			45	19	19	1	5	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	X	1	Total Ca 1 1	0	0

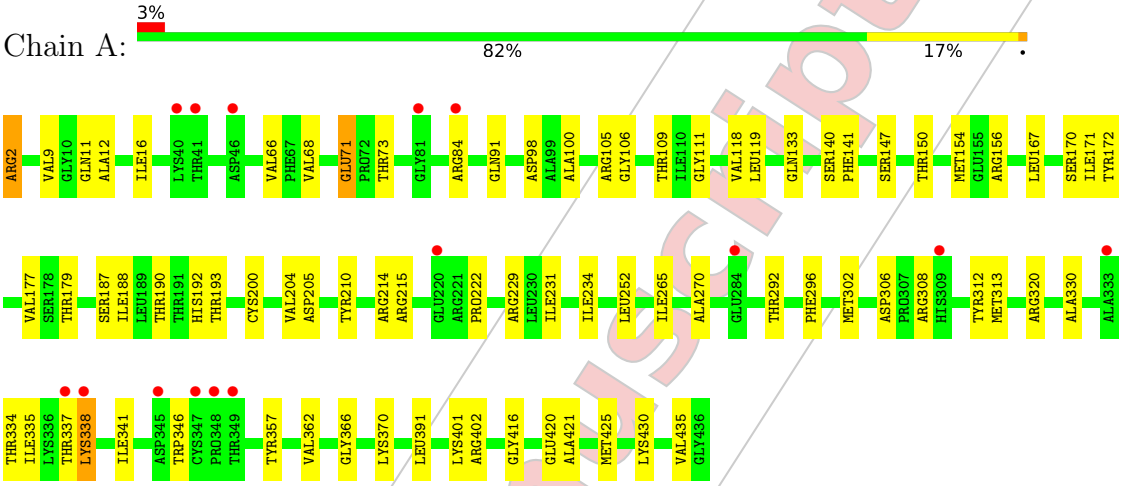
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	S	421	Total O 421 421	0	0

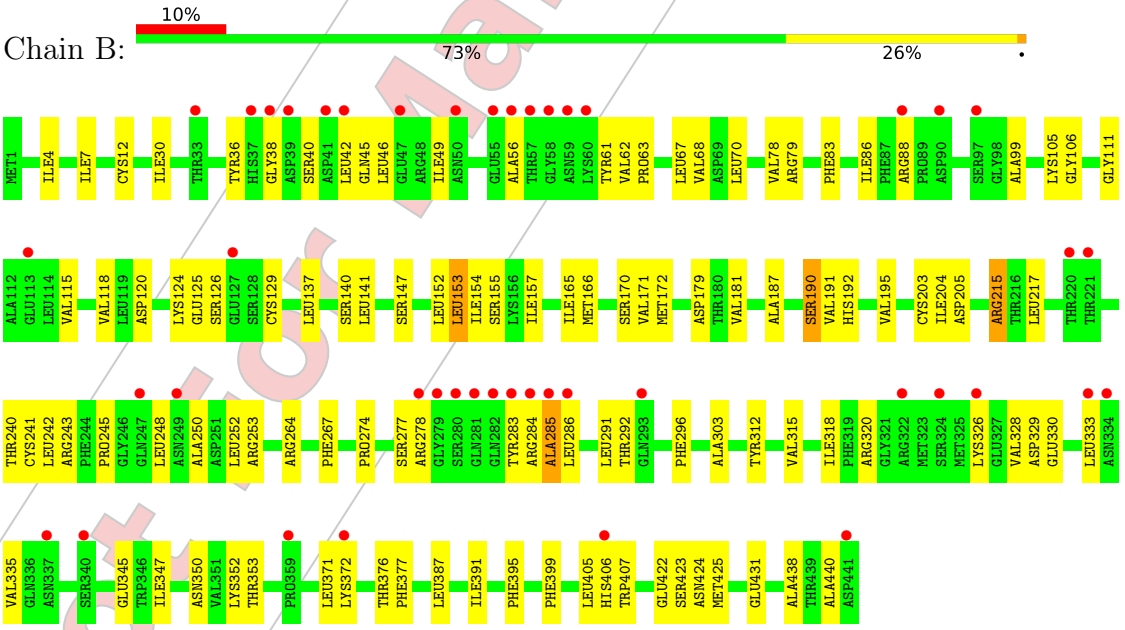
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

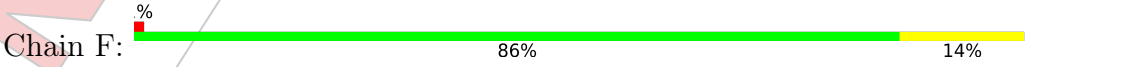
• Molecule 1: Tubulin alpha-1B chain

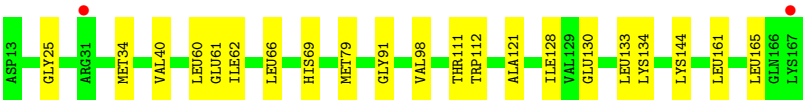


• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Designed Ankyrin Repeat Protein (DARPIN) D1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.23Å 90.94Å 82.43Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	13.00 – 2.00 15.04 – 1.74	Depositor EDS
% Data completeness (in resolution range)	94.4 (13.00-2.00) 67.9 (15.04-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.155 , 0.206 0.174 , 0.204	Depositor DCC
R_{free} test set	1038 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16106	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GAO, GDP, GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.71	0/3487	0.85	0/4739
2	B	0.69	2/3425 (0.1%)	0.82	5/4641 (0.1%)
3	F	0.62	0/1178	0.81	0/1601
All	All	0.69	2/8090 (0.0%)	0.84	5/10981 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	1	5
All	All	1	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	431[A]	GLU	C-N	-9.49	1.12	1.34
2	B	431[B]	GLU	C-N	-9.49	1.12	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	283	TYR	CB-CA-C	9.83	130.06	110.40
2	B	153	LEU	O-C-N	8.62	136.49	122.70
2	B	153	LEU	CA-C-N	-5.88	104.27	117.20
2	B	179	ASP	CB-CG-OD1	-5.36	113.48	118.30
2	B	179	ASP	CB-CG-OD2	5.11	122.89	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	283	TYR	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	215	ARG	Sidechain
1	A	320	ARG	Sidechain
1	A	402	ARG	Sidechain
1	A	84	ARG	Sidechain
2	B	152	LEU	Mainchain
2	B	215	ARG	Sidechain
2	B	243	ARG	Sidechain
2	B	278	ARG	Sidechain
2	B	79	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3396	3290	3280	52	1
2	B	3349	3197	3195	76	0
3	F	1159	1163	1162	18	0
4	X	32	12	12	1	0
5	X	1	0	0	0	0
6	X	28	12	12	0	0
7	X	26	19	0	3	0
8	X	1	0	0	0	0
9	S	421	0	0	9	1
All	All	8413	7693	7661	146	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LEU:HD23	2:B:250:ALA:HB2	1.42	0.98
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.65	0.79
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.75	0.68
1:A:330:ALA:O	1:A:334:THR:HG23	1.95	0.67
3:F:79:MET:CE	3:F:111:THR:HG21	2.23	0.67
2:B:118:VAL:HG11	2:B:153:LEU:HD21	1.76	0.67
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.80	0.64
3:F:34:MET:HE3	3:F:66:LEU:HD23	1.80	0.63
2:B:328:VAL:HG12	2:B:353:THR:HG21	1.82	0.61
2:B:46:LEU:HD11	2:B:61:TYR:CZ	2.35	0.61
2:B:318:ILE:CG2	2:B:376:THR:HB	2.31	0.60
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.31	0.60
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.84	0.60
1:A:204:VAL:HG11	1:A:231:ILE:HG12	1.84	0.59
1:A:177:VAL:HG13	1:A:177:VAL:O	2.03	0.58
2:B:318:ILE:HG23	2:B:318:ILE:O	2.03	0.58
2:B:46:LEU:HD21	2:B:61:TYR:OH	2.04	0.58
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.35	0.57
7:X:604:GAO:C11	7:X:604:GAO:O1	2.53	0.57
1:A:416:GLY:O	1:A:420:GLU:HG3	2.04	0.57
1:A:188:ILE:HG23	1:A:425:MET:HG2	1.86	0.57
3:F:79:MET:HE1	3:F:111:THR:HG21	1.85	0.57
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.87	0.56
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.88	0.56
2:B:106:GLY:O	2:B:111:GLY:HA3	2.05	0.56
2:B:274:PRO:HG2	2:B:371:LEU:HD22	1.88	0.56
3:F:60:LEU:HD11	3:F:98:VAL:HG21	1.86	0.56
2:B:68:VAL:HG11	2:B:118:VAL:HG21	1.87	0.56
2:B:352:LYS:HB2	7:X:604:GAO:C17	2.37	0.55
2:B:153:LEU:O	2:B:157:ILE:HG13	2.07	0.55
3:F:61:GLU:HB2	9:S:155:HOH:O	2.07	0.54
2:B:217:LEU:HD13	2:B:277:SER:OG	2.08	0.54
2:B:345:GLU:HG3	2:B:440:ALA:HB2	1.90	0.53
3:F:34:MET:HE2	3:F:40:VAL:HG21	1.90	0.53
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.43	0.53
2:B:63:PRO:CD	2:B:86:ILE:HG13	2.39	0.53
1:A:312:TYR:CE2	1:A:341:ILE:HG23	2.44	0.53
2:B:46:LEU:HD11	2:B:61:TYR:CE2	2.43	0.53
2:B:83:PHE:O	2:B:86:ILE:HG22	2.07	0.53
3:F:79:MET:HE3	3:F:111:THR:HG21	1.90	0.52
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.89	0.52
2:B:7:ILE:O	2:B:137:LEU:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.44	0.52
1:A:362:VAL:HG12	9:S:549:HOH:O	2.09	0.52
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.92	0.52
1:A:337:THR:O	1:A:338:LYS:CB	2.58	0.52
2:B:284:ARG:O	2:B:285:ALA:HB3	2.09	0.52
2:B:326:LYS:O	2:B:330:GLU:HG3	2.10	0.52
3:F:34:MET:CE	3:F:69:HIS:HB2	2.40	0.52
2:B:30:ILE:HD13	2:B:30:ILE:N	2.25	0.52
2:B:318:ILE:HG23	2:B:376:THR:HB	1.94	0.50
2:B:12:CYS:CB	2:B:140:SER:HB3	2.42	0.50
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.46	0.50
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.46	0.50
2:B:120:ASP:O	2:B:124:LYS:HD2	2.12	0.50
3:F:130:GLU:O	3:F:134:LYS:HG2	2.11	0.50
2:B:315:VAL:HG11	2:B:377:PHE:CE1	2.46	0.50
1:A:306:ASP:OD1	1:A:308:ARG:HD3	2.11	0.50
2:B:141:LEU:HD21	2:B:170:SER:HB3	1.94	0.50
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.52	0.50
2:B:315:VAL:CG1	2:B:377:PHE:CE1	2.95	0.49
2:B:67:LEU:CD2	2:B:78:VAL:HG11	2.42	0.49
7:X:604:GAO:C15	7:X:604:GAO:S	3.00	0.49
3:F:34:MET:HE2	3:F:40:VAL:CG2	2.42	0.49
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.94	0.48
1:A:265:ILE:O	1:A:265:ILE:HG13	2.13	0.48
3:F:34:MET:CE	3:F:66:LEU:HD23	2.43	0.48
2:B:12:CYS:HB3	2:B:140:SER:HB3	1.96	0.48
1:A:106:GLY:O	1:A:111:GLY:HA3	2.14	0.47
1:A:193:THR:HG23	9:S:550:HOH:O	2.14	0.47
2:B:192:HIS:CE1	2:B:424:ASN:HD22	2.32	0.47
2:B:46:LEU:HA	2:B:49:ILE:HB	1.97	0.47
2:B:67:LEU:HD22	2:B:78:VAL:HG11	1.97	0.47
2:B:406:HIS:CE1	2:B:407:TRP:CD1	3.02	0.47
1:A:401:LYS:HE3	2:B:438:ALA:HB1	1.96	0.47
1:A:234:ILE:HG21	1:A:302:MET:SD	2.55	0.47
1:A:292:THR:HG22	1:A:335:ILE:HD12	1.97	0.47
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.33	0.47
3:F:34:MET:HE1	3:F:69:HIS:HB2	1.97	0.47
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.96	0.46
2:B:312:TYR:CZ	2:B:377:PHE:CZ	3.04	0.46
1:A:430:LYS:HE2	9:S:569:HOH:O	2.15	0.46
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.46
1:A:362:VAL:HA	9:S:567:HOH:O	2.15	0.46
1:A:229:ARG:CD	1:A:366:GLY:HA2	2.46	0.46
2:B:147:SER:HB2	2:B:190:SER:OG	2.15	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.46
3:F:34:MET:HE1	3:F:66:LEU:HA	1.98	0.45
2:B:312:TYR:CE1	2:B:377:PHE:CZ	3.05	0.45
1:A:100:ALA:HB2	2:B:253:ARG:HD2	1.98	0.45
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.98	0.45
1:A:119:LEU:CD1	1:A:156:ARG:NH2	2.80	0.45
2:B:205:ASP:CB	2:B:303:ALA:HA	2.46	0.45
2:B:241:CYS:O	2:B:250:ALA:HB3	2.16	0.45
1:A:296:PHE:CE1	1:A:335:ILE:HD13	2.52	0.45
3:F:112:TRP:C	3:F:144:LYS:HG3	2.37	0.45
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.52	0.45
2:B:88:ARG:NH1	2:B:125:GLU:OE2	2.50	0.45
2:B:70:LEU:HD21	2:B:111:GLY:HA2	1.99	0.45
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.99	0.44
1:A:179:THR:HG21	9:S:175:HOH:O	2.17	0.44
1:A:362:VAL:HG21	1:A:370:LYS:NZ	2.33	0.44
1:A:362:VAL:HA	9:S:549:HOH:O	2.16	0.44
2:B:63:PRO:HD2	2:B:86:ILE:HG13	2.00	0.44
2:B:126:SER:O	2:B:129:CYS:HB2	2.17	0.44
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.44
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.99	0.43
2:B:399:PHE:CE1	2:B:405:LEU:HD11	2.53	0.43
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.48	0.43
1:A:150:THR:O	1:A:154:MET:HG2	2.18	0.43
1:A:270:ALA:HB3	1:A:302:MET:CE	2.45	0.43
2:B:328:VAL:CG1	2:B:353:THR:HG21	2.47	0.43
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.00	0.43
2:B:296:PHE:CZ	2:B:377:PHE:HE1	2.37	0.43
1:A:71:GLU:OE1	1:A:73:THR:HG23	2.19	0.42
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.54	0.42
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.00	0.42
2:B:88:ARG:NH1	2:B:125:GLU:CD	2.73	0.42
2:B:172:MET:HE2	2:B:203:CYS:HA	2.02	0.42
1:A:105:ARG:HA	1:A:109:THR:OG1	2.20	0.42
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.42
1:A:346:TRP:CZ2	1:A:435:VAL:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:25:GLY:HA2	3:F:62:ILE:HD12	2.01	0.42
3:F:91:GLY:HA2	3:F:128:ILE:CD1	2.50	0.42
2:B:240:THR:OG1	2:B:320:ARG:HD2	2.20	0.42
2:B:42:LEU:CA	2:B:45:GLN:N	2.83	0.41
1:A:313:MET:SD	1:A:435:VAL:HG11	2.61	0.41
2:B:387:LEU:HD23	2:B:387:LEU:C	2.40	0.41
2:B:329:ASP:O	2:B:333:LEU:HD13	2.19	0.41
2:B:391:ILE:HG22	2:B:425:MET:HE1	2.03	0.41
2:B:4:ILE:CD1	2:B:242:LEU:HD13	2.51	0.41
1:A:11:GLN:HB2	9:S:39:HOH:O	2.20	0.41
1:A:68[A]:VAL:HG11	1:A:118:VAL:HG21	2.03	0.41
2:B:187:ALA:O	2:B:191:VAL:HG23	2.21	0.41
1:A:66:VAL:HG22	1:A:91:GLN:OE1	2.21	0.41
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.61	0.41
2:B:99:ALA:O	2:B:105:LYS:HD2	2.21	0.41
3:F:133:LEU:HD11	3:F:165:LEU:HD23	2.02	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.03	0.40
2:B:181:VAL:HG22	9:S:372:HOH:O	2.21	0.40
2:B:195:VAL:HG13	2:B:264:ARG:HG2	2.02	0.40
2:B:115:VAL:HG23	2:B:153:LEU:HD13	2.02	0.40
1:A:179:THR:HG23	4:X:501:GTP:H2'	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:OH	9:S:101:HOH:O[1_456]	2.00	0.20

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/435 (100%)	426 (98%)	9 (2%)	1 (0%)	47	44
2	B	428/430 (100%)	410 (96%)	15 (4%)	3 (1%)	22	16
3	F	154/155 (99%)	152 (99%)	2 (1%)	0	100	100
All	All	1018/1020 (100%)	988 (97%)	26 (3%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	LYS
2	B	285	ALA
2	B	245	PRO
2	B	56	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/366 (100%)	365 (100%)	1 (0%)	92	95
2	B	363/371 (98%)	357 (98%)	6 (2%)	60	65
3	F	121/120 (101%)	121 (100%)	0	100	100
All	All	850/857 (99%)	843 (99%)	7 (1%)	81	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
2	B	40	SER
2	B	155	SER
2	B	190	SER
2	B	215	ARG
2	B	372	LYS
2	B	423	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
2	B	300	ASN
2	B	331	GLN
2	B	406	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic and 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GDP	X	503	-	24,30,30	1.38	5 (20%)	30,47,47	0.80	1 (3%)
4	GTP	X	501	5	26,34,34	1.07	2 (7%)	32,54,54	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	X	503	-	-	6/12/32/32	0/3/3/3
4	GTP	X	501	5	-	5/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	503	GDP	PB-O3B	-4.09	1.39	1.54
6	X	503	GDP	C5-C6	-3.04	1.41	1.47
4	X	501	GTP	C5-C6	-2.76	1.41	1.47
6	X	503	GDP	C8-N7	-2.28	1.31	1.35
4	X	501	GTP	C8-N7	-2.21	1.31	1.35
6	X	503	GDP	PB-O2B	-2.11	1.46	1.54
6	X	503	GDP	C5-C4	-2.00	1.38	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	503	GDP	O6-C6-C5	2.17	128.60	124.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	501	GTP	C5'-O5'-PA-O1A
4	X	501	GTP	C5'-O5'-PA-O2A
6	X	503	GDP	C5'-O5'-PA-O1A
6	X	503	GDP	C5'-O5'-PA-O2A
6	X	503	GDP	C4'-C5'-O5'-PA
6	X	503	GDP	PB-O3A-PA-O1A
4	X	501	GTP	PB-O3B-PG-O3G
6	X	503	GDP	PA-O3A-PB-O3B
4	X	501	GTP	C5'-O5'-PA-O3A
6	X	503	GDP	C5'-O5'-PA-O3A
4	X	501	GTP	C4'-C5'-O5'-PA

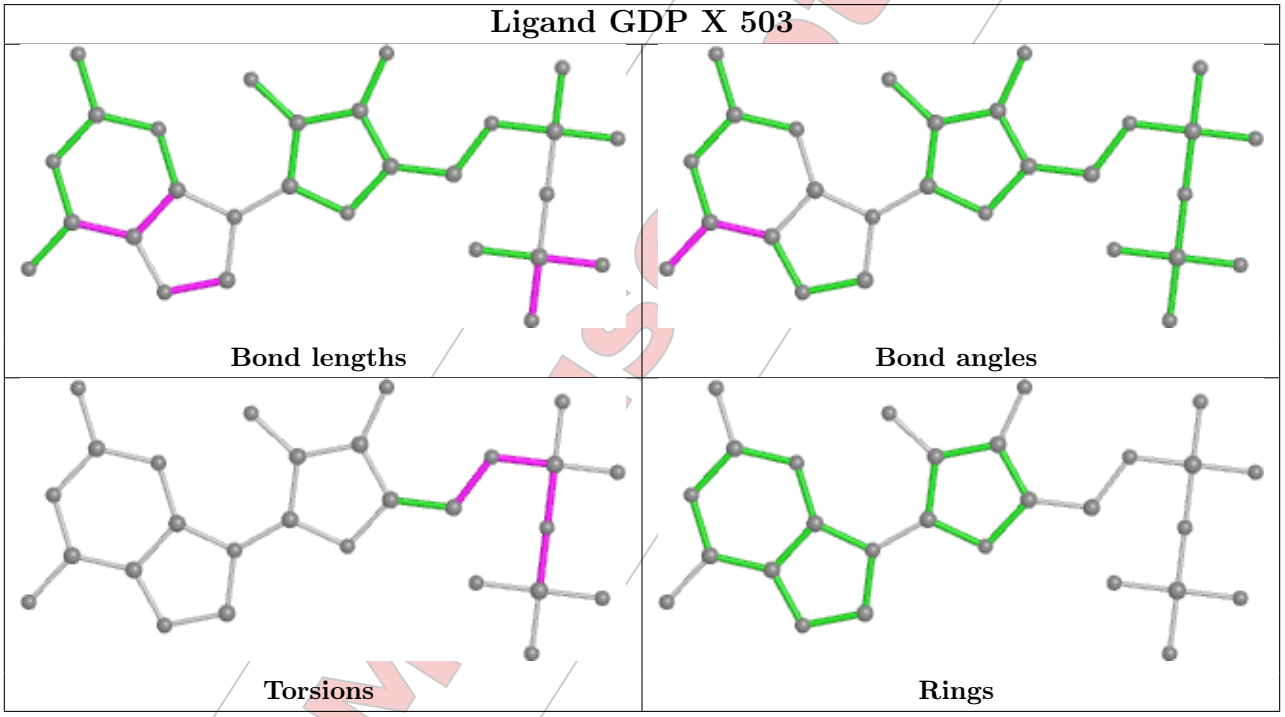
There are no ring outliers.

1 monomer is involved in 1 short contact:

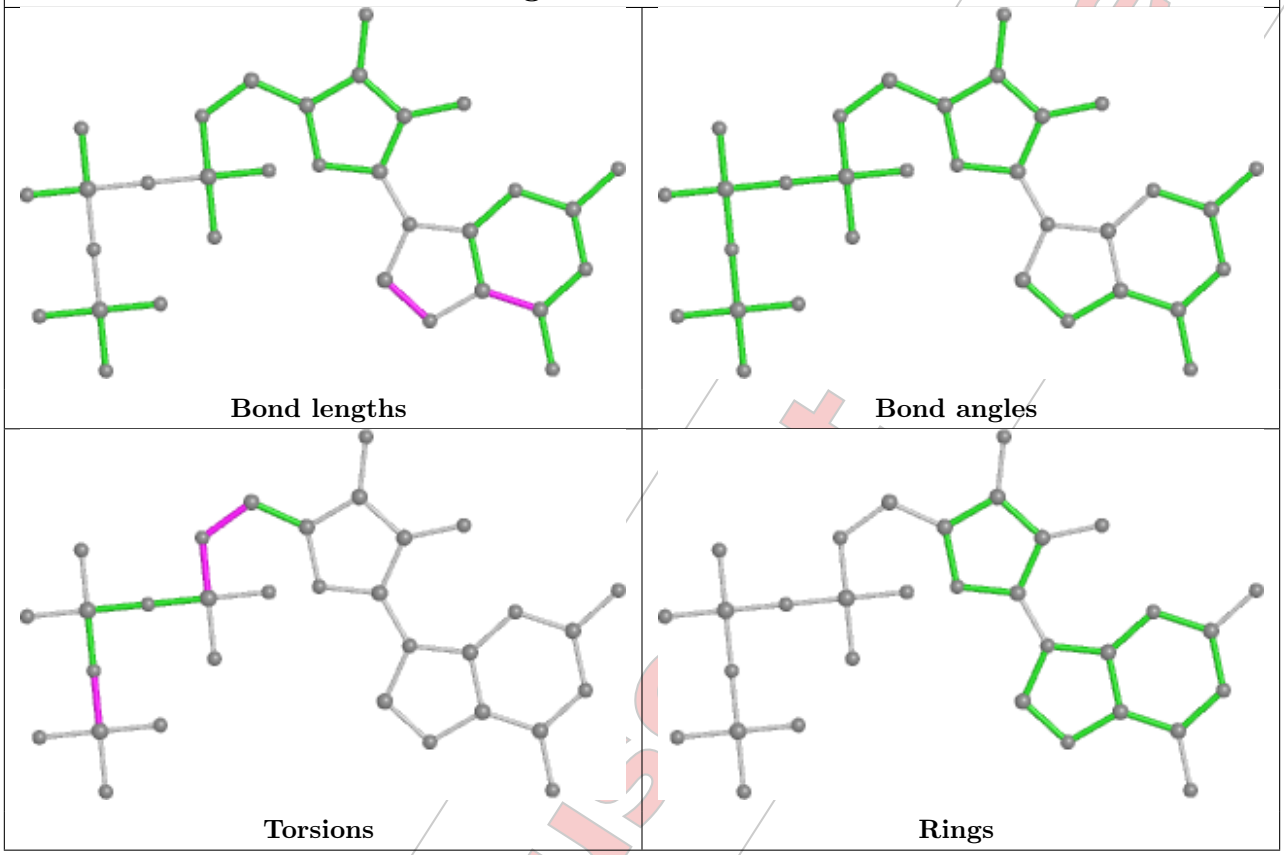
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP X 503



Ligand GTP X 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	42:LEU	C	45:GLN	N	3.44
1	B	431[A]:GLU	C	432:TYR	N	1.12
1	B	431[B]:GLU	C	432:TYR	N	1.12

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	435/435 (100%)	-0.28	15 (3%) 45 44	10, 22, 51, 87	0
2	B	430/430 (100%)	0.36	44 (10%) 6 6	15, 37, 74, 120	0
3	F	155/155 (100%)	-0.34	2 (1%) 77 76	15, 23, 46, 62	0
All	All	1020/1020 (100%)	-0.02	61 (5%) 21 20	10, 27, 64, 120	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	281	GLN	8.8
1	A	337	THR	8.2
2	B	285	ALA	7.7
2	B	280	SER	6.9
2	B	247	GLN	6.6
2	B	283	TYR	5.8
2	B	37	HIS	5.7
2	B	38	GLY	5.4
2	B	279	GLY	5.4
2	B	57	THR	5.4
2	B	282	GLN	5.3
2	B	41	ASP	5.2
2	B	56	ALA	5.1
2	B	333	LEU	4.9
2	B	39	ASP	4.4
2	B	441	ASP	4.0
1	A	41	THR	3.9
1	A	46	ASP	3.9
2	B	284	ARG	3.8
1	A	40	LYS	3.8
1	A	348	PRO	3.7
2	B	88	ARG	3.5
2	B	337	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	338	LYS	3.4
2	B	406	HIS	3.3
2	B	33	THR	3.2
1	A	345	ASP	3.2
2	B	322	ARG	3.0
2	B	42	LEU	3.0
2	B	59	ASN	3.0
2	B	286	LEU	3.0
2	B	326	LYS	2.9
3	F	31	ARG	2.9
3	F	167	LYS	2.9
1	A	220	GLU	2.9
2	B	220	THR	2.8
1	A	349	THR	2.8
2	B	278	ARG	2.8
1	A	84	ARG	2.7
1	A	347	CYS	2.6
2	B	324	SER	2.6
2	B	58	GLY	2.6
1	A	284	GLU	2.6
2	B	113	GLU	2.5
2	B	249	ASN	2.5
2	B	293	GLN	2.4
2	B	97	SER	2.4
2	B	50	ASN	2.4
2	B	359	PRO	2.3
1	A	309	HIS	2.3
2	B	90	ASP	2.3
2	B	334	ASN	2.2
2	B	60	LYS	2.2
1	A	333	ALA	2.2
2	B	55	GLU	2.2
2	B	47	GLU	2.2
2	B	127	GLU	2.1
1	A	81	GLY	2.1
2	B	221	THR	2.1
2	B	372	LYS	2.0
2	B	340	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

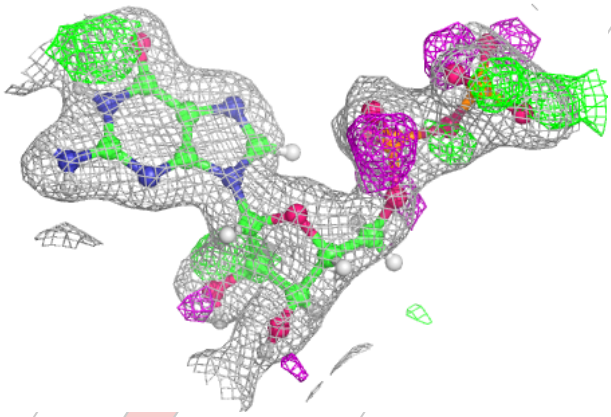
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

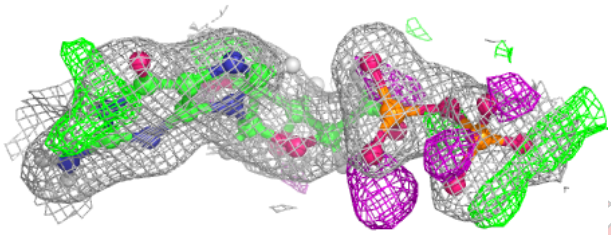
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	X	502	1/?	0.93	0.10	10,10,10,10	0
6	GDP	X	503	28/?	0.93	0.12	12,24,33,34	0
7	GAO	X	604	26/?	0.93	0.12	27,46,72,87	0
8	CA	X	605	1/?	0.96	0.04	39,39,39,39	0
4	GTP	X	501	32/?	0.97	0.09	8,13,15,18	0

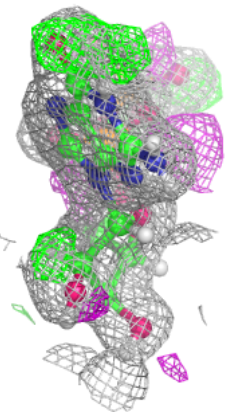
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP X 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

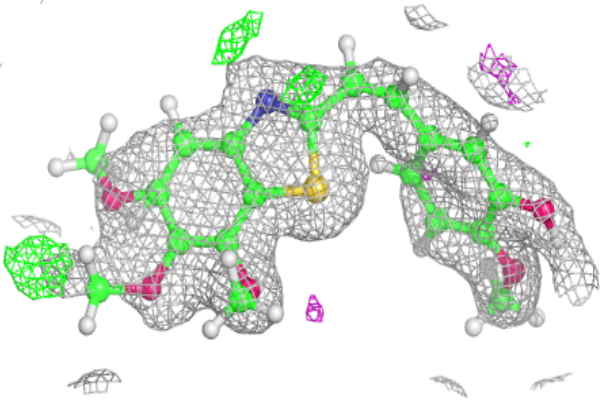


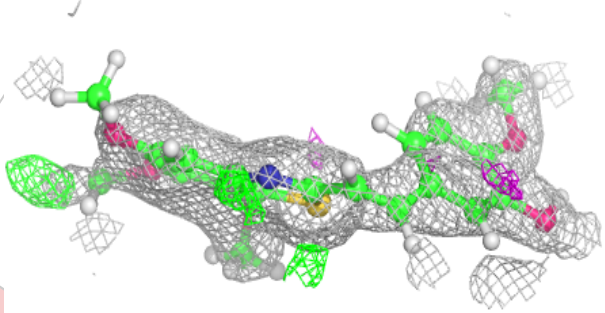


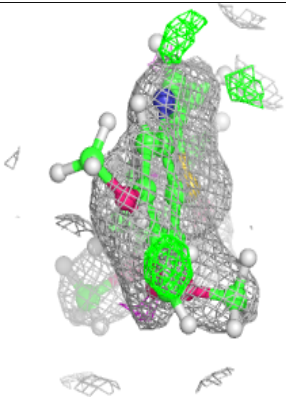


Electron density around GAO X 604:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

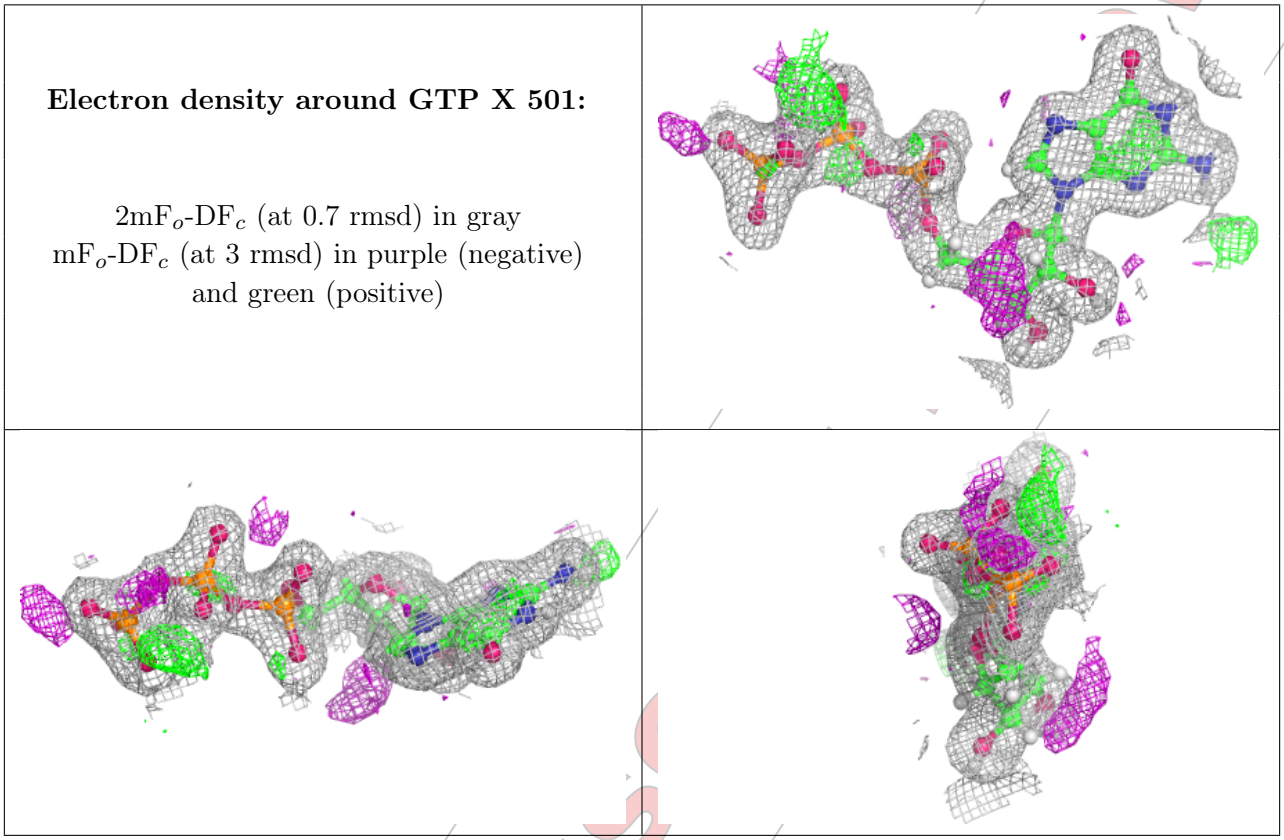






Electron density around GTP X 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2023 – 08:12 am GMT

Deposition ID : D_1292128590

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

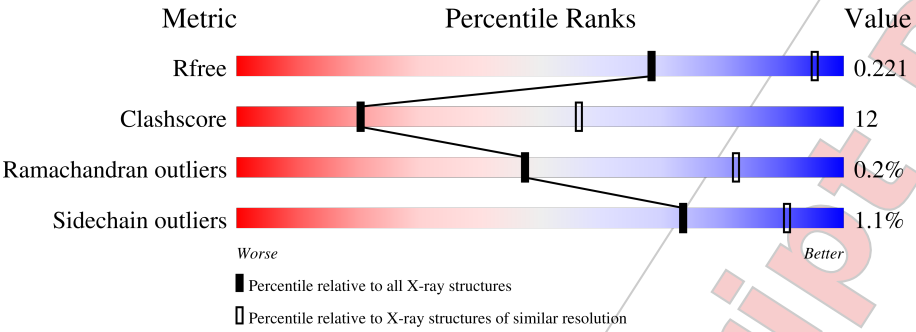
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	439	72% 27%
2	B	423	77% 23%
3	C	440	77% 22%
4	D	421	69% 31%
5	E	121	79% 21% .
6	F	320	70% 28% .

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34647 atoms, of which 17104 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	439	6913	2214	3431	582	661	25	0	13	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	423	6646	2126	3271	569	653	27	1	9	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	440	6893	2205	3412	587	665	24	0	10	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	421	6533	2091	3211	561	642	28	5	4	0

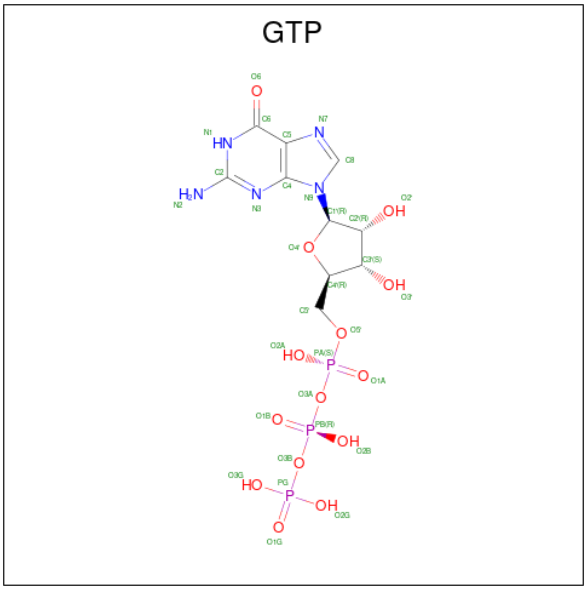
- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	121	2032	621	1026	182	198	5	0	1	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	320	5281	1711	2641	437	478	14	13	5	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	X	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
7	X	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

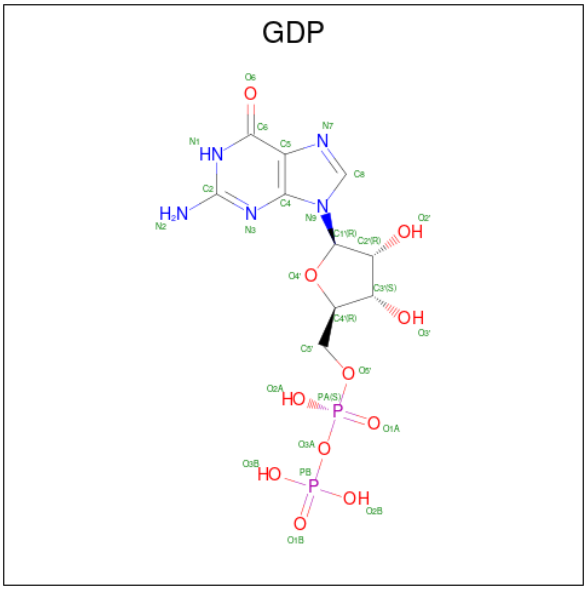
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	X	1	Total	Ca	0	0
			1	1		
9	X	1	Total	Ca	0	0
			1	1		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

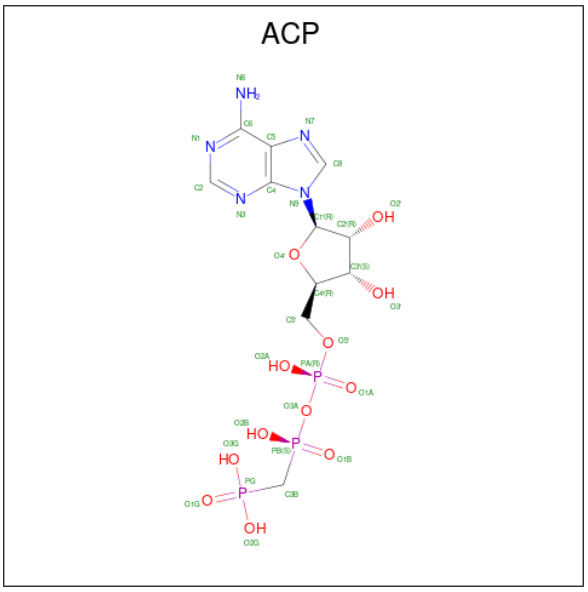


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	X	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
10	X	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 11 is a ligand with the chemical component id COL but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for COL. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	X	1	Total	C	H	N	O	0	0
			54	22	25	1	6		
11	X	1	Total	C	H	N	O	0	0
			54	22	25	1	6		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
12	X	1	45	11	14	5	12	3	0	0

- Molecule 13 is water.

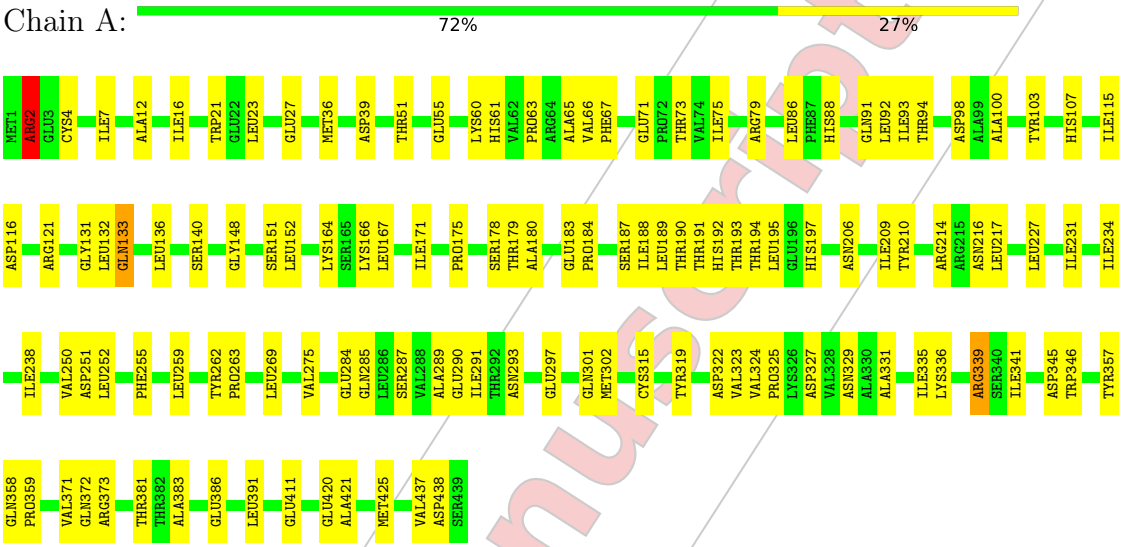
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	S	22	22	22	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

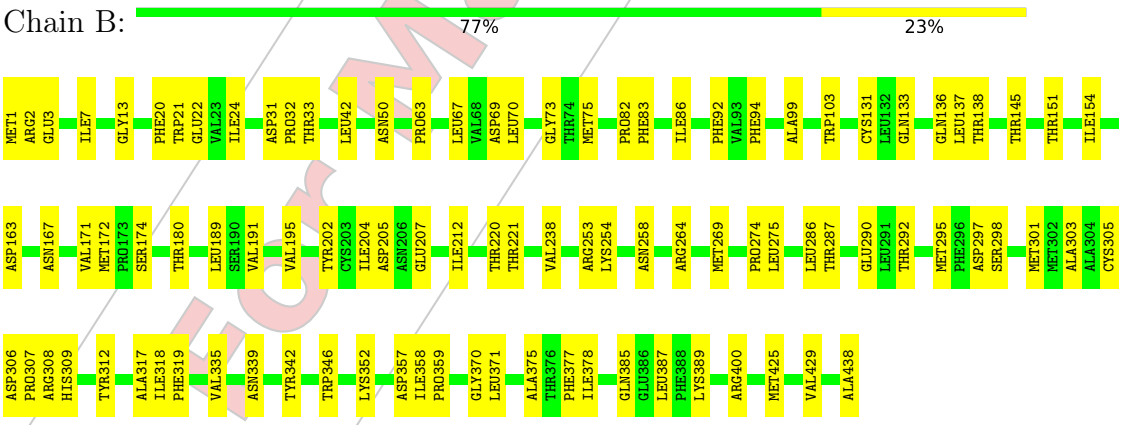
- Molecule 1:

Chain A:



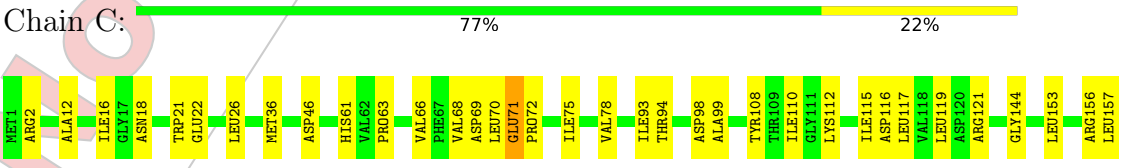
- Molecule 2:

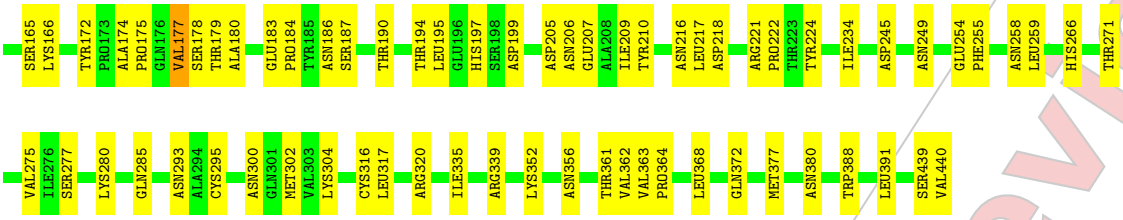
Chain B:



- Molecule 3:

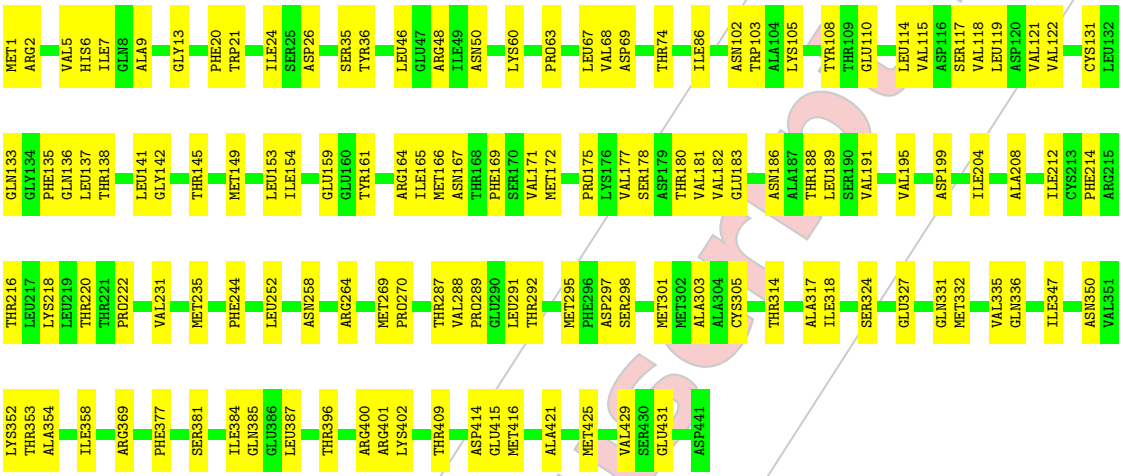
Chain C:





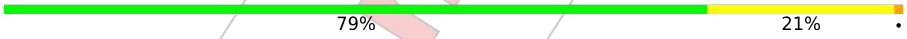
- Molecule 4:

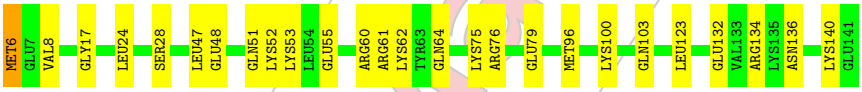
Chain D:



- Molecule 5:

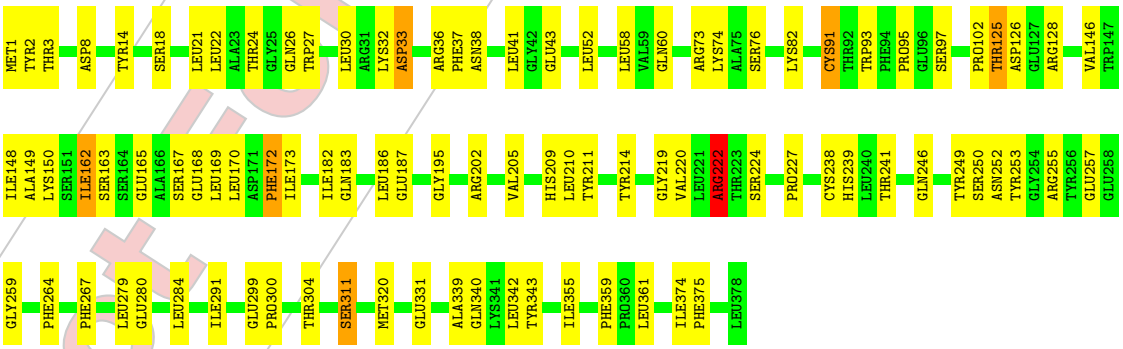
Chain E:





- Molecule 6:

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.71Å 160.61Å 180.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.18 – 3.00 15.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.18-3.00) 69.5 (15.22-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.20Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.163 , 0.214 0.176 , 0.221	Depositor DCC
R_{free} test set	2000 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 73.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34647	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACP, COL, GDP, CA, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/3599	0.54	0/4888
2	B	0.41	0/3473	0.57	0/4704
3	C	0.44	0/3589	0.56	0/4874
4	D	0.36	0/3407	0.53	0/4618
5	E	0.41	0/1017	0.51	0/1349
6	F	0.36	0/2712	0.54	0/3663
All	All	0.39	0/17797	0.55	0/24096

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
3	C	0	3
4	D	0	1
6	F	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
1	A	339	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	264	ARG	Sidechain
3	C	2	ARG	Sidechain
3	C	221	ARG	Sidechain
3	C	339	ARG	Sidechain
4	D	401	ARG	Sidechain
6	F	222	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3482	3431	3430	99	0
2	B	3375	3271	3268	87	0
3	C	3481	3412	3409	68	0
4	D	3322	3211	3210	103	0
5	E	1006	1026	1026	20	0
6	F	2640	2641	2641	68	0
7	X	64	24	24	0	0
8	X	4	0	0	0	0
9	X	2	0	0	0	0
10	X	56	24	24	2	0
11	X	58	50	0	5	0
12	X	31	14	14	1	0
13	S	22	0	0	0	0
All	All	17543	17104	17046	428	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (428) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:128:ARG:HE	6:F:170:LEU:HD22	1.37	0.88
1:A:381:THR:HG22	1:A:383:ALA:H	1.41	0.86
4:D:118:VAL:HG21	4:D:153:LEU:HD21	1.56	0.84
4:D:175:PRO:HA	4:D:178:SER:HB2	1.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:125:THR:HG22	6:F:126:ASP:HA	1.61	0.82
6:F:149:ALA:HB2	6:F:182:ILE:HG12	1.63	0.81
2:B:1:MET:N	2:B:131:CYS:HB3	1.96	0.80
1:A:166:LYS:HE2	1:A:197:HIS:O	1.84	0.78
3:C:75:ILE:HD12	3:C:94:THR:HG22	1.66	0.78
1:A:2:ARG:NH2	1:A:250[A]:VAL:HG13	2.00	0.77
1:A:357:TYR:CE2	5:E:17:GLY:HA2	2.21	0.76
2:B:75:MET:CE	2:B:94:PHE:HB3	2.15	0.76
2:B:136:GLN:HA	2:B:167:ASN:O	1.86	0.76
6:F:339:ALA:HB3	6:F:342:LEU:HD13	1.68	0.76
2:B:1:MET:H2	2:B:131:CYS:HB3	1.51	0.76
4:D:352:LYS:HG3	11:X:511:COL:C4	2.16	0.75
3:C:177:VAL:HG21	3:C:206:ASN:HB3	1.69	0.74
1:A:2:ARG:HH21	1:A:250[A]:VAL:HG13	1.53	0.74
1:A:75:ILE:HG23	1:A:92:LEU:HD12	1.69	0.73
6:F:202:ARG:HB3	6:F:220:VAL:HG12	1.71	0.72
3:C:18:ASN:HD21	3:C:78:VAL:HG22	1.54	0.72
1:A:67:PHE:HB2	1:A:92:LEU:HD13	1.71	0.72
4:D:385:GLN:HB2	4:D:429:VAL:HG13	1.70	0.72
3:C:119:LEU:HD11	3:C:156:ARG:HB3	1.71	0.71
1:A:297:GLU:HG2	1:A:339:ARG:HH22	1.55	0.71
2:B:83:PHE:O	2:B:86:ILE:HG22	1.90	0.71
3:C:93:ILE:HD11	3:C:121:ARG:HG3	1.71	0.70
4:D:142:GLY:HA3	10:X:509:GDP:H4'	1.74	0.69
3:C:70:LEU:HD13	3:C:110:ILE:CG2	2.22	0.69
5:E:48:GLU:HG2	5:E:52:LYS:HE3	1.75	0.69
1:A:63:PRO:CG	1:A:86:LEU:HD21	2.23	0.68
1:A:329:ASN:HB3	5:E:6:MET:HE1	1.75	0.68
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.74	0.68
2:B:75:MET:HE3	2:B:94:PHE:HB3	1.76	0.67
3:C:175:PRO:HA	3:C:179:THR:CG2	2.25	0.67
4:D:63:PRO:HD3	4:D:86:ILE:HG12	1.75	0.67
6:F:219:GLY:HA3	6:F:264:PHE:CZ	2.30	0.67
6:F:320:MET:HE1	12:X:512:ACP:N3	2.09	0.67
4:D:105:LYS:HD3	4:D:110:GLU:HG3	1.78	0.66
4:D:191:VAL:HG11	4:D:425:MET:HE2	1.78	0.66
1:A:4:CYS:SG	1:A:252:LEU:HD21	2.35	0.66
1:A:371:VAL:HG12	1:A:373:ARG:H	1.61	0.66
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.79	0.65
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.31	0.64
4:D:171:VAL:HA	4:D:204:ILE:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:292:THR:HG22	4:D:335:VAL:HG21	1.78	0.64
4:D:2:ARG:HB3	4:D:133:GLN:HE21	1.63	0.63
4:D:214:PHE:O	4:D:218:LYS:HA	1.99	0.63
4:D:103:TRP:CE3	4:D:189:LEU:HD13	2.34	0.63
4:D:204:ILE:HD13	4:D:231:VAL:HG13	1.79	0.63
6:F:128:ARG:NE	6:F:170:LEU:HD22	2.12	0.63
3:C:175:PRO:HA	3:C:179:THR:HG21	1.81	0.63
6:F:209:HIS:CD2	6:F:210:LEU:HG	2.35	0.62
1:A:293:ASN:ND2	1:A:339:ARG:HH21	1.98	0.62
6:F:246:GLN:O	6:F:253:TYR:HB2	1.98	0.62
2:B:287:THR:HG22	2:B:290:GLU:CG	2.29	0.62
3:C:216:ASN:HB3	3:C:275:VAL:O	2.00	0.62
6:F:374:ILE:HD11	6:F:375:PHE:CE2	2.34	0.62
1:A:357:TYR:CD2	5:E:17:GLY:HA2	2.34	0.62
2:B:317:ALA:C	2:B:318:ILE:HD12	2.19	0.62
2:B:287:THR:HG23	2:B:290:GLU:H	1.63	0.61
4:D:118:VAL:CG2	4:D:153:LEU:HD21	2.29	0.61
3:C:12:ALA:O	3:C:16:ILE:HG12	2.00	0.61
4:D:269[B]:MET:CE	4:D:305:CYS:HB2	2.30	0.61
4:D:269[B]:MET:HE1	4:D:305:CYS:HB2	1.83	0.61
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.36	0.60
4:D:141:LEU:HD12	4:D:172:MET:HE3	1.81	0.60
1:A:63:PRO:HG2	1:A:86:LEU:HD21	1.83	0.60
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.32	0.60
3:C:165:SER:HA	3:C:199:ASP:OD2	2.02	0.60
1:A:285:GLN:HG3	1:A:372[B]:GLN:OE1	2.01	0.60
2:B:274:PRO:HB3	2:B:286:LEU:HD12	1.84	0.60
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.17	0.60
2:B:191:VAL:O	2:B:195:VAL:HG23	2.02	0.60
2:B:318:ILE:HD11	11:X:506:COL:C16	2.32	0.60
6:F:91:CYS:SG	6:F:93:TRP:CD2	2.96	0.59
6:F:165:GLU:HG2	6:F:167:SER:H	1.68	0.59
6:F:14:TYR:HB3	6:F:41:LEU:HD13	1.85	0.59
1:A:190:THR:O	1:A:194:THR:HG22	2.03	0.58
3:C:180:ALA:HB1	4:D:258:ASN:OD1	2.03	0.58
2:B:370:GLY:O	2:B:371:LEU:HD23	2.03	0.58
1:A:324:VAL:HG23	1:A:327:ASP:H	1.68	0.58
4:D:188:THR:HG22	4:D:421:ALA:HB1	1.86	0.58
4:D:6:HIS:CD2	4:D:21:TRP:HE1	2.22	0.58
6:F:148:ILE:HB	6:F:162:ILE:HG23	1.85	0.58
4:D:396:THR:O	4:D:400:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:ARG:HD2	3:C:439:SER:HB3	1.87	0.57
3:C:166:LYS:HE2	3:C:197:HIS:O	2.04	0.57
3:C:271:THR:HG23	3:C:300:ASN:O	2.04	0.57
2:B:163:ASP:O	2:B:253:ARG:NH2	2.37	0.57
1:A:322:ASP:O	1:A:373:ARG:NH1	2.36	0.57
4:D:20:PHE:CZ	4:D:24:ILE:HD13	2.39	0.57
3:C:440:VAL:HG12	3:C:440:VAL:O	2.05	0.57
2:B:292:THR:HG22	2:B:319:PHE:CZ	2.40	0.56
1:A:227:LEU:O	1:A:231:ILE:HG13	2.06	0.56
4:D:318:ILE:HG13	4:D:354:ALA:HB3	1.87	0.56
5:E:96:MET:O	5:E:100:LYS:HB2	2.06	0.56
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.87	0.56
4:D:358:ILE:O	4:D:358:ILE:HG13	2.04	0.56
4:D:141:LEU:HD12	4:D:172:MET:CE	2.35	0.56
3:C:75:ILE:HD12	3:C:94:THR:CG2	2.35	0.56
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	1.87	0.56
4:D:180:THR:HG22	4:D:181:VAL:N	2.20	0.56
4:D:220:THR:O	4:D:222:PRO:HD3	2.06	0.56
6:F:202:ARG:HB3	6:F:220:VAL:CG1	2.36	0.56
4:D:118:VAL:O	4:D:122:VAL:HG13	2.05	0.56
2:B:308:ARG:HG2	2:B:342:TYR:CE2	2.41	0.55
3:C:209:ILE:HD11	3:C:302:MET:SD	2.46	0.55
4:D:244:PHE:CZ	4:D:358:ILE:HD11	2.40	0.55
6:F:214:TYR:HB3	6:F:375:PHE:HB3	1.87	0.55
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.87	0.55
2:B:1:MET:HE1	2:B:50[B]:ASN:HB2	1.88	0.55
3:C:18:ASN:ND2	3:C:78:VAL:HG22	2.20	0.55
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.89	0.55
1:A:325:PRO:O	1:A:329:ASN:ND2	2.40	0.55
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.07	0.55
6:F:149:ALA:CB	6:F:182:ILE:HG12	2.35	0.55
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.71	0.54
3:C:361:THR:HG22	3:C:362:VAL:N	2.22	0.54
3:C:21:TRP:CZ3	3:C:63:PRO:HB3	2.42	0.54
4:D:69:ASP:HA	4:D:145:THR:HG21	1.90	0.54
1:A:88:HIS:N	1:A:91:GLN:OE1	2.36	0.54
1:A:167:LEU:HD22	1:A:252:LEU:HD12	1.89	0.54
5:E:60:ARG:O	5:E:64:GLN:HG3	2.08	0.54
2:B:151:THR:HA	2:B:154:ILE:HD12	1.90	0.54
5:E:51:GLN:O	5:E:55:GLU:HG3	2.08	0.54
4:D:332:MET:O	4:D:336:GLN:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22[A]:GLU:OE2	2:B:82:PRO:HG2	2.08	0.53
6:F:21:LEU:HD22	6:F:27:TRP:CD2	2.43	0.53
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.90	0.53
3:C:218:ASP:OD2	3:C:280:LYS:HE3	2.09	0.53
3:C:259:LEU:O	3:C:380:ASN:ND2	2.39	0.53
4:D:115:VAL:O	4:D:119:LEU:HG	2.08	0.53
1:A:289:ALA:HA	1:A:331:ALA:HB2	1.91	0.53
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.74	0.53
3:C:254:GLU:HG2	3:C:352:LYS:HE2	1.90	0.53
4:D:108:TYR:O	5:E:134:ARG:NH1	2.41	0.53
1:A:151:SER:HB2	1:A:193:THR:CG2	2.37	0.53
1:A:437:VAL:HG12	1:A:438:ASP:N	2.23	0.53
6:F:74:LYS:HE3	6:F:331:GLU:OE1	2.09	0.53
4:D:20:PHE:CD1	4:D:235:MET:HE2	2.43	0.53
4:D:141:LEU:HD12	4:D:172:MET:SD	2.49	0.53
4:D:9:ALA:O	4:D:13:GLY:HA3	2.08	0.53
6:F:8:ASP:HB2	6:F:43:GLU:HA	1.91	0.53
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.44	0.53
3:C:70:LEU:HD13	3:C:110:ILE:HG22	1.89	0.53
2:B:22[B]:GLU:HG3	2:B:83:PHE:CE1	2.44	0.52
3:C:190:THR:O	3:C:194[B]:THR:HG23	2.09	0.52
4:D:288:VAL:HG12	4:D:331:GLN:HG3	1.91	0.52
2:B:220:THR:HG23	2:B:221:THR:HG22	1.91	0.52
4:D:103:TRP:HB2	4:D:186:ASN:OD1	2.09	0.52
6:F:73:ARG:HB2	6:F:76[B]:SER:OG	2.09	0.52
4:D:2:ARG:HB3	4:D:133:GLN:NE2	2.24	0.52
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.44	0.52
2:B:286:LEU:HD22	2:B:290:GLU:CB	2.39	0.52
2:B:295:MET:SD	2:B:375:ALA:HB1	2.49	0.52
3:C:187:SER:HB3	3:C:391:LEU:HD21	1.91	0.52
3:C:317:LEU:HD23	3:C:377:MET:HG3	1.92	0.52
2:B:69:ASP:HA	2:B:145:THR:HG21	1.93	0.51
4:D:183:GLU:OE2	10:X:509:GDP:H3'	2.10	0.51
6:F:146:VAL:HG23	6:F:187:GLU:OE2	2.10	0.51
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.30	0.51
3:C:36:MET:HB3	3:C:61:HIS:CE1	2.45	0.51
4:D:324:SER:OG	4:D:327:GLU:HB2	2.10	0.51
2:B:286:LEU:HD22	2:B:290:GLU:HB3	1.92	0.51
3:C:69:ASP:O	3:C:94:THR:HA	2.10	0.51
4:D:165:ILE:HA	4:D:199:ASP:OD2	2.10	0.51
2:B:346:TRP:HE1	2:B:438:ALA:CB	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:OD2	2:B:33:THR:HG22	2.10	0.51
3:C:293[B]:ASN:CG	3:C:335:ILE:HD11	2.31	0.51
4:D:26:ASP:OD2	4:D:369:ARG:HD3	2.11	0.51
4:D:269[A]:MET:CE	4:D:305:CYS:HB2	2.41	0.51
2:B:352:LYS:HG3	11:X:506:COL:C4	2.41	0.51
4:D:180:THR:HG22	4:D:182:VAL:H	1.74	0.51
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.93	0.51
6:F:32:LYS:HG3	6:F:33:ASP:N	2.25	0.50
3:C:271:THR:HG21	3:C:295[B]:CYS:HA	1.93	0.50
6:F:21:LEU:HD22	6:F:27:TRP:CE2	2.46	0.50
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.25	0.50
1:A:107:HIS:CD2	1:A:152:LEU:HB2	2.46	0.50
1:A:191:THR:O	1:A:195:LEU:HB2	2.12	0.50
2:B:238:VAL:HG22	2:B:378:ILE:HD11	1.94	0.50
4:D:1:MET:O	4:D:131:CYS:HB3	2.11	0.50
2:B:7:ILE:O	2:B:137:LEU:HA	2.12	0.50
2:B:269:MET:HE1	2:B:301:MET:HG3	1.94	0.50
3:C:115:ILE:HG23	3:C:116:ASP:N	2.26	0.50
3:C:210:TYR:CE1	3:C:222:PRO:HD2	2.46	0.50
5:E:132:GLU:O	5:E:136:ASN:HB2	2.11	0.50
1:A:79:ARG:NH2	1:A:94:THR:HG21	2.26	0.50
2:B:1:MET:HB2	2:B:3:GLU:OE2	2.12	0.50
3:C:175:PRO:HA	3:C:179:THR:HG22	1.94	0.50
2:B:137:LEU:CD2	2:B:154:ILE:HD11	2.42	0.50
6:F:148:ILE:HG12	6:F:150:LYS:HG2	1.92	0.50
4:D:287:THR:OG1	4:D:289:PRO:HD2	2.11	0.49
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.94	0.49
2:B:180:THR:HA	3:C:258:ASN:HD21	1.75	0.49
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.95	0.49
3:C:46:ASP:OD1	3:C:46:ASP:N	2.43	0.49
4:D:67:LEU:N	4:D:67:LEU:HD12	2.27	0.49
2:B:1:MET:HE1	2:B:50[A]:ASN:HB3	1.93	0.49
4:D:20:PHE:O	4:D:24:ILE:HG12	2.13	0.49
2:B:67:LEU:N	2:B:67:LEU:HD12	2.27	0.49
1:A:36:MET:HB3	1:A:61:HIS:NE2	2.27	0.49
6:F:304:THR:HG21	6:F:311:SER:HB2	1.95	0.49
3:C:119:LEU:HD11	3:C:156:ARG:CB	2.42	0.49
2:B:287:THR:HG22	2:B:290:GLU:HG3	1.92	0.49
2:B:295:MET:CG	2:B:377:PHE:HB2	2.43	0.49
6:F:339:ALA:HB3	6:F:342:LEU:CD1	2.39	0.49
4:D:138:THR:HG22	4:D:169:PHE:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:297:ASP:OD1	4:D:298:SER:N	2.46	0.49
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.41	0.49
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.48	0.49
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.48	0.49
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.95	0.49
2:B:346:TRP:HE1	2:B:438:ALA:HB3	1.78	0.49
3:C:186:ASN:O	3:C:190:THR:HG22	2.12	0.49
4:D:5:VAL:HB	4:D:135:PHE:CD2	2.48	0.49
1:A:255:PHE:O	1:A:259:LEU:HB2	2.13	0.48
2:B:274:PRO:HB3	2:B:286:LEU:CD1	2.42	0.48
2:B:318:ILE:HD12	2:B:318:ILE:N	2.28	0.48
3:C:99:ALA:HB3	3:C:144:GLY:HA3	1.95	0.48
3:C:271:THR:HG21	3:C:295[A]:CYS:HA	1.94	0.48
6:F:102:PRO:HB3	6:F:173:ILE:CG2	2.44	0.48
6:F:205:VAL:CG2	6:F:291:ILE:HD13	2.43	0.48
2:B:191:VAL:HG11	2:B:425:MET:HE2	1.96	0.48
2:B:202:TYR:CZ	2:B:238:VAL:HG11	2.49	0.48
3:C:108:TYR:O	3:C:112:LYS:HG2	2.13	0.48
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.48	0.48
3:C:174:ALA:HB1	3:C:207:GLU:HB2	1.95	0.48
1:A:252:LEU:HD22	1:A:252:LEU:H	1.78	0.48
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.48
4:D:287:THR:CB	4:D:289:PRO:HD2	2.44	0.48
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.94	0.48
1:A:180:ALA:HB1	2:B:258:ASN:OD1	2.12	0.48
1:A:339:ARG:HB2	1:A:341:ILE:HD11	1.96	0.48
3:C:70:LEU:HD13	3:C:110:ILE:HG21	1.93	0.48
6:F:102:PRO:HA	6:F:173:ILE:HG22	1.96	0.48
6:F:168:GLU:OE1	6:F:168:GLU:N	2.39	0.48
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.96	0.47
1:A:336:LYS:HD3	1:A:336:LYS:O	2.14	0.47
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.49	0.47
2:B:31:ASP:CG	2:B:33:THR:HG22	2.34	0.47
4:D:172:MET:HE2	4:D:387:LEU:HD21	1.96	0.47
4:D:347:ILE:HG22	4:D:350:ASN:HB3	1.95	0.47
2:B:357:ASP:O	2:B:359:PRO:HD3	2.14	0.47
4:D:269[A]:MET:HE1	4:D:305:CYS:HB2	1.97	0.47
6:F:250:SER:C	6:F:253:TYR:H	2.17	0.47
1:A:115:ILE:HG23	1:A:116:ASP:N	2.30	0.47
6:F:3:THR:HB	6:F:30:LEU:HD11	1.97	0.47
1:A:2:ARG:O	1:A:51[A]:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:VAL:HB	4:D:425:MET:CE	2.45	0.47
4:D:191:VAL:O	4:D:195:VAL:HG23	2.14	0.47
4:D:314:THR:HB	11:X:511:COL:C6	2.43	0.47
1:A:383:ALA:O	1:A:386:GLU:HG3	2.14	0.47
1:A:209[B]:ILE:HG13	1:A:227:LEU:HD22	1.96	0.47
3:C:71:GLU:HG2	3:C:98:ASP:HB3	1.96	0.47
6:F:36:ARG:HA	6:F:58:LEU:CD1	2.44	0.47
1:A:71:GLU:OE1	1:A:73:THR:HG22	2.15	0.46
4:D:177:VAL:HG12	4:D:177:VAL:O	2.15	0.46
4:D:381:SER:O	4:D:384[B]:ILE:HG22	2.15	0.46
4:D:402:LYS:HE2	4:D:415:GLU:OE2	2.14	0.46
1:A:91:GLN:C	1:A:92:LEU:HD22	2.36	0.46
1:A:175:PRO:HA	1:A:179:THR:OG1	2.15	0.46
4:D:136:GLN:HA	4:D:167:ASN:O	2.15	0.46
6:F:148:ILE:HG23	6:F:148:ILE:O	2.16	0.46
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.97	0.46
4:D:295:MET:HG3	4:D:377:PHE:HB2	1.97	0.46
2:B:1:MET:HE1	2:B:50[B]:ASN:CB	2.45	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
6:F:280:GLU:HA	6:F:284[B]:LEU:HB2	1.97	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.51	0.46
3:C:363:VAL:HG23	3:C:364:PRO:HD2	1.97	0.46
4:D:36:TYR:CD1	4:D:46:LEU:HD21	2.50	0.46
3:C:249:ASN:ND2	3:C:356[A]:ASN:OD1	2.49	0.46
4:D:159:GLU:HG3	5:E:123:LEU:HD13	1.98	0.46
2:B:75:MET:HG2	2:B:94:PHE:CD2	2.51	0.46
2:B:287:THR:CG2	2:B:290:GLU:H	2.28	0.46
4:D:154:ILE:HG23	4:D:166:MET:HG2	1.98	0.46
6:F:253:TYR:OH	6:F:259:GLY:HA2	2.17	0.45
1:A:335:ILE:C	1:A:335:ILE:HD12	2.37	0.45
4:D:115:VAL:HG23	4:D:153:LEU:CD2	2.47	0.45
4:D:7:ILE:O	4:D:137:LEU:HA	2.16	0.45
4:D:414:ASP:OD2	4:D:416:MET:HB2	2.16	0.45
6:F:186:LEU:HD12	6:F:320:MET:HG2	1.99	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.45
6:F:195:GLY:O	6:F:227:PRO:HB3	2.16	0.45
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.98	0.45
1:A:341:ILE:N	1:A:341:ILE:HD12	2.32	0.45
2:B:335:VAL:O	2:B:339:ASN:ND2	2.41	0.45
3:C:217:LEU:HD21	3:C:368:LEU:HD23	1.99	0.45
4:D:409:THR:O	5:E:140:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.99	0.45
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.99	0.45
4:D:161:TYR:HB3	4:D:164:ARG:CG	2.47	0.45
4:D:301:MET:C	4:D:303:ALA:H	2.20	0.45
1:A:23:LEU:O	1:A:27:GLU:HG3	2.17	0.45
6:F:253:TYR:CZ	6:F:259:GLY:HA2	2.52	0.45
6:F:267:PHE:CD2	6:F:279:LEU:HD13	2.51	0.45
3:C:177:VAL:CG2	3:C:206:ASN:HB3	2.45	0.45
4:D:244:PHE:CZ	4:D:358:ILE:CD1	3.00	0.45
6:F:165:GLU:HB3	6:F:168:GLU:OE2	2.17	0.45
1:A:2:ARG:NE	1:A:251:ASP:HB3	2.32	0.44
6:F:168:GLU:HG2	6:F:169:LEU:N	2.32	0.44
6:F:202:ARG:NH2	6:F:222:ARG:HH12	2.15	0.44
2:B:1:MET:HE1	2:B:50[A]:ASN:CB	2.46	0.44
6:F:37:PHE:O	6:F:60:GLN:HG2	2.18	0.44
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.00	0.44
4:D:119:LEU:O	4:D:122:VAL:HG22	2.18	0.44
5:E:53:LYS:HE2	5:E:53:LYS:HB3	1.84	0.44
3:C:285:GLN:OE1	3:C:372:GLN:NE2	2.50	0.44
1:A:75:ILE:CG2	1:A:92:LEU:HD12	2.45	0.44
1:A:287:SER:OG	1:A:290:GLU:HG3	2.17	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
3:C:172:TYR:HB3	3:C:205:ASP:HA	2.00	0.44
4:D:295:MET:CG	4:D:377:PHE:HB2	2.48	0.44
2:B:42:LEU:HD12	2:B:358:ILE:HD11	1.99	0.44
2:B:172:MET:HE2	2:B:172:MET:HB3	1.92	0.44
5:E:6:MET:HG2	5:E:24:LEU:CD2	2.48	0.44
6:F:205:VAL:HG21	6:F:291:ILE:HD13	2.00	0.44
6:F:299:GLU:N	6:F:300:PRO:HD2	2.33	0.44
4:D:117:SER:O	4:D:121:VAL:HG23	2.17	0.44
4:D:48:ARG:HD3	4:D:48:ARG:HA	1.77	0.43
6:F:148:ILE:HG13	6:F:162:ILE:HG12	1.98	0.43
3:C:183:GLU:N	3:C:184:PRO:CD	2.82	0.43
3:C:234:ILE:HD12	3:C:234:ILE:N	2.33	0.43
5:E:48:GLU:O	5:E:52:LYS:HG3	2.18	0.43
1:A:217:LEU:HD21	1:A:275:VAL:HG12	2.00	0.43
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.53	0.43
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.33	0.43
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.43
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.01	0.43
4:D:35:SER:OG	4:D:60:LYS:HE3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:LYS:NZ	6:F:97:SER:O	2.48	0.43
1:A:234:ILE:O	1:A:238:ILE:HG13	2.19	0.43
1:A:411:GLU:O	5:E:61:ARG:HD3	2.18	0.43
2:B:63:PRO:HD3	2:B:86:ILE:HG12	2.00	0.43
2:B:275:LEU:HD23	2:B:275:LEU:HA	1.76	0.43
2:B:287:THR:HG22	2:B:290:GLU:CB	2.48	0.43
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.19	0.43
6:F:37:PHE:HZ	6:F:52:LEU:CD2	2.32	0.43
6:F:238:CYS:HG	6:F:239:HIS:CE1	2.35	0.43
6:F:172:PHE:HD1	6:F:172:PHE:O	2.01	0.43
6:F:284[A]:LEU:HD12	6:F:284[A]:LEU:HA	1.78	0.43
2:B:305:CYS:O	2:B:307:PRO:HD3	2.19	0.43
3:C:388:TRP:HA	3:C:388:TRP:CE3	2.54	0.43
6:F:2:TYR:CE1	6:F:359:PHE:HB3	2.53	0.43
1:A:55:GLU:HA	1:A:60:LYS:O	2.18	0.43
2:B:287:THR:HG22	2:B:290:GLU:HB2	2.00	0.43
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.59	0.42
5:E:75:LYS:O	5:E:79:GLU:HG3	2.19	0.42
2:B:286:LEU:HD23	2:B:286:LEU:HA	1.84	0.42
4:D:9:ALA:HA	4:D:68:VAL:O	2.19	0.42
4:D:258:ASN:HB3	11:X:511:COL:C4	2.49	0.42
1:A:100:ALA:HA	2:B:254:LYS:CG	2.49	0.42
1:A:285:GLN:OE1	1:A:285:GLN:N	2.51	0.42
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.37	0.42
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.42
3:C:72:PRO:CG	4:D:1:MET:CE	2.96	0.42
4:D:114:LEU:HG	4:D:114:LEU:O	2.18	0.42
4:D:208:ALA:O	4:D:212:ILE:HG13	2.19	0.42
6:F:18:SER:O	6:F:22:LEU:HG	2.19	0.42
1:A:39:ASP:OD2	1:A:61:HIS:HE1	2.03	0.42
4:D:50:ASN:HD22	4:D:50:ASN:H	1.68	0.42
4:D:212:ILE:O	4:D:216:THR:HB	2.19	0.42
6:F:24:THR:HG22	6:F:26:GLN:HG3	2.02	0.42
4:D:317:ALA:O	4:D:353:THR:HA	2.20	0.42
2:B:20:PHE:CE2	2:B:24:ILE:HD13	2.55	0.42
1:A:93:ILE:HD11	1:A:121:ARG:CG	2.45	0.42
1:A:319:TYR:HB3	1:A:323:VAL:HG21	2.01	0.42
1:A:345:ASP:HB3	5:E:28:SER:HB2	2.01	0.42
3:C:277:SER:OG	3:C:280:LYS:HG3	2.20	0.42
4:D:292:THR:CG2	4:D:335:VAL:HG21	2.46	0.42
5:E:76:ARG:HA	5:E:76:ARG:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:264:ARG:NE	4:D:431:GLU:OE2	2.52	0.41
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.86	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.41
4:D:102:ASN:HD22	4:D:105:LYS:HG3	1.84	0.41
4:D:165:ILE:HG21	4:D:252:LEU:HB3	2.02	0.41
5:E:47:LEU:HD23	5:E:47:LEU:O	2.21	0.41
6:F:21:LEU:HD21	6:F:355:ILE:HG21	2.03	0.41
6:F:38:ASN:O	6:F:60:GLN:HA	2.20	0.41
6:F:95:PRO:HB2	6:F:183:GLN:CG	2.50	0.41
1:A:209[A]:ILE:HG22	1:A:227:LEU:CD2	2.49	0.41
3:C:22:GLU:O	3:C:26:LEU:HG	2.20	0.41
3:C:117:LEU:HD21	3:C:121:ARG:NH2	2.35	0.41
3:C:178:SER:HB2	3:C:224:TYR:OH	2.20	0.41
3:C:361:THR:CG2	3:C:362:VAL:N	2.84	0.41
3:C:153:LEU:O	3:C:157:LEU:HG	2.20	0.41
4:D:414:ASP:N	4:D:414:ASP:OD1	2.53	0.41
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.50	0.41
1:A:151:SER:HB2	1:A:193:THR:HG22	2.00	0.41
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	2.01	0.41
3:C:72:PRO:HG2	4:D:1:MET:CE	2.51	0.41
3:C:255:PHE:CD1	3:C:316:CYS:HB3	2.56	0.41
6:F:168:GLU:O	6:F:172:PHE:HB2	2.21	0.41
3:C:304:LYS:HE3	3:C:304:LYS:HB2	1.95	0.41
4:D:115:VAL:HG23	4:D:153:LEU:HD23	2.02	0.41
4:D:172:MET:HG3	4:D:387:LEU:HD11	2.02	0.41
4:D:270:PRO:HA	4:D:377:PHE:O	2.20	0.41
6:F:224:SER:HB2	6:F:241:THR:HG22	2.03	0.41
1:A:132:LEU:O	1:A:164:LYS:NZ	2.51	0.41
1:A:358:GLN:HA	1:A:359:PRO:HD3	1.95	0.41
4:D:291:LEU:HD12	4:D:291:LEU:HA	1.86	0.41
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	2.02	0.41
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.92	0.41
1:A:437:VAL:CG1	1:A:438:ASP:N	2.84	0.41
3:C:72:PRO:HG2	4:D:1:MET:HE1	2.03	0.41
5:E:6:MET:HE3	5:E:6:MET:HB3	1.84	0.41
6:F:24:THR:CG2	6:F:361:LEU:HD13	2.50	0.41
3:C:66:VAL:HG12	3:C:68[A]:VAL:HG23	2.02	0.41
6:F:252:ASN:ND2	6:F:255:ARG:HD2	2.36	0.41
6:F:279:LEU:HG	6:F:284[B]:LEU:HG	2.03	0.41
6:F:340:GLN:HA	6:F:343:TYR:HD2	1.86	0.41
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:MET:HE2	4:D:235:MET:HB3	1.94	0.40
1:A:133:GLN:HB2	1:A:252:LEU:HD23	2.04	0.40
1:A:183:GLU:N	1:A:184:PRO:CD	2.85	0.40
1:A:192:HIS:NE2	1:A:420[A]:GLU:HG2	2.36	0.40
6:F:24:THR:HG23	6:F:361:LEU:HD13	2.03	0.40
3:C:195:LEU:HD12	3:C:266:HIS:CE1	2.57	0.40
4:D:387:LEU:HD23	4:D:387:LEU:C	2.41	0.40
6:F:24:THR:HG22	6:F:26:GLN:H	1.86	0.40
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.57	0.40
4:D:145:THR:O	4:D:149:MET:HB3	2.20	0.40
2:B:205:ASP:HB3	2:B:303:ALA:HA	2.03	0.40
4:D:287:THR:HB	4:D:289:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/439 (102%)	431 (96%)	17 (4%)	2 (0%)	34	72
2	B	428/423 (101%)	406 (95%)	21 (5%)	1 (0%)	47	82
3	C	448/440 (102%)	432 (96%)	15 (3%)	1 (0%)	47	82
4	D	421/421 (100%)	400 (95%)	20 (5%)	1 (0%)	47	82
5	E	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
6	F	310/320 (97%)	288 (93%)	22 (7%)	0	100	100
All	All	2175/2164 (100%)	2073 (95%)	97 (4%)	5 (0%)	47	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	177	VAL

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Mol	Chain	Res	Type
1	A	178	SER
4	D	74	THR
2	B	73	GLY
1	A	131	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/370 (103%)	379 (99%)	3 (1%)	81	93
2	B	374/366 (102%)	374 (100%)	0	100	100
3	C	381/371 (103%)	379 (100%)	2 (0%)	88	96
4	D	367/364 (101%)	367 (100%)	0	100	100
5	E	110/109 (101%)	106 (96%)	4 (4%)	35	70
6	F	294/289 (102%)	282 (96%)	12 (4%)	30	67
All	All	1908/1869 (102%)	1887 (99%)	21 (1%)	73	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	133	GLN
1	A	284	GLU
3	C	71	GLU
3	C	245	ASP
5	E	6	MET
5	E	8	VAL
5	E	62	LYS
5	E	103	GLN
6	F	1	MET
6	F	33	ASP
6	F	91	CYS
6	F	125	THR
6	F	162	ILE

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Mol	Chain	Res	Type
6	F	163	SER
6	F	172	PHE
6	F	211	TYR
6	F	222	ARG
6	F	249	TYR
6	F	257	GLU
6	F	311	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
2	B	167	ASN
4	D	136	GLN
4	D	167	ASN
6	F	333	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic and 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GTP	X	501	8	26,34,34	1.00	2 (7%)	32,54,54	0.72	1 (3%)
10	GDP	X	504	8	24,30,30	1.00	2 (8%)	30,47,47	0.66	1 (3%)
7	GTP	X	507	8	26,34,34	1.01	2 (7%)	32,54,54	0.69	1 (3%)
10	GDP	X	509	8	24,30,30	1.00	3 (12%)	30,47,47	0.68	1 (3%)
12	ACP	X	512	-	27,33,33	0.91	1 (3%)	32,52,52	0.97	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GTP	X	501	8	-	4/18/38/38	0/3/3/3
10	GDP	X	504	8	-	4/12/32/32	0/3/3/3
7	GTP	X	507	8	-	5/18/38/38	0/3/3/3
10	GDP	X	509	8	-	5/12/32/32	0/3/3/3
12	ACP	X	512	-	-	6/15/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	509	GDP	C5-C6	-2.78	1.41	1.47
7	X	507	GTP	C5-C6	-2.72	1.41	1.47
10	X	504	GDP	C5-C6	-2.69	1.41	1.47
7	X	501	GTP	C5-C6	-2.67	1.42	1.47
12	X	512	ACP	PB-O2B	-2.44	1.50	1.56
7	X	507	GTP	C8-N7	-2.15	1.31	1.35
10	X	509	GDP	C8-N7	-2.12	1.31	1.35
10	X	504	GDP	C8-N7	-2.11	1.31	1.35
7	X	501	GTP	C8-N7	-2.10	1.31	1.35
10	X	509	GDP	C5-C4	-2.01	1.37	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	X	512	ACP	O1G-PG-C3B	-2.53	105.80	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	X	512	ACP	C3'-C2'-C1'	2.43	104.63	100.98
12	X	512	ACP	C5-C6-N6	2.19	123.67	120.35
10	X	509	GDP	O6-C6-C5	2.09	128.46	124.37
7	X	507	GTP	O6-C6-C5	2.06	128.39	124.37
7	X	501	GTP	O6-C6-C5	2.06	128.39	124.37
10	X	504	GDP	O6-C6-C5	2.05	128.37	124.37

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	501	GTP	C5'-O5'-PA-O1A
7	X	507	GTP	C5'-O5'-PA-O1A
10	X	504	GDP	C5'-O5'-PA-O1A
10	X	509	GDP	C5'-O5'-PA-O1A
12	X	512	ACP	PG-C3B-PB-O1B
12	X	512	ACP	PG-C3B-PB-O2B
12	X	512	ACP	PG-C3B-PB-O3A
12	X	512	ACP	C5'-O5'-PA-O3A
12	X	512	ACP	PB-O3A-PA-O5'
10	X	509	GDP	C5'-O5'-PA-O3A
10	X	509	GDP	PB-O3A-PA-O2A
7	X	501	GTP	C5'-O5'-PA-O2A
7	X	507	GTP	C5'-O5'-PA-O2A
10	X	504	GDP	C5'-O5'-PA-O2A
10	X	509	GDP	C5'-O5'-PA-O2A
12	X	512	ACP	C5'-O5'-PA-O1A
7	X	501	GTP	PB-O3B-PG-O3G
7	X	507	GTP	PB-O3B-PG-O3G
7	X	501	GTP	C5'-O5'-PA-O3A
7	X	507	GTP	C5'-O5'-PA-O3A
10	X	504	GDP	C5'-O5'-PA-O3A
7	X	507	GTP	PB-O3A-PA-O1A
10	X	504	GDP	PB-O3A-PA-O2A
10	X	509	GDP	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	509	GDP	2	0

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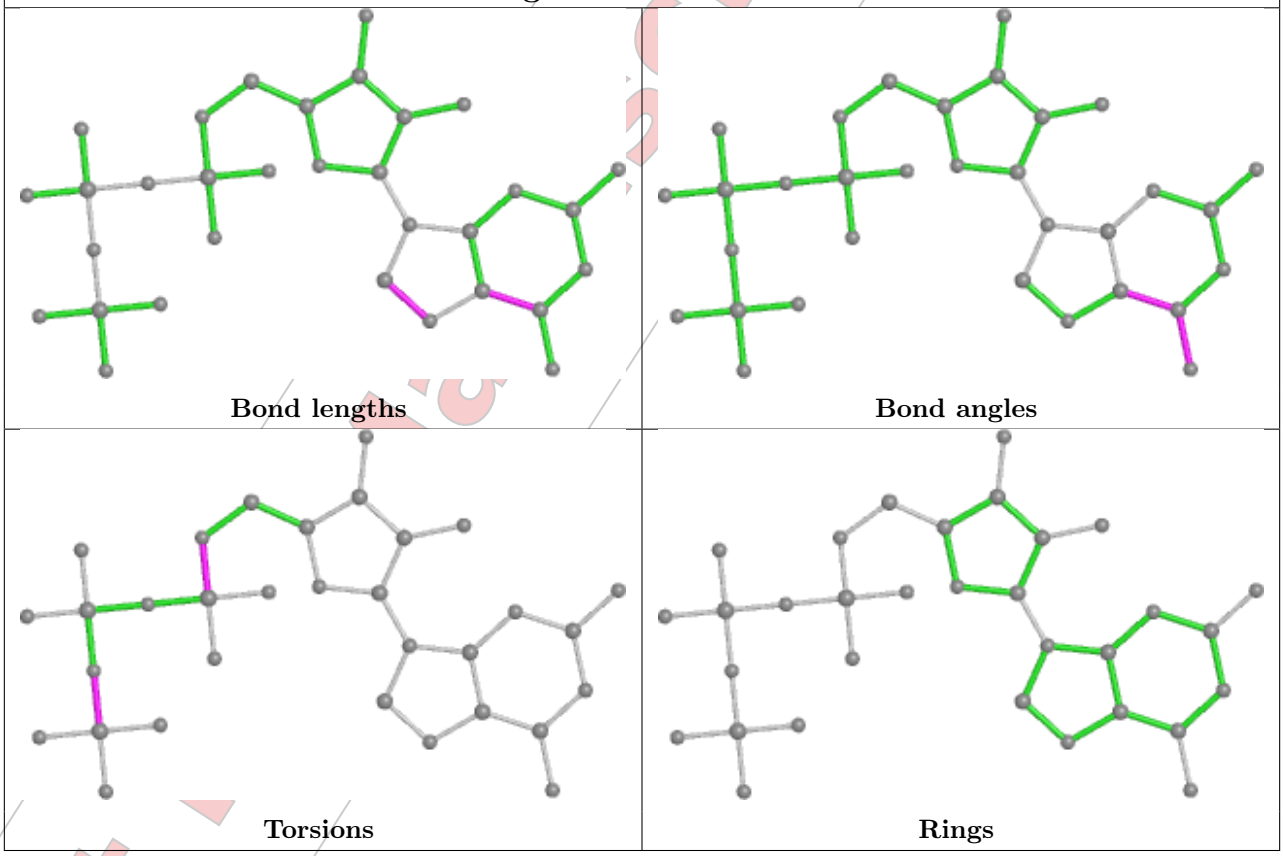
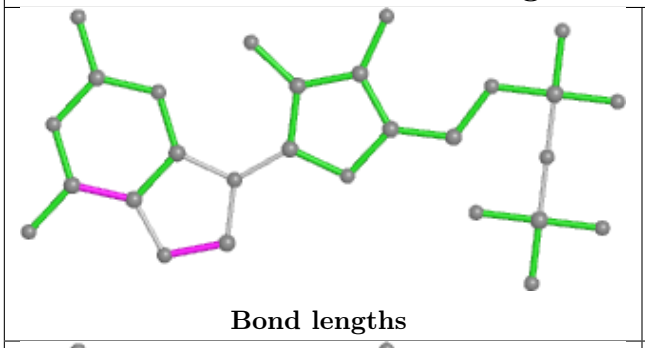
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	X	512	ACP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

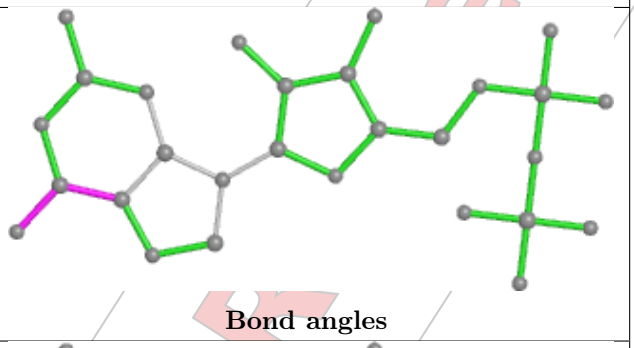
Ligand GTP X 501



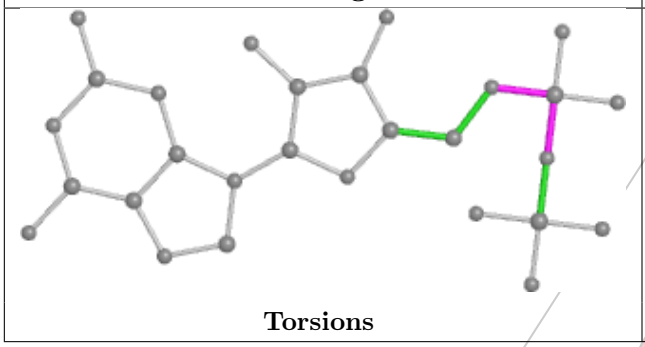
Ligand GDP X 504



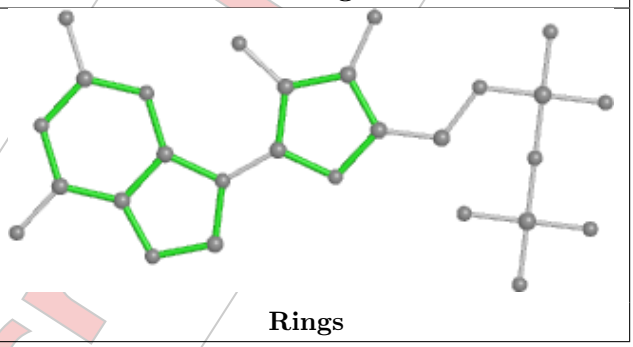
Bond lengths



Bond angles

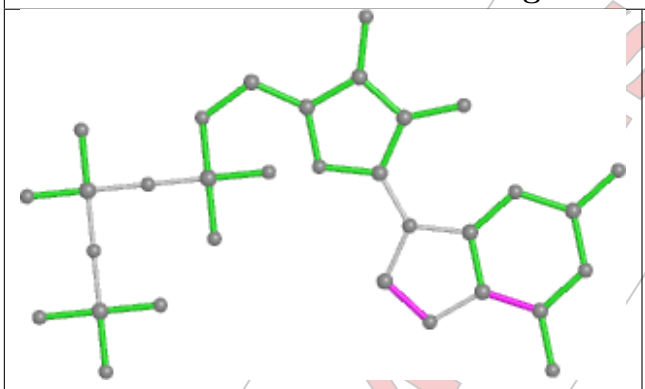


Torsions

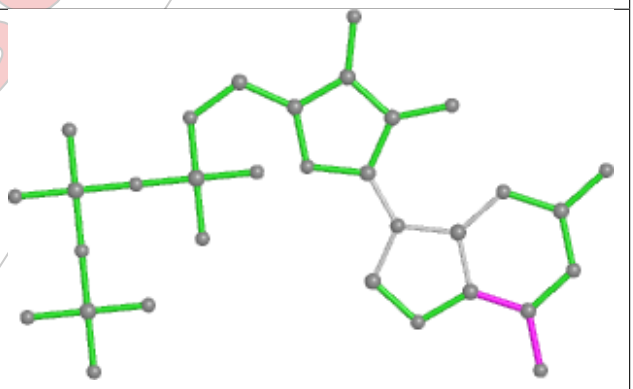


Rings

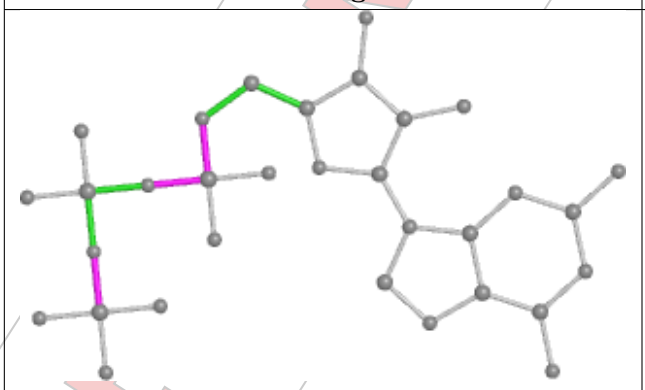
Ligand GTP X 507



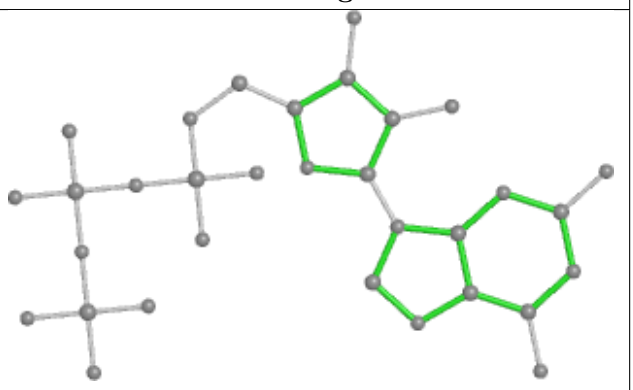
Bond lengths



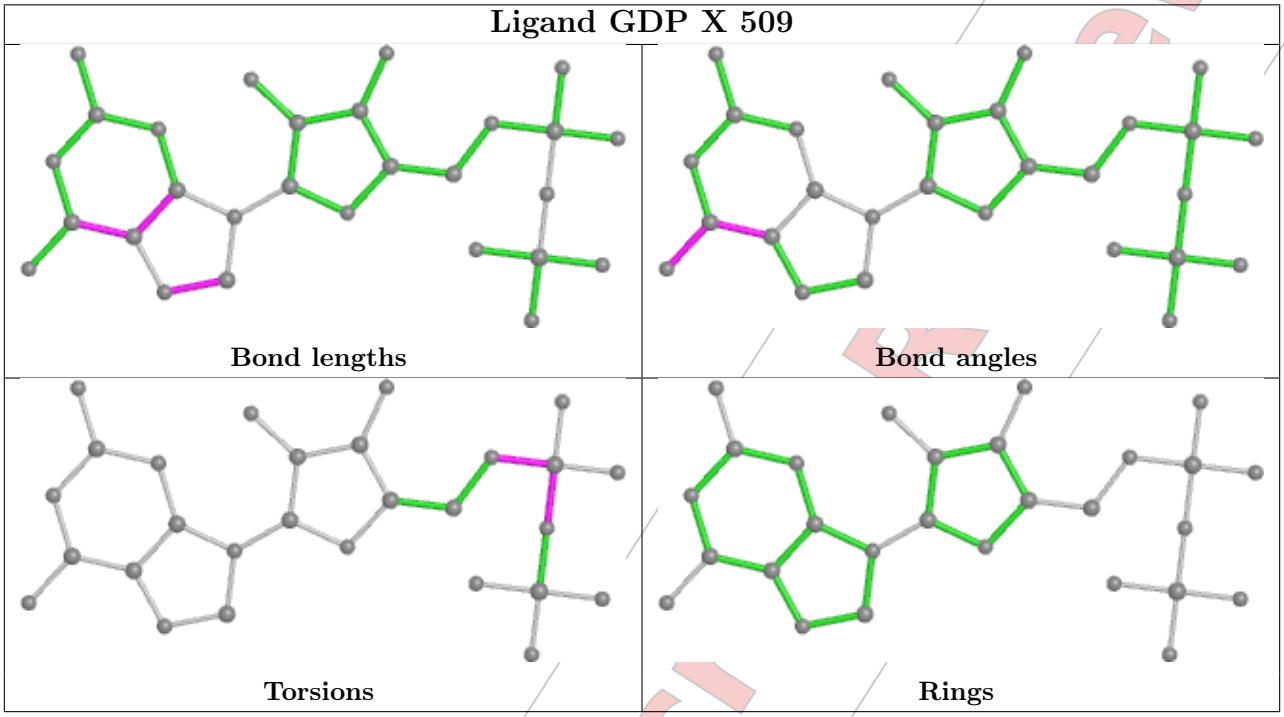
Bond angles

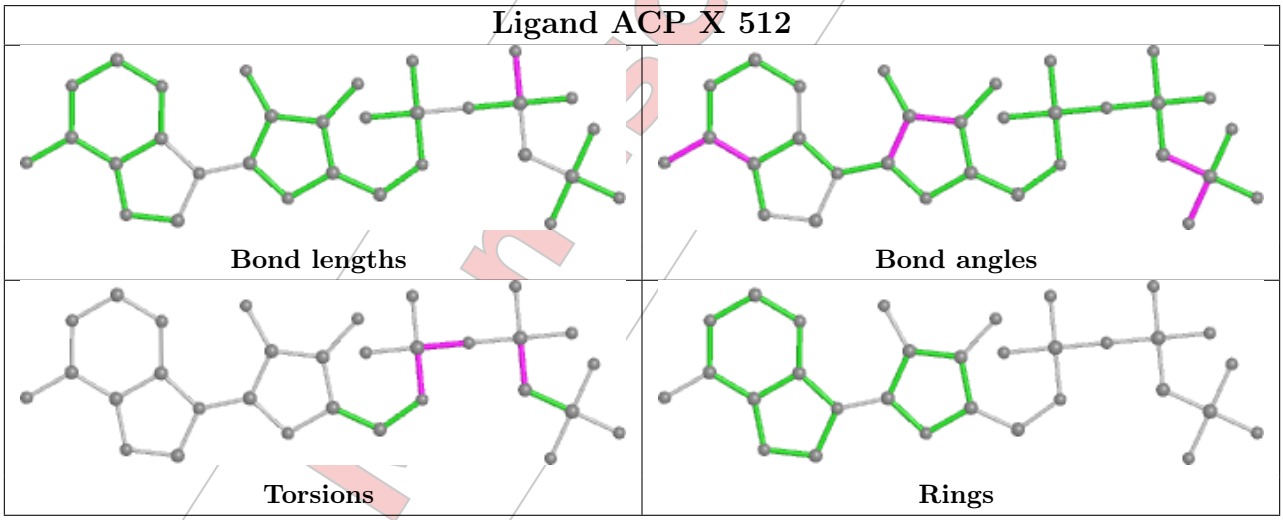


Torsions



Rings





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	6
5	E	1

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Mol	Chain	Number of breaks
4	D	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.70
1	F	362:ALA	C	373:SER	N	19.68
1	F	102:PRO	C	125:THR	N	12.42
1	F	151:SER	C	162:ILE	N	11.70
1	D	275:LEU	C	286:LEU	N	11.66
1	F	136:ASN	C	144:GLY	N	11.08
1	B	276:THR	C	282:GLN	N	8.40
1	F	173:ILE	C	179:VAL	N	8.40
1	F	231:ALA	C	235:ASP	N	6.52

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

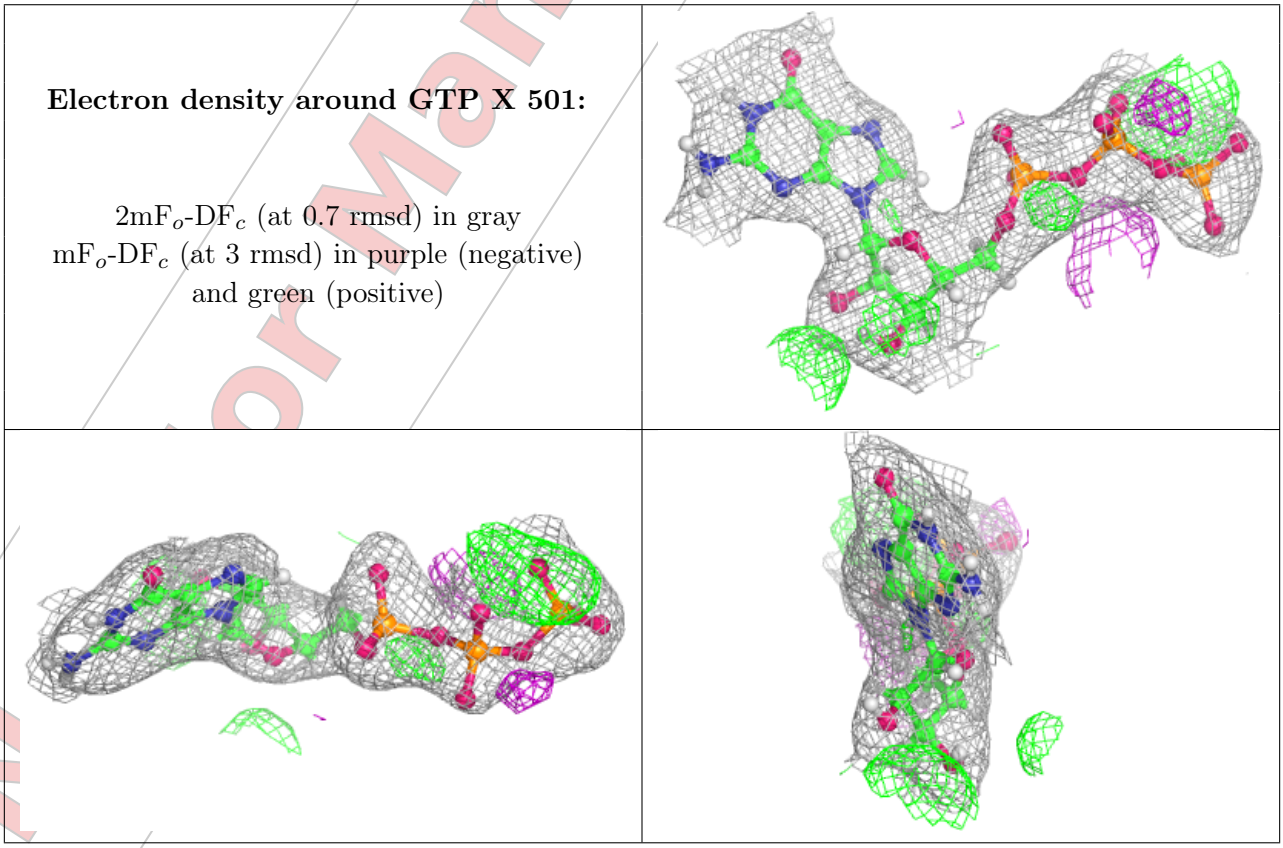
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

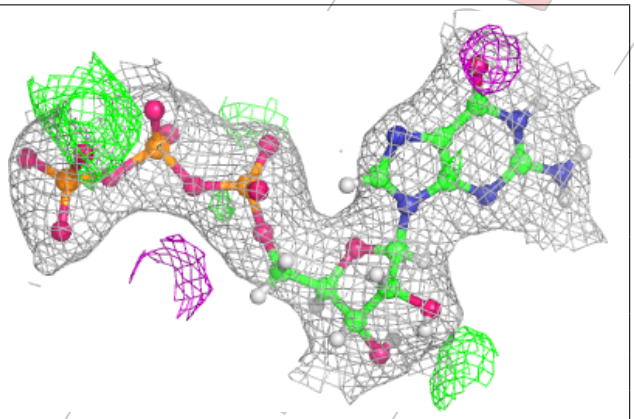
Electron density around GTP X 501:

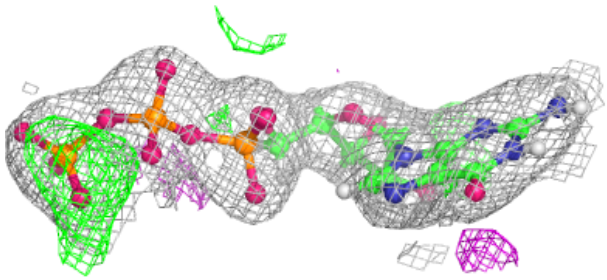
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

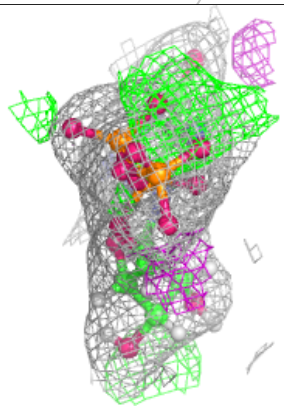


Electron density around GTP X 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

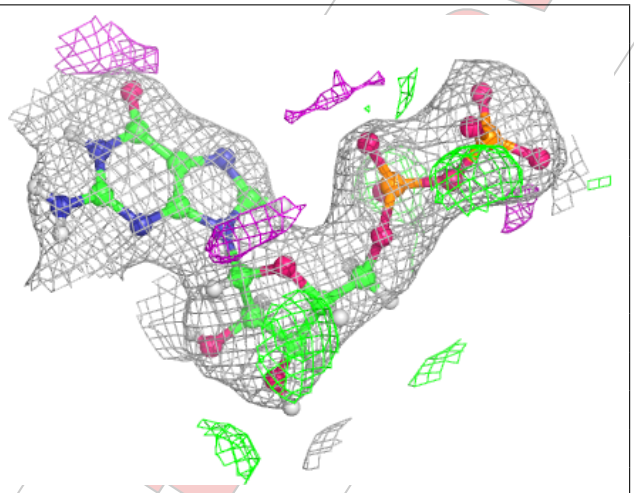


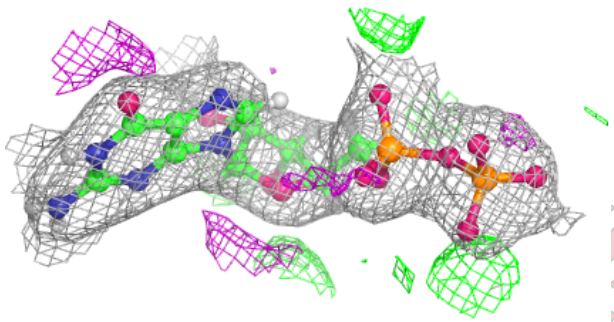


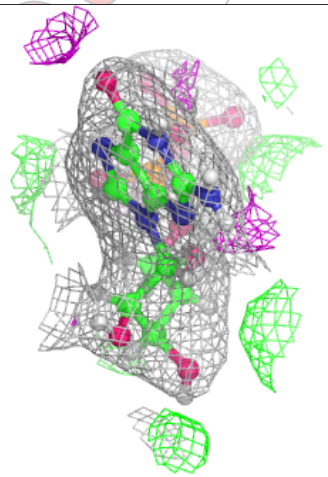


Electron density around GDP X 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

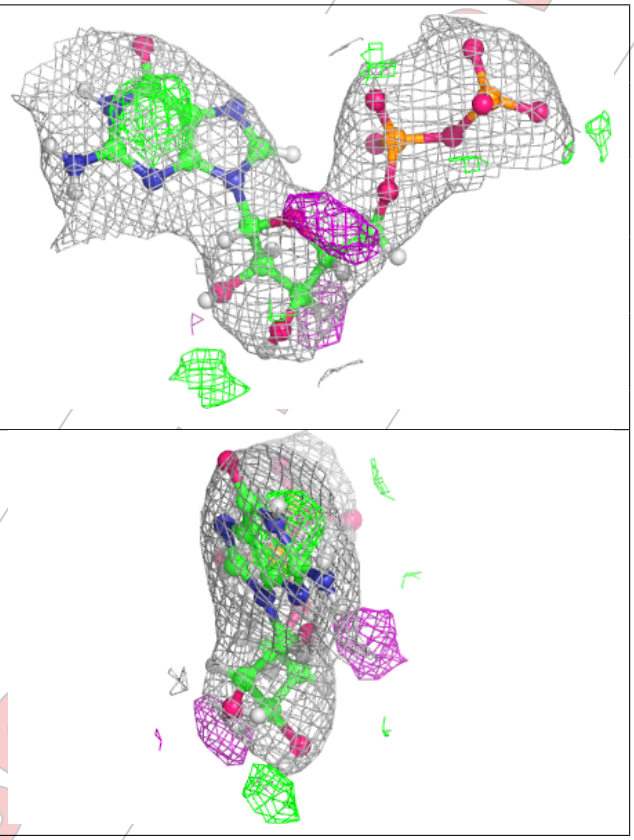






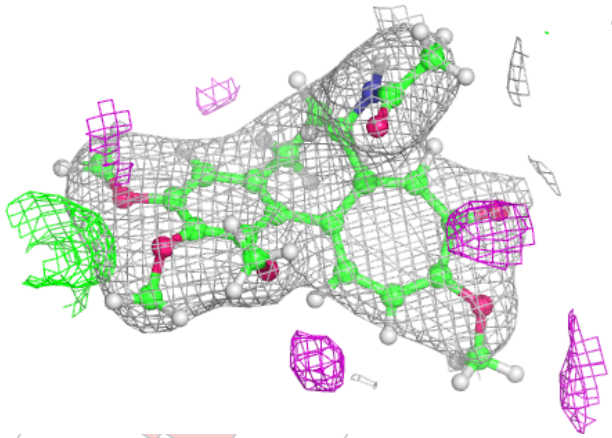
Electron density around GDP X 509:

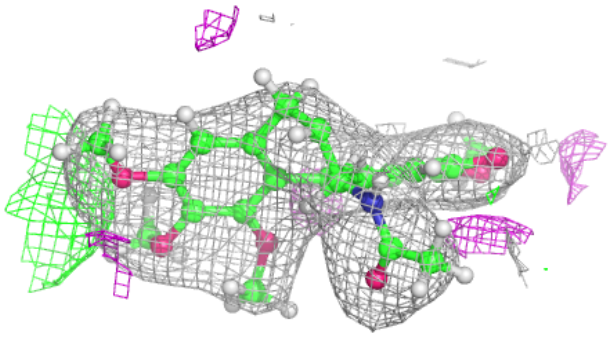
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

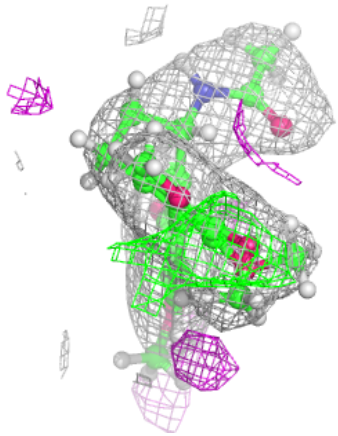


Electron density around COL X 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

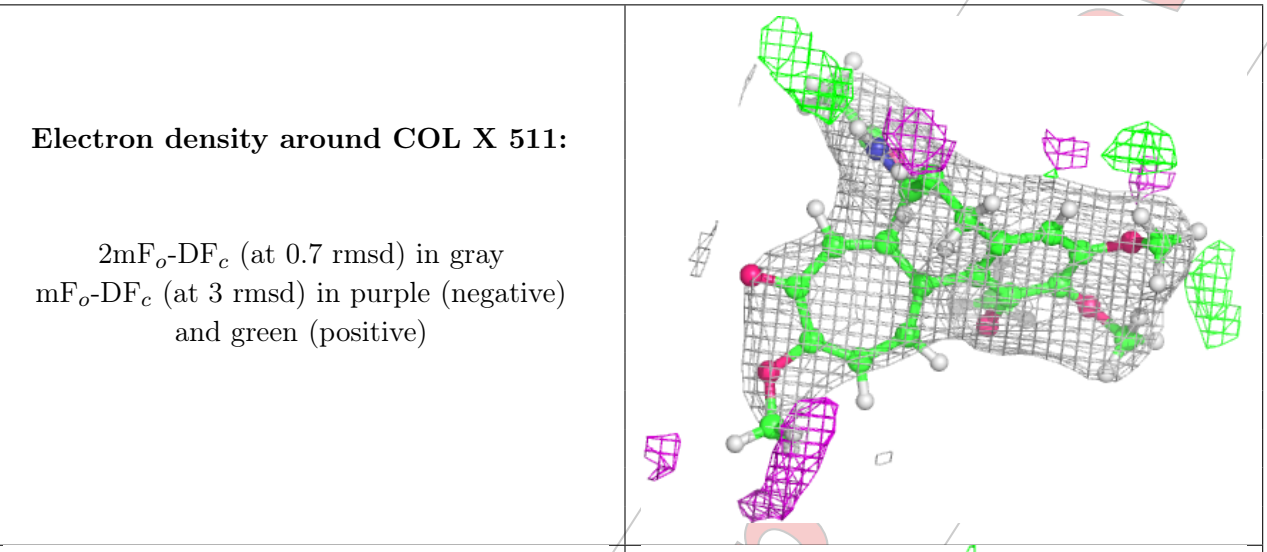


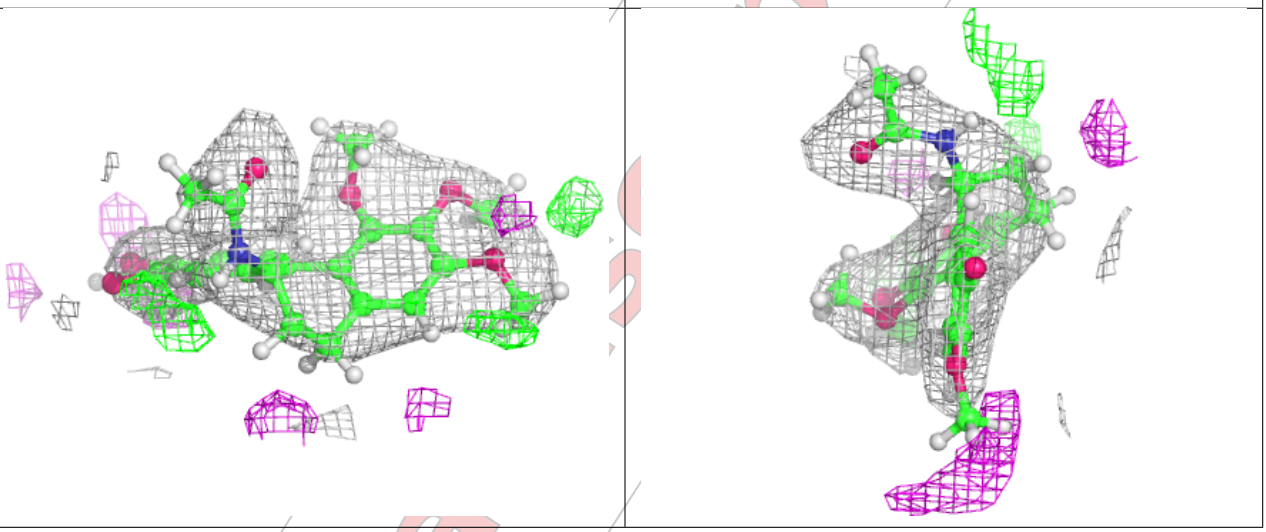




Electron density around COL X 511:

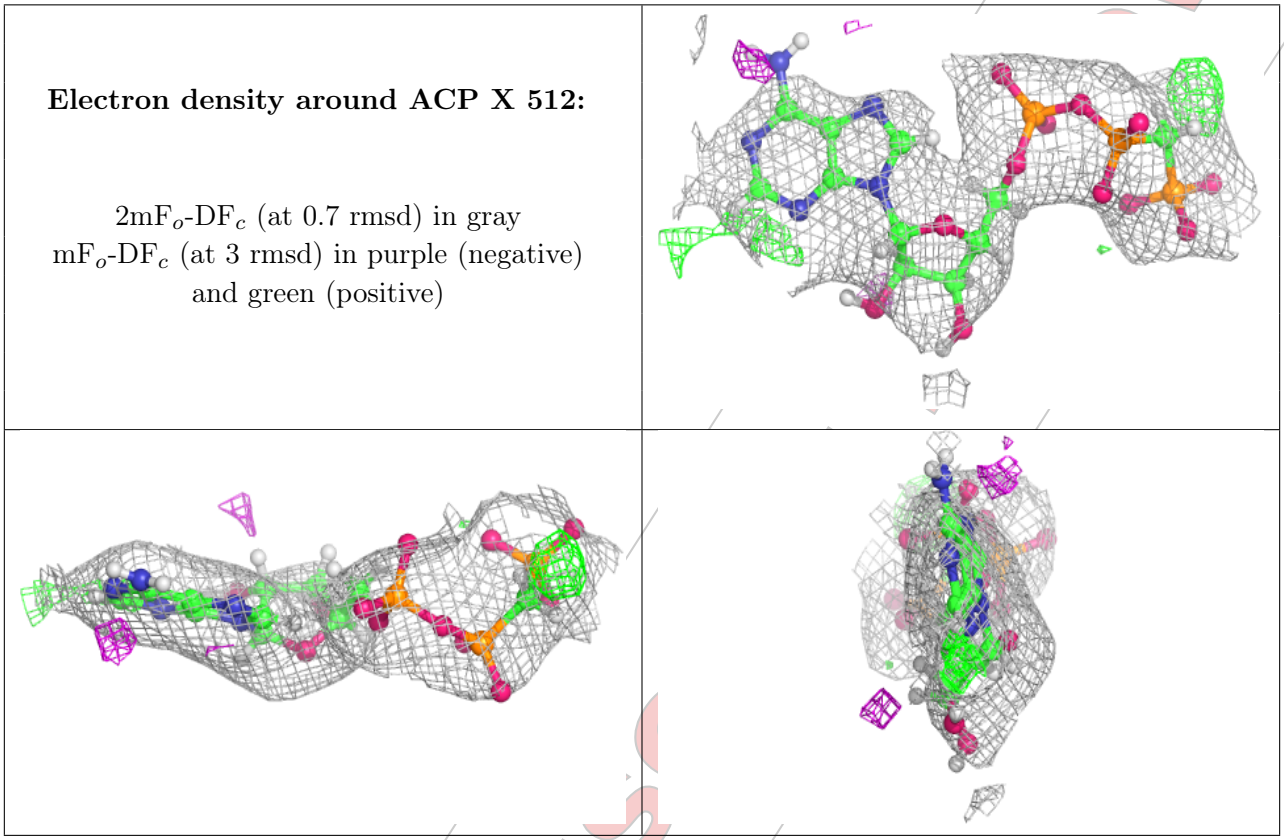
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around ACP X 512:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2023 – 06:12 pm GMT

Deposition ID : D_1292128578

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

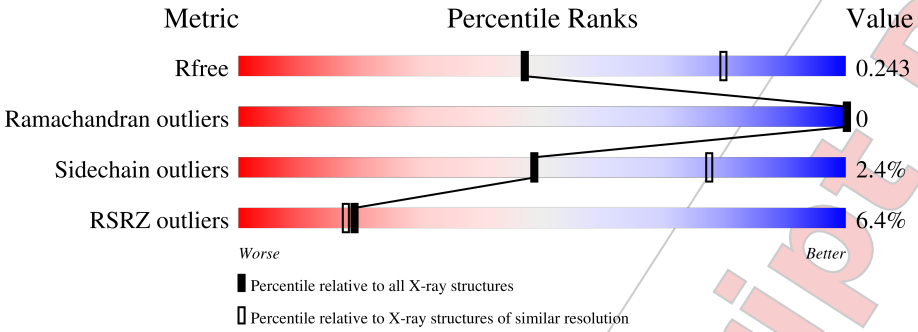
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	4% 99% .
2	B	425	4% 99% .
3	C	440	% 98% .
4	D	427	6% 98% .
5	E	123	11% 97% .
6	F	332	17% 95% 5%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17569 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3436	2173	584	656	23	0	1	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3360	2111	574	649	26	2	2	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	440	3440	2177	584	656	23	0	1	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	427	3358	2107	574	651	26	2	1	0

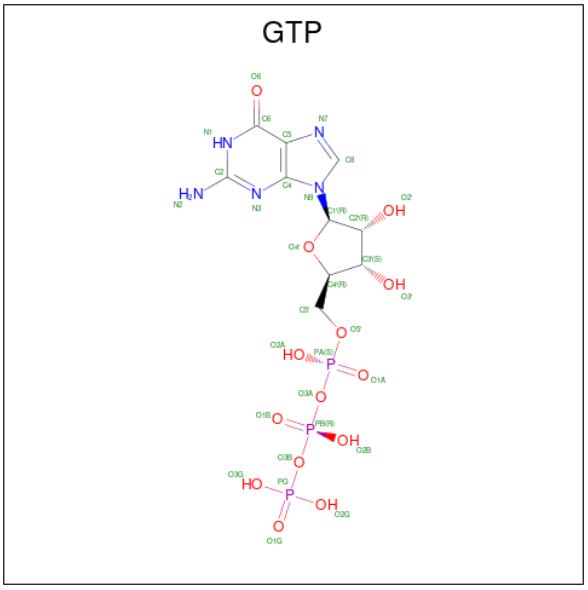
- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	123	1014	625	183	201	5	0	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	332	Total	C	N	O	S	0	1	0
			2714	1740	464	495	15			

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
7	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		

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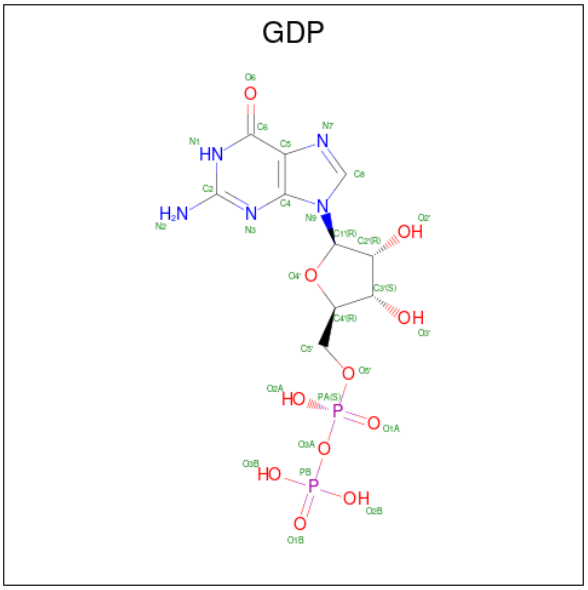
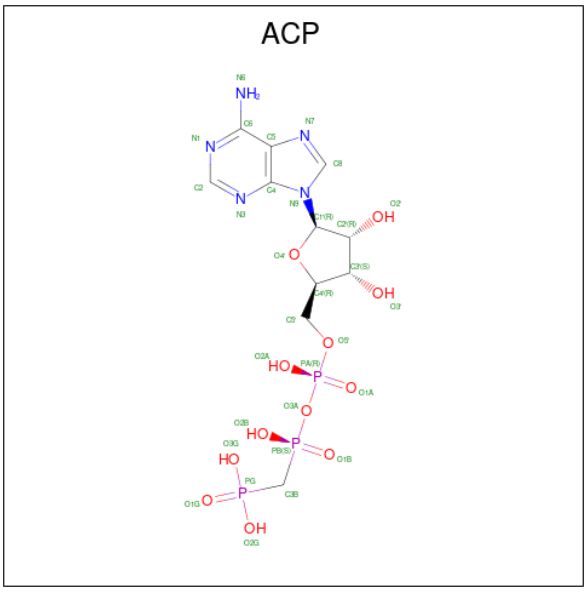
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Ca 1 1	0	0

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O P 28 10 5 11 2	0	0
10	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

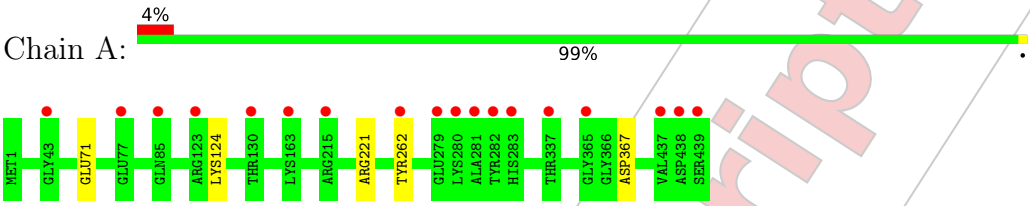
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	S	91	Total	O	0	0
			91	91		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

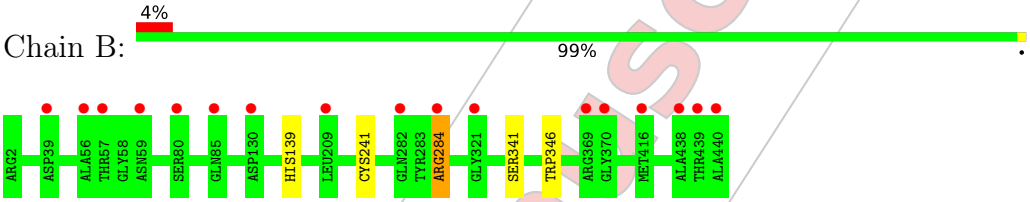
- Molecule 1:

Chain A:



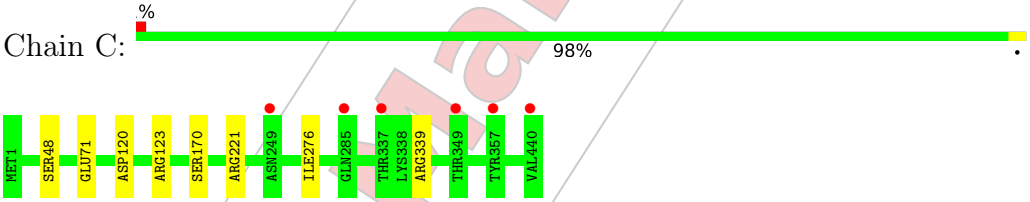
- Molecule 2:

Chain B:



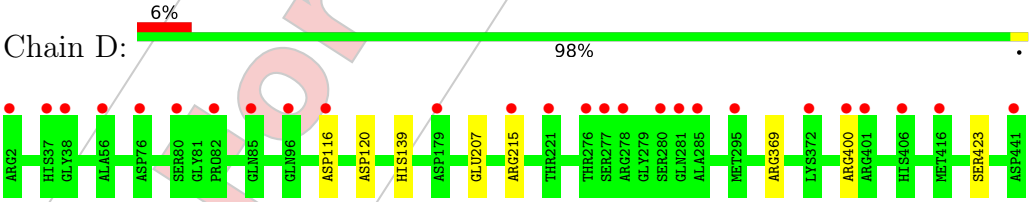
- Molecule 3:

Chain C:



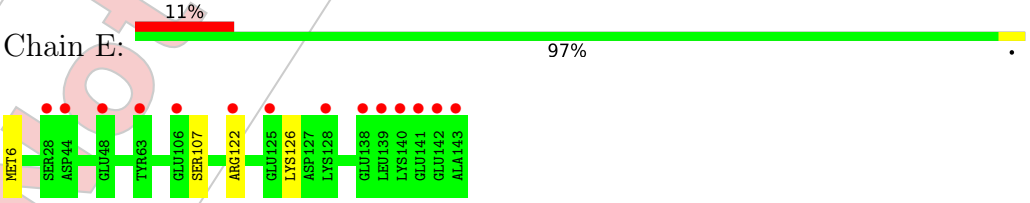
- Molecule 4:

Chain D:



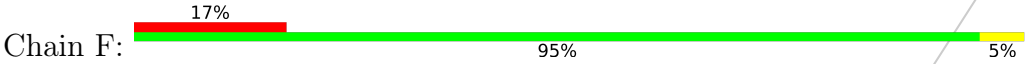
- Molecule 5:

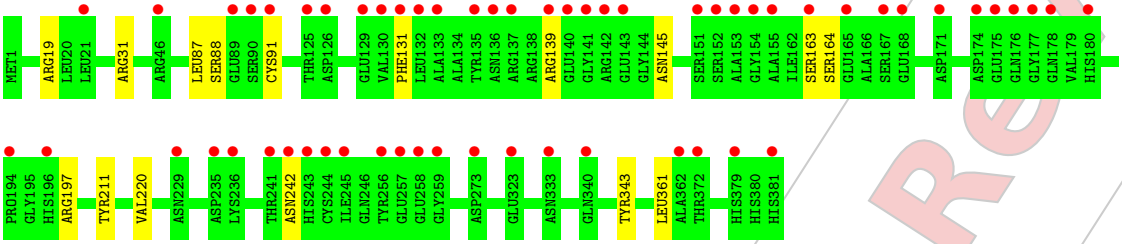
Chain E:



• Molecule 6:

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.53Å 160.48Å 181.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.20 – 2.70 15.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.20-2.70) 99.9 (15.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.69Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.186 , 0.234 0.198 , 0.243	Depositor DCC
R_{free} test set	627 reflections (0.74%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 79.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17569	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACP, GTP, MG, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/3514	0.50	0/4770
2	B	0.28	0/3437	0.48	0/4655
3	C	0.26	0/3521	0.47	0/4780
4	D	0.27	0/3431	0.47	0/4645
5	E	0.23	0/1022	0.41	0/1356
6	F	0.27	0/2777	0.49	0/3750
All	All	0.27	0/17702	0.48	0/23956

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	284	ARG	Sidechain
3	C	221	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3436	0	3343	0	0
2	B	3360	0	3238	0	0
3	C	3440	0	3353	0	0
4	D	3358	0	3232	0	0
5	E	1014	0	1029	0	0
6	F	2714	0	2682	0	0
7	A	32	0	12	0	0
7	C	32	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	0	0
11	F	31	0	14	0	0
12	S	91	0	0	0	0
All	All	17569	0	16939	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/439 (100%)	423 (97%)	15 (3%)	0	100	100
2	B	423/425 (100%)	409 (97%)	14 (3%)	0	100	100
3	C	439/440 (100%)	425 (97%)	14 (3%)	0	100	100
4	D	423/427 (99%)	406 (96%)	17 (4%)	0	100	100
5	E	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
6	F	321/332 (97%)	302 (94%)	19 (6%)	0	100	100
All	All	2163/2186 (99%)	2082 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/370 (100%)	366 (99%)	5 (1%)	69	87
2	B	369/367 (100%)	364 (99%)	5 (1%)	67	86
3	C	372/371 (100%)	365 (98%)	7 (2%)	57	82
4	D	367/368 (100%)	359 (98%)	8 (2%)	52	79
5	E	110/110 (100%)	106 (96%)	4 (4%)	35	64
6	F	298/297 (100%)	282 (95%)	16 (5%)	22	47
All	All	1887/1883 (100%)	1842 (98%)	45 (2%)	49	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	124	LYS
1	A	221	ARG
1	A	262	TYR
1	A	367	ASP
2	B	139	HIS
2	B	241	CYS

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Mol	Chain	Res	Type
2	B	284	ARG
2	B	341	SER
2	B	346	TRP
3	C	48	SER
3	C	71	GLU
3	C	120	ASP
3	C	123	ARG
3	C	170	SER
3	C	276	ILE
3	C	339	ARG
4	D	116	ASP
4	D	120	ASP
4	D	139	HIS
4	D	207	GLU
4	D	215	ARG
4	D	369	ARG
4	D	400	ARG
4	D	423	SER
5	E	6	MET
5	E	107	SER
5	E	122	ARG
5	E	126	LYS
6	F	19	ARG
6	F	31	ARG
6	F	87	LEU
6	F	88	SER
6	F	91	CYS
6	F	131	PHE
6	F	139	ARG
6	F	145	ASN
6	F	163	SER
6	F	164	SER
6	F	197	ARG
6	F	211	TYR
6	F	220	VAL
6	F	242	ASN
6	F	343	TYR
6	F	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	285	GLN
1	A	301	GLN
2	B	424	ASN
3	C	133	GLN
3	C	256	GLN
4	D	50	ASN
4	D	101	ASN
5	E	51	GLN
5	E	91	ASN
6	F	348	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GTP	C	501	8	26,34,34	1.01	2 (7%)	32,54,54	0.68	1 (3%)
7	GTP	A	501	8	26,34,34	1.01	2 (7%)	32,54,54	0.69	1 (3%)
11	ACP	F	401	-	27,33,33	0.91	1 (3%)	32,52,52	0.82	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	GDP	B	501	8	24,30,30	1.00	2 (8%)	30,47,47	0.65	1 (3%)
10	GDP	D	501	-	24,30,30	0.98	2 (8%)	30,47,47	0.68	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GTP	C	501	8	-	6/18/38/38	0/3/3/3
7	GTP	A	501	8	-	5/18/38/38	0/3/3/3
11	ACP	F	401	-	-	4/15/38/38	0/3/3/3
10	GDP	B	501	8	-	3/12/32/32	0/3/3/3
10	GDP	D	501	-	-	2/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	501	GTP	C5-C6	-2.72	1.41	1.47
10	D	501	GDP	C5-C6	-2.71	1.41	1.47
10	B	501	GDP	C5-C6	-2.68	1.42	1.47
7	C	501	GTP	C5-C6	-2.67	1.42	1.47
11	F	401	ACP	PB-O2B	-2.46	1.50	1.56
7	C	501	GTP	C8-N7	-2.16	1.31	1.35
10	B	501	GDP	C8-N7	-2.14	1.31	1.35
7	A	501	GTP	C8-N7	-2.10	1.31	1.35
10	D	501	GDP	C8-N7	-2.08	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	401	ACP	C5-C6-N6	2.27	123.81	120.35
11	F	401	ACP	O1G-PG-C3B	-2.11	106.69	111.24
7	C	501	GTP	O6-C6-C5	2.07	128.41	124.37
7	A	501	GTP	O6-C6-C5	2.07	128.41	124.37
10	D	501	GDP	O6-C6-C5	2.06	128.39	124.37
10	B	501	GDP	O6-C6-C5	2.03	128.33	124.37

There are no chirality outliers.

All (20) torsion outliers are listed below:

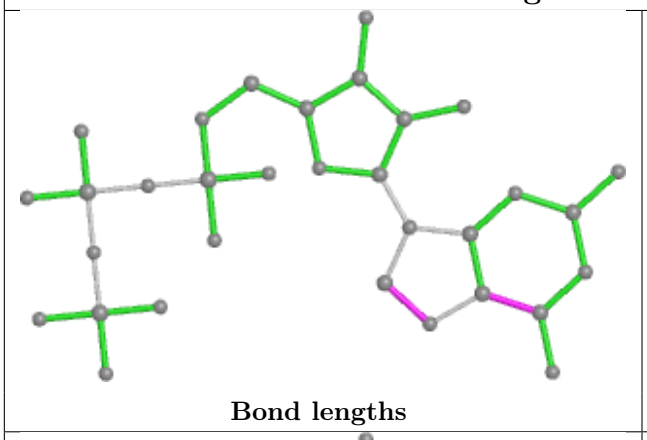
Mol	Chain	Res	Type	Atoms
7	A	501	GTP	C5'-O5'-PA-O1A
7	C	501	GTP	PB-O3B-PG-O3G
7	C	501	GTP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-C3B-PG-O1G
7	A	501	GTP	PB-O3B-PG-O2G
7	A	501	GTP	PB-O3B-PG-O3G
7	A	501	GTP	C5'-O5'-PA-O3A
7	C	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
7	A	501	GTP	C5'-O5'-PA-O2A
7	C	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-C3B-PG-O2G
10	B	501	GDP	C5'-O5'-PA-O3A
7	C	501	GTP	PB-O3A-PA-O1A
7	C	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A

There are no ring outliers.

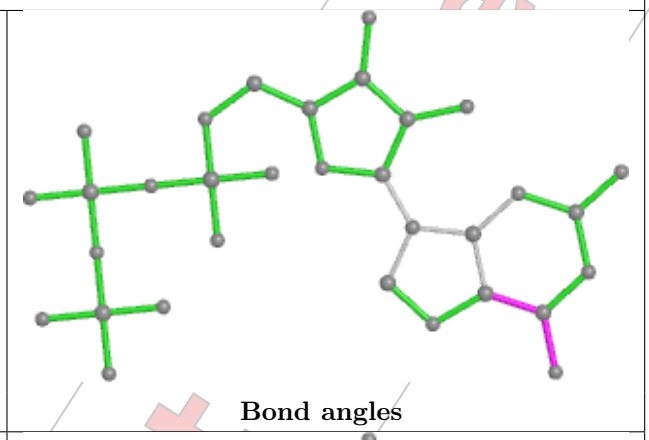
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

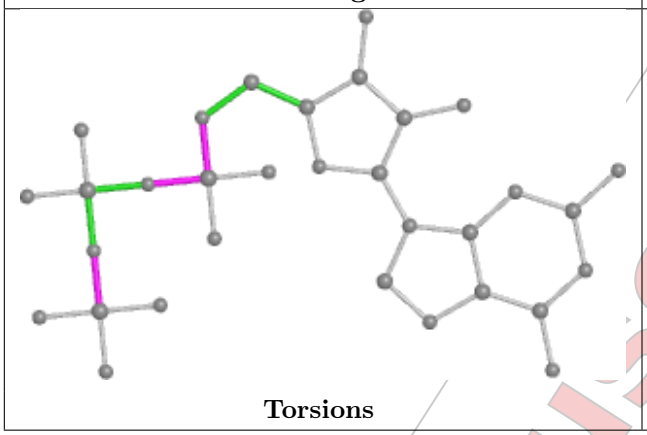
Ligand GTP C 501



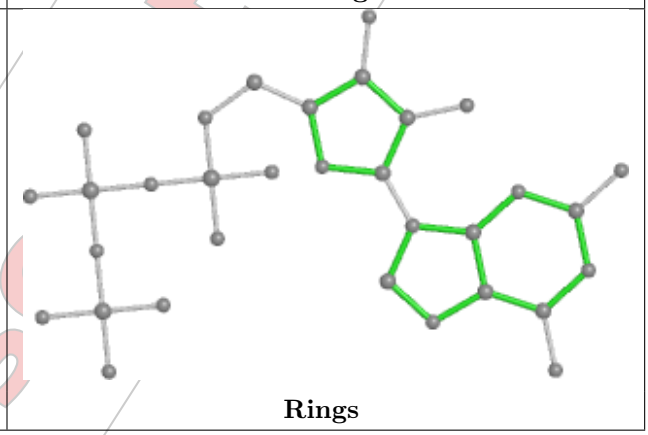
Bond lengths



Bond angles

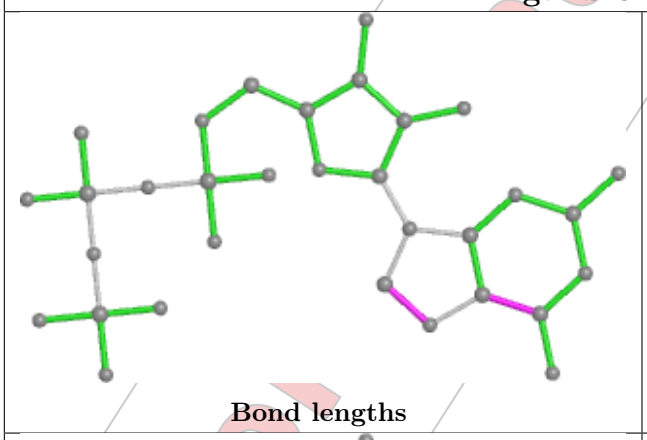


Torsions

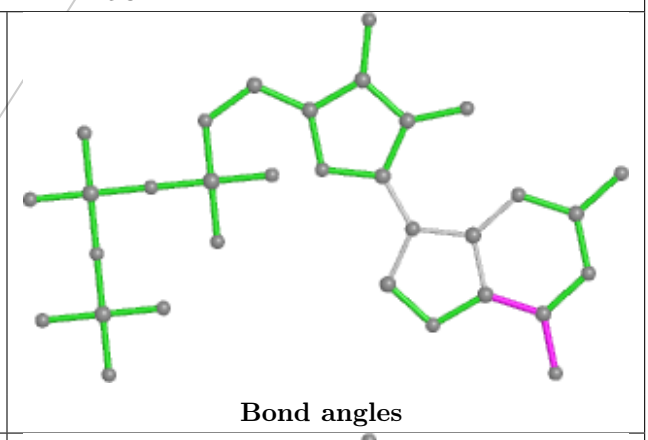


Rings

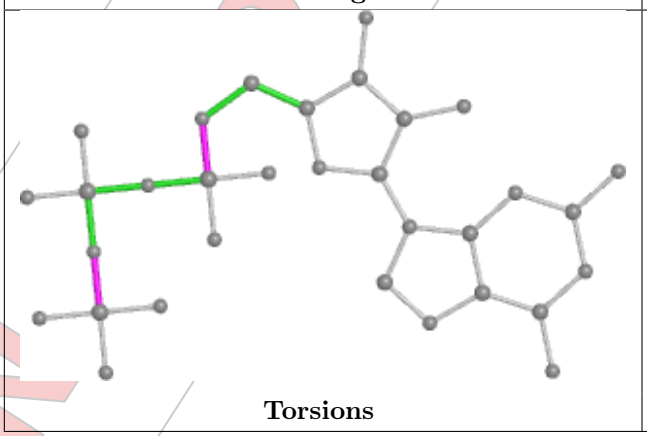
Ligand GTP A 501



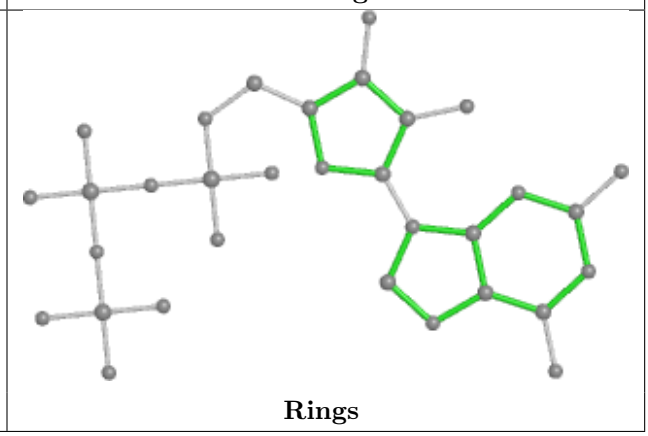
Bond lengths



Bond angles

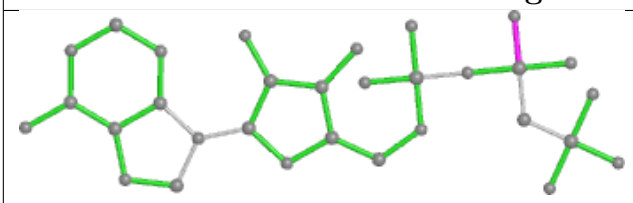


Torsions

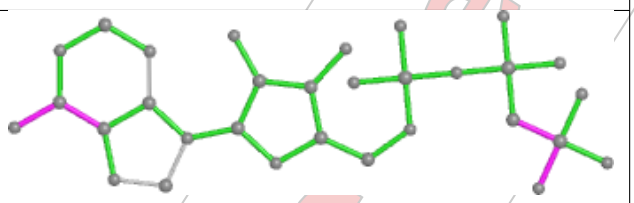


Rings

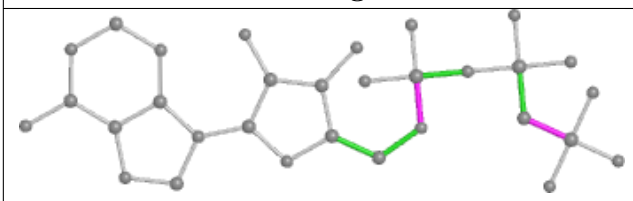
Ligand ACP F 401



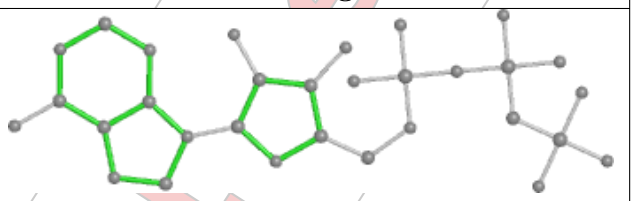
Bond lengths



Bond angles

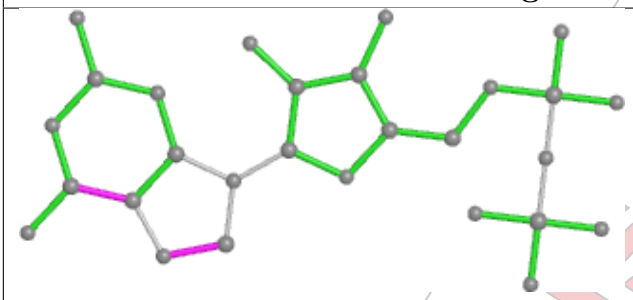


Torsions

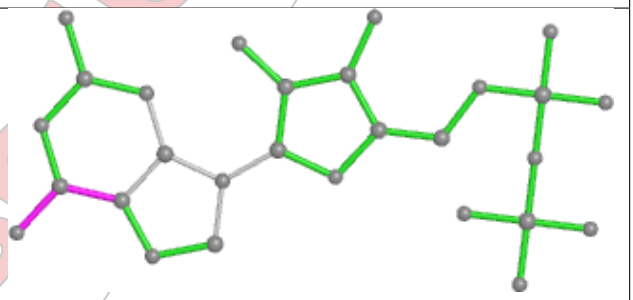


Rings

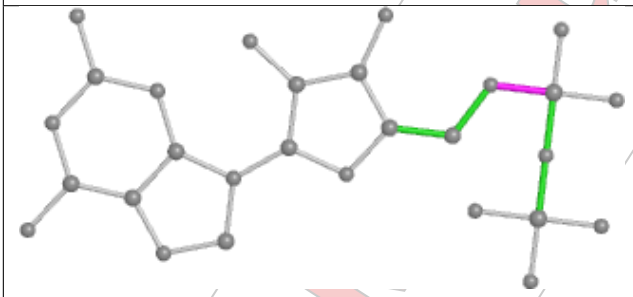
Ligand GDP B 501



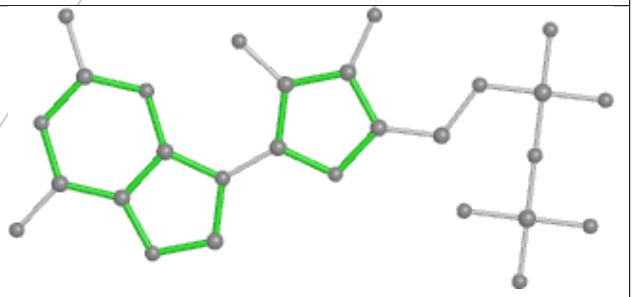
Bond lengths



Bond angles

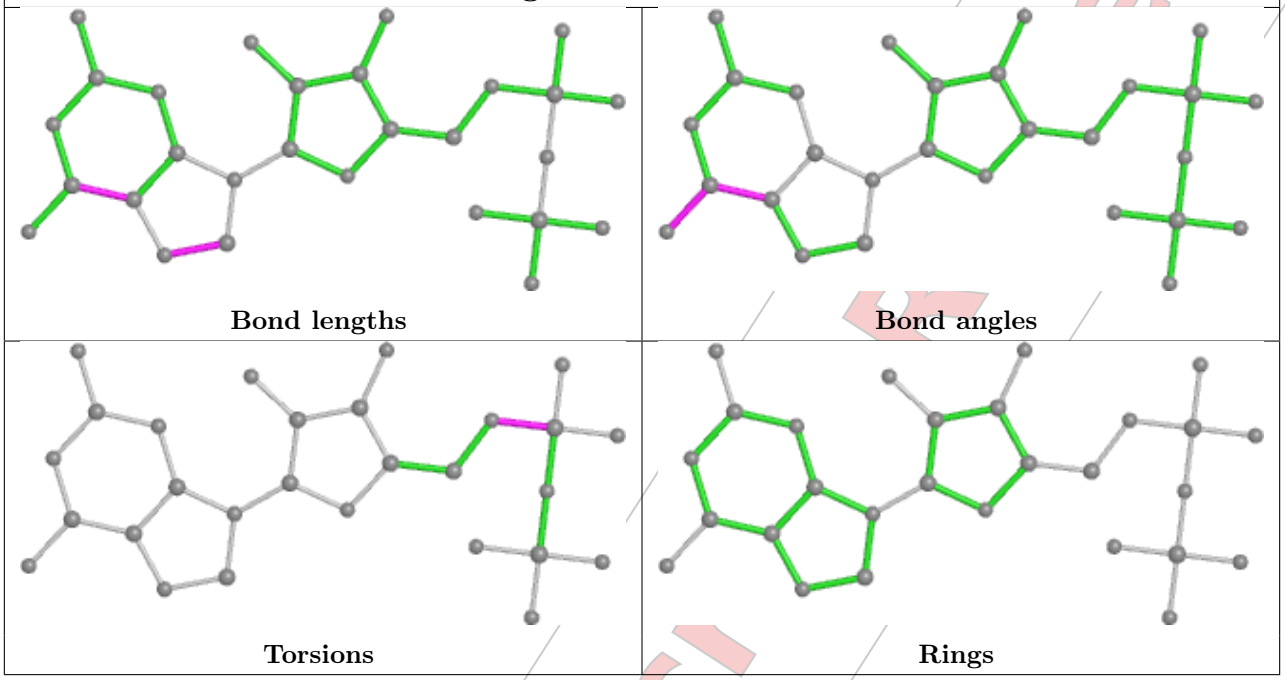


Torsions



Rings

Ligand GDP D 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	5
5	E	1
2	B	1
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.44
1	F	362:ALA	C	372:THR	N	16.72
1	F	155:ALA	C	162:ILE	N	13.81
1	F	102:PRO	C	125:THR	N	12.29
1	F	246:GLN	C	256:TYR	N	11.47
1	B	277:SER	C	282:GLN	N	7.96
1	D	281:GLN	C	285:ALA	N	6.39
1	F	231:ALA	C	235:ASP	N	6.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	439/439 (100%)	-0.06	18 (4%) 37 36	39, 68, 116, 239	0
2	B	425/425 (100%)	-0.00	17 (4%) 38 37	40, 63, 111, 163	4 (0%)
3	C	440/440 (100%)	-0.21	6 (1%) 75 77	38, 55, 96, 133	0
4	D	427/427 (100%)	0.20	26 (6%) 21 20	41, 80, 131, 181	3 (0%)
5	E	123/123 (100%)	0.69	14 (11%) 5 4	53, 80, 144, 173	0
6	F	332/332 (100%)	0.79	58 (17%) 1 1	57, 95, 172, 218	0
All	All	2186/2186 (100%)	0.14	139 (6%) 19 18	38, 72, 135, 239	7 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	285	ALA	11.1
6	F	372	THR	10.0
6	F	154	GLY	8.9
6	F	155	ALA	8.8
5	E	143	ALA	8.3
6	F	137	ARG	8.3
6	F	142	ARG	7.5
1	A	439	SER	7.5
1	A	438	ASP	6.7
6	F	244	CYS	6.7
6	F	133	ALA	6.6
6	F	153	ALA	6.1
5	E	142	GLU	6.1
6	F	236	LYS	6.0
1	A	282	TYR	5.8
4	D	179	ASP	5.8
6	F	132	LEU	5.6
6	F	242	ASN	5.4
5	E	139	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
6	F	143	GLU	5.0
6	F	140	GLU	4.9
6	F	152	SER	4.8
6	F	125	THR	4.7
2	B	80	SER	4.7
5	E	48	GLU	4.4
6	F	176	GLN	4.4
4	D	416	MET	4.3
6	F	171	ASP	4.3
6	F	381	HIS	4.1
6	F	175	GLU	4.1
5	E	28	SER	4.1
4	D	280	SER	4.0
5	E	138	GLU	4.0
3	C	440	VAL	3.8
6	F	245	ILE	3.7
4	D	278	ARG	3.7
4	D	441	ASP	3.6
5	E	141	GLU	3.6
6	F	131	PHE	3.6
4	D	295	MET	3.6
6	F	141	GLY	3.6
4	D	277	SER	3.6
5	E	128	LYS	3.6
4	D	215	ARG	3.5
2	B	59	ASN	3.5
6	F	168	GLU	3.5
6	F	229	ASN	3.5
6	F	135	TYR	3.5
4	D	281	GLN	3.5
1	A	280	LYS	3.4
4	D	401	ARG	3.3
4	D	276	THR	3.3
2	B	370	GLY	3.3
6	F	139	ARG	3.2
6	F	21	LEU	3.2
6	F	90	SER	3.2
1	A	281	ALA	3.2
1	A	163	LYS	3.2
2	B	321	GLY	3.2
2	B	57	THR	3.1
4	D	400	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	438	ALA	3.1
6	F	243	HIS	3.1
2	B	56	ALA	3.1
6	F	174	ASP	3.1
5	E	140	LYS	3.1
6	F	89	GLU	3.0
2	B	39	ASP	3.0
1	A	262	TYR	3.0
4	D	82	PRO	3.0
6	F	130	VAL	3.0
6	F	256	TYR	3.0
2	B	369	ARG	3.0
4	D	406	HIS	2.9
4	D	76	ASP	2.9
1	A	283	HIS	2.9
2	B	85	GLN	2.9
1	A	437	VAL	2.9
6	F	333	ASN	2.9
6	F	259	GLY	2.9
6	F	177	GLY	2.8
1	A	365	GLY	2.8
6	F	167	SER	2.8
4	D	85	GLN	2.8
4	D	116	ASP	2.8
4	D	80	SER	2.7
6	F	46	ARG	2.7
1	A	77	GLU	2.7
4	D	96	GLN	2.7
6	F	136	ASN	2.7
6	F	194	PRO	2.7
2	B	282	GLN	2.7
6	F	180	HIS	2.7
6	F	163	SER	2.7
6	F	165	GLU	2.6
5	E	44	ASP	2.6
6	F	91	CYS	2.6
2	B	416	MET	2.6
4	D	37	HIS	2.6
6	F	178	GLN	2.6
3	C	249	ASN	2.6
3	C	349	THR	2.5
6	F	258	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	439	THR	2.5
5	E	125	GLU	2.5
6	F	379	HIS	2.5
1	A	123	ARG	2.5
2	B	284	ARG	2.5
1	A	279	GLU	2.5
1	A	130	THR	2.5
4	D	2[A]	ARG	2.4
4	D	38	GLY	2.4
6	F	126	ASP	2.4
6	F	235	ASP	2.4
6	F	362	ALA	2.4
1	A	215	ARG	2.4
3	C	357	TYR	2.3
1	A	337	THR	2.3
6	F	151	SER	2.3
4	D	372	LYS	2.3
1	A	43	GLY	2.3
5	E	63	TYR	2.3
6	F	241	THR	2.3
2	B	130	ASP	2.3
2	B	209	LEU	2.2
5	E	122	ARG	2.2
6	F	129	GLU	2.2
6	F	323	GLU	2.1
2	B	440	ALA	2.1
4	D	221	THR	2.1
3	C	285	GLN	2.1
4	D	56	ALA	2.1
5	E	106	GLU	2.1
6	F	257	GLU	2.0
1	A	85	GLN	2.0
6	F	340	GLN	2.0
6	F	196	HIS	2.0
6	F	273	ASP	2.0
3	C	337	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

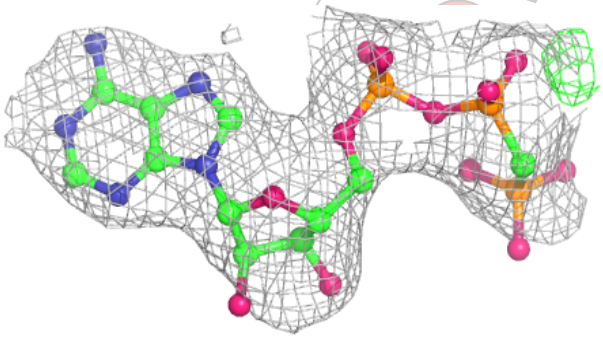
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

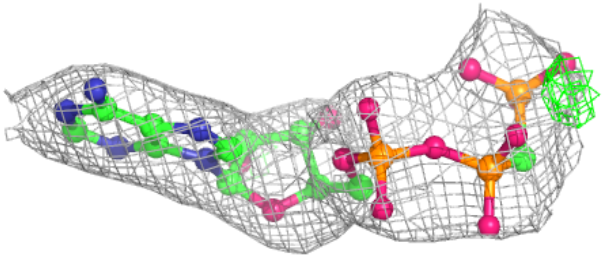
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	ACP	F	401	31/?	0.92	0.13	92,115,145,162	0
10	GDP	D	501	28/?	0.94	0.16	66,76,101,113	0
9	CA	A	503	1/?	0.94	0.06	89,89,89,89	0
8	MG	A	502	1/?	0.96	0.08	44,44,44,44	0
9	CA	C	503	1/?	0.96	0.04	72,72,72,72	0
10	GDP	B	501	28/?	0.97	0.15	34,50,64,71	0
7	GTP	A	501	32/?	0.97	0.15	37,50,68,79	0
8	MG	B	502	1/?	0.97	0.24	57,57,57,57	0
8	MG	C	502	1/?	0.98	0.09	45,45,45,45	0
7	GTP	C	501	32/?	0.98	0.12	36,46,62,72	0

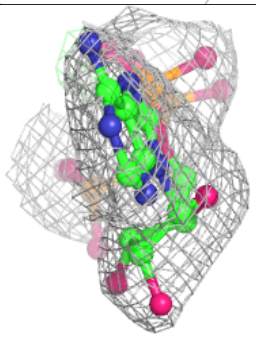
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ACP F 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

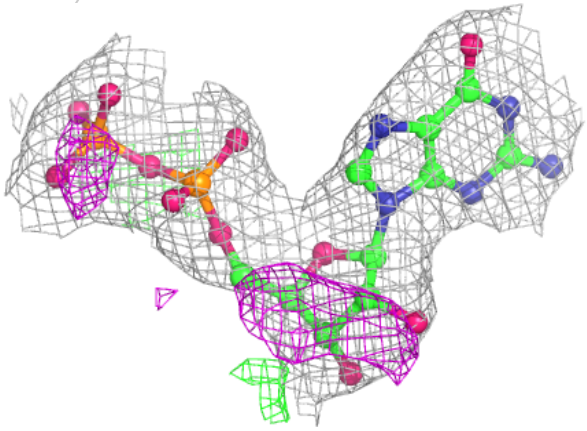


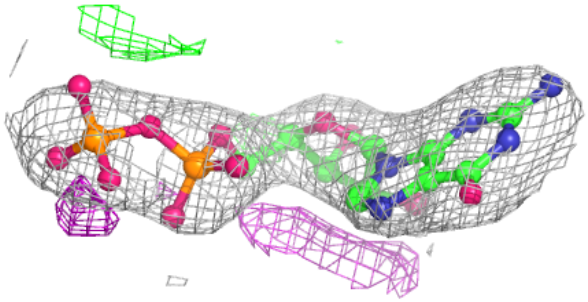


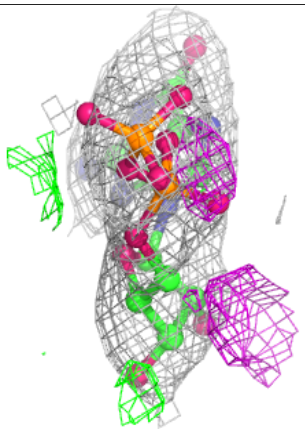


Electron density around GDP D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

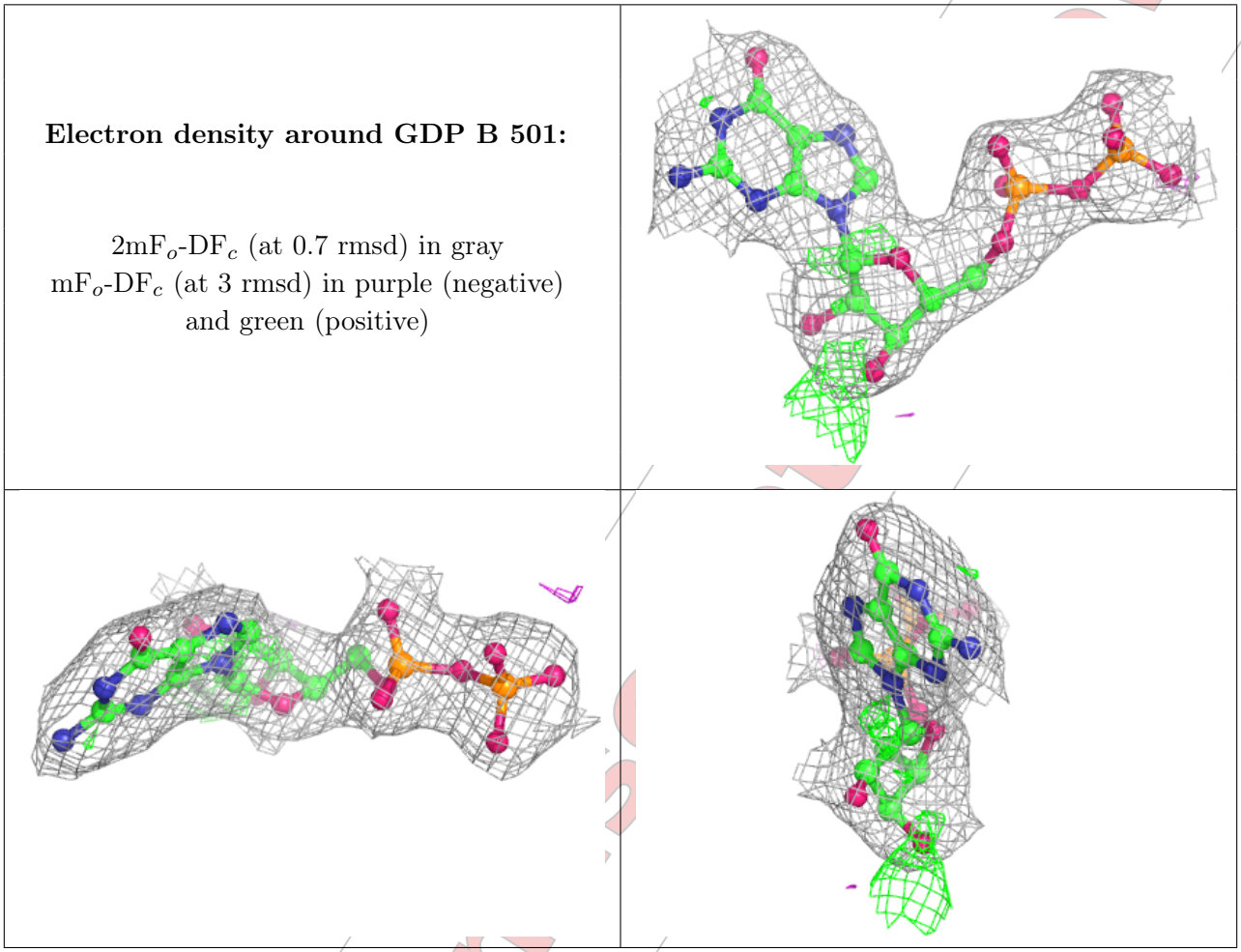






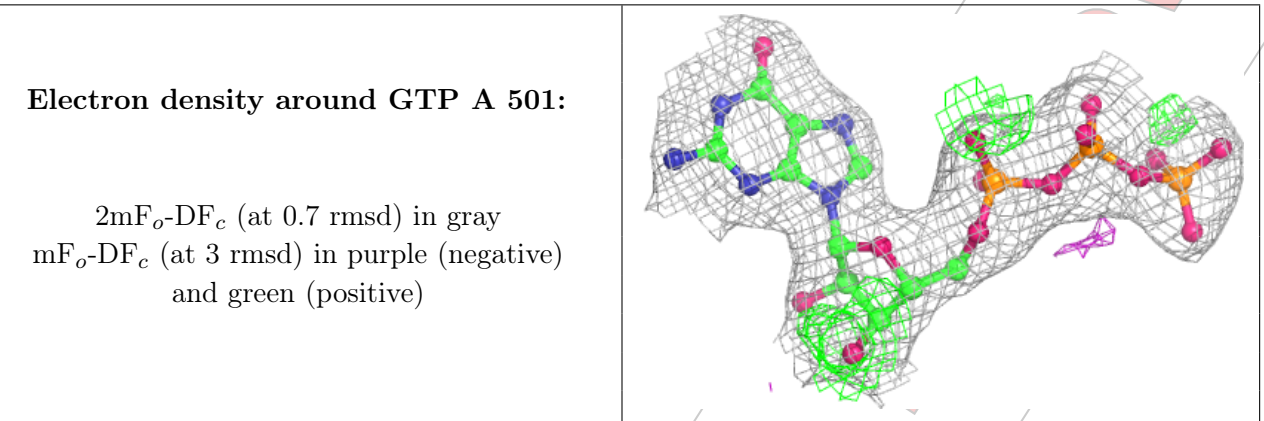
Electron density around GDP B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



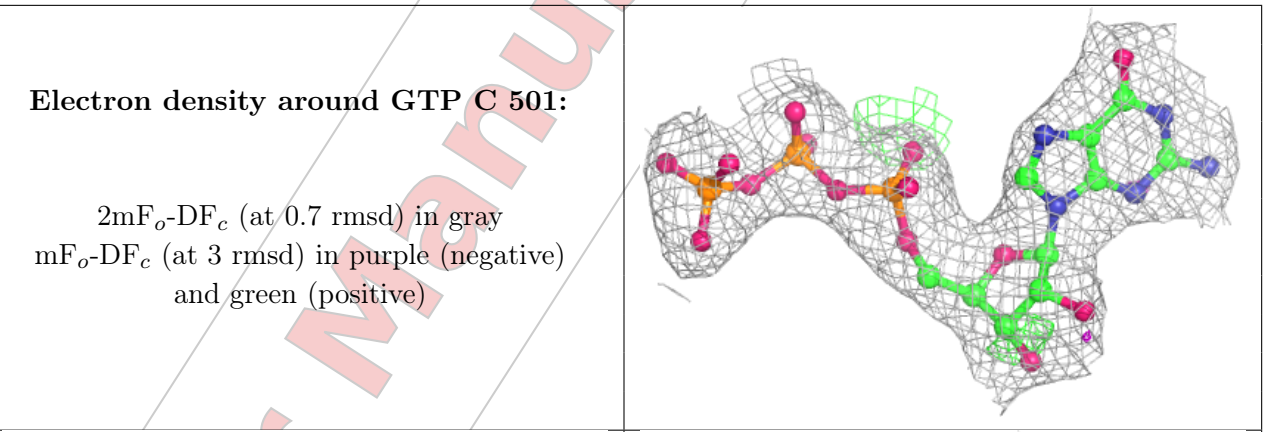
Electron density around GTP A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2023 – 07:04 pm GMT

Deposition ID : D_1292128529

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

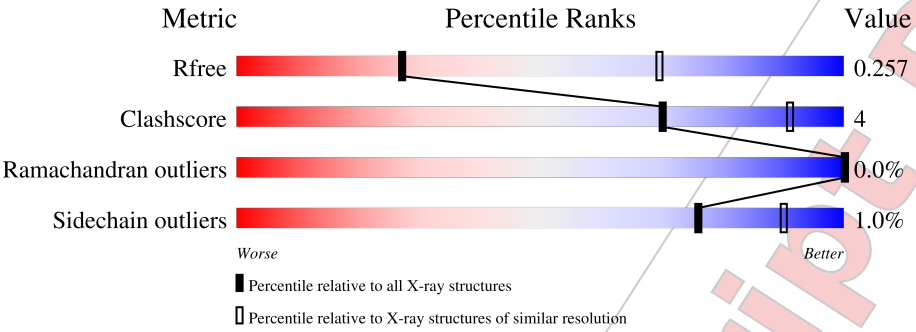
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	437	92% 7%
2	B	427	94% 6%
3	C	440	94% 6%
4	D	421	90% 10%
5	E	121	96% .
6	F	336	84% 14% .

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34471 atoms, of which 16974 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	437	6749	2163	3333	581	650	22	0	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	427	6600	2110	3239	576	649	26	0	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	440	6789	2175	3352	584	656	22	0	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	421	6497	2080	3188	562	640	27	0	0	0

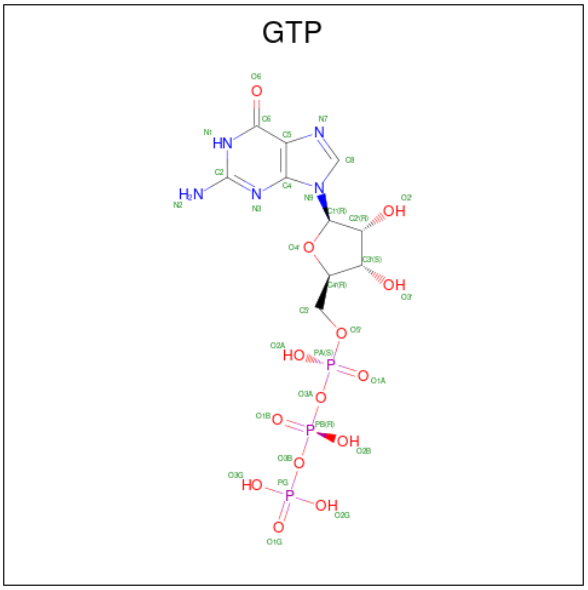
- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	121	2036	623	1026	184	198	5	0	1	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	336	5495	1773	2734	473	501	14	0	0	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	X	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
7	X	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
7	X	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

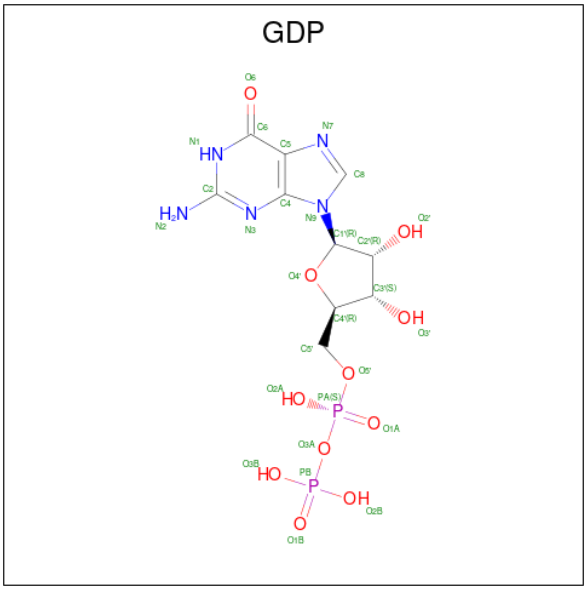
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	X	1	Total	Ca	0	0
			1	1		
9	X	1	Total	Ca	0	0
			1	1		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

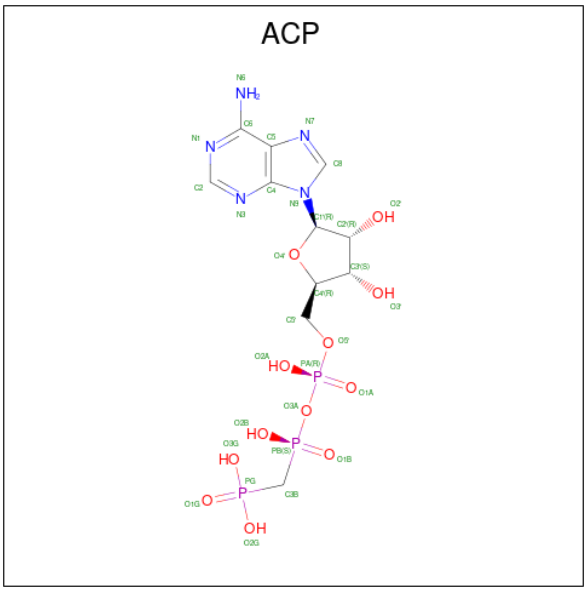


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
10	X	1	40	10	12	5	11	2	0	0

- Molecule 11 is a ligand with the chemical component id ANS but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for ANS. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	H	N	O		
11	X	1	84	32	1	40	2	9	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	X	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 13 is water.

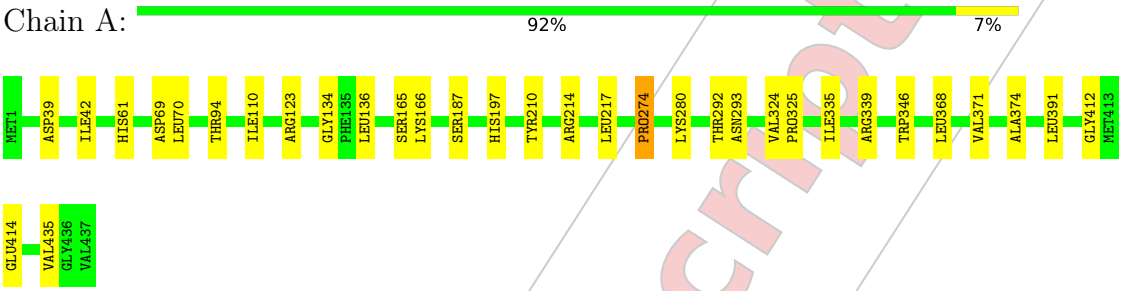
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	G	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

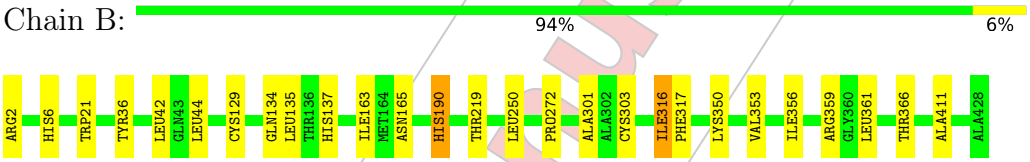
- Molecule 1:

Chain A:



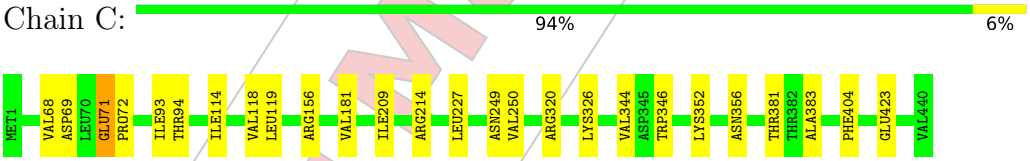
- Molecule 2:

Chain B:



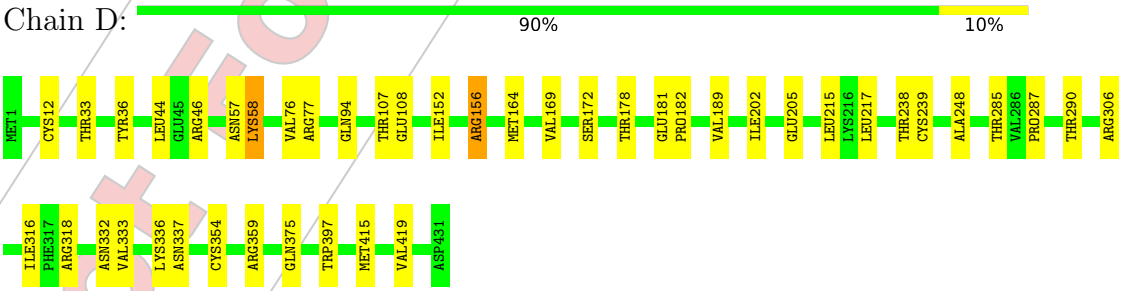
- Molecule 3:

Chain C:



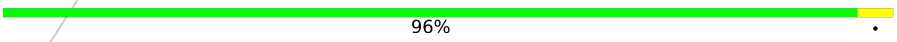
- Molecule 4:

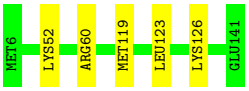
Chain D:



- Molecule 5:

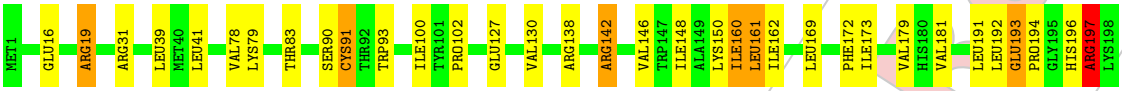
Chain E:





• Molecule 6:

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.06Å 159.61Å 180.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.10 – 3.20 15.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.10-3.20) 87.7 (15.10-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 2.51Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.200 , 0.241 0.218 , 0.257	Depositor DCC
R_{free} test set	2000 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	34471	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GTP, MG, ACP, ANS, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/3494	0.51	0/4743
2	B	0.28	0/3436	0.51	0/4654
3	C	0.29	0/3515	0.51	0/4772
4	D	0.28	0/3382	0.51	0/4581
5	E	0.26	0/1019	0.48	0/1352
6	F	0.31	0/2823	0.54	0/3813
All	All	0.29	0/17669	0.51	0/23915

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
6	F	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	156	ARG	Sidechain
4	D	359	ARG	Sidechain
6	F	19	ARG	Sidechain
6	F	193	GLU	Peptide
6	F	197	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3333	3330	22	0
2	B	3361	3239	3238	16	0
3	C	3437	3352	3348	14	0
4	D	3309	3188	3189	26	0
5	E	1010	1026	1024	3	0
6	F	2761	2734	2733	46	0
7	X	92	36	36	1	0
8	X	3	0	0	0	0
9	X	2	0	0	0	0
10	X	28	12	12	0	0
11	X	44	40	2	4	0
12	X	31	14	14	0	0
13	G	3	0	0	0	0
All	All	17497	16974	16926	125	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:ILE:HD12	6:F:173:ILE:HD13	1.55	0.89
1:A:42:ILE:HD12	1:A:42:ILE:O	1.86	0.75
6:F:192:LEU:HD23	6:F:193:GLU:N	2.05	0.72
6:F:192:LEU:HD22	6:F:197:ARG:NE	2.07	0.68
1:A:293:ASN:ND2	1:A:339:ARG:HH21	1.97	0.63
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.81	0.63
6:F:161:LEU:HD23	6:F:172:PHE:CD2	2.35	0.62
6:F:161:LEU:C	6:F:161:LEU:HD12	2.20	0.60
6:F:160:ILE:HG21	6:F:240:LEU:HD21	1.82	0.60
6:F:161:LEU:HD12	6:F:162:ILE:N	2.17	0.59
6:F:192:LEU:HD23	6:F:192:LEU:C	2.23	0.59
6:F:90:SER:O	6:F:91:CYS:C	2.40	0.59
6:F:377:LYS:HD2	6:F:377:LYS:H	1.67	0.59
11:X:510:ANS:C25	11:X:510:ANS:CL	2.88	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:ILE:HD12	2:B:356:ILE:H	1.68	0.58
4:D:156:ARG:HG2	5:E:123:LEU:HD11	1.85	0.58
6:F:192:LEU:HD21	6:F:194:PRO:HD2	1.85	0.57
6:F:240:LEU:HD12	6:F:240:LEU:N	2.20	0.56
1:A:187:SER:CB	1:A:391:LEU:HD21	2.34	0.56
3:C:381:THR:HG22	3:C:383:ALA:H	1.70	0.56
4:D:57:ASN:ND2	4:D:57:ASN:O	2.38	0.56
3:C:344:VAL:HG21	3:C:346:TRP:CE2	2.42	0.54
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.88	0.54
4:D:215:LEU:HB3	4:D:217:LEU:HD23	1.90	0.54
6:F:213:ILE:HD11	6:F:296:MET:CE	2.37	0.53
1:A:414:GLU:OE2	5:E:60:ARG:NH2	2.42	0.53
6:F:197:ARG:HH22	6:F:256:TYR:CB	2.22	0.53
4:D:332:ASN:OD1	4:D:336:LYS:HE3	2.09	0.53
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.90	0.52
4:D:239:CYS:SG	4:D:316:ILE:HD12	2.50	0.52
1:A:274:PRO:HD3	1:A:374:ALA:HA	1.90	0.52
4:D:107:THR:OG1	4:D:108:GLU:N	2.43	0.52
6:F:199:PHE:CD1	6:F:221:LEU:HD23	2.45	0.51
4:D:290:THR:HG22	4:D:333:VAL:HG21	1.93	0.51
6:F:161:LEU:HD21	6:F:169:LEU:HD23	1.92	0.51
4:D:306:ARG:NH2	4:D:337:ASN:OD1	2.44	0.50
2:B:135:LEU:HG	2:B:137:HIS:ND1	2.27	0.50
3:C:209:ILE:HG22	3:C:227:LEU:HD22	1.92	0.50
6:F:162:ILE:N	6:F:162:ILE:HD12	2.26	0.50
1:A:346:TRP:CZ2	1:A:435:VAL:HG13	2.46	0.50
4:D:215:LEU:CB	4:D:217:LEU:HD23	2.42	0.49
1:A:412:GLY:O	5:E:60:ARG:NH1	2.46	0.49
4:D:36:TYR:CE2	4:D:44:LEU:HD11	2.48	0.49
3:C:68:VAL:HG21	3:C:118:VAL:HG21	1.93	0.49
6:F:79:LYS:O	6:F:83:THR:HG23	2.12	0.49
2:B:301:ALA:O	2:B:303:CYS:N	2.43	0.48
4:D:318:ARG:HA	4:D:354:CYS:O	2.14	0.48
2:B:42:LEU:HD13	2:B:356:ILE:HD11	1.96	0.48
6:F:197:ARG:HH22	6:F:256:TYR:HB2	1.78	0.48
4:D:189:VAL:HG11	4:D:415:MET:HE2	1.95	0.47
6:F:146:VAL:HG11	6:F:233:PHE:CE1	2.49	0.47
3:C:249:ASN:OD1	3:C:356:ASN:ND2	2.47	0.47
4:D:397:TRP:CZ3	11:X:510:ANS:O5	2.67	0.47
6:F:192:LEU:HD11	6:F:262:MET:CE	2.44	0.47
6:F:161:LEU:HD23	6:F:172:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:THR:HG21	3:C:326:LYS:HA	1.97	0.47
6:F:127:GLU:HB2	6:F:130:VAL:CG1	2.45	0.47
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.49	0.47
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.50	0.46
4:D:178:THR:HA	11:X:510:ANS:C25	2.45	0.46
6:F:160:ILE:CG2	6:F:240:LEU:HD21	2.46	0.46
3:C:119:LEU:HD11	3:C:156:ARG:HB3	1.97	0.46
3:C:181:VAL:HG11	3:C:404:PHE:CZ	2.51	0.46
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.46	0.46
4:D:285:THR:HB	4:D:287:PRO:HD2	1.98	0.46
2:B:356:ILE:HD12	2:B:356:ILE:N	2.31	0.46
4:D:152:ILE:HG23	4:D:164:MET:HG2	1.97	0.45
6:F:16:GLU:OE2	6:F:19:ARG:CZ	2.65	0.45
1:A:39:ASP:OD2	1:A:61:HIS:HE1	2.00	0.45
4:D:181:GLU:N	4:D:182:PRO:HD2	2.32	0.45
6:F:148:ILE:HD11	6:F:160:ILE:HD12	1.97	0.45
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.99	0.45
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.99	0.45
4:D:33:THR:C	4:D:58:LYS:HZ1	2.20	0.45
6:F:191:LEU:HD13	6:F:196:HIS:CE1	2.52	0.44
1:A:136:LEU:HD12	1:A:136:LEU:N	2.33	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.44
3:C:250:VAL:HG11	3:C:352:LYS:HE3	1.99	0.44
6:F:271:LEU:HD23	6:F:275:LEU:HD12	1.99	0.44
2:B:135:LEU:HD23	2:B:137:HIS:CE1	2.52	0.44
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.53	0.44
4:D:172:SER:OG	4:D:205:GLU:OE1	2.30	0.44
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.99	0.44
6:F:150:LYS:HG2	6:F:160:ILE:HD11	1.99	0.43
6:F:346:LEU:C	6:F:346:LEU:HD13	2.38	0.43
3:C:344:VAL:HG21	3:C:346:TRP:CZ2	2.52	0.43
6:F:226:GLU:OE1	6:F:226:GLU:N	2.51	0.43
6:F:78:VAL:HG21	6:F:181:VAL:HG21	2.00	0.43
6:F:102:PRO:HD2	6:F:179:VAL:HA	2.00	0.43
6:F:161:LEU:HD11	6:F:169:LEU:HD23	1.99	0.43
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.49	0.43
6:F:91:CYS:SG	6:F:93:TRP:CE2	3.12	0.43
4:D:169:VAL:HA	4:D:202:ILE:O	2.19	0.43
1:A:324:VAL:CG2	1:A:325:PRO:HD2	2.48	0.42
1:A:324:VAL:HG23	1:A:325:PRO:HD2	2.01	0.42
4:D:238:THR:HB	4:D:316:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:LEU:HD21	6:F:41:LEU:HD21	2.00	0.42
2:B:316:ILE:HG23	2:B:366:THR:HB	2.01	0.42
3:C:93:ILE:HG22	3:C:114:ILE:HD11	2.02	0.42
6:F:221:LEU:O	6:F:261:GLU:HA	2.19	0.42
2:B:2:ARG:HA	2:B:129:CYS:O	2.20	0.42
4:D:46:ARG:NH2	4:D:248:ALA:O	2.52	0.42
11:X:510:ANS:C2	11:X:510:ANS:C29	2.97	0.42
6:F:214:TYR:HB3	6:F:375:PHE:HB3	2.02	0.41
6:F:240:LEU:N	6:F:240:LEU:CD1	2.82	0.41
2:B:317:PHE:O	2:B:353:VAL:HA	2.20	0.41
3:C:320:ARG:HA	3:C:356:ASN:O	2.20	0.41
4:D:94:GLN:OE1	4:D:94:GLN:N	2.47	0.41
6:F:298:ILE:HD12	6:F:302:ILE:HD13	2.02	0.41
6:F:213:ILE:CD1	6:F:296:MET:CE	2.98	0.41
6:F:138:ARG:O	6:F:142:ARG:N	2.53	0.41
3:C:71:GLU:HG2	3:C:72:PRO:HD2	2.03	0.41
6:F:148:ILE:HD11	6:F:160:ILE:CD1	2.51	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
3:C:69:ASP:O	3:C:94:THR:HA	2.21	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.40
6:F:256:TYR:CD1	6:F:256:TYR:N	2.89	0.40
2:B:134:GLN:HA	2:B:165:ASN:O	2.20	0.40
6:F:93:TRP:O	6:F:328:TRP:HA	2.22	0.40
6:F:161:LEU:HD11	6:F:169:LEU:CD2	2.51	0.40
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.40
1:A:134:GLY:HA3	1:A:165:SER:O	2.22	0.40
4:D:12:CYS:HB2	7:X:509:GTP:C8	2.55	0.40
4:D:76:VAL:HG23	4:D:77:ARG:N	2.37	0.40
4:D:375:GLN:HB2	4:D:419:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/437 (100%)	422 (97%)	13 (3%)	0	100	100
2	B	425/427 (100%)	416 (98%)	9 (2%)	0	100	100
3	C	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
4	D	417/421 (99%)	407 (98%)	10 (2%)	0	100	100
5	E	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
6	F	326/336 (97%)	309 (95%)	16 (5%)	1 (0%)	41	74
All	All	2159/2182 (99%)	2096 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	91	CYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/368 (100%)	365 (99%)	3 (1%)	81	93
2	B	369/369 (100%)	365 (99%)	4 (1%)	73	88
3	C	371/371 (100%)	368 (99%)	3 (1%)	81	93
4	D	364/364 (100%)	363 (100%)	1 (0%)	92	96
5	E	110/109 (101%)	107 (97%)	3 (3%)	44	75
6	F	303/303 (100%)	298 (98%)	5 (2%)	60	83
All	All	1885/1884 (100%)	1866 (99%)	19 (1%)	76	90

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	274	PRO
1	A	280	LYS
2	B	190	HIS

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Mol	Chain	Res	Type
2	B	316	ILE
2	B	350	LYS
2	B	359	ARG
3	C	71	GLU
3	C	214	ARG
3	C	423	GLU
4	D	58	LYS
5	E	52	LYS
5	E	119	MET
5	E	126	LYS
6	F	31	ARG
6	F	142	ARG
6	F	160	ILE
6	F	161	LEU
6	F	197	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
2	B	8	GLN
2	B	134	GLN
2	B	375	GLN
2	B	426	GLN
3	C	101	ASN
4	D	14	ASN
4	D	134	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic and 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	ACP	X	511	-	27,33,33	0.86	1 (3%)	32,52,52	1.57	2 (6%)
7	GTP	X	509	-	24,30,34	1.08	3 (12%)	30,47,54	0.88	1 (3%)
7	GTP	X	506	8	26,34,34	1.07	3 (11%)	32,54,54	0.77	0
7	GTP	X	501	8	26,34,34	1.08	3 (11%)	32,54,54	0.75	0
10	GDP	X	504	8	24,30,30	1.04	3 (12%)	30,47,47	0.69	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ACP	X	511	-	-	6/15/38/38	0/3/3/3
7	GTP	X	509	-	-	4/12/32/38	0/3/3/3
7	GTP	X	506	8	-	5/18/38/38	0/3/3/3
7	GTP	X	501	8	-	4/18/38/38	0/3/3/3
10	GDP	X	504	8	-	3/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	X	511	ACP	PB-O3A	3.41	1.62	1.58
7	X	509	GTP	C5-C6	-2.99	1.41	1.47
7	X	501	GTP	C5-C6	-2.95	1.41	1.47
7	X	506	GTP	C5-C6	-2.91	1.41	1.47
10	X	504	GDP	C5-C6	-2.74	1.41	1.47
7	X	501	GTP	C8-N7	-2.25	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	506	GTP	C8-N7	-2.20	1.31	1.35
7	X	509	GTP	C8-N7	-2.20	1.31	1.35
7	X	506	GTP	C5-C4	-2.13	1.37	1.43
10	X	504	GDP	C8-N7	-2.10	1.31	1.35
7	X	501	GTP	C5-C4	-2.10	1.37	1.43
10	X	504	GDP	C5-C4	-2.01	1.37	1.43
7	X	509	GTP	C5-C4	-2.00	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	X	511	ACP	PB-O3A-PA	-7.10	110.06	132.56
12	X	511	ACP	C5-C6-N6	2.31	123.86	120.35
7	X	509	GTP	O2B-PB-O1B	2.26	119.53	110.68
10	X	504	GDP	O6-C6-C5	2.10	128.48	124.37

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	501	GTP	C5'-O5'-PA-O3A
7	X	501	GTP	C5'-O5'-PA-O2A
7	X	506	GTP	C5'-O5'-PA-O3A
7	X	506	GTP	C5'-O5'-PA-O2A
7	X	509	GTP	C5'-O5'-PA-O1A
7	X	509	GTP	C5'-O5'-PA-O2A
10	X	504	GDP	PA-O3A-PB-O3B
10	X	504	GDP	C5'-O5'-PA-O3A
12	X	511	ACP	PB-C3B-PG-O1G
12	X	511	ACP	PB-C3B-PG-O3G
12	X	511	ACP	PG-C3B-PB-O1B
12	X	511	ACP	PG-C3B-PB-O3A
12	X	511	ACP	O4'-C4'-C5'-O5'
7	X	506	GTP	C4'-C5'-O5'-PA
7	X	509	GTP	C4'-C5'-O5'-PA
12	X	511	ACP	C3'-C4'-C5'-O5'
7	X	501	GTP	C4'-C5'-O5'-PA
7	X	506	GTP	C5'-O5'-PA-O1A
10	X	504	GDP	C5'-O5'-PA-O2A
7	X	501	GTP	PA-O3A-PB-O2B
7	X	506	GTP	PA-O3A-PB-O2B
7	X	509	GTP	C5'-O5'-PA-O3A

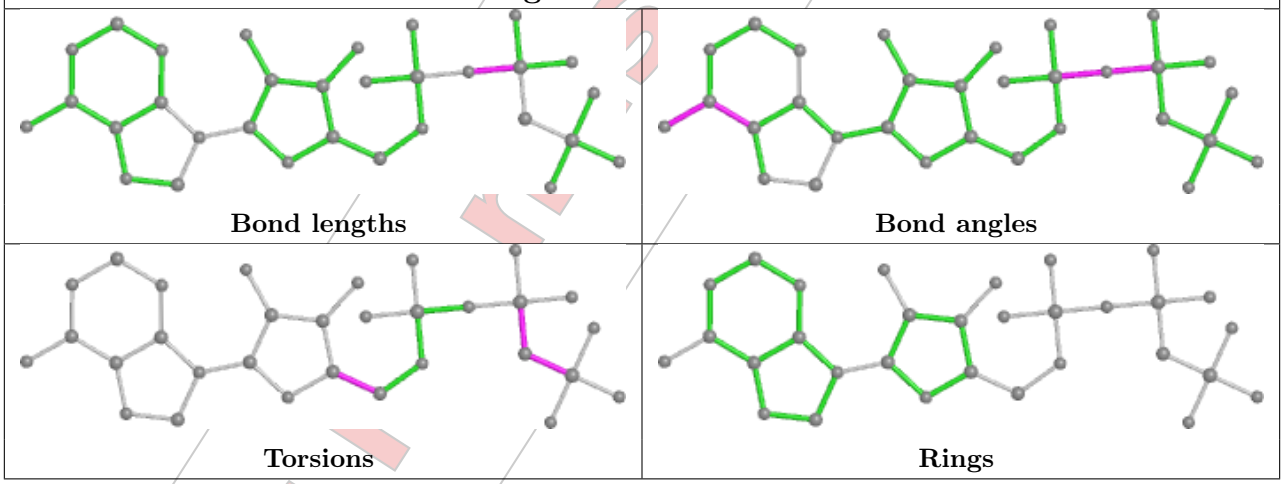
There are no ring outliers.

1 monomer is involved in 1 short contact:

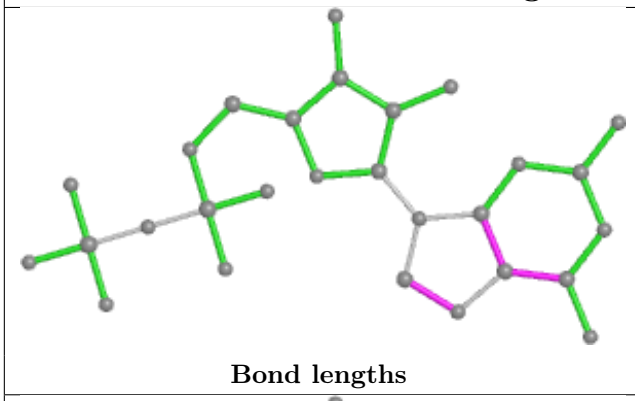
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	X	509	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

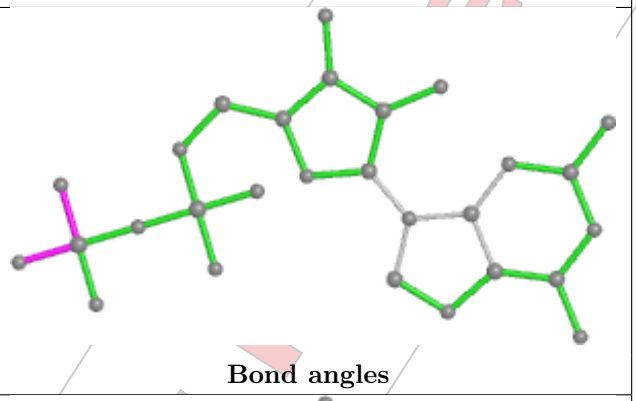
Ligand ACP X 511



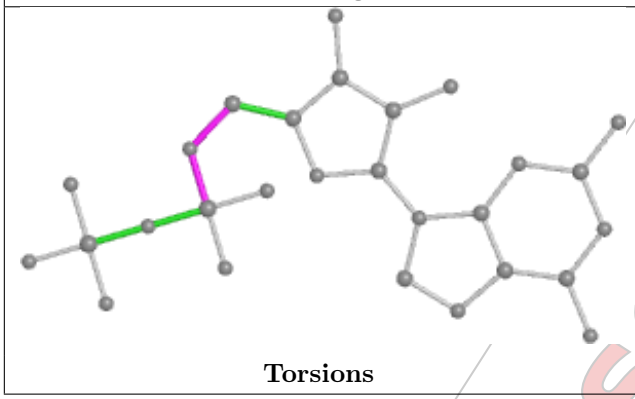
Ligand GTP X 509



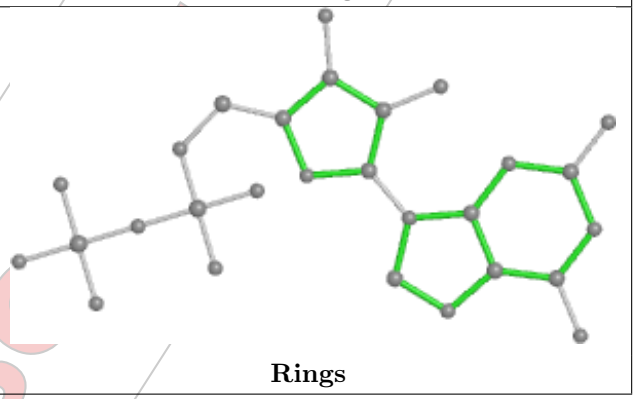
Bond lengths



Bond angles

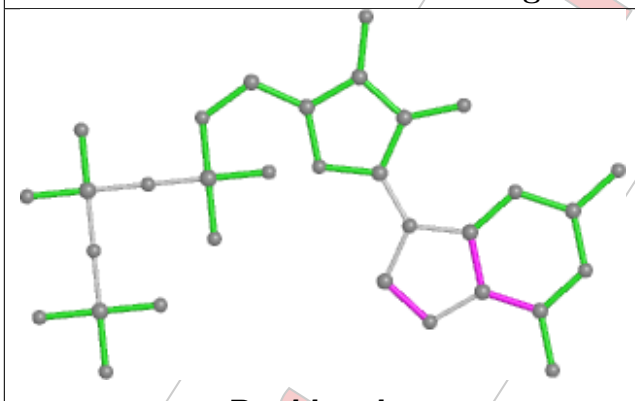


Torsions

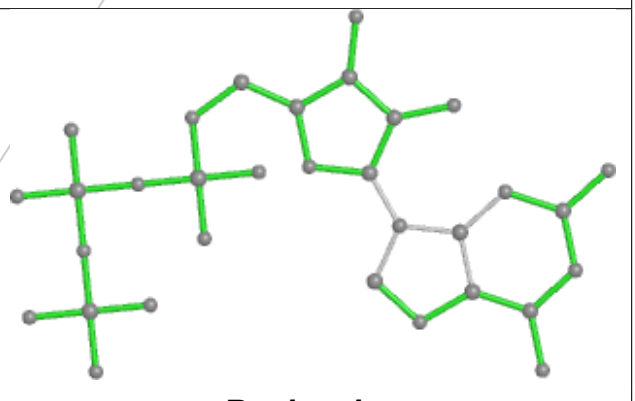


Rings

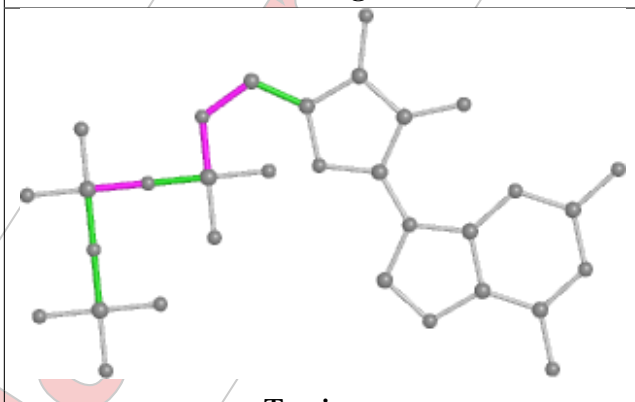
Ligand GTP X 506



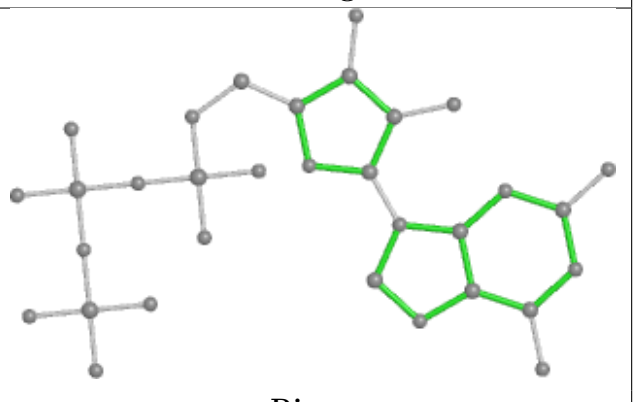
Bond lengths



Bond angles

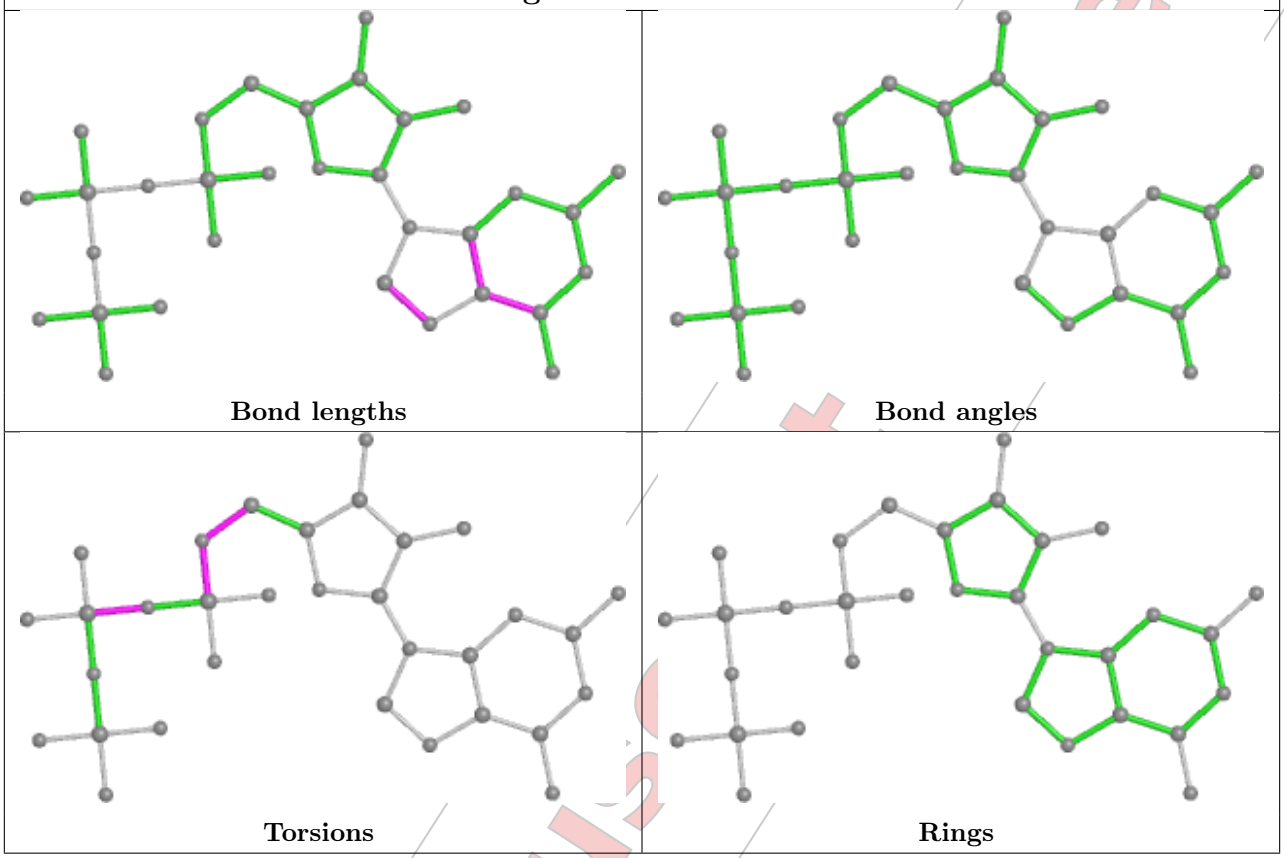


Torsions

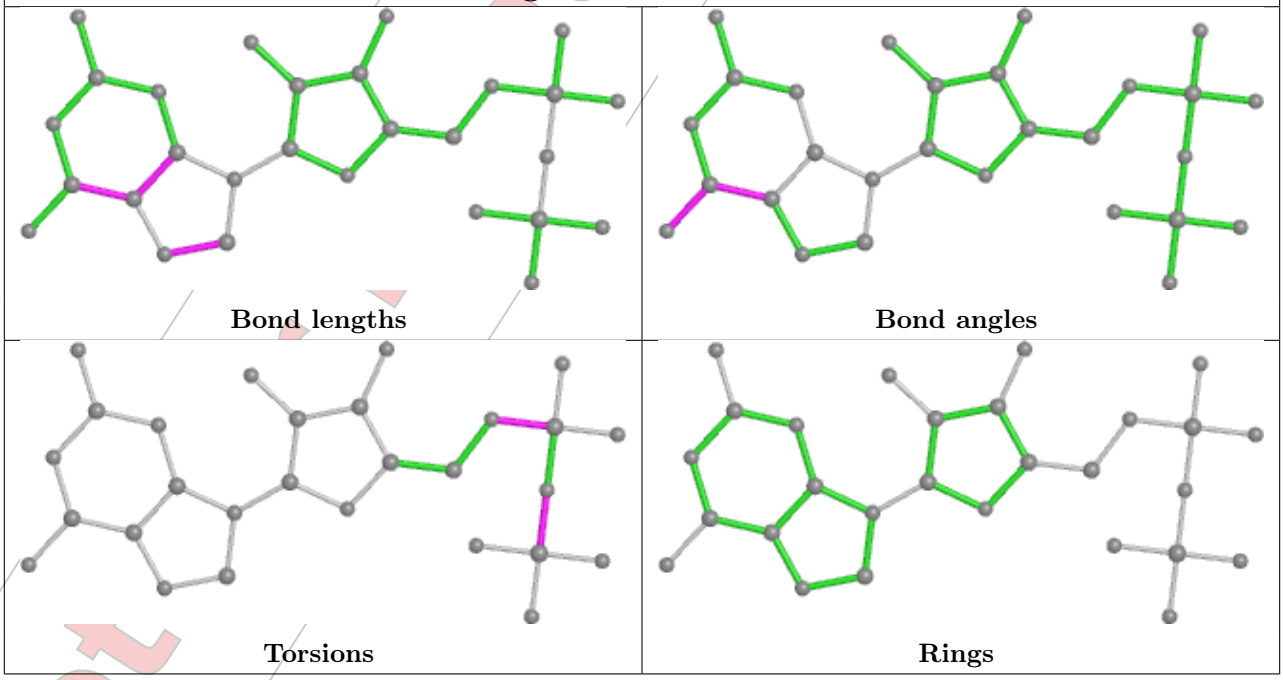


Rings

Ligand GTP X 501



Ligand GDP X 504



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	4
5	E	1
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.06
1	F	362:ALA	C	372:THR	N	20.68
1	F	103:THR	C	126:ASP	N	11.71
1	D	273:LEU	C	284:LEU	N	11.29
1	F	247:LYS	C	252:ASN	N	9.41
1	F	150:LYS	C	160:ILE	N	6.42

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

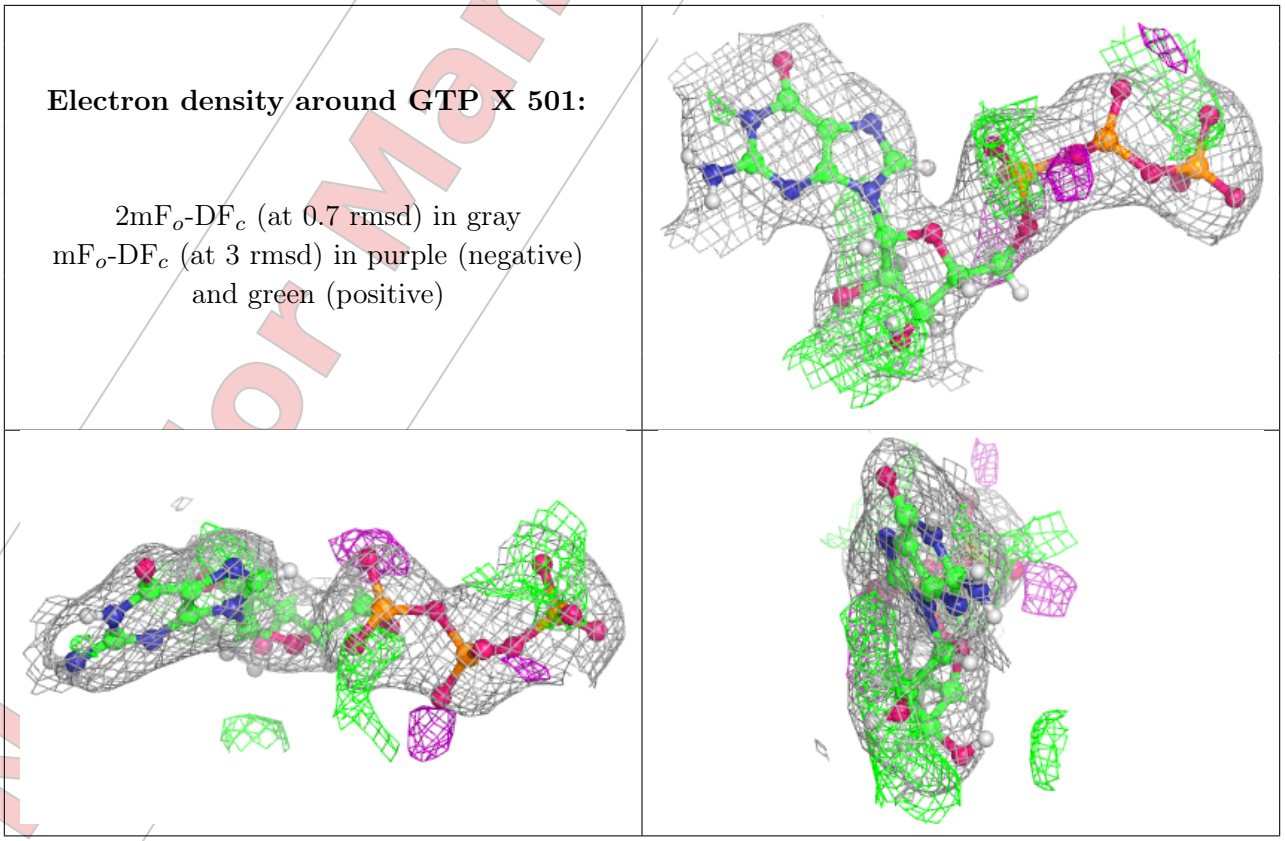
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

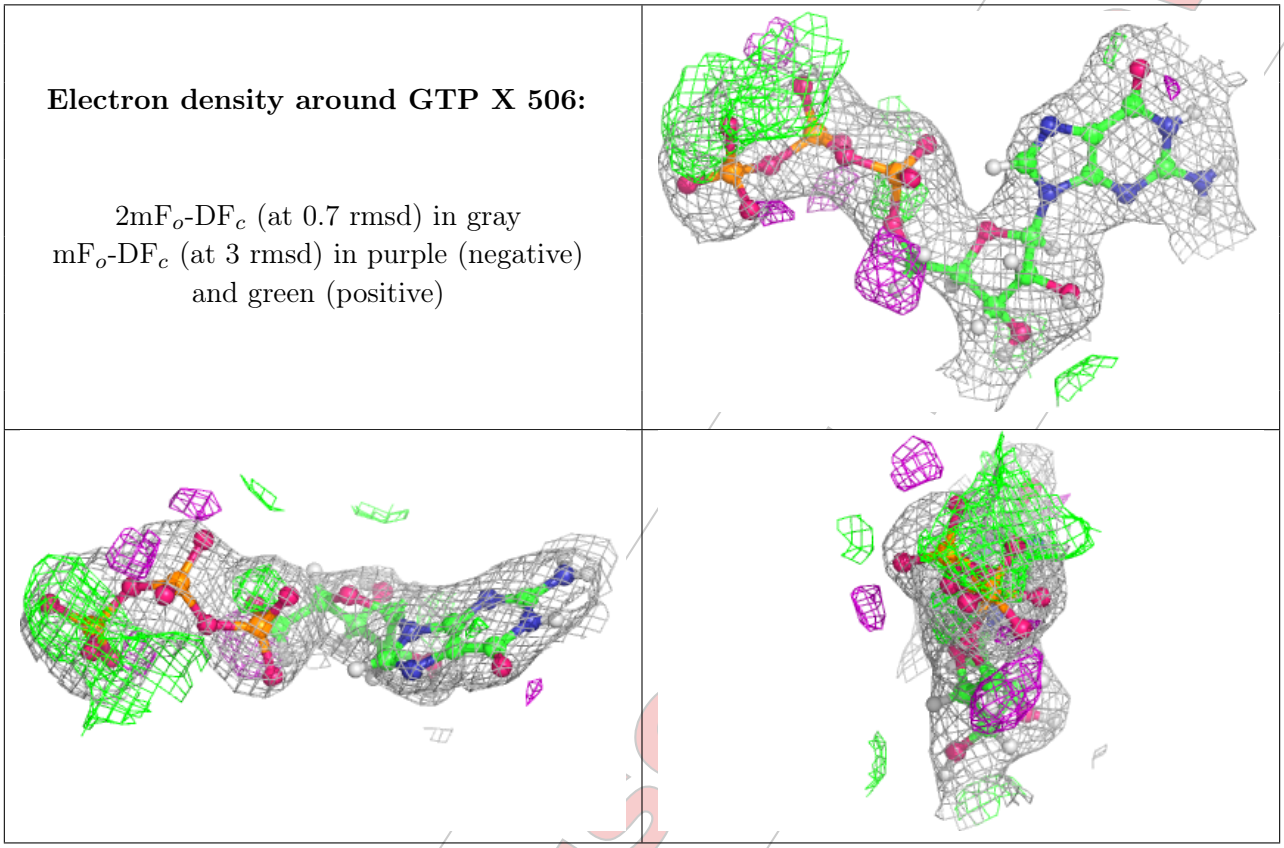
Electron density around GTP X 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



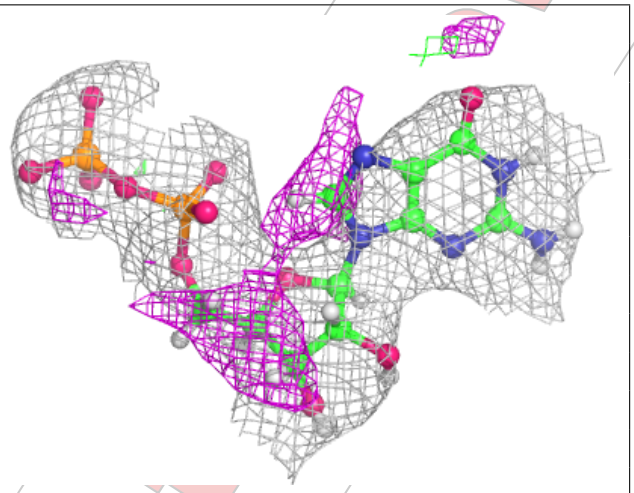
Electron density around GTP X 506:

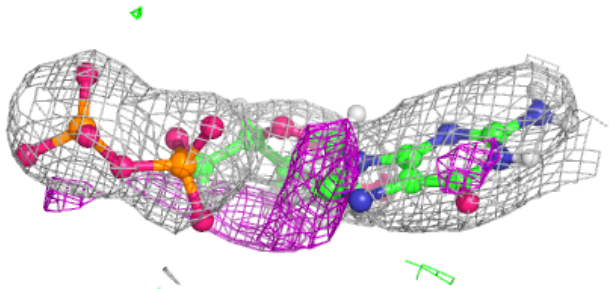
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

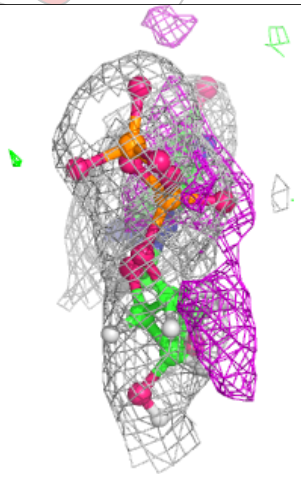


Electron density around GTP X 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

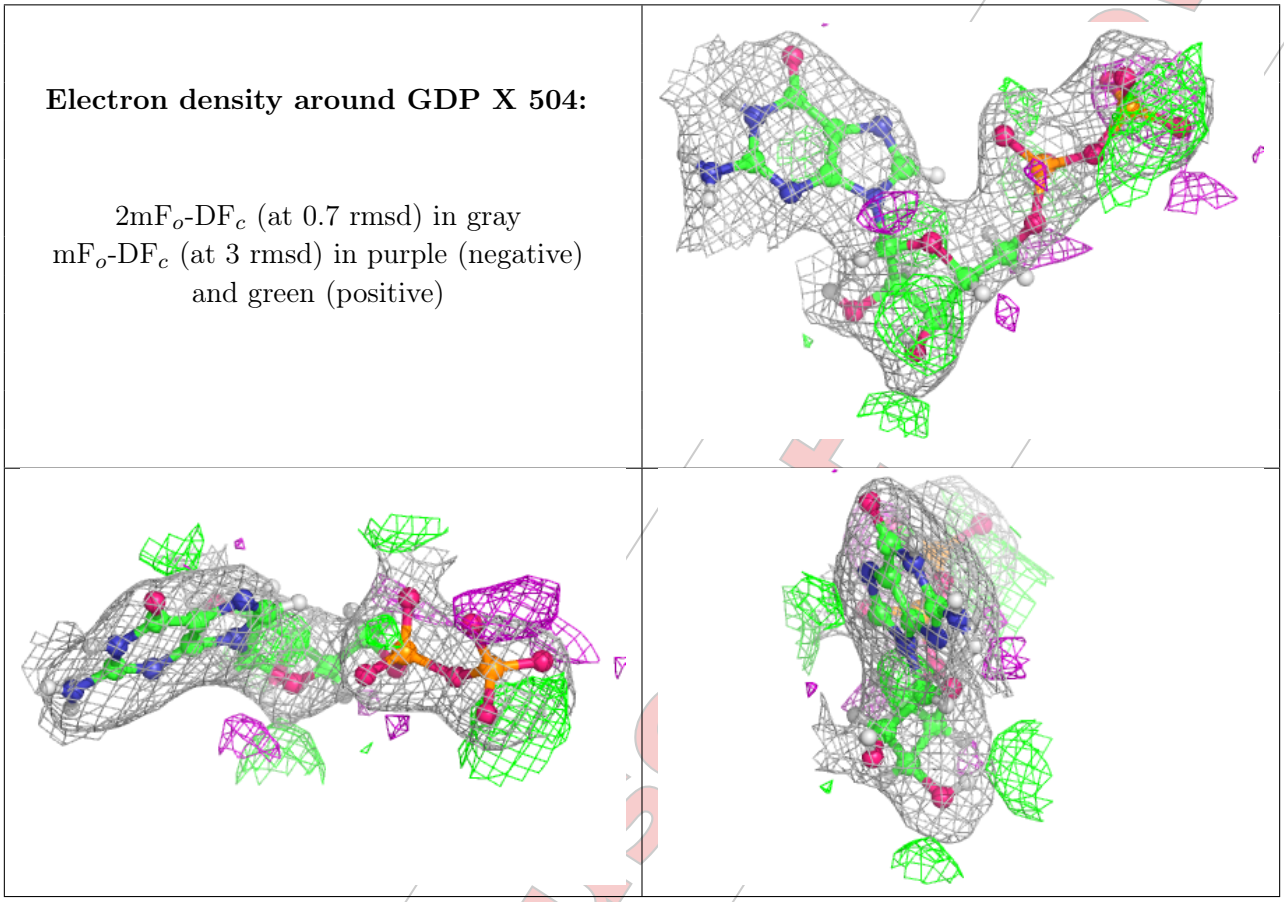






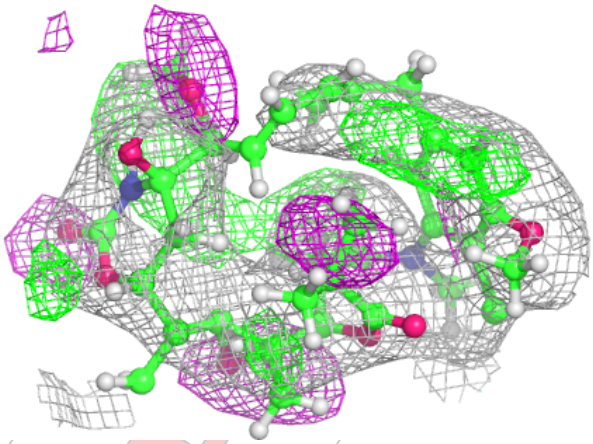
Electron density around GDP X 504:

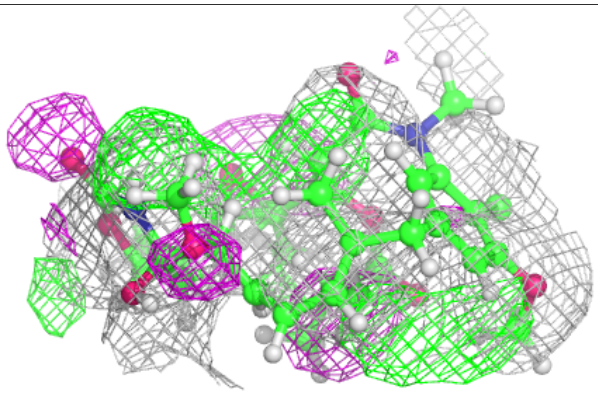
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

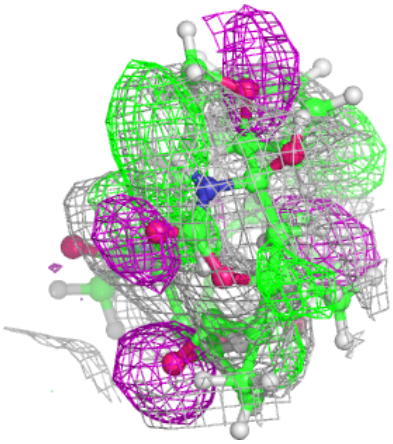


Electron density around ANS X 510:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

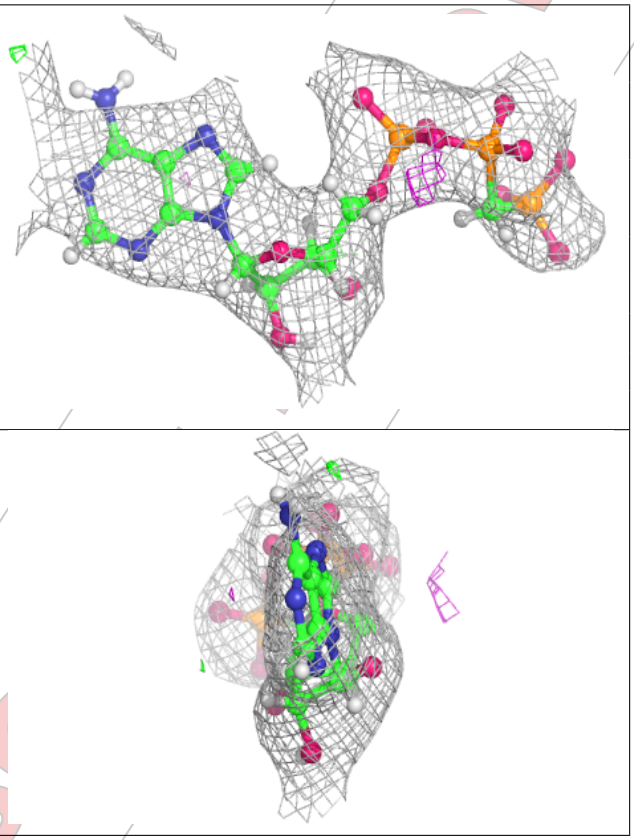






Electron density around ACP X 511:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2023 – 09:54 pm GMT

Deposition ID : D_1292128635

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

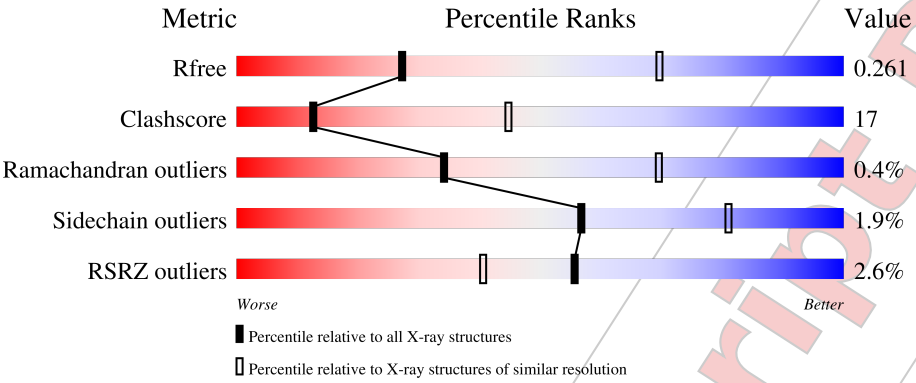
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	% 69% 30%
2	C	440	65% 33%
3	D	424	3% 63% 37%
4	E	120	3% 76% 24%

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Mol	Chain	Length	Quality of chain
5	F	331	9% 64% 33%
6	B	428	75% 25%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17637 atoms, of which 58 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3465	2200	584	657	24	5	9	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	440	3466	2197	584	662	23	4	7	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	424	3343	2102	567	646	28	6	4	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	120	991	612	180	194	5	0	0	0

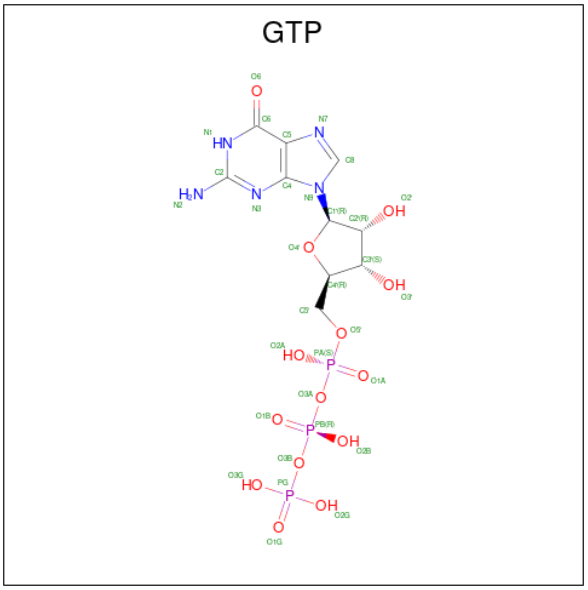
- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	331	2729	1762	457	496	14	5	4	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	B	428	3370	2118	576	649	27	6	2	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	X	1	Total C N O P 32 10 5 14 3	0	0
7	X	1	Total C N O P 32 10 5 14 3	0	0

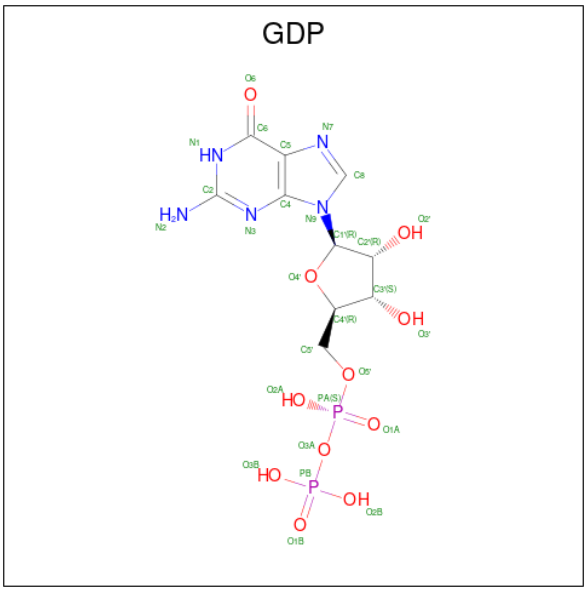
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	X	1	Total Mg 1 1	0	0
8	X	1	Total Mg 1 1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

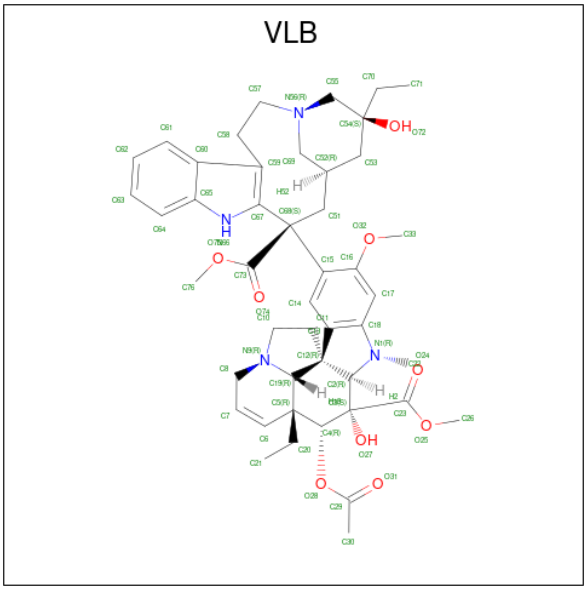
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	X	1	Total Ca 1 1	0	0
9	X	1	Total Ca 1 1	0	0

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	X	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
10	X	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula: $C_{46}H_{58}N_4O_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	X	1	Total	C	H	N	O	0	0
			117	46	58	4	9		

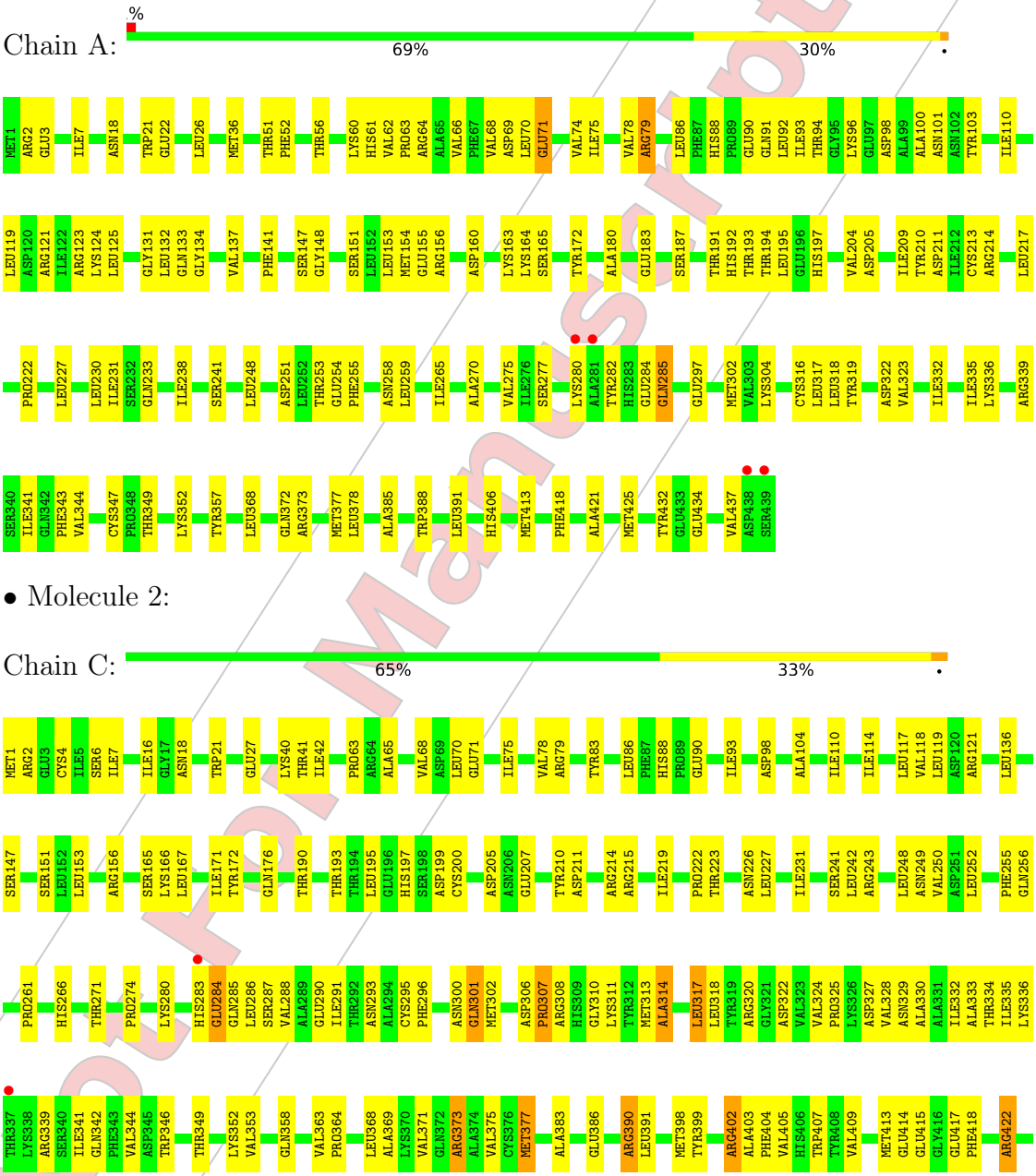
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	S	32	Total O 32 32	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

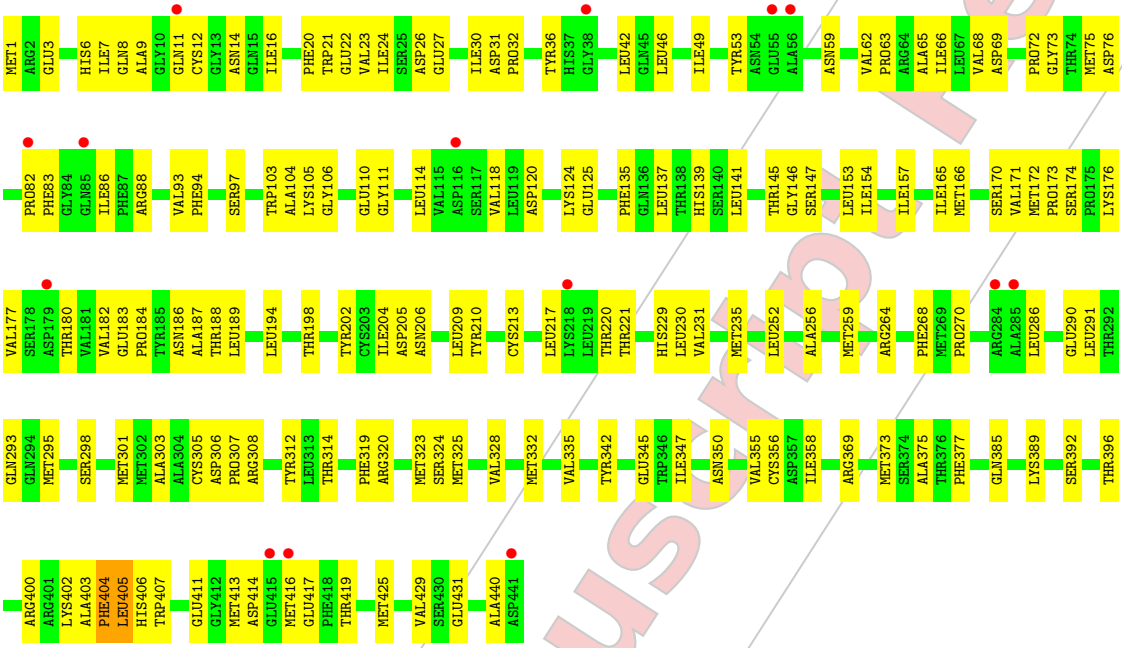
- Molecule 1:



- Molecule 2:

• Molecule 3:

Chain D:

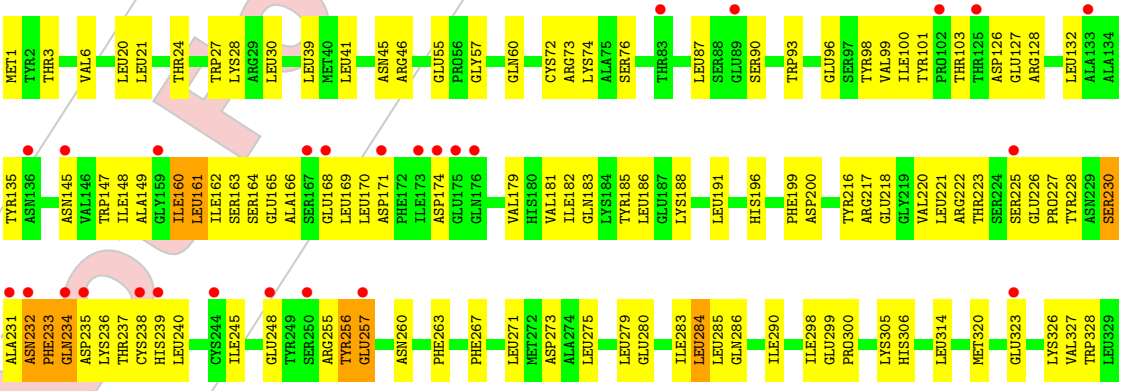


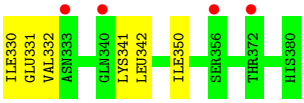
• Molecule 4:

Chain E:

• Molecule 5:

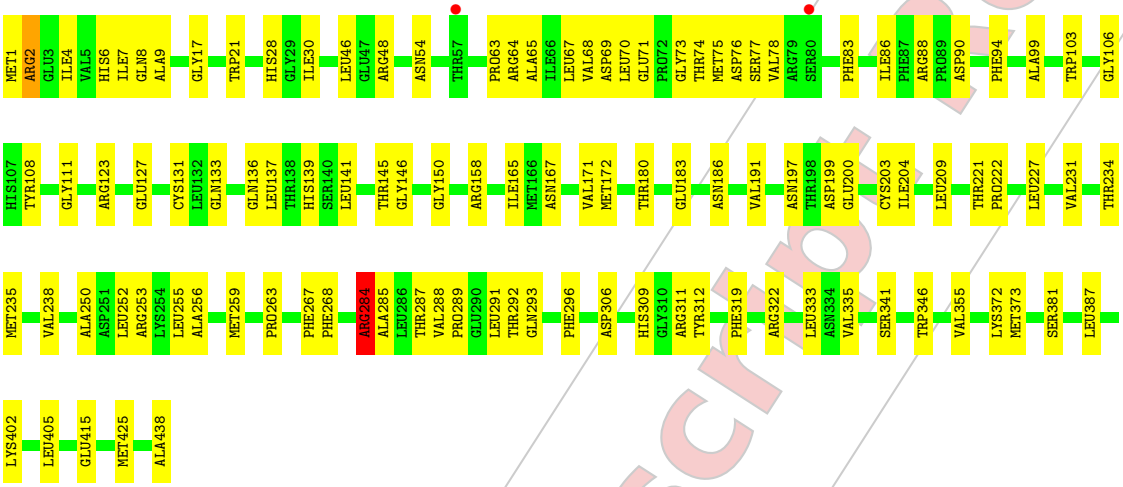
Chain F:





• Molecule 6:

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.39Å 159.74Å 182.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.13 – 3.20 15.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.13-3.20) 76.0 (15.13-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.79 (at 2.51Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.200 , 0.248 0.217 , 0.261	Depositor DCC
R_{free} test set	1999 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17637	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VLB, GDP, MG, GTP, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.32	0/3571	0.59	0/4849
2	C	0.47	0/3565	0.66	0/4842
3	D	0.32	0/3428	0.59	0/4645
4	E	0.34	0/999	0.65	0/1325
5	F	0.38	0/2802	0.62	0/3789
6	B	0.34	0/3451	0.63	0/4675
All	All	0.37	0/17816	0.62	0/24125

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	5
6	B	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain
6	B	284	ARG	Sidechain
2	C	243	ARG	Sidechain
2	C	373	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	C	390	ARG	Sidechain
2	C	402	ARG	Sidechain
2	C	422	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3465	0	3402	121	0
2	C	3466	0	3393	120	1
3	D	3343	0	3231	139	0
4	E	991	0	1012	27	1
5	F	2729	0	2715	92	0
6	B	3370	0	3250	85	0
7	X	64	0	24	1	0
8	X	2	0	0	0	0
9	X	2	0	0	0	0
10	X	56	0	24	4	0
11	X	59	58	58	15	0
12	S	32	0	0	3	0
All	All	17579	58	17109	577	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:HB3	1:A:280:LYS:HG3	1.35	1.07
6:B:2:ARG:HD3	6:B:133:GLN:HG2	1.41	1.02
3:D:141:LEU:HD11	3:D:170:SER:HB3	1.46	0.95
5:F:233:PHE:HA	5:F:239:HIS:CE1	2.02	0.95
3:D:402:LYS:HE3	3:D:405:LEU:CD1	1.97	0.94
5:F:132:LEU:HD21	5:F:170:LEU:HD11	1.50	0.94
5:F:263:PHE:HE2	5:F:341:LYS:HD3	1.34	0.93
2:C:293:ASN:HA	2:C:335:ILE:HD11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:402:LYS:HG3	3:D:405:LEU:HD13	1.53	0.91
1:A:317:LEU:HD21	1:A:377:MET:HE2	1.53	0.91
3:D:402:LYS:CG	3:D:405:LEU:HD13	2.03	0.89
2:C:88:HIS:NE2	2:C:90:GLU:HG3	1.88	0.89
2:C:274:PRO:HG2	2:C:371:VAL:HG11	1.54	0.88
5:F:226:GLU:HG3	5:F:227:PRO:HD2	1.57	0.86
3:D:402:LYS:HE3	3:D:405:LEU:HD11	1.58	0.86
3:D:402:LYS:CE	3:D:405:LEU:HD11	2.06	0.86
3:D:402:LYS:CE	3:D:405:LEU:CD1	2.55	0.84
4:E:126:LYS:HE2	4:E:126:LYS:HA	1.59	0.84
6:B:221:THR:HA	11:X:505:VLB:H761	1.59	0.83
2:C:176:GLN:HE22	2:C:207:GLU:HG3	1.42	0.83
2:C:328:VAL:HG11	2:C:353:VAL:HG11	1.60	0.83
3:D:298:SER:HB2	3:D:307:PRO:HD2	1.60	0.82
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.61	0.82
6:B:285:ALA:HB2	6:B:372:LYS:HE3	1.60	0.82
1:A:277:SER:HB3	1:A:280:LYS:CG	2.10	0.80
2:C:430:LYS:HE2	2:C:434:GLU:OE2	1.82	0.79
2:C:93:ILE:HD11	2:C:121:ARG:HG3	1.65	0.78
5:F:326:LYS:HE2	5:F:328:TRP:CZ2	2.18	0.78
3:D:20:PHE:HB2	3:D:235:MET:CE	2.13	0.78
1:A:357:TYR:CE2	4:E:17:GLY:HA2	2.18	0.77
5:F:257:GLU:HB3	5:F:260:ASN:HA	1.65	0.77
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.19	0.76
5:F:20:LEU:O	5:F:24:THR:HG23	1.85	0.76
1:A:317:LEU:HD21	1:A:377:MET:CE	2.16	0.75
1:A:132:LEU:O	1:A:164:LYS:HE3	1.86	0.75
1:A:209:ILE:HD11	1:A:302:MET:HE3	1.67	0.75
1:A:154:MET:HG3	1:A:194:THR:HG23	1.68	0.74
3:D:319:PHE:HB3	3:D:323:MET:CE	2.17	0.74
1:A:209:ILE:HD11	1:A:302:MET:CE	2.18	0.74
3:D:26:ASP:OD2	3:D:369:ARG:HD2	1.88	0.74
3:D:345:GLU:HG2	3:D:440:ALA:HB2	1.70	0.73
6:B:83:PHE:O	6:B:86:ILE:HG12	1.89	0.72
6:B:221:THR:HA	11:X:505:VLB:C76	2.19	0.72
1:A:277:SER:HB3	1:A:280:LYS:HE3	1.72	0.72
2:C:386:GLU:O	2:C:390:ARG:HG3	1.90	0.72
2:C:329:ASN:HD21	11:X:505:VLB:H66	1.36	0.71
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.72	0.71
1:A:154:MET:HE2	1:A:154:MET:HA	1.72	0.71
6:B:165:ILE:HG21	6:B:252:LEU:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:MET:HE3	3:D:166:MET:HA	1.71	0.71
6:B:83:PHE:HD2	6:B:86:ILE:HD13	1.55	0.71
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.73	0.71
2:C:271:THR:HG21	2:C:295:CYS:HA	1.72	0.70
1:A:62:VAL:HG23	1:A:86:LEU:O	1.91	0.70
5:F:305:LYS:HG2	5:F:306:HIS:CD2	2.26	0.70
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.73	0.70
1:A:332:ILE:O	1:A:335:ILE:HG13	1.91	0.70
3:D:259:MET:HE2	3:D:259:MET:HA	1.73	0.70
3:D:319:PHE:HB3	3:D:323:MET:HE1	1.72	0.70
1:A:56:THR:CG2	1:A:60:LYS:HB3	2.23	0.69
3:D:402:LYS:CE	3:D:405:LEU:HD13	2.22	0.69
3:D:406:HIS:CD2	3:D:407:TRP:HD1	2.10	0.69
3:D:165:ILE:HG21	3:D:252:LEU:HB3	1.73	0.69
3:D:137:LEU:HD23	3:D:154:ILE:HD11	1.75	0.69
1:A:339:ARG:HB2	1:A:341:ILE:HD11	1.74	0.68
2:C:332:ILE:HB	11:X:505:VLB:H303	1.76	0.68
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.24	0.68
1:A:277:SER:CB	1:A:280:LYS:HG3	2.18	0.68
2:C:274:PRO:CG	2:C:371:VAL:HG11	2.24	0.67
3:D:105:LYS:HG2	3:D:411:GLU:OE2	1.95	0.67
11:X:505:VLB:C22	11:X:505:VLB:H262	2.24	0.67
1:A:270:ALA:O	1:A:302:MET:HG2	1.95	0.67
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.09	0.66
6:B:6:HIS:CD2	6:B:21:TRP:HE1	2.13	0.66
5:F:103:THR:HG22	5:F:174:ASP:OD1	1.95	0.66
6:B:8:GLN:NE2	6:B:17:GLY:HA3	2.09	0.66
1:A:22:GLU:O	1:A:26:LEU:HD13	1.95	0.66
3:D:20:PHE:HB2	3:D:235:MET:HE3	1.76	0.66
5:F:162:ILE:HD11	5:F:234:GLN:N	2.11	0.66
2:C:252:LEU:HG	2:C:256:GLN:HE21	1.58	0.66
2:C:318:LEU:HD12	2:C:318:LEU:N	2.11	0.66
1:A:277:SER:CB	1:A:280:LYS:HE3	2.25	0.66
3:D:259:MET:HE2	3:D:314:THR:HB	1.78	0.66
5:F:314:LEU:HD22	5:F:350:ILE:HD11	1.76	0.66
2:C:40:LYS:O	2:C:42:ILE:HG13	1.95	0.66
6:B:306:ASP:HB3	6:B:309:HIS:ND1	2.11	0.65
5:F:73:ARG:HB2	5:F:76:SER:HB2	1.78	0.65
6:B:136:GLN:HA	6:B:167:ASN:O	1.96	0.65
2:C:317:LEU:HG	2:C:377:MET:HG3	1.79	0.65
2:C:322:ASP:HB3	2:C:373:ARG:HH21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:213:CYS:HA	3:D:217:LEU:HB2	1.78	0.65
5:F:263:PHE:CE2	5:F:341:LYS:HD3	2.25	0.65
2:C:301:GLN:HE22	2:C:307:PRO:HG2	1.62	0.64
1:A:336:LYS:HG2	4:E:24:LEU:HD23	1.79	0.64
3:D:286:LEU:HB2	3:D:290:GLU:OE1	1.96	0.64
2:C:431:ASP:O	2:C:435:VAL:HG13	1.98	0.64
5:F:101:TYR:CE1	5:F:126:ASP:HB3	2.33	0.64
2:C:271:THR:HG23	2:C:300:ASN:O	1.96	0.64
3:D:20:PHE:CZ	3:D:24:ILE:HD13	2.33	0.64
3:D:402:LYS:HE3	3:D:405:LEU:HD13	1.77	0.64
3:D:402:LYS:HE2	3:D:405:LEU:HD11	1.78	0.64
6:B:292:THR:HG22	6:B:335:VAL:HG21	1.80	0.64
4:E:68:LEU:HD11	6:B:158:ARG:NH2	2.12	0.64
3:D:83:PHE:O	3:D:86:ILE:HG22	1.98	0.63
3:D:411:GLU:OE1	4:E:137:LYS:HE2	1.98	0.63
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.80	0.63
5:F:98:TYR:HA	5:F:127:GLU:OE2	1.99	0.63
2:C:274:PRO:CB	2:C:286:LEU:HD12	2.28	0.63
6:B:2:ARG:HA	6:B:131:CYS:O	1.97	0.63
6:B:88:ARG:NH1	6:B:90:ASP:HB2	2.14	0.63
3:D:325:MET:SD	3:D:355:VAL:HG21	2.39	0.63
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.79	0.62
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.80	0.62
1:A:172:TYR:HE1	1:A:391:LEU:HD22	1.64	0.62
2:C:211:ASP:HB3	2:C:215:ARG:NH1	2.15	0.62
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.30	0.62
5:F:237:THR:H	5:F:240:LEU:HD12	1.65	0.62
2:C:432:TYR:O	2:C:435:VAL:HG22	2.00	0.62
4:E:46:SER:O	4:E:50:ILE:HD13	2.00	0.62
11:X:505:VLB:H572	11:X:505:VLB:H511	1.80	0.61
3:D:106:GLY:O	3:D:111:GLY:HA3	2.00	0.61
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.41	0.61
3:D:22:GLU:HG2	3:D:83:PHE:CD2	2.34	0.61
3:D:141:LEU:HA	3:D:147:SER:HB3	1.81	0.61
5:F:57:GLY:HA3	6:B:333:LEU:HD13	1.83	0.61
6:B:191:VAL:HG11	6:B:425:MET:CE	2.31	0.61
5:F:185:TYR:HE1	5:F:228:TYR:HH	1.46	0.61
1:A:155:GLU:HA	1:A:197:HIS:CD2	2.36	0.61
3:D:396:THR:O	3:D:400:ARG:HB2	2.01	0.61
5:F:3:THR:HB	5:F:30:LEU:HD11	1.83	0.61
2:C:176:GLN:NE2	2:C:207:GLU:HG3	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:73:GLY:O	6:B:75:MET:N	2.35	0.60
2:C:255:PHE:CE1	2:C:352:LYS:HG2	2.37	0.60
1:A:172:TYR:CE1	1:A:391:LEU:HD22	2.37	0.60
1:A:56:THR:HG22	1:A:60:LYS:HB3	1.84	0.60
2:C:4[A]:CYS:SG	2:C:136:LEU:HG	2.42	0.60
3:D:194:LEU:HD22	3:D:198:THR:HG21	1.84	0.60
6:B:2:ARG:HD3	6:B:133:GLN:CG	2.22	0.60
11:X:505:VLB:H262	11:X:505:VLB:N1	2.16	0.60
2:C:165:SER:HA	2:C:199:ASP:OD2	2.02	0.59
2:C:166:LYS:HE2	2:C:197:HIS:O	2.01	0.59
2:C:274:PRO:HB3	2:C:286:LEU:HD12	1.85	0.59
3:D:103:TRP:HB2	3:D:186:ASN:OD1	2.01	0.59
2:C:335:ILE:CG2	2:C:341:ILE:HD11	2.32	0.59
4:E:126:LYS:HE2	4:E:126:LYS:CA	2.29	0.59
5:F:100:ILE:HG12	5:F:128:ARG:HA	1.82	0.59
11:X:505:VLB:C67	11:X:505:VLB:H691	2.33	0.59
1:A:163:LYS:O	1:A:164:LYS:HD2	2.03	0.59
6:B:171:VAL:HA	6:B:204:ILE:O	2.03	0.59
1:A:56:THR:HG21	1:A:60:LYS:HB3	1.85	0.59
3:D:12:CYS:O	3:D:16:ILE:HG12	2.03	0.59
4:E:45:PRO:HB3	4:E:49:GLU:OE1	2.03	0.59
5:F:220:VAL:HG12	5:F:263:PHE:CE1	2.38	0.58
1:A:69:ASP:O	1:A:94:THR:HA	2.04	0.58
2:C:223:THR:O	2:C:227:LEU:HD13	2.03	0.58
6:B:200:GLU:OE2	6:B:256:ALA:HB2	2.02	0.58
2:C:311:LYS:HG2	2:C:342:GLN:HG2	1.84	0.58
2:C:405:VAL:O	2:C:409:VAL:HG23	2.03	0.58
3:D:66:ILE:HD11	3:D:125:GLU:HG3	1.86	0.58
5:F:165:GLU:O	5:F:168:GLU:HG2	2.04	0.58
2:C:261:PRO:HG3	2:C:313:MET:CE	2.33	0.58
4:E:47:LEU:O	4:E:51:GLN:HG2	2.03	0.58
5:F:186:LEU:HD21	5:F:328:TRP:CD1	2.38	0.58
6:B:69:ASP:O	6:B:94:PHE:HA	2.04	0.58
2:C:88:HIS:CD2	2:C:90:GLU:HG3	2.39	0.58
3:D:6:HIS:CD2	3:D:21:TRP:HE1	2.22	0.58
5:F:326:LYS:HE2	5:F:328:TRP:CH2	2.39	0.58
3:D:145:THR:N	10:X:508:GDP:O2B	2.37	0.57
3:D:118:VAL:HG11	3:D:153:LEU:HD11	1.86	0.57
3:D:183:GLU:HB2	3:D:184:PRO:HD3	1.85	0.57
3:D:205:ASP:O	3:D:209:LEU:HD22	2.04	0.57
2:C:195:LEU:HD12	2:C:266:HIS:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:VAL:HA	3:D:204:ILE:O	2.05	0.57
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.39	0.57
2:C:119:LEU:HD11	2:C:156:ARG:HB3	1.87	0.57
5:F:199:PHE:HB3	5:F:223:THR:HG22	1.87	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.56
2:C:75:ILE:HG22	2:C:79:ARG:NH1	2.19	0.56
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.05	0.56
1:A:163:LYS:HD2	1:A:163:LYS:N	2.20	0.56
3:D:392:SER:O	3:D:396:THR:HG22	2.05	0.56
2:C:248:LEU:HD13	11:X:505:VLB:H61	1.87	0.56
3:D:206:ASN:HA	3:D:209:LEU:HD23	1.87	0.56
1:A:180:ALA:O	1:A:183:GLU:HG3	2.06	0.56
3:D:295:MET:CE	3:D:375:ALA:HB1	2.36	0.56
3:D:347:ILE:HG22	3:D:350:ASN:HB3	1.88	0.56
1:A:277:SER:HB3	1:A:280:LYS:CE	2.36	0.56
3:D:332:MET:O	3:D:335:VAL:HG12	2.05	0.56
3:D:97:SER:HB2	3:D:110:GLU:HG2	1.87	0.56
3:D:204:ILE:HD12	3:D:204:ILE:N	2.21	0.56
5:F:46:ARG:HB3	5:F:46:ARG:CZ	2.36	0.56
3:D:188:THR:HG23	3:D:425:MET:HE3	1.88	0.55
2:C:311:LYS:HE3	2:C:436:GLY:O	2.05	0.55
3:D:291:LEU:HD11	3:D:373:MET:HG3	1.88	0.55
2:C:271:THR:CG2	2:C:295:CYS:HA	2.37	0.55
2:C:368:LEU:HD12	2:C:369:ALA:H	1.71	0.55
1:A:137:VAL:HG21	1:A:154:MET:CE	2.36	0.55
3:D:209:LEU:HD12	3:D:230:LEU:HB2	1.88	0.55
3:D:402:LYS:HG2	3:D:405:LEU:HD22	1.87	0.55
5:F:163:SER:HB3	5:F:169:LEU:HD11	1.89	0.55
6:B:158:ARG:NH1	6:B:197:ASN:OD1	2.39	0.55
2:C:151[B]:SER:HB3	2:C:193:THR:HG21	1.88	0.55
6:B:311:ARG:NH1	6:B:341:SER:O	2.38	0.55
3:D:259:MET:CE	3:D:314:THR:HB	2.36	0.54
2:C:287:SER:H	2:C:290:GLU:HG3	1.72	0.54
2:C:172:TYR:HB3	2:C:205:ASP:HA	1.90	0.54
2:C:301:GLN:NE2	2:C:307:PRO:HG2	2.22	0.54
2:C:88:HIS:CD2	2:C:90:GLU:H	2.25	0.54
3:D:205:ASP:HB3	3:D:303:ALA:HA	1.90	0.54
3:D:290:GLU:O	3:D:293:GLN:HG2	2.06	0.54
5:F:245:ILE:HG22	5:F:245:ILE:O	2.07	0.54
1:A:56:THR:CG2	1:A:60:LYS:H	2.20	0.54
1:A:357:TYR:CD2	4:E:17:GLY:HA2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:30:ILE:HD12	6:B:30:ILE:N	2.23	0.54
2:C:151[A]:SER:HB2	2:C:193:THR:HG21	1.90	0.54
2:C:261:PRO:HG3	2:C:313:MET:HE2	1.90	0.54
3:D:264:ARG:NE	3:D:431:GLU:OE2	2.41	0.54
3:D:286:LEU:H	3:D:286:LEU:HD23	1.72	0.54
3:D:8:GLN:NE2	3:D:14:ASN:HA	2.23	0.54
3:D:416:MET:O	3:D:419:THR:N	2.40	0.54
5:F:162:ILE:C	5:F:162:ILE:HD12	2.28	0.54
2:C:414:GLU:O	2:C:417[B]:GLU:HG3	2.08	0.54
6:B:21:TRP:CZ2	6:B:65:ALA:HB2	2.43	0.54
3:D:20:PHE:HB2	3:D:235:MET:HE1	1.90	0.53
1:A:90:GLU:O	1:A:121:ARG:HD2	2.09	0.53
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.53
2:C:344:VAL:HG21	2:C:346:TRP:CE2	2.44	0.53
3:D:402:LYS:HE2	3:D:405:LEU:CD1	2.36	0.53
3:D:7:ILE:O	3:D:137:LEU:HA	2.08	0.53
6:B:21:TRP:CZ3	6:B:63:PRO:HB3	2.44	0.53
1:A:339:ARG:HB2	1:A:341:ILE:CD1	2.39	0.53
2:C:332:ILE:O	2:C:336:LYS:HG3	2.08	0.53
4:E:105:MET:HE2	4:E:105:MET:HA	1.91	0.53
1:A:372[B]:GLN:OE1	1:A:373:ARG:NH1	2.42	0.53
5:F:171:ASP:HA	5:F:174:ASP:HB2	1.91	0.53
2:C:434:GLU:HA	2:C:437:VAL:HG23	1.91	0.52
5:F:74:LYS:NZ	5:F:331:GLU:OE1	2.41	0.52
6:B:319:PHE:O	6:B:355:VAL:HA	2.09	0.52
1:A:191:THR:O	1:A:195:LEU:HB2	2.09	0.52
2:C:214:ARG:HG2	2:C:219:ILE:O	2.08	0.52
5:F:147:TRP:HB3	5:F:182:ILE:HG23	1.91	0.52
5:F:280:GLU:HA	5:F:284[A]:LEU:HB2	1.91	0.52
6:B:221:THR:CA	11:X:505:VLB:H761	2.36	0.52
2:C:117:LEU:HD11	2:C:121:ARG:CZ	2.40	0.52
2:C:335:ILE:HG23	2:C:339:ARG:HD2	1.90	0.52
1:A:66[B]:VAL:HG23	1:A:125:LEU:HD12	1.92	0.52
2:C:151[B]:SER:HB3	2:C:193:THR:CG2	2.40	0.52
1:A:96:LYS:N	1:A:96:LYS:HD2	2.25	0.52
2:C:21:TRP:CZ3	2:C:63:PRO:HB3	2.45	0.52
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.90	0.52
2:C:151[A]:SER:HB2	2:C:193:THR:CG2	2.40	0.52
3:D:312:TYR:CE1	3:D:377:PHE:HZ	2.28	0.52
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.10	0.52
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:MET:HA	3:D:166:MET:CE	2.40	0.52
6:B:4:ILE:O	6:B:64:ARG:HD2	2.09	0.52
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.51
3:D:22:GLU:HG2	3:D:83:PHE:HD2	1.75	0.51
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.90	0.51
3:D:153:LEU:O	3:D:157:ILE:HG13	2.10	0.51
3:D:320:ARG:O	3:D:373:MET:HA	2.10	0.51
5:F:87:LEU:O	5:F:90:SER:HB2	2.10	0.51
5:F:93:TRP:CZ3	5:F:290:ILE:HG23	2.46	0.51
5:F:225:SER:HB2	5:F:260:ASN:HD21	1.76	0.51
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.41	0.51
3:D:11:GLN:HB3	10:X:508:GDP:O2A	2.10	0.51
3:D:49:ILE:HG13	3:D:53:TYR:HD2	1.74	0.51
5:F:255:ARG:HD3	5:F:256:TYR:CZ	2.45	0.51
1:A:434:GLU:O	1:A:437:VAL:HG12	2.10	0.51
3:D:176:LYS:HD3	3:D:210:TYR:CD2	2.46	0.51
6:B:83:PHE:CD2	6:B:86:ILE:HD13	2.43	0.51
2:C:200:CYS:HA	2:C:266:HIS:HB2	1.93	0.51
2:C:227:LEU:O	2:C:231:ILE:HG13	2.10	0.51
1:A:96:LYS:HD2	1:A:96:LYS:H	1.75	0.51
2:C:313:MET:O	2:C:314:ALA:HB2	2.10	0.51
3:D:319:PHE:HB2	3:D:355:VAL:HG12	1.94	0.50
5:F:233:PHE:HA	5:F:239:HIS:NE2	2.23	0.50
5:F:279:LEU:HD12	5:F:283:ILE:HB	1.93	0.50
6:B:289:PRO:O	6:B:293:GLN:HG2	2.11	0.50
2:C:70:LEU:HD13	2:C:110:ILE:CG2	2.41	0.50
2:C:318:LEU:HD12	2:C:318:LEU:H	1.74	0.50
5:F:162:ILE:HD13	5:F:233:PHE:HB2	1.92	0.50
11:X:505:VLB:C73	11:X:505:VLB:O32	2.60	0.50
1:A:317:LEU:CD2	1:A:377:MET:HE2	2.34	0.50
1:A:251:ASP:OD1	1:A:253:THR:HB	2.11	0.50
6:B:322:ARG:O	6:B:373:MET:HE2	2.11	0.50
6:B:48:ARG:NH2	6:B:250:ALA:O	2.41	0.50
2:C:296:PHE:HB3	2:C:339:ARG:HD3	1.93	0.50
6:B:172:MET:HG3	6:B:387:LEU:HD11	1.92	0.50
3:D:59:ASN:O	3:D:59:ASN:ND2	2.45	0.50
6:B:83:PHE:HB3	6:B:86:ILE:CD1	2.42	0.50
3:D:259:MET:HA	3:D:259:MET:CE	2.40	0.49
3:D:301:MET:HA	3:D:301:MET:HE2	1.92	0.49
1:A:277:SER:HB3	1:A:280:LYS:CD	2.41	0.49
3:D:403:ALA:O	3:D:405:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:148:ILE:O	5:F:182:ILE:HG12	2.12	0.49
6:B:7:ILE:O	6:B:137:LEU:HA	2.12	0.49
2:C:320:ARG:CG	2:C:358:GLN:O	2.59	0.49
3:D:12:CYS:SG	3:D:171:VAL:HG21	2.51	0.49
11:X:505:VLB:H64	11:X:505:VLB:H211	1.95	0.49
1:A:123:ARG:HH22	1:A:160:ASP:HB3	1.76	0.49
2:C:295:CYS:SG	2:C:375:VAL:HG13	2.52	0.49
2:C:306:ASP:OD2	2:C:308:ARG:NH2	2.45	0.49
3:D:416:MET:O	3:D:417:GLU:C	2.49	0.49
6:B:123:ARG:O	6:B:127:GLU:HG2	2.13	0.49
2:C:241:SER:HA	2:C:249:ASN:HD21	1.77	0.49
5:F:162:ILE:HD11	5:F:233:PHE:C	2.33	0.49
2:C:252:LEU:O	2:C:256:GLN:HG3	2.12	0.49
2:C:274:PRO:HB2	2:C:286:LEU:HD12	1.93	0.49
3:D:88:ARG:NH2	12:S:29:HOH:O	2.44	0.49
5:F:163:SER:HB3	5:F:169:LEU:CD1	2.43	0.49
1:A:227:LEU:O	1:A:231:ILE:HG13	2.12	0.49
2:C:117:LEU:HD11	2:C:121:ARG:NH2	2.27	0.49
4:E:131:GLU:OE1	4:E:131:GLU:HA	2.13	0.49
2:C:324:VAL:HG22	2:C:327:ASP:OD2	2.13	0.49
1:A:71:GLU:OE2	1:A:74:VAL:HG23	2.13	0.48
2:C:40:LYS:O	2:C:42:ILE:N	2.46	0.48
2:C:383:ALA:O	2:C:386:GLU:HG3	2.13	0.48
3:D:146:GLY:N	10:X:508:GDP:O2B	2.40	0.48
6:B:312:TYR:CD1	6:B:381:SER:HB2	2.48	0.48
3:D:345:GLU:CG	3:D:440:ALA:HB2	2.40	0.48
1:A:154:MET:HG3	1:A:194:THR:CG2	2.39	0.48
2:C:241:SER:HB2	2:C:250:VAL:O	2.13	0.48
4:E:76:ARG:NH1	4:E:79:GLU:OE2	2.46	0.48
6:B:54:ASN:OD1	6:B:64:ARG:NH2	2.46	0.48
6:B:204:ILE:HD13	6:B:231:VAL:HG13	1.95	0.48
6:B:231:VAL:O	6:B:235:MET:HG3	2.14	0.48
5:F:135:TYR:OH	5:F:164:SER:O	2.25	0.48
2:C:377:MET:HE3	2:C:377:MET:HB3	1.83	0.48
5:F:99:VAL:HG23	5:F:126:ASP:HB2	1.95	0.48
5:F:299:GLU:N	5:F:300:PRO:HD2	2.28	0.48
1:A:68[A]:VAL:HG22	1:A:93:ILE:HB	1.93	0.48
1:A:141:PHE:O	1:A:147:SER:HB3	2.14	0.48
6:B:284:ARG:O	6:B:284:ARG:HG3	2.14	0.48
1:A:151:SER:HB2	1:A:193:THR:CG2	2.43	0.48
3:D:104:ALA:HB2	3:D:413:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:180:THR:O	6:B:183:GLU:HG3	2.14	0.48
2:C:68[B]:VAL:HG21	2:C:118:VAL:HG21	1.95	0.48
5:F:179:VAL:HG13	5:F:179:VAL:O	2.14	0.47
6:B:74:THR:O	6:B:78:VAL:HG23	2.13	0.47
6:B:83:PHE:HB3	6:B:86:ILE:HD11	1.95	0.47
1:A:88:HIS:O	1:A:91:GLN:HG2	2.13	0.47
2:C:403:ALA:O	2:C:404:PHE:HB2	2.14	0.47
3:D:22:GLU:OE2	3:D:82:PRO:HG2	2.14	0.47
3:D:385:GLN:O	3:D:389:LYS:HG3	2.14	0.47
2:C:288:VAL:O	2:C:291:ILE:HG12	2.13	0.47
5:F:161:LEU:HD12	5:F:169:LEU:HD21	1.97	0.47
3:D:30:ILE:HD12	3:D:30:ILE:N	2.29	0.47
4:E:50:ILE:HD12	4:E:50:ILE:N	2.29	0.47
6:B:191:VAL:HG11	6:B:425:MET:HE2	1.93	0.47
2:C:6:SER:O	2:C:65:ALA:HA	2.15	0.47
2:C:147:SER:HB2	2:C:190:THR:HB	1.96	0.47
2:C:283:HIS:O	2:C:284:GLU:HB2	2.14	0.47
2:C:284:GLU:OE2	2:C:286:LEU:HD21	2.14	0.47
5:F:271:LEU:HD23	5:F:275[A]:LEU:HD23	1.95	0.47
6:B:200:GLU:HB3	6:B:268:PHE:CE2	2.50	0.47
2:C:328:VAL:O	2:C:332:ILE:HG13	2.15	0.47
3:D:308:ARG:HG3	3:D:342:TYR:CZ	2.50	0.47
3:D:319:PHE:HB3	3:D:323:MET:HE3	1.95	0.47
4:E:53:LYS:HE3	4:E:53:LYS:HB2	1.72	0.47
5:F:267:PHE:O	5:F:271:LEU:HG	2.15	0.47
3:D:411:GLU:OE1	4:E:137:LYS:CE	2.63	0.47
5:F:326:LYS:HE2	5:F:328:TRP:CE2	2.48	0.47
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.96	0.47
1:A:79:ARG:HG2	1:A:92:LEU:HD13	1.95	0.47
1:A:241:SER:HB2	1:A:248:LEU:O	2.15	0.47
2:C:83:TYR:HD2	2:C:86:LEU:HD22	1.79	0.47
1:A:3:GLU:HG2	1:A:64:ARG:HH21	1.79	0.47
3:D:286:LEU:HD23	3:D:286:LEU:N	2.30	0.47
3:D:355:VAL:HG23	3:D:355:VAL:O	2.14	0.47
3:D:49:ILE:HG13	3:D:53:TYR:CD2	2.49	0.46
6:B:296:PHE:CE1	6:B:335:VAL:HG11	2.50	0.46
1:A:204:VAL:HG13	1:A:302:MET:HE3	1.97	0.46
3:D:9:ALA:HA	3:D:68:VAL:O	2.15	0.46
5:F:98:TYR:O	5:F:181:VAL:HG23	2.15	0.46
5:F:148:ILE:HG12	5:F:149:ALA:N	2.30	0.46
5:F:196:HIS:O	5:F:228:TYR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:70:LEU:HD12	6:B:99:ALA:HB2	1.97	0.46
6:B:291:LEU:HD11	6:B:373:MET:HB3	1.96	0.46
2:C:27:GLU:CD	2:C:320:ARG:HH22	2.19	0.46
3:D:62:VAL:HG11	3:D:88:ARG:HG3	1.97	0.46
5:F:221:LEU:HD12	5:F:221:LEU:N	2.30	0.46
5:F:283:ILE:HG23	5:F:327:VAL:CG2	2.45	0.46
3:D:174:SER:O	3:D:177:VAL:HG12	2.15	0.46
3:D:320:ARG:HA	3:D:356:CYS:O	2.16	0.46
5:F:283:ILE:HG23	5:F:327:VAL:HG21	1.97	0.46
6:B:141:LEU:HD12	6:B:172:MET:CE	2.45	0.46
6:B:346:TRP:HE1	6:B:438:ALA:HB3	1.81	0.46
6:B:402:LYS:HE2	6:B:415:GLU:OE1	2.16	0.46
2:C:313:MET:HE2	2:C:346:TRP:HH2	1.81	0.46
3:D:220:THR:HG22	3:D:221:THR:HG23	1.97	0.46
3:D:406:HIS:CD2	3:D:407:TRP:CD1	2.98	0.46
5:F:132:LEU:HD21	5:F:170:LEU:CD1	2.34	0.46
5:F:162:ILE:CD1	5:F:233:PHE:HB2	2.44	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.51	0.46
6:B:292:THR:HG22	6:B:335:VAL:CG2	2.44	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.46
1:A:258:ASN:OD1	1:A:352:LYS:HE2	2.16	0.46
3:D:135:PHE:HB2	3:D:166:MET:CE	2.46	0.46
5:F:320:MET:HE1	12:S:42:HOH:O	2.15	0.46
6:B:172:MET:HE2	6:B:387:LEU:HD21	1.98	0.46
2:C:287:SER:H	2:C:290:GLU:CG	2.29	0.46
3:D:20:PHE:CE2	3:D:24:ILE:HD13	2.51	0.46
2:C:335:ILE:O	2:C:336:LYS:C	2.53	0.46
3:D:406:HIS:NE2	3:D:407:TRP:CD1	2.83	0.46
6:B:75:MET:O	6:B:76:ASP:C	2.54	0.46
1:A:2:ARG:O	1:A:133:GLN:NE2	2.42	0.46
5:F:72:CYS:HA	5:F:332:VAL:O	2.15	0.46
6:B:145:THR:N	10:X:504:GDP:O2B	2.49	0.46
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.51	0.45
2:C:16:ILE:CD1	2:C:171:ILE:HD11	2.46	0.45
2:C:136:LEU:HD23	2:C:167:LEU:HB2	1.98	0.45
5:F:200:ASP:O	5:F:221:LEU:HA	2.16	0.45
6:B:405:LEU:HD12	6:B:405:LEU:HA	1.80	0.45
3:D:69:ASP:HA	3:D:145:THR:HG21	1.98	0.45
1:A:155:GLU:HA	1:A:197:HIS:HD2	1.81	0.45
3:D:141:LEU:HB3	3:D:187:ALA:HA	1.98	0.45
5:F:235:ASP:O	5:F:236:LYS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:N	1:A:341:ILE:HD12	2.30	0.45
2:C:88:HIS:HD2	2:C:90:GLU:HB2	1.82	0.45
3:D:103:TRP:CE3	3:D:189:LEU:HD13	2.51	0.45
4:E:44:ASP:HA	4:E:45:PRO:HD3	1.76	0.45
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.46	0.45
3:D:295:MET:HE2	3:D:377:PHE:HB2	1.98	0.45
2:C:328:VAL:CG1	2:C:353:VAL:HG11	2.40	0.45
5:F:286:GLN:O	5:F:290:ILE:HG13	2.16	0.45
6:B:21:TRP:CE3	6:B:63:PRO:HB3	2.52	0.45
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.41	0.45
4:E:126:LYS:CA	4:E:126:LYS:CE	2.95	0.45
6:B:67:LEU:N	6:B:67:LEU:HD12	2.32	0.45
5:F:199:PHE:CD2	5:F:221:LEU:HD23	2.52	0.45
1:A:2:ARG:HB3	1:A:131:GLY:O	2.17	0.45
1:A:357:TYR:OH	4:E:18:GLN:HG3	2.16	0.45
2:C:287:SER:N	2:C:290:GLU:HG3	2.32	0.45
6:B:209:LEU:HB3	6:B:227:LEU:HG	1.98	0.45
2:C:287:SER:H	2:C:290:GLU:CD	2.21	0.44
4:E:82:VAL:HG11	6:B:108:TYR:CG	2.52	0.44
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.53	0.44
5:F:191:LEU:HD13	5:F:196:HIS:CE1	2.53	0.44
5:F:320:MET:CE	12:S:42:HOH:O	2.65	0.44
6:B:9:ALA:HA	6:B:68:VAL:O	2.17	0.44
3:D:385:GLN:HB2	3:D:429:VAL:HG13	1.98	0.44
6:B:1:MET:HE2	6:B:1:MET:HA	1.99	0.44
6:B:222:PRO:HD2	11:X:505:VLB:H762	1.99	0.44
1:A:258:ASN:HB2	1:A:259:LEU:HD22	1.99	0.44
6:B:165:ILE:HA	6:B:199:ASP:OD2	2.17	0.44
3:D:36:TYR:CD1	3:D:46:LEU:HD11	2.53	0.44
2:C:7:ILE:HG21	2:C:153:LEU:HD21	1.99	0.44
3:D:137:LEU:HG	3:D:139:HIS:ND1	2.32	0.44
5:F:320:MET:HE2	5:F:330:ILE:HG13	1.99	0.44
1:A:322:ASP:HB3	1:A:373:ARG:HH21	1.83	0.44
3:D:402:LYS:HG2	3:D:402:LYS:O	2.18	0.44
4:E:7:GLU:O	4:E:22:VAL:HA	2.17	0.44
5:F:135:TYR:HE1	5:F:145:ASN:HB3	1.83	0.44
1:A:52:PHE:O	1:A:64:ARG:HG3	2.17	0.43
1:A:413:MET:CE	1:A:418:PHE:CE1	3.01	0.43
2:C:219:ILE:HD13	2:C:226:ASN:ND2	2.33	0.43
3:D:135:PHE:HB2	3:D:166:MET:HE3	2.00	0.43
3:D:404:PHE:C	3:D:406:HIS:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:284[A]:LEU:HD12	5:F:284[A]:LEU:HA	1.76	0.43
6:B:106:GLY:O	6:B:111:GLY:HA3	2.18	0.43
6:B:319:PHE:HB2	6:B:355:VAL:HG22	2.01	0.43
2:C:18:ASN:OD1	2:C:78:VAL:HG22	2.18	0.43
2:C:330:ALA:O	2:C:333:ALA:HB3	2.18	0.43
3:D:23:VAL:O	3:D:27:GLU:HG3	2.18	0.43
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.34	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.43
2:C:407:TRP:CH2	3:D:256:ALA:HB1	2.53	0.43
3:D:69:ASP:O	3:D:94:PHE:HA	2.18	0.43
3:D:194:LEU:CD2	3:D:198:THR:HG21	2.48	0.43
11:X:505:VLB:H762	11:X:505:VLB:H512	1.99	0.43
3:D:73:GLY:HA2	3:D:76:ASP:HB2	1.99	0.43
3:D:180:THR:O	3:D:182:VAL:N	2.46	0.43
2:C:93:ILE:HG22	2:C:114:ILE:HD11	2.01	0.43
2:C:335:ILE:HG22	2:C:341:ILE:HD11	2.00	0.43
3:D:104:ALA:HB2	3:D:413:MET:HE1	2.01	0.43
1:A:56:THR:HG22	1:A:60:LYS:N	2.34	0.43
2:C:250:VAL:HG11	2:C:352:LYS:HE2	2.00	0.43
5:F:21:LEU:HD22	5:F:27:TRP:NE1	2.34	0.43
5:F:45:ASN:C	5:F:46:ARG:HG2	2.39	0.43
3:D:21:TRP:CZ3	3:D:63:PRO:HB3	2.53	0.43
5:F:231:ALA:O	5:F:232:ASN:HB3	2.17	0.43
5:F:286:GLN:OE1	5:F:327:VAL:HG23	2.18	0.43
3:D:21:TRP:CZ2	3:D:65:ALA:HB2	2.53	0.43
3:D:93:VAL:HG12	3:D:114:LEU:HD11	2.01	0.43
6:B:203:CYS:SG	6:B:267:PHE:HB3	2.59	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.42
5:F:257:GLU:HB3	5:F:260:ASN:CA	2.43	0.42
6:B:146:GLY:O	6:B:150:GLY:HA3	2.17	0.42
6:B:285:ALA:HB2	6:B:372:LYS:CE	2.42	0.42
3:D:204:ILE:HG21	3:D:231:VAL:HG22	2.01	0.42
3:D:268:PHE:O	3:D:270:PRO:HD3	2.19	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.54	0.42
2:C:398:MET:HE3	3:D:347:ILE:HG23	2.00	0.42
2:C:399:TYR:O	2:C:402:ARG:HD3	2.19	0.42
2:C:422:ARG:HD2	2:C:422:ARG:HA	1.74	0.42
3:D:172:MET:HA	3:D:173:PRO:HD3	1.91	0.42
1:A:285:GLN:CG	1:A:372[B]:GLN:CD	2.88	0.42
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:MET:O	2:C:2:ARG:HB2	2.20	0.42
2:C:415:GLU:O	2:C:418:PHE:HB2	2.19	0.42
3:D:120:ASP:O	3:D:124:LYS:HG3	2.19	0.42
3:D:298:SER:HB2	3:D:306:ASP:OD1	2.18	0.42
3:D:298:SER:CB	3:D:307:PRO:HD2	2.42	0.42
3:D:414:ASP:OD1	3:D:414:ASP:N	2.43	0.42
5:F:248:GLU:O	5:F:248:GLU:HG2	2.19	0.42
6:B:103:TRP:HB2	6:B:186:ASN:OD1	2.18	0.42
2:C:333:ALA:O	2:C:334:THR:C	2.57	0.42
6:B:30:ILE:HD12	6:B:30:ILE:H	1.84	0.42
1:A:2:ARG:CB	1:A:133:GLN:HG2	2.47	0.42
1:A:70:LEU:HB2	1:A:98:ASP:HA	2.01	0.42
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.54	0.42
3:D:303:ALA:O	3:D:305:CYS:N	2.51	0.42
4:E:137:LYS:NZ	4:E:140:LYS:NZ	2.67	0.42
1:A:75:ILE:O	1:A:79:ARG:HG3	2.20	0.42
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.02	0.42
4:E:60:ARG:O	4:E:64:GLN:HG2	2.20	0.42
5:F:1:MET:CE	5:F:28:LYS:HB2	2.50	0.42
5:F:271:LEU:C	5:F:273:ASP:H	2.22	0.42
6:B:141:LEU:HD12	6:B:172:MET:SD	2.59	0.42
6:B:158:ARG:NH1	6:B:197:ASN:HA	2.34	0.42
6:B:387:LEU:C	6:B:387:LEU:HD23	2.40	0.42
1:A:406:HIS:CD2	6:B:263:PRO:HD3	2.55	0.42
5:F:188:LYS:O	5:F:323:GLU:HG3	2.20	0.42
5:F:298:ILE:C	5:F:300:PRO:HD2	2.40	0.42
1:A:238:ILE:HG12	1:A:378:LEU:HD21	2.02	0.42
3:D:31:ASP:HB2	3:D:32:PRO:HD2	2.02	0.42
3:D:205:ASP:O	3:D:209:LEU:CD2	2.68	0.42
5:F:6:VAL:HG22	5:F:41:LEU:HD12	2.02	0.42
5:F:279:LEU:HG	5:F:284[A]:LEU:HD22	2.00	0.42
5:F:279:LEU:HG	5:F:284[B]:LEU:HG	2.01	0.42
6:B:46:LEU:HD23	6:B:46:LEU:HA	1.90	0.42
6:B:234:THR:O	6:B:238:VAL:HG13	2.20	0.42
2:C:104:ALA:HB2	2:C:413:MET:HG3	2.02	0.41
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.41
2:C:98:ASP:HB2	7:X:506:GTP:O3G	2.20	0.41
2:C:210:TYR:CZ	2:C:222:PRO:HD2	2.56	0.41
5:F:160:ILE:HG13	5:F:240:LEU:HD21	2.01	0.41
1:A:357:TYR:OH	4:E:18:GLN:NE2	2.44	0.41
2:C:296:PHE:CB	2:C:339:ARG:HD3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:42:LEU:HB3	3:D:358:ILE:HD11	2.02	0.41
5:F:217:ARG:HG3	5:F:218:GLU:HG2	2.01	0.41
2:C:430:LYS:O	2:C:434:GLU:HG3	2.19	0.41
3:D:404:PHE:C	3:D:406:HIS:N	2.74	0.41
5:F:55:GLU:HB2	5:F:60:GLN:HE21	1.85	0.41
1:A:100:ALA:HB2	6:B:253:ARG:HD2	2.03	0.41
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.55	0.41
1:A:213:CYS:O	1:A:217:LEU:HB2	2.20	0.41
2:C:90:GLU:HB3	2:C:121:ARG:HD2	2.03	0.41
5:F:98:TYR:HB3	5:F:127:GLU:HG3	2.02	0.41
1:A:372[B]:GLN:HG3	1:A:373:ARG:CZ	2.50	0.41
1:A:255:PHE:O	1:A:259:LEU:HD23	2.20	0.41
5:F:96:GLU:O	5:F:183:GLN:HA	2.21	0.41
2:C:328:VAL:HG11	11:X:505:VLB:H63	2.02	0.41
4:E:46:SER:O	4:E:50:ILE:CD1	2.68	0.41
1:A:56:THR:HG22	1:A:60:LYS:H	1.86	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.57	0.41
4:E:24:LEU:HD12	4:E:24:LEU:N	2.36	0.41
2:C:285:GLN:HE21	2:C:373:ARG:HH12	1.68	0.40
2:C:308:ARG:C	2:C:310:GLY:H	2.25	0.40
3:D:36:TYR:CE1	3:D:46:LEU:CD1	3.04	0.40
3:D:202:TYR:O	3:D:204:ILE:HD12	2.21	0.40
3:D:324:SER:O	3:D:328:VAL:HG23	2.21	0.40
5:F:216:TYR:OH	5:F:342:LEU:HD22	2.21	0.40
6:B:191:VAL:CG1	6:B:425:MET:CE	2.97	0.40
1:A:335:ILE:HD12	1:A:336:LYS:N	2.37	0.40
5:F:39:LEU:HD21	5:F:41:LEU:HD21	2.03	0.40
5:F:135:TYR:CE2	5:F:166:ALA:HB2	2.56	0.40
6:B:255:LEU:HD12	6:B:259:MET:HG2	2.03	0.40
3:D:1:MET:HG3	3:D:3:GLU:OE2	2.21	0.40
4:E:8:VAL:O	4:E:9:ILE:HD13	2.22	0.40
6:B:28:HIS:HB2	6:B:30:ILE:CD1	2.52	0.40
6:B:287:THR:O	6:B:288:VAL:C	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:322:ASP:OD2	4:E:98:LYS:NZ[4_455]	1.92	0.28

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/439 (102%)	426 (96%)	18 (4%)	2 (0%)	34	69
2	C	445/440 (101%)	415 (93%)	27 (6%)	3 (1%)	22	61
3	D	424/424 (100%)	402 (95%)	20 (5%)	2 (0%)	29	67
4	E	116/120 (97%)	113 (97%)	3 (3%)	0	100	100
5	F	323/331 (98%)	295 (91%)	26 (8%)	2 (1%)	25	64
6	B	428/428 (100%)	415 (97%)	13 (3%)	0	100	100
All	All	2182/2182 (100%)	2066 (95%)	107 (5%)	9 (0%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	41	THR
2	C	284	GLU
3	D	404	PHE
5	F	230	SER
1	A	284	GLU
2	C	314	ALA
1	A	282	TYR
3	D	72	PRO
5	F	232	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	378/370 (102%)	375 (99%)	3 (1%)	81 93
2	C	378/371 (102%)	364 (96%)	14 (4%)	34 68
3	D	369/366 (101%)	366 (99%)	3 (1%)	81 93
4	E	108/108 (100%)	106 (98%)	2 (2%)	57 81
5	F	303/299 (101%)	292 (96%)	11 (4%)	35 69
6	B	369/370 (100%)	364 (99%)	5 (1%)	67 86
All	All	1905/1884 (101%)	1867 (98%)	38 (2%)	57 80

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	124	LYS
1	A	285	GLN
2	C	71	GLU
2	C	242	LEU
2	C	280	LYS
2	C	301	GLN
2	C	302	MET
2	C	307	PRO
2	C	317	LEU
2	C	325	PRO
2	C	349	THR
2	C	363[A]	VAL
2	C	363[B]	VAL
2	C	377	MET
2	C	391	LEU
2	C	439	SER
3	D	75	MET
3	D	229	HIS
3	D	405	LEU
4	E	61	ARG
4	E	106	GLU
5	F	160	ILE
5	F	161	LEU
5	F	222	ARG
5	F	230	SER
5	F	233	PHE
5	F	234	GLN
5	F	238	CYS
5	F	256	TYR

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Mol	Chain	Res	Type
5	F	257	GLU
5	F	284[A]	LEU
5	F	284[B]	LEU
6	B	2	ARG
6	B	71	GLU
6	B	77	SER
6	B	139	HIS
6	B	284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	88	HIS
2	C	256	GLN
2	C	329	ASN
2	C	342	GLN
3	D	349	ASN
5	F	229	ASN
5	F	232	ASN
5	F	234	GLN
5	F	260	ASN
6	B	8	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	GDP	X	508	-	24,30,30	0.90	1 (4%)	30,47,47	1.16	4 (13%)
7	GTP	X	506	8	26,34,34	1.01	3 (11%)	32,54,54	0.73	1 (3%)
11	VLB	X	505	-	63,67,67	4.03	24 (38%)	79,108,108	2.76	36 (45%)
10	GDP	X	504	-	24,30,30	0.99	1 (4%)	30,47,47	0.99	2 (6%)
7	GTP	X	501	8	26,34,34	0.99	3 (11%)	32,54,54	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GDP	X	508	-	-	3/12/32/32	0/3/3/3
7	GTP	X	506	8	-	7/18/38/38	0/3/3/3
11	VLB	X	505	-	-	12/38/131/131	0/7/9/9
10	GDP	X	504	-	-	2/12/32/32	0/3/3/3
7	GTP	X	501	8	-	5/18/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	505	VLB	C68-C73	25.35	1.74	1.53
11	X	505	VLB	C58-C59	-8.42	1.37	1.52
11	X	505	VLB	C57-N56	6.44	1.62	1.47
11	X	505	VLB	O75-C76	-5.51	1.32	1.45
11	X	505	VLB	O32-C33	-5.13	1.27	1.42
11	X	505	VLB	C68-C15	-3.94	1.40	1.54
11	X	505	VLB	O25-C26	-3.77	1.36	1.45
11	X	505	VLB	C5-C6	-3.73	1.44	1.51
11	X	505	VLB	C68-C67	-3.66	1.50	1.53
11	X	505	VLB	C69-N56	3.17	1.52	1.46
11	X	505	VLB	C20-C5	-3.17	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	505	VLB	C70-C54	3.05	1.58	1.53
11	X	505	VLB	O28-C4	-2.94	1.38	1.44
11	X	505	VLB	C69-C52	2.93	1.56	1.52
11	X	505	VLB	C57-C58	-2.90	1.44	1.52
11	X	505	VLB	C21-C20	2.75	1.63	1.51
7	X	506	GTP	C5-C6	-2.69	1.41	1.47
7	X	501	GTP	C5-C6	-2.67	1.42	1.47
10	X	504	GDP	C6-N1	-2.65	1.33	1.37
11	X	505	VLB	O74-C73	2.63	1.26	1.20
11	X	505	VLB	C19-N9	2.58	1.51	1.47
11	X	505	VLB	O75-C73	2.43	1.37	1.33
11	X	505	VLB	C14-C13	-2.32	1.36	1.39
11	X	505	VLB	O27-C3	-2.31	1.38	1.42
10	X	508	GDP	C6-N1	-2.27	1.34	1.37
11	X	505	VLB	C59-C67	-2.17	1.36	1.39
7	X	501	GTP	C8-N7	-2.13	1.31	1.35
7	X	506	GTP	C8-N7	-2.13	1.31	1.35
11	X	505	VLB	C60-C65	-2.06	1.37	1.42
7	X	506	GTP	C5-C4	-2.04	1.37	1.43
11	X	505	VLB	C51-C68	2.01	1.58	1.56
7	X	501	GTP	C5-C4	-2.00	1.38	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	X	505	VLB	O32-C16-C15	7.16	123.91	116.58
11	X	505	VLB	O25-C23-C3	7.07	124.10	112.22
11	X	505	VLB	O72-C54-C70	-5.59	99.11	108.75
11	X	505	VLB	C3-C2-N1	-5.58	105.13	112.81
11	X	505	VLB	O75-C73-C68	5.47	119.54	111.32
11	X	505	VLB	C33-O32-C16	-5.25	109.60	117.53
11	X	505	VLB	C22-N1-C2	-4.86	107.35	119.21
11	X	505	VLB	C22-N1-C18	-4.86	105.32	120.84
11	X	505	VLB	O32-C16-C17	-4.76	115.93	124.12
11	X	505	VLB	C58-C57-N56	4.56	123.62	113.44
11	X	505	VLB	C57-C58-C59	4.42	122.65	114.30
11	X	505	VLB	O75-C73-O74	-4.34	116.33	123.93
11	X	505	VLB	O24-C23-C3	-3.88	117.91	123.94
11	X	505	VLB	C19-C5-C6	3.84	112.21	108.28
11	X	505	VLB	C13-C18-N1	3.83	115.33	110.98
11	X	505	VLB	O28-C29-C30	3.53	117.58	111.09
11	X	505	VLB	C17-C18-N1	-3.53	122.69	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	X	505	VLB	O25-C23-O24	-3.39	117.99	123.93
11	X	505	VLB	C18-N1-C2	-3.33	104.57	109.03
11	X	505	VLB	C63-C64-C65	-3.30	115.34	120.08
11	X	505	VLB	C52-C69-N56	3.28	116.42	111.28
11	X	505	VLB	C62-C61-C60	-3.15	116.52	120.89
11	X	505	VLB	C14-C15-C16	2.89	120.91	116.78
11	X	505	VLB	C8-N9-C19	-2.87	104.99	112.50
11	X	505	VLB	C4-C3-C2	-2.62	103.84	109.23
11	X	505	VLB	C76-O75-C73	-2.54	111.65	115.94
11	X	505	VLB	C53-C54-C55	2.48	112.33	109.29
11	X	505	VLB	C69-N56-C55	-2.47	108.06	111.01
10	X	504	GDP	C8-N7-C5	2.44	107.64	102.99
10	X	508	GDP	C3'-C2'-C1'	2.38	104.57	100.98
11	X	505	VLB	C4-O28-C29	-2.38	113.98	117.65
11	X	505	VLB	C7-C8-N9	-2.33	105.47	111.03
11	X	505	VLB	C17-C16-C15	-2.25	120.13	122.20
10	X	508	GDP	C5-C6-N1	2.25	117.92	113.95
10	X	508	GDP	O3B-PB-O3A	2.21	112.05	104.64
10	X	508	GDP	C8-N7-C5	2.19	107.16	102.99
11	X	505	VLB	C61-C60-C65	2.17	121.05	118.17
11	X	505	VLB	C54-C53-C52	2.16	116.37	110.02
11	X	505	VLB	O28-C29-O31	-2.10	118.80	122.96
11	X	505	VLB	C53-C52-C69	2.08	111.15	108.72
10	X	504	GDP	PA-O3A-PB	-2.05	125.80	132.83
7	X	506	GTP	O6-C6-C5	2.03	128.34	124.37
11	X	505	VLB	C4-C3-C23	2.01	115.98	110.85

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	501	GTP	PB-O3B-PG-O2G
7	X	501	GTP	C5'-O5'-PA-O1A
7	X	506	GTP	C5'-O5'-PA-O1A
10	X	504	GDP	C5'-O5'-PA-O3A
10	X	504	GDP	C5'-O5'-PA-O2A
10	X	508	GDP	C5'-O5'-PA-O1A
10	X	508	GDP	C5'-O5'-PA-O2A
11	X	505	VLB	C68-C73-O75-C76
11	X	505	VLB	C3-C23-O25-C26
11	X	505	VLB	O24-C23-O25-C26
11	X	505	VLB	O74-C73-O75-C76

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Mol	Chain	Res	Type	Atoms
11	X	505	VLB	C30-C29-O28-C4
11	X	505	VLB	C17-C16-O32-C33
11	X	505	VLB	O31-C29-O28-C4
11	X	505	VLB	C15-C16-O32-C33
7	X	506	GTP	PB-O3A-PA-O1A
10	X	508	GDP	C5'-O5'-PA-O3A
7	X	501	GTP	C5'-O5'-PA-O2A
7	X	506	GTP	C5'-O5'-PA-O2A
7	X	506	GTP	C4'-C5'-O5'-PA
11	X	505	VLB	C58-C57-N56-C55
11	X	505	VLB	C15-C68-C73-O75
11	X	505	VLB	C15-C68-C73-O74
7	X	501	GTP	PB-O3B-PG-O3G
7	X	501	GTP	C5'-O5'-PA-O3A
7	X	506	GTP	C5'-O5'-PA-O3A
7	X	506	GTP	C3'-C4'-C5'-O5'
7	X	506	GTP	PB-O3A-PA-O2A
11	X	505	VLB	C21-C20-C5-C4

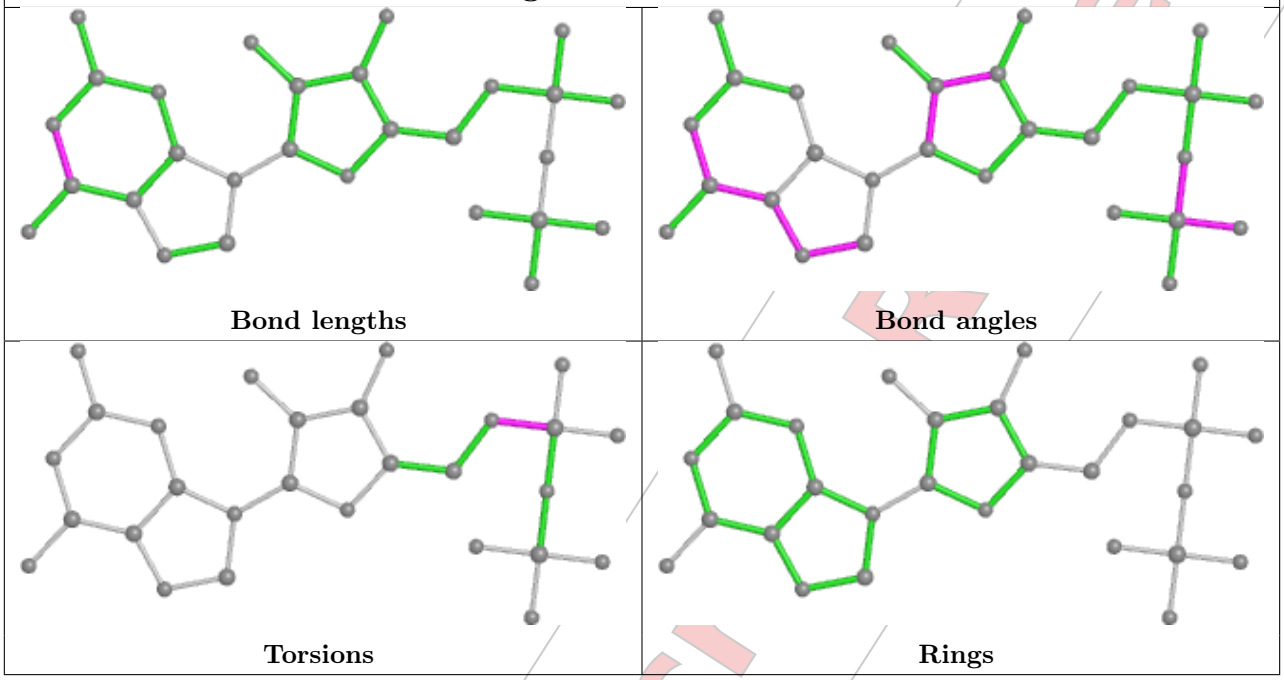
There are no ring outliers.

4 monomers are involved in 20 short contacts:

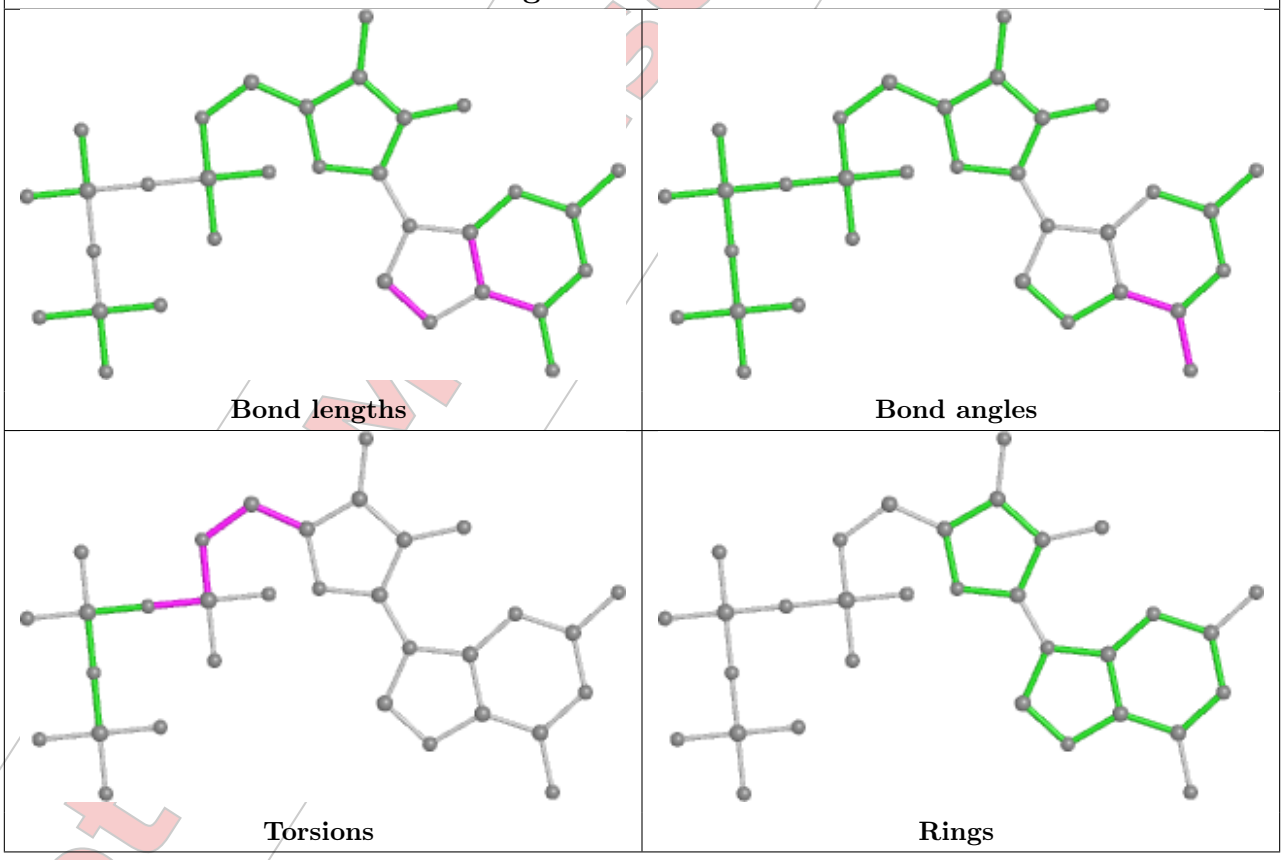
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	508	GDP	3	0
7	X	506	GTP	1	0
11	X	505	VLB	15	0
10	X	504	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

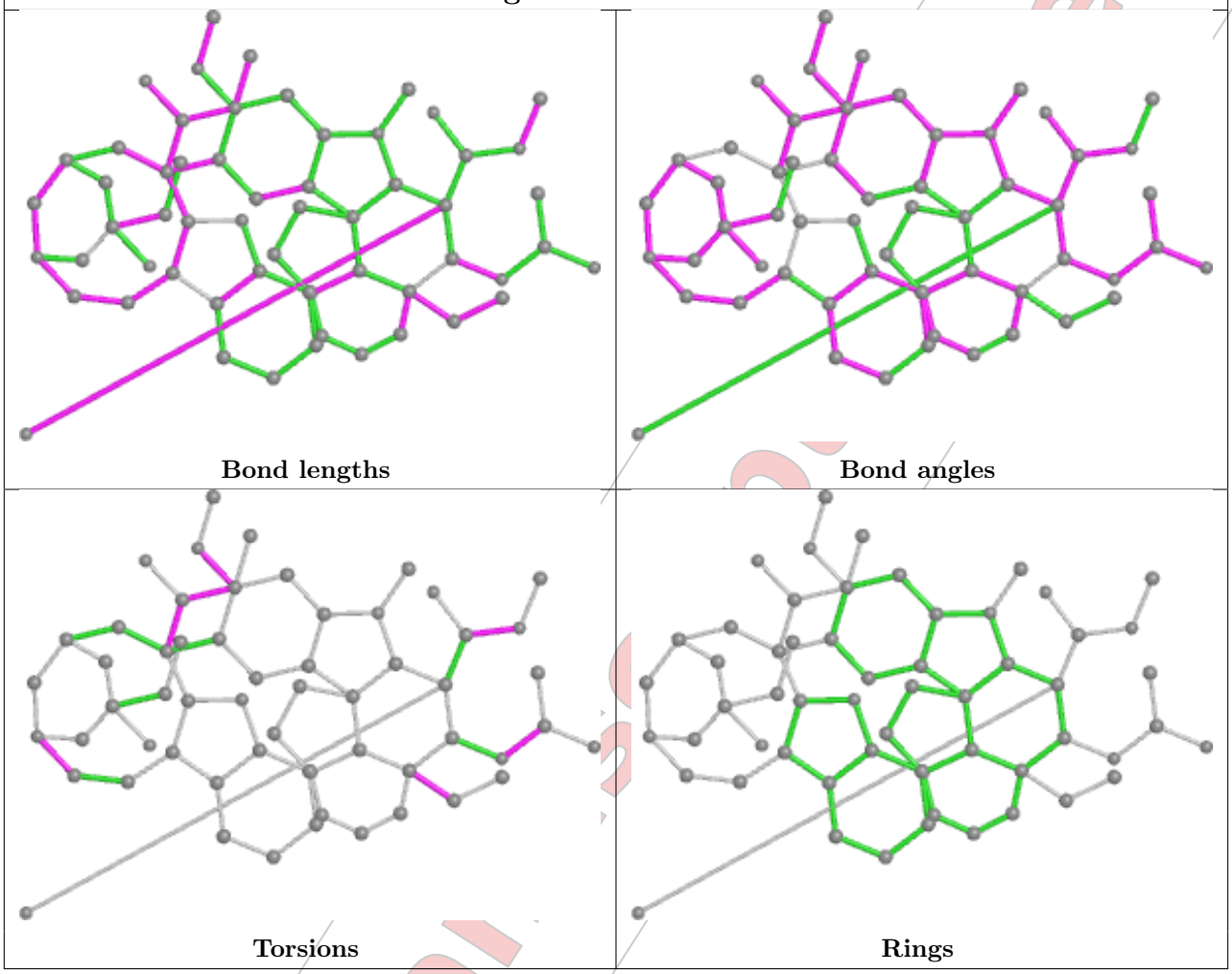
Ligand GDP X 508



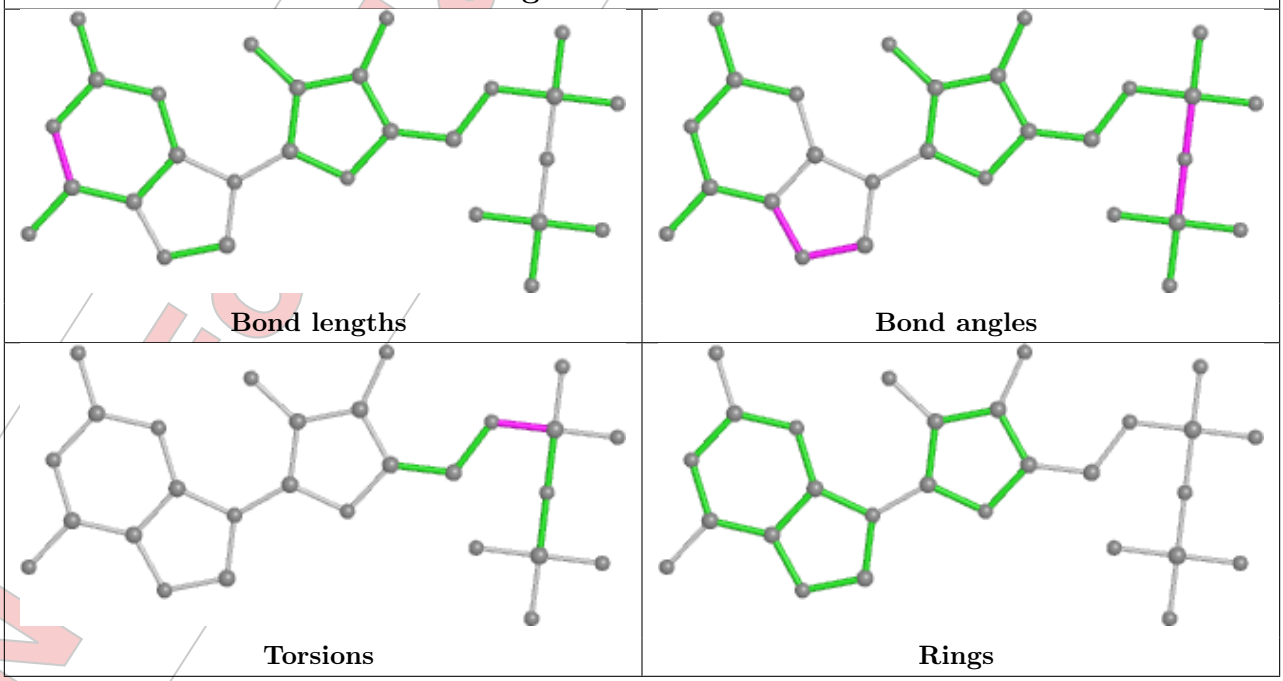
Ligand GTP X 506



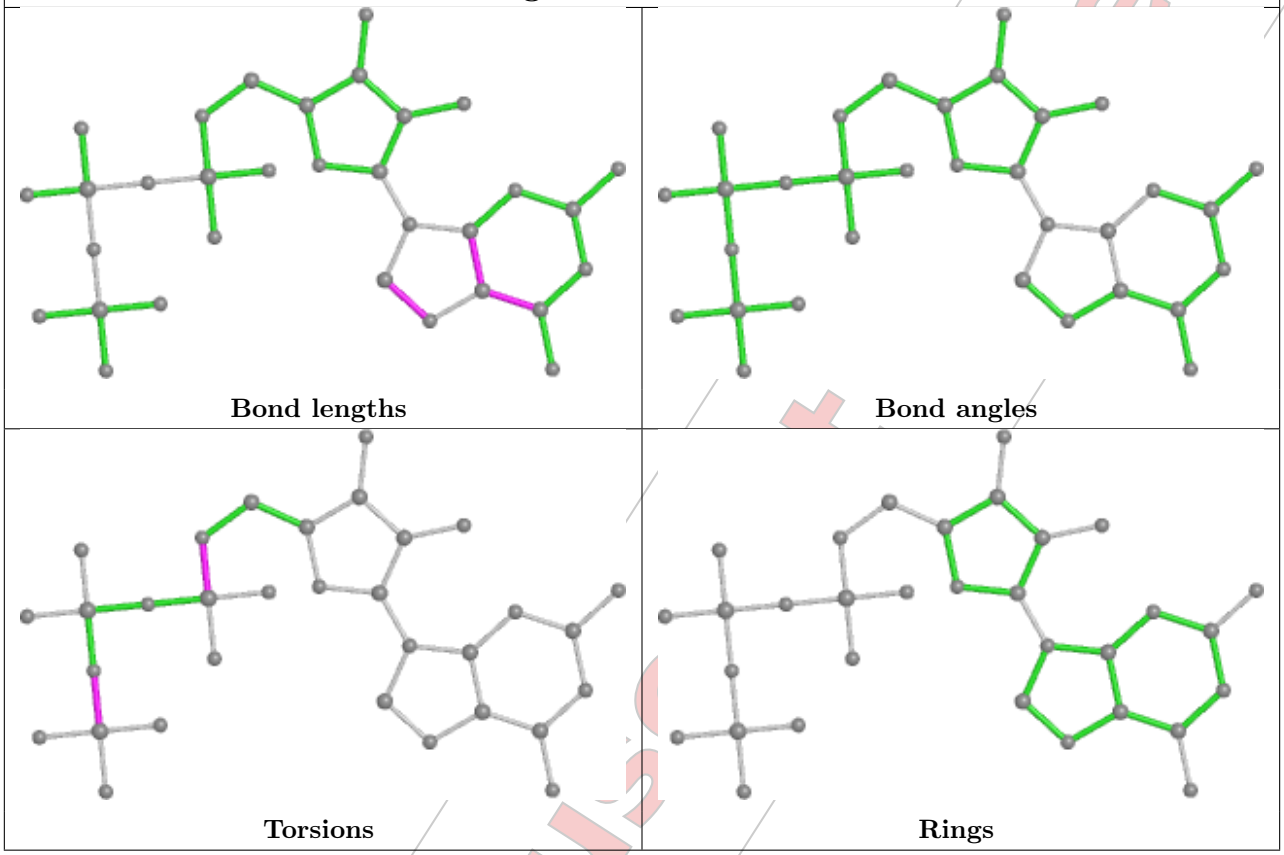
Ligand VLB X 505



Ligand GDP X 504



Ligand GTP X 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	F	5
4	E	1
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.56
1	F	362:ALA	C	372:THR	N	20.09
1	F	103:THR	C	125:THR	N	13.23
1	D	276:THR	C	284:ARG	N	10.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	250:SER	C	255:ARG	N	9.11
1	F	149:ALA	C	159:GLY	N	8.13
1	F	137:ARG	C	144:GLY	N	7.47

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	439/439 (100%)	-0.38	4 (0%) 84 75	36, 65, 112, 259	0
2	C	440/440 (100%)	-0.49	2 (0%) 91 86	24, 50, 88, 226	0
3	D	424/424 (100%)	-0.14	14 (3%) 46 30	41, 82, 130, 180	1 (0%)
4	E	120/120 (100%)	0.02	4 (3%) 46 30	47, 82, 130, 153	0
5	F	331/331 (100%)	0.26	31 (9%) 8 4	51, 97, 172, 212	0
6	B	428/428 (100%)	-0.46	2 (0%) 91 86	24, 54, 97, 150	4 (0%)
All	All	2182/2182 (100%)	-0.25	57 (2%) 56 40	24, 68, 134, 259	5 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	175	GLU	8.8
1	A	439	SER	7.3
5	F	238	CYS	6.5
5	F	257	GLU	5.6
5	F	232	ASN	5.3
5	F	372	THR	5.0
5	F	102	PRO	4.6
5	F	231	ALA	4.4
3	D	56	ALA	4.0
5	F	167	SER	4.0
5	F	248	GLU	4.0
4	E	138	GLU	3.9
5	F	176	GLN	3.9
3	D	415	GLU	3.7
3	D	179	ASP	3.6
4	E	103	GLN	3.4
5	F	174	ASP	3.3
5	F	168	GLU	3.2
5	F	125	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	441	ASP	3.1
3	D	285	ALA	3.0
5	F	171	ASP	3.0
5	F	133	ALA	3.0
5	F	234	GLN	2.9
3	D	55	GLU	2.9
5	F	83	THR	2.9
6	B	80	SER	2.9
3	D	11	GLN	2.8
5	F	323	GLU	2.8
5	F	136	ASN	2.8
3	D	218	LYS	2.8
5	F	89	GLU	2.7
5	F	145	ASN	2.7
5	F	340	GLN	2.7
5	F	173	ILE	2.7
5	F	250	SER	2.7
1	A	438	ASP	2.6
3	D	82	PRO	2.6
6	B	57	THR	2.5
3	D	284	ARG	2.5
3	D	416	MET	2.4
5	F	235	ASP	2.3
5	F	244	CYS	2.3
5	F	356	SER	2.2
2	C	337	THR	2.2
5	F	159	GLY	2.2
2	C	283	HIS	2.2
1	A	280	LYS	2.2
5	F	333	ASN	2.2
4	E	140	LYS	2.2
5	F	225	SER	2.2
5	F	239	HIS	2.1
3	D	116	ASP	2.1
3	D	38	GLY	2.1
1	A	281	ALA	2.1
3	D	85	GLN	2.0
4	E	128	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

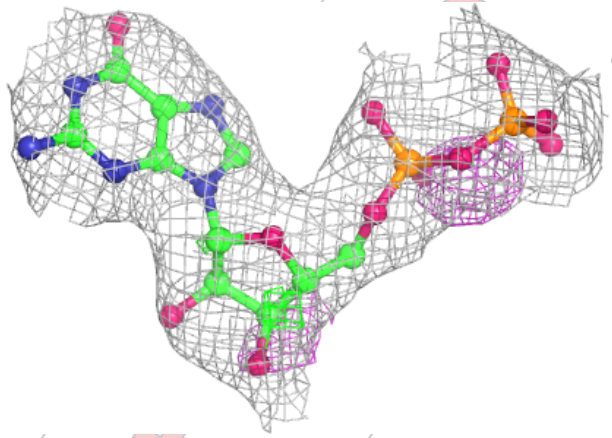
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

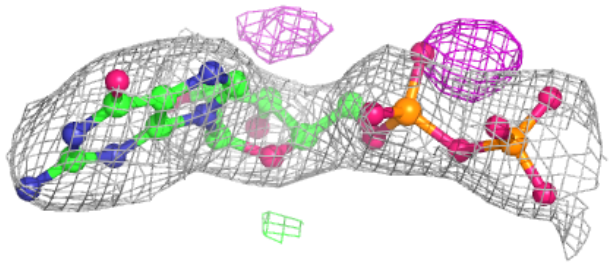
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	GDP	X	508	28/?	0.89	0.16	74,78,89,101	0
8	MG	X	507	1/?	0.91	0.40	41,41,41,41	0
11	VLB	X	505	59/?	0.91	0.15	38,47,55,59	0
8	MG	X	502	1/?	0.92	0.29	45,45,45,45	0
7	GTP	X	501	32/?	0.94	0.17	49,51,55,55	0
9	CA	X	509	1/?	0.95	0.17	30,30,30,30	0
10	GDP	X	504	28/?	0.95	0.13	36,41,43,44	0
7	GTP	X	506	32/?	0.95	0.14	41,45,48,48	0
9	CA	X	503	1/?	0.95	0.08	91,91,91,91	0

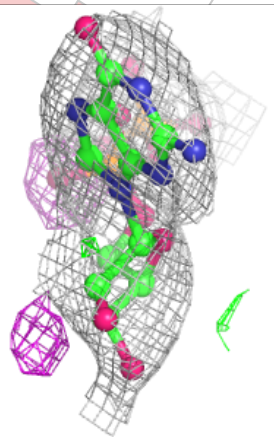
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP X 508:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

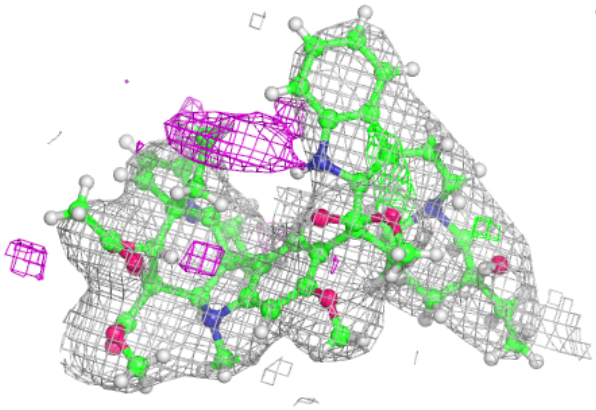


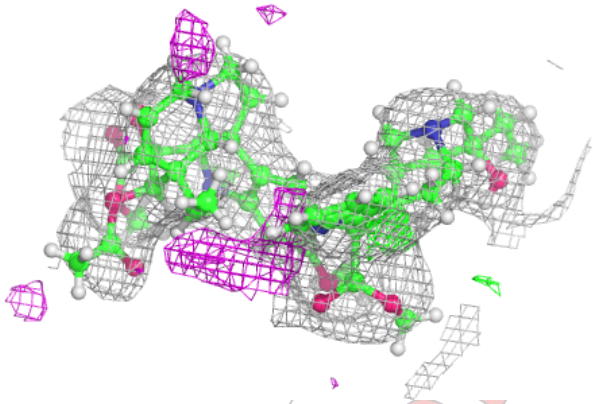


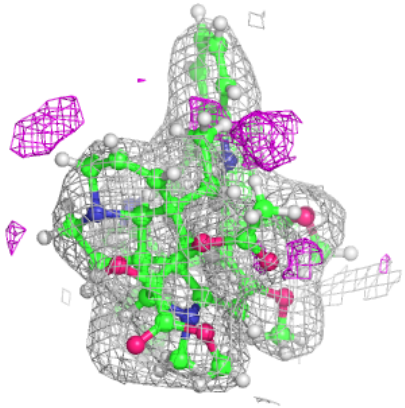


Electron density around VLB X 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

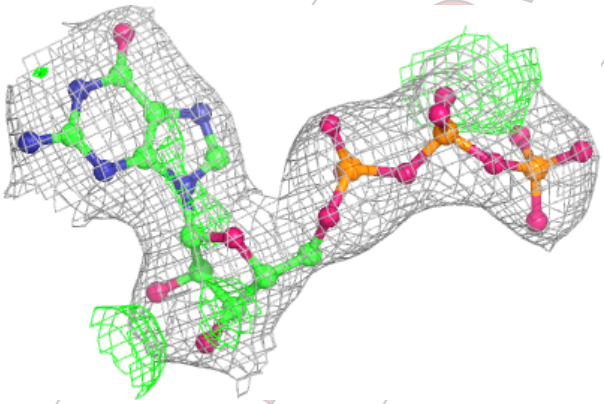


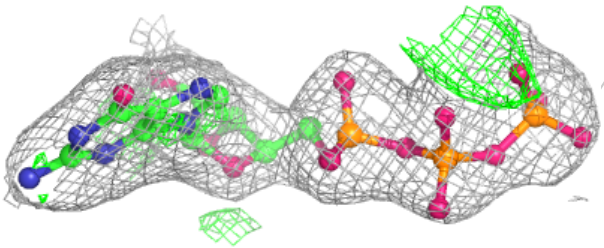


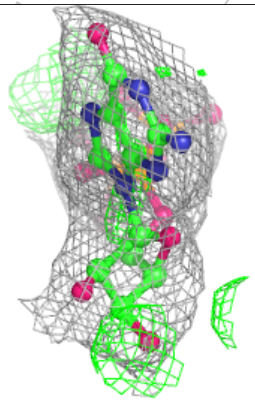


Electron density around GTP X 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

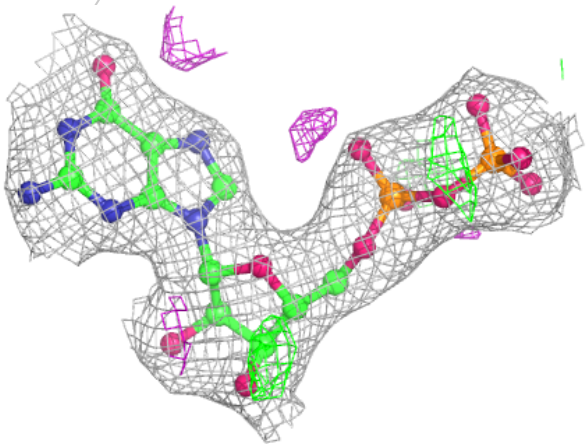


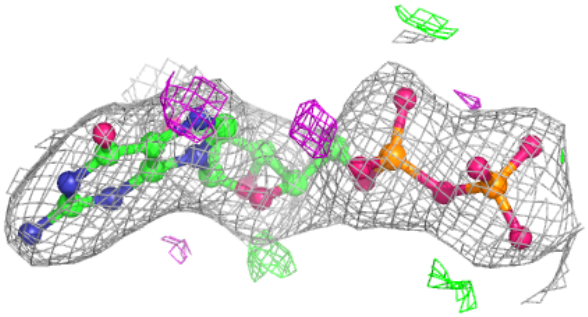


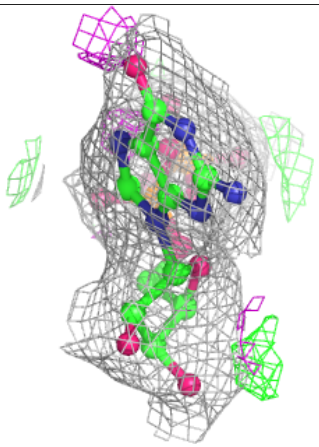


Electron density around GDP X 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

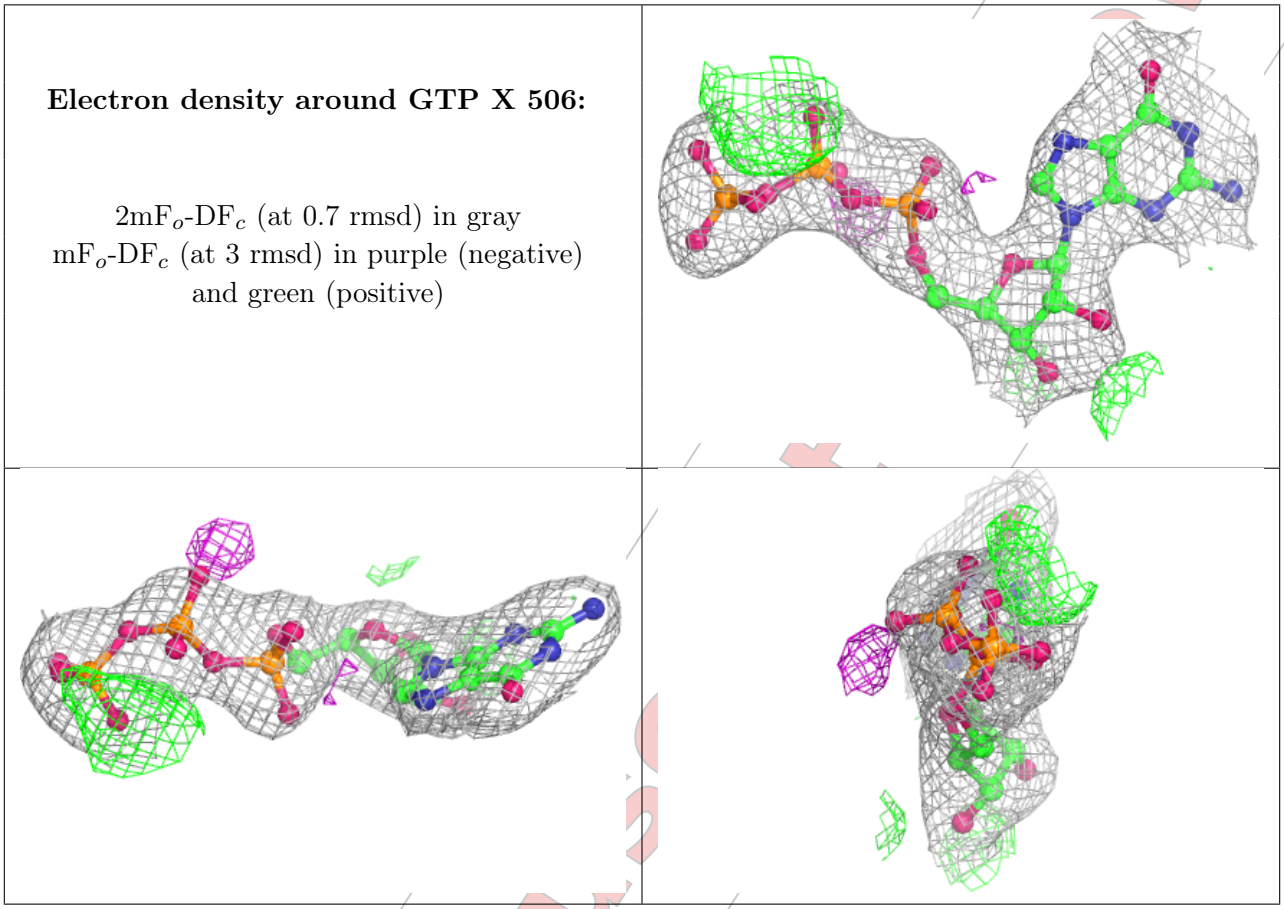






Electron density around GTP X 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2023 – 07:39 pm GMT

Deposition ID : D_1292128601

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

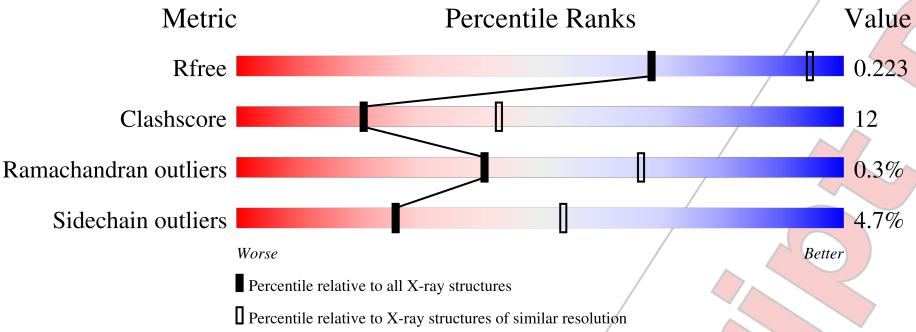
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	439	72% 26% .
2	B	428	70% 28% .
3	C	440	82% 18%
4	D	431	68% 29% .
5	E	121	78% 21% .
6	F	320	69% 29% .

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34805 atoms, of which 17172 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	439	6888	2204	3414	585	661	24	0	10	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	428	6733	2148	3317	581	660	27	2	11	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	440	6884	2203	3405	586	666	24	0	10	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	431	6705	2140	3299	580	658	28	0	4	0

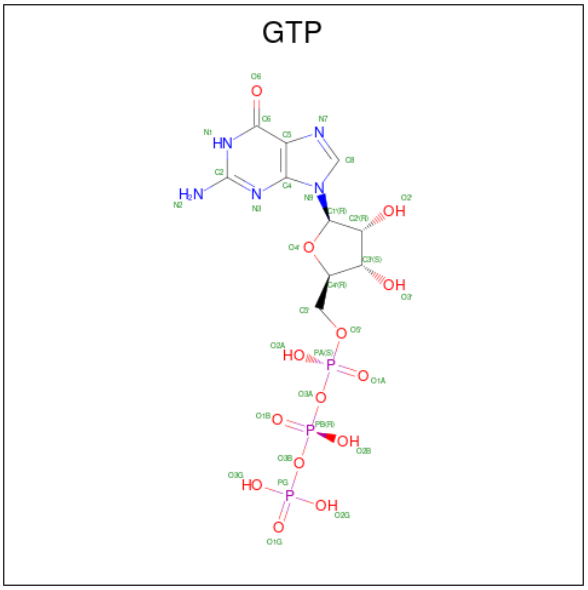
- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	121	2046	625	1035	182	198	6	0	2	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	320	5269	1707	2633	437	478	14	0	4	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	X	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
7	X	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

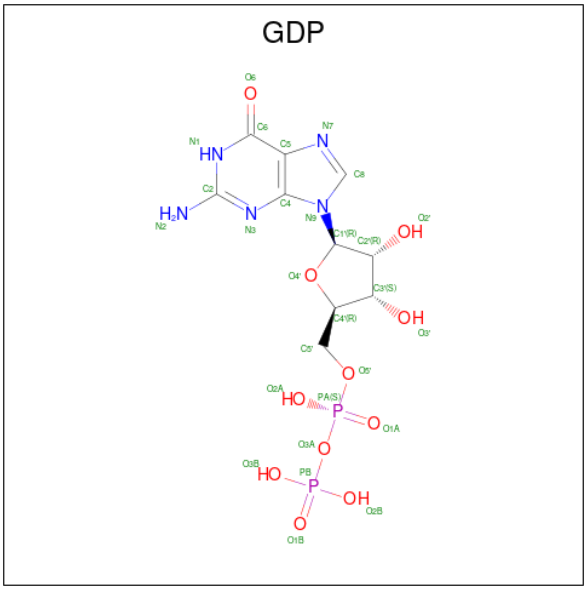
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	X	1	Total	Ca	0	0
			1	1		
9	X	1	Total	Ca	0	0
			1	1		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

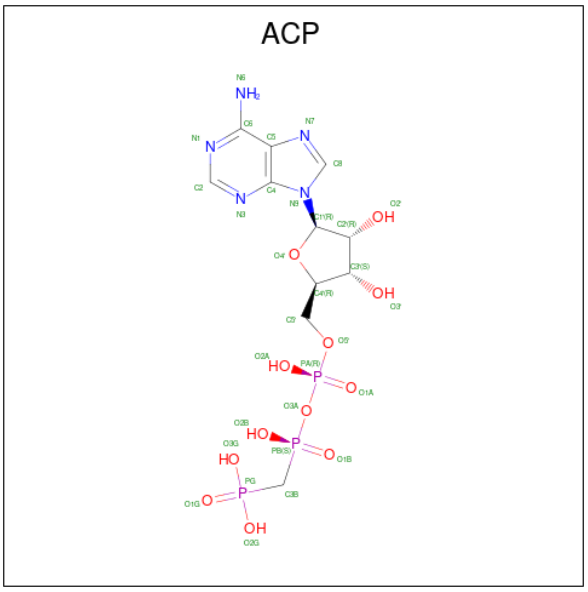


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
10	X	1	40	10	12	5	11	2	0	0
			Total	C	H	N	O	P		
10	X	1	40	10	12	5	11	2	0	0

- Molecule 11 is a ligand with the chemical component id SQB but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for SQB. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	H	N	O		
11	X	1	31	1	17	7	2	4	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	X	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	G	30	Total	O	0	0
			30	30		

3 Residue-property plots (i)

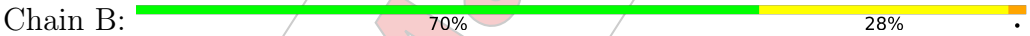
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

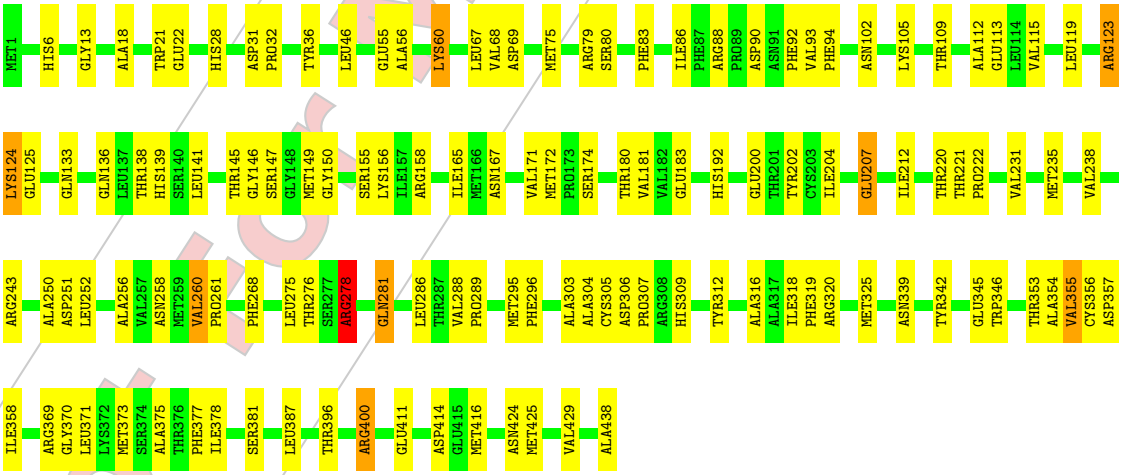
- Molecule 1:

Chain A:

- Molecule 2:

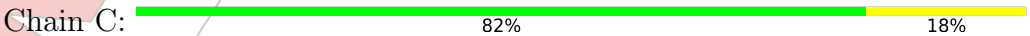
Chain B:





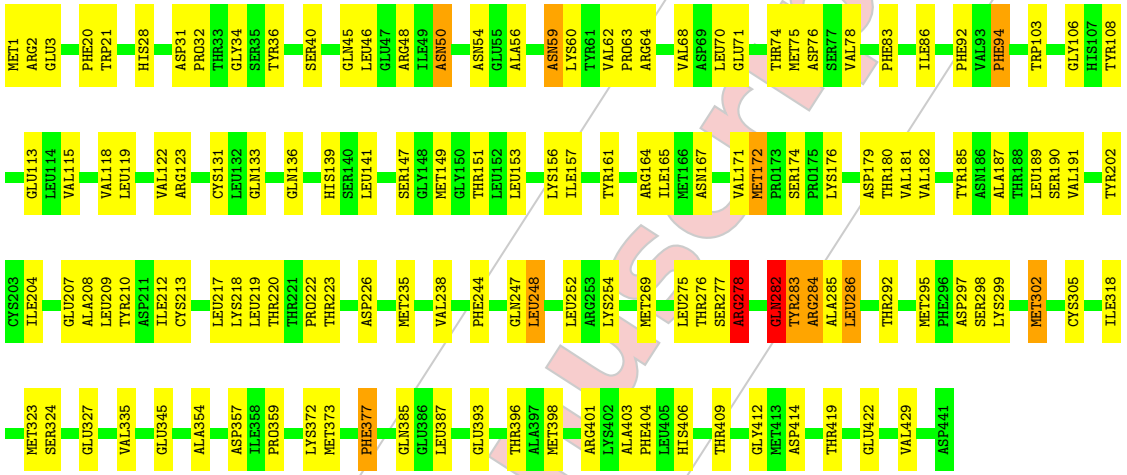
- Molecule 3:

Chain C:



- Molecule 4:

Chain D:

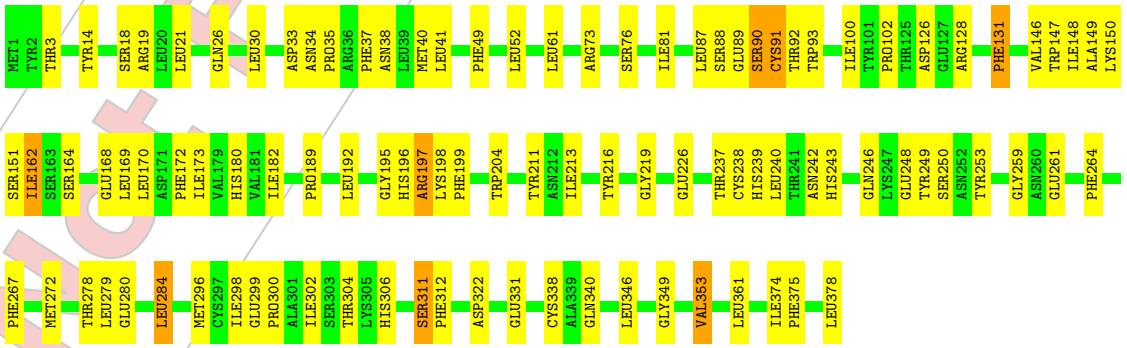


- Molecule 5:

Chain E:

- Molecule 6:

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.65Å 160.33Å 180.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.35 – 2.70 15.37 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.35-2.70) 56.8 (15.37-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1764.17 (at 2.03Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.168 , 0.217 0.184 , 0.223	Depositor DCC
R_{free} test set	1974 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å^2)	-9.9	Xtriage
Anisotropy	-0.596	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 71.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	34805	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, GTP, GDP, MG, SQB, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/3582	0.49	0/4864
2	B	0.36	0/3527	0.55	0/4776
3	C	0.33	0/3593	0.51	0/4878
4	D	0.33	0/3493	0.53	0/4733
5	E	0.25	0/1025	0.44	0/1359
6	F	0.34	0/2705	0.54	0/3653
All	All	0.32	0/17925	0.52	0/24263

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
3	C	0	2
4	D	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	A	214	ARG	Sidechain
2	B	123	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	278	ARG	Sidechain
3	C	243	ARG	Sidechain
3	C	320	ARG	Sidechain
4	D	278	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3474	3414	3412	96	0
2	B	3416	3317	3309	95	0
3	C	3479	3405	3392	47	0
4	D	3406	3299	3298	106	0
5	E	1011	1035	1035	26	0
6	F	2636	2633	2632	68	0
7	X	64	24	24	2	0
8	X	4	0	0	0	0
9	X	2	0	0	0	0
10	X	56	24	24	1	0
11	X	24	7	0	9	0
12	X	31	14	14	2	0
13	G	30	0	0	1	0
All	All	17633	17172	17140	423	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.47	0.93
4:D:181:VAL:O	4:D:398:MET:HE1	1.84	0.78
2:B:256:ALA:O	2:B:260:VAL:HG13	1.85	0.76
6:F:248:GLU:HG2	6:F:249:TYR:CD1	2.19	0.76
4:D:292:THR:HG22	4:D:335:VAL:HG21	1.68	0.75
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:293[B]:ASN:OD1	3:C:335:ILE:HD11	1.87	0.75
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.69	0.74
2:B:83:PHE:O	2:B:86:ILE:HG22	1.87	0.74
6:F:3:THR:HG23	6:F:38:ASN:H	1.53	0.73
2:B:156:LYS:HE2	5:E:76:ARG:NE	2.03	0.73
4:D:180:THR:HG22	4:D:182:VAL:H	1.52	0.73
6:F:278:THR:HG22	6:F:280:GLU:H	1.53	0.72
2:B:268:PHE:HB3	2:B:378:ILE:CG2	2.19	0.72
4:D:133:GLN:HE21	4:D:252:LEU:H	1.36	0.72
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.08	0.72
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.72	0.72
1:A:70:LEU:HD23	1:A:145:THR:OG1	1.90	0.71
2:B:378:ILE:N	2:B:378:ILE:HD12	2.05	0.71
4:D:180:THR:CG2	4:D:182:VAL:HG22	2.20	0.71
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.73	0.71
2:B:325:MET:HG3	2:B:355:VAL:HG21	1.74	0.69
2:B:370:GLY:O	2:B:371:LEU:HD12	1.92	0.69
4:D:147:SER:O	4:D:151:THR:HG23	1.92	0.69
2:B:221:THR:HG23	2:B:221:THR:O	1.92	0.69
4:D:324:SER:OG	4:D:327:GLU:HB2	1.92	0.68
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.74	0.68
4:D:75:MET:HG2	4:D:92:PHE:HD2	1.58	0.68
4:D:118:VAL:HG11	4:D:153:LEU:HD21	1.75	0.67
3:C:119:LEU:HD11	3:C:156:ARG:HB3	1.77	0.67
6:F:100:ILE:HD13	6:F:173:ILE:HD13	1.76	0.67
4:D:286:LEU:HD13	4:D:373:MET:HG2	1.77	0.66
4:D:385:GLN:HB2	4:D:429:VAL:HG13	1.78	0.65
6:F:248:GLU:HG2	6:F:249:TYR:CE1	2.30	0.65
1:A:40:LYS:HE3	1:A:40:LYS:CA	2.26	0.65
1:A:104:ALA:HB2	1:A:413:MET:CE	2.27	0.65
1:A:386:GLU:O	1:A:390:ARG:HG3	1.97	0.65
6:F:298:ILE:HD12	6:F:302:ILE:HD13	1.78	0.65
2:B:378:ILE:HD12	2:B:378:ILE:H	1.61	0.64
6:F:149:ALA:O	6:F:150:LYS:HD2	1.97	0.63
1:A:286:LEU:HD22	1:A:286:LEU:H	1.63	0.63
1:A:339:ARG:HB2	1:A:341:ILE:HD11	1.80	0.63
4:D:174:SER:HB2	4:D:207:GLU:HB2	1.80	0.63
2:B:268:PHE:HB3	2:B:378:ILE:HG23	1.81	0.63
3:C:254:GLU:HG2	3:C:352:LYS:HE2	1.80	0.63
1:A:81:GLY:O	1:A:84:ARG:HG2	1.99	0.63
5:E:57:ALA:HA	5:E:60:ARG:NH1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HG22	1:A:347:CYS:HB2	1.82	0.62
4:D:56:ALA:HB3	4:D:60:LYS:HB2	1.81	0.62
6:F:149:ALA:HB2	6:F:182:ILE:HG12	1.82	0.62
1:A:285:GLN:HG3	1:A:372[B]:GLN:OE1	1.99	0.62
4:D:59:ASN:O	4:D:59:ASN:ND2	2.28	0.61
4:D:136:GLN:HA	4:D:167:ASN:O	2.00	0.61
1:A:40:LYS:HE3	1:A:40:LYS:HA	1.82	0.61
4:D:118:VAL:CG1	4:D:153:LEU:HD21	2.31	0.61
1:A:177:VAL:HG12	7:X:501:GTP:O2'	2.01	0.61
2:B:316:ALA:HB1	11:X:506:SQB:C16	2.31	0.61
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.83	0.61
2:B:378:ILE:HD11	11:X:506:SQB:BR	2.57	0.60
4:D:403:ALA:HB1	4:D:404:PHE:HD1	1.66	0.60
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.82	0.60
3:C:187:SER:HB3	3:C:391:LEU:HD21	1.83	0.60
6:F:148:ILE:HB	6:F:162:ILE:HG23	1.82	0.60
6:F:237:THR:HG21	6:F:249:TYR:O	2.01	0.60
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.82	0.60
3:C:93:ILE:HD11	3:C:121:ARG:HG3	1.84	0.60
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.36	0.60
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	1.84	0.59
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.02	0.59
2:B:69:ASP:O	2:B:94:PHE:HA	2.03	0.59
4:D:171:VAL:HA	4:D:204:ILE:O	2.03	0.59
6:F:195:GLY:HA3	6:F:197:ARG:HD3	1.83	0.59
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.84	0.59
4:D:20:PHE:HB2	4:D:235:MET:HE2	1.83	0.58
4:D:36:TYR:CE2	4:D:46:LEU:HD11	2.37	0.58
4:D:393:GLU:O	4:D:396:THR:HG22	2.02	0.58
4:D:179:ASP:HB2	10:X:509:GDP:H3'	1.85	0.58
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
1:A:336:LYS:C	1:A:336:LYS:HD3	2.23	0.58
6:F:3:THR:HG23	6:F:38:ASN:N	2.17	0.58
1:A:2:ARG:CB	1:A:133:GLN:HG2	2.33	0.58
6:F:100:ILE:HD11	6:F:180:HIS:HB2	1.84	0.58
2:B:318:ILE:HG12	11:X:506:SQB:BR	2.59	0.58
5:E:6:MET:HG2	5:E:24:LEU:CD2	2.34	0.58
4:D:223:THR:HG22	4:D:226:ASP:OD2	2.04	0.57
6:F:213:ILE:HG22	6:F:378[B]:LEU:HD12	1.84	0.57
1:A:336:LYS:HD3	1:A:336:LYS:O	2.04	0.57
6:F:374:ILE:HD11	6:F:375:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:ARG:HG2	4:D:164:ARG:HH11	1.67	0.57
4:D:209:LEU:HD21	4:D:302:MET:HG3	1.87	0.57
1:A:151:SER:HB2	1:A:193:THR:CG2	2.35	0.57
4:D:269[B]:MET:CE	4:D:305:CYS:HB2	2.35	0.57
4:D:180:THR:HG21	4:D:182:VAL:HG22	1.87	0.57
6:F:3:THR:OG1	6:F:30:LEU:HD11	2.04	0.57
2:B:13:GLY:CA	2:B:138[B]:THR:HG22	2.27	0.56
6:F:259:GLY:O	6:F:261:GLU:HG3	2.05	0.56
1:A:344:VAL:CG2	1:A:347:CYS:HB2	2.35	0.56
3:C:277:SER:OG	3:C:280:LYS:HG3	2.05	0.56
4:D:172:MET:HE2	4:D:172:MET:N	2.21	0.56
4:D:212:ILE:HG22	4:D:217:LEU:HD23	1.86	0.56
1:A:344:VAL:HG21	1:A:346:TRP:CE2	2.41	0.56
4:D:141:LEU:HD22	4:D:190:SER:HB3	1.87	0.56
5:E:9:ILE:HD13	5:E:23:ILE:HD12	1.87	0.56
2:B:295:MET:HE3	2:B:296:PHE:CE1	2.40	0.56
6:F:278:THR:HG22	6:F:280:GLU:N	2.19	0.56
4:D:113:GLU:OE2	4:D:113:GLU:HA	2.06	0.56
4:D:103:TRP:CE3	4:D:189:LEU:HD13	2.41	0.55
4:D:74:THR:O	4:D:78:VAL:HG13	2.06	0.55
6:F:304:THR:HG21	6:F:311:SER:HB2	1.87	0.55
2:B:102:ASN:HB3	2:B:105[A]:LYS:HG3	1.88	0.55
4:D:133:GLN:NE2	4:D:252:LEU:H	2.04	0.55
6:F:146:VAL:HG22	6:F:164:SER:OG	2.06	0.55
4:D:161:TYR:HB3	4:D:164:ARG:HG3	1.88	0.55
4:D:284:ARG:NH2	4:D:285:ALA:H	2.04	0.55
4:D:180:THR:HG22	4:D:182:VAL:HG22	1.88	0.55
2:B:202:TYR:CE1	2:B:238:VAL:HG21	2.42	0.55
6:F:280:GLU:HA	6:F:284[A]:LEU:HB2	1.89	0.55
4:D:75:MET:HG2	4:D:92:PHE:CD2	2.40	0.54
6:F:100:ILE:HD12	6:F:100:ILE:O	2.07	0.54
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.89	0.54
6:F:213:ILE:CG2	6:F:378[B]:LEU:HD12	2.38	0.54
2:B:86:ILE:HG12	2:B:86:ILE:O	2.08	0.54
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.37	0.54
2:B:295:MET:SD	2:B:375:ALA:HB1	2.48	0.54
1:A:33:ASP:OD1	1:A:35:GLN:HG2	2.08	0.54
6:F:374:ILE:HD11	6:F:375:PHE:CZ	2.43	0.54
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.90	0.53
5:E:6:MET:HG2	5:E:24:LEU:HD22	1.90	0.53
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:49:PHE:HA	6:F:52:LEU:HD12	1.89	0.53
2:B:318:ILE:HA	2:B:354:ALA:O	2.09	0.53
3:C:154:MET:HG3	3:C:194[A]:THR:HG23	1.90	0.53
2:B:56:ALA:HB3	2:B:60:LYS:HG2	1.91	0.53
1:A:433:GLU:O	1:A:437:VAL:HB	2.08	0.53
2:B:67:LEU:N	2:B:67:LEU:HD12	2.24	0.53
2:B:69:ASP:HB2	2:B:75:MET:HE3	1.91	0.53
4:D:218:LYS:O	4:D:219:LEU:HD23	2.09	0.53
4:D:164:ARG:HG2	4:D:164:ARG:NH1	2.24	0.53
2:B:75:MET:HG3	2:B:94:PHE:HD1	1.75	0.53
2:B:158[B]:ARG:CZ	5:E:68:LEU:HD11	2.38	0.52
2:B:316:ALA:HB1	11:X:506:SQB:O3	2.08	0.52
6:F:61:LEU:HD11	6:F:312:PHE:HD1	1.74	0.52
4:D:34:GLY:CA	4:D:86:ILE:HD11	2.38	0.52
4:D:50:ASN:H	4:D:50:ASN:ND2	2.06	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.52
1:A:283:HIS:HD2	1:A:284:GLU:O	1.92	0.52
3:C:96:LYS:HB2	3:C:96:LYS:NZ	2.25	0.52
3:C:271:THR:HG23	3:C:300:ASN:O	2.10	0.52
4:D:286:LEU:HD12	4:D:286:LEU:O	2.09	0.52
6:F:128:ARG:CZ	6:F:170:LEU:HD22	2.40	0.52
3:C:21:TRP:CZ3	3:C:63:PRO:HB3	2.45	0.52
3:C:147:SER:HB2	3:C:190:THR:HB	1.91	0.52
6:F:100:ILE:HA	6:F:126:ASP:HB2	1.90	0.52
3:C:99:ALA:HB3	3:C:144:GLY:HA3	1.92	0.52
4:D:220:THR:O	4:D:222:PRO:HD3	2.09	0.52
2:B:124:LYS:HD3	2:B:125:GLU:HG2	1.92	0.51
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.10	0.51
4:D:21:TRP:CZ3	4:D:63:PRO:HB3	2.44	0.51
6:F:204:TRP:CZ2	6:F:338:CYS:HA	2.45	0.51
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.10	0.51
5:E:57:ALA:HA	5:E:60:ARG:HH11	1.75	0.51
6:F:242:ASN:O	6:F:246:GLN:HG2	2.11	0.51
3:C:192:HIS:HD1	3:C:424:ASP:CB	2.24	0.51
4:D:372:LYS:HD3	4:D:373:MET:HE3	1.93	0.51
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.46	0.51
3:C:79:ARG:HG2	3:C:92:LEU:HD12	1.92	0.51
6:F:102:PRO:HB3	6:F:173:ILE:CG2	2.40	0.51
2:B:220:THR:O	2:B:222:PRO:HD3	2.11	0.51
4:D:20:PHE:HB2	4:D:235:MET:CE	2.41	0.51
4:D:75:MET:SD	4:D:94:PHE:HB3	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:248:LEU:HD12	4:D:354:ALA:HB2	1.93	0.51
6:F:168:GLU:O	6:F:172:PHE:HB2	2.11	0.51
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.46	0.50
2:B:105[A]:LYS:HA	2:B:109:THR:OG1	2.11	0.50
4:D:403:ALA:HB1	4:D:404:PHE:CD1	2.45	0.50
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.12	0.50
1:A:401:LYS:HE3	2:B:438:ALA:HB1	1.93	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.52	0.50
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.47	0.50
2:B:276:THR:HG21	2:B:371:LEU:HD11	1.93	0.50
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.25	0.50
5:E:9:ILE:HD13	5:E:23:ILE:CD1	2.40	0.50
2:B:180:THR:O	2:B:183:GLU:HG3	2.12	0.50
4:D:176:LYS:HD3	4:D:210:TYR:CD2	2.46	0.50
2:B:112:ALA:O	2:B:115:VAL:HG12	2.12	0.50
3:C:180:ALA:HB3	3:C:183:GLU:HG3	1.93	0.50
3:C:75:ILE:HD12	3:C:94:THR:HG22	1.93	0.50
3:C:245:ASP:N	3:C:245:ASP:OD1	2.42	0.50
3:C:176:GLN:HE22	3:C:207:GLU:HG3	1.77	0.50
1:A:265:ILE:O	1:A:265:ILE:HG22	2.12	0.49
1:A:297:GLU:OE2	6:F:306:HIS:ND1	2.44	0.49
3:C:177:VAL:HG12	3:C:177:VAL:O	2.12	0.49
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.93	0.49
4:D:31:ASP:HB2	4:D:32:PRO:CD	2.42	0.49
5:E:81:GLU:O	5:E:84[B]:GLN:HG2	2.12	0.49
5:E:135:LYS:HE2	5:E:139:LEU:HD11	1.94	0.49
4:D:269[B]:MET:HE1	4:D:305:CYS:HB2	1.94	0.49
6:F:219:GLY:HA3	6:F:264:PHE:CZ	2.48	0.49
6:F:246:GLN:O	6:F:250:SER:OG	2.30	0.49
1:A:40:LYS:HE3	1:A:40:LYS:O	2.11	0.49
6:F:198:LYS:HG2	6:F:199:PHE:H	1.77	0.49
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.48	0.49
2:B:425:MET:O	2:B:429:VAL:HG23	2.12	0.49
3:C:210:TYR:CZ	3:C:222:PRO:HD2	2.47	0.49
2:B:318:ILE:CG1	11:X:506:SQB:BR	3.16	0.49
6:F:91:CYS:C	6:F:93:TRP:H	2.16	0.49
1:A:283:HIS:CD2	1:A:284:GLU:O	2.65	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.48
6:F:14:TYR:HB3	6:F:41:LEU:HD13	1.95	0.48
6:F:49:PHE:HA	6:F:52:LEU:CD1	2.43	0.48
2:B:105[B]:LYS:HA	2:B:109:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:PRO:HG2	3:C:87:PHE:CE1	2.48	0.48
3:C:183:GLU:N	3:C:184:PRO:CD	2.77	0.48
4:D:119:LEU:O	4:D:123:ARG:HG3	2.12	0.48
4:D:318:ILE:HG22	13:G:58:HOH:O	2.13	0.48
6:F:102:PRO:HB3	6:F:173:ILE:HG22	1.93	0.48
2:B:75:MET:HG3	2:B:94:PHE:CD1	2.48	0.48
2:B:105[A]:LYS:HE2	2:B:411:GLU:OE2	2.13	0.48
2:B:346:TRP:HE1	2:B:438:ALA:HB3	1.78	0.48
4:D:278:ARG:CZ	4:D:278:ARG:HB3	2.43	0.48
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.48	0.48
2:B:320:ARG:HA	2:B:356:CYS:O	2.13	0.48
2:B:378:ILE:CD1	11:X:506:SQB:BR	3.17	0.48
2:B:28:HIS:NE2	2:B:243:ARG:HD2	2.29	0.48
6:F:128:ARG:NH2	6:F:170:LEU:HD22	2.29	0.48
4:D:153:LEU:O	4:D:157:ILE:HD12	2.14	0.48
4:D:286:LEU:HD13	4:D:373:MET:CG	2.41	0.48
6:F:26:GLN:NE2	6:F:361:LEU:HD22	2.27	0.48
1:A:67:PHE:HB2	1:A:92:LEU:HD12	1.96	0.48
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.94	0.48
2:B:156:LYS:HE2	5:E:76:ARG:HE	1.75	0.48
2:B:369:ARG:HD2	2:B:370:GLY:N	2.29	0.48
4:D:213:CYS:HA	4:D:217:LEU:HB2	1.96	0.48
1:A:210:TYR:CE2	1:A:214:ARG:HD3	2.49	0.47
6:F:243:HIS:NE2	6:F:253:TYR:OH	2.46	0.47
1:A:355:ILE:O	5:E:17:GLY:HA3	2.13	0.47
3:C:282:TYR:O	3:C:283:HIS:CB	2.62	0.47
4:D:275:LEU:O	4:D:277:SER:N	2.47	0.47
1:A:114:ILE:HD12	1:A:117:LEU:HB3	1.96	0.47
1:A:329:ASN:HD21	5:E:8:VAL:HG21	1.80	0.47
4:D:31:ASP:HB2	4:D:32:PRO:HD2	1.95	0.47
2:B:318:ILE:HG23	11:X:506:SQB:BR	2.69	0.47
6:F:34:ASN:OD1	6:F:35:PRO:HD2	2.14	0.47
1:A:23:LEU:O	1:A:27:GLU:HG3	2.14	0.47
2:B:260:VAL:O	2:B:260:VAL:HG22	2.14	0.47
4:D:103:TRP:HD1	4:D:147:SER:OG	1.98	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.49	0.47
2:B:250:ALA:HB1	11:X:506:SQB:C5	2.45	0.47
2:B:258:ASN:HB3	11:X:506:SQB:C11	2.43	0.47
3:C:192:HIS:CG	3:C:421:ALA:HA	2.50	0.47
3:C:343:PHE:HB2	3:C:349:THR:HG22	1.95	0.47
4:D:218:LYS:C	4:D:219:LEU:HD23	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:238:CYS:SG	6:F:239:HIS:CD2	3.08	0.47
1:A:357:TYR:OH	5:E:18:GLN:NE2	2.47	0.47
2:B:133:GLN:OE1	2:B:251:ASP:HB2	2.14	0.47
2:B:221:THR:O	2:B:221:THR:CG2	2.61	0.47
2:B:286:LEU:N	2:B:286:LEU:HD12	2.29	0.47
1:A:187:SER:CB	1:A:391:LEU:HD21	2.45	0.46
4:D:406:HIS:HA	4:D:409:THR:OG1	2.15	0.46
1:A:177:VAL:HG11	1:A:224:TYR:HE1	1.80	0.46
1:A:404:PHE:CD1	2:B:261:PRO:HA	2.50	0.46
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.79	0.46
4:D:165:ILE:HG21	4:D:252:LEU:HB3	1.97	0.46
4:D:282:GLN:C	4:D:284:ARG:H	2.19	0.46
3:C:177:VAL:HG11	3:C:224:TYR:CE1	2.51	0.46
4:D:108:TYR:O	5:E:134:ARG:HD3	2.14	0.46
4:D:185:TYR:OH	4:D:398:MET:HB3	2.15	0.46
2:B:146:GLY:O	2:B:150:GLY:HA3	2.16	0.46
3:C:66:VAL:HG12	3:C:68[A]:VAL:HG23	1.98	0.46
1:A:154:MET:HG3	1:A:194:THR:HG23	1.98	0.46
6:F:91:CYS:O	6:F:93:TRP:N	2.47	0.46
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.81	0.46
6:F:267:PHE:CD2	6:F:279:LEU:HD13	2.51	0.46
1:A:40:LYS:HA	1:A:40:LYS:CE	2.43	0.46
1:A:151:SER:HB2	1:A:193:THR:HG22	1.97	0.46
1:A:158:SER:OG	1:A:166:LYS:HE3	2.16	0.46
1:A:335:ILE:C	1:A:335:ILE:HD12	2.36	0.46
1:A:285:GLN:HE21	1:A:373:ARG:NH1	2.13	0.46
2:B:181:VAL:HG13	3:C:258:ASN:ND2	2.31	0.46
2:B:318:ILE:O	2:B:318:ILE:HD12	2.16	0.46
6:F:216:TYR:CE1	6:F:374:ILE:HD13	2.51	0.46
2:B:305:CYS:O	2:B:307:PRO:HD3	2.15	0.45
4:D:297:ASP:OD2	4:D:299:LYS:HB2	2.16	0.45
4:D:387:LEU:HD23	4:D:387:LEU:C	2.36	0.45
6:F:131:PHE:C	6:F:131:PHE:CD2	2.89	0.45
6:F:189:PRO:HA	6:F:322:ASP:HA	1.98	0.45
1:A:214:ARG:HG2	1:A:219:ILE:O	2.16	0.45
1:A:117:LEU:HD11	1:A:121:ARG:HH11	1.81	0.45
4:D:106:GLY:O	4:D:149:MET:HB2	2.17	0.45
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.98	0.45
4:D:180:THR:CG2	4:D:181:VAL:N	2.79	0.45
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.17	0.45
2:B:18:ALA:O	2:B:22[A]:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ASP:O	3:C:80:THR:HG23	2.16	0.45
3:C:344:VAL:HG21	3:C:346:TRP:CE2	2.52	0.45
4:D:141:LEU:HD12	4:D:172:MET:SD	2.56	0.45
4:D:401:ARG:O	4:D:401:ARG:HG3	2.15	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.17	0.45
3:C:69:ASP:O	3:C:94:THR:HA	2.17	0.45
3:C:282:TYR:O	3:C:283:HIS:HB2	2.17	0.45
4:D:357:ASP:O	4:D:359:PRO:HD3	2.17	0.45
4:D:48:ARG:NH1	4:D:244:PHE:O	2.50	0.45
5:E:9:ILE:HG12	5:E:21:GLU:HB3	1.99	0.45
1:A:5:ILE:HD12	1:A:132:LEU:HD11	1.99	0.44
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.51	0.44
3:C:2:ARG:HA	3:C:131:GLY:O	2.17	0.44
6:F:151:SER:HB2	6:F:180:HIS:CD2	2.52	0.44
4:D:181:VAL:HG22	4:D:398:MET:HE1	2.00	0.44
4:D:282:GLN:C	4:D:284:ARG:N	2.70	0.44
6:F:18:SER:HA	6:F:21:LEU:HD12	1.99	0.44
2:B:358:ILE:HD13	2:B:358:ILE:N	2.32	0.44
2:B:303:ALA:O	2:B:305:CYS:N	2.50	0.44
2:B:414[A]:ASP:OD1	2:B:416:MET:HB2	2.18	0.44
1:A:3:GLU:O	1:A:133:GLN:HG3	2.17	0.44
1:A:114:ILE:HD12	1:A:114:ILE:O	2.18	0.44
1:A:312:TYR:O	1:A:344:VAL:HG13	2.16	0.44
1:A:332:ILE:HD13	5:E:22:VAL:HG11	2.00	0.44
2:B:278:ARG:H	2:B:278:ARG:HG2	1.52	0.44
4:D:292:THR:CG2	4:D:335:VAL:HG21	2.44	0.44
4:D:3:GLU:O	4:D:133:GLN:HB3	2.17	0.44
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.00	0.44
6:F:299:GLU:N	6:F:300:PRO:HD2	2.33	0.44
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.33	0.43
2:B:396:THR:O	2:B:400:ARG:HB2	2.18	0.43
3:C:115:ILE:HG23	3:C:116:ASP:N	2.33	0.43
3:C:177:VAL:HG12	7:X:507:GTP:O2'	2.18	0.43
6:F:340:GLN:OE1	6:F:340:GLN:HA	2.17	0.43
1:A:262:TYR:CE1	1:A:346:TRP:CH2	3.06	0.43
6:F:331:GLU:CD	12:X:511:ACP:H3B1	2.39	0.43
2:B:400:ARG:HA	2:B:400:ARG:NE	2.34	0.43
4:D:56:ALA:HB2	4:D:62:VAL:HG23	2.01	0.43
6:F:81:ILE:O	6:F:87:LEU:O	2.35	0.43
3:C:204:VAL:HG11	3:C:231:ILE:HG12	2.00	0.43
5:E:14:CYS:SG	5:E:15:THR:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:OD1	1:A:329:ASN:N	2.51	0.43
4:D:1:MET:O	4:D:131:CYS:HB3	2.18	0.43
2:B:136:GLN:HA	2:B:167:ASN:O	2.19	0.43
4:D:118:VAL:O	4:D:122:VAL:HG23	2.19	0.43
3:C:90:GLU:CD	3:C:90:GLU:H	2.23	0.43
4:D:269[B]:MET:HE3	4:D:305:CYS:HB2	2.01	0.43
4:D:295:MET:HG2	4:D:377:PHE:HB2	2.01	0.43
5:E:6:MET:HE3	5:E:22:VAL:HG21	2.01	0.43
5:E:130:ALA:C	5:E:134:ARG:HH21	2.22	0.43
3:C:119:LEU:HD11	3:C:156:ARG:CB	2.47	0.42
4:D:28:HIS:HA	4:D:45:GLN:HB3	2.00	0.42
6:F:226:GLU:HB2	6:F:238:CYS:HB3	2.00	0.42
1:A:2:ARG:HB2	1:A:133:GLN:HG2	2.01	0.42
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.38	0.42
5:E:9:ILE:HG13	5:E:10:GLU:HG3	2.00	0.42
1:A:70:LEU:CD2	1:A:145:THR:HG23	2.49	0.42
1:A:153:LEU:HD12	1:A:153:LEU:O	2.19	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.89	0.42
2:B:113:GLU:H	2:B:113:GLU:HG2	1.47	0.42
2:B:288:VAL:N	2:B:289:PRO:CD	2.82	0.42
6:F:100:ILE:CD1	6:F:173:ILE:HD13	2.47	0.42
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.55	0.42
1:A:347:CYS:C	5:E:27:PRO:HB3	2.40	0.42
4:D:34:GLY:HA2	4:D:86:ILE:HD11	2.01	0.42
4:D:208:ALA:O	4:D:212:ILE:HG13	2.19	0.42
6:F:102:PRO:HA	6:F:173:ILE:HG22	2.00	0.42
1:A:255:PHE:O	1:A:259:LEU:HB2	2.19	0.42
2:B:68:VAL:HA	2:B:93:VAL:O	2.19	0.42
4:D:48:ARG:HG3	4:D:48:ARG:HH11	1.84	0.42
4:D:187:ALA:O	4:D:191:VAL:HG23	2.19	0.42
6:F:349:GLY:O	6:F:353:VAL:HG13	2.19	0.42
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.42
5:E:76:ARG:NH1	5:E:76:ARG:HG2	2.35	0.42
1:A:7:ILE:HG23	1:A:66[B]:VAL:CG1	2.50	0.42
1:A:7:ILE:HD13	1:A:122:ILE:HD11	2.02	0.42
1:A:75:ILE:HD12	1:A:94:THR:HG22	2.01	0.42
1:A:313:MET:HG2	1:A:346:TRP:CH2	2.55	0.42
2:B:345:GLU:OE2	2:B:345:GLU:N	2.48	0.42
5:E:6:MET:HE3	5:E:6:MET:HB3	1.84	0.42
2:B:123:ARG:O	2:B:124:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.48	0.41
2:B:268:PHE:HB3	2:B:378:ILE:HG22	2.01	0.41
3:C:306:ASP:OD1	3:C:308:ARG:HG2	2.20	0.41
6:F:37:PHE:CE1	6:F:40:MET:HB2	2.55	0.41
3:C:101:ASN:HD21	4:D:254:LYS:HE2	1.84	0.41
4:D:48:ARG:NH1	4:D:48:ARG:HG3	2.35	0.41
4:D:202:TYR:CZ	4:D:238:VAL:CG1	3.03	0.41
2:B:231:VAL:O	2:B:235:MET:HG3	2.20	0.41
3:C:343:PHE:CB	3:C:349:THR:HG22	2.51	0.41
6:F:216:TYR:CD2	6:F:346:LEU:HD13	2.55	0.41
1:A:43:GLY:HA2	1:A:55:GLU:HB3	2.02	0.41
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.20	0.41
4:D:2:ARG:NE	4:D:2:ARG:HA	2.36	0.41
4:D:40:SER:O	4:D:45:GLN:HG3	2.20	0.41
4:D:54:ASN:OD1	4:D:64:ARG:NE	2.53	0.41
6:F:88:SER:C	6:F:90:SER:N	2.72	0.41
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.55	0.41
3:C:96:LYS:HB2	3:C:96:LYS:HZ3	1.86	0.41
6:F:280:GLU:HA	6:F:284[B]:LEU:HB2	2.03	0.41
4:D:282:GLN:HB2	4:D:283:TYR:H	1.58	0.41
1:A:119:LEU:HD12	1:A:156:ARG:NH2	2.35	0.41
3:C:177:VAL:O	3:C:177:VAL:CG1	2.69	0.41
6:F:242:ASN:ND2	12:X:511:ACP:O2B	2.51	0.41
5:E:90:ASN:O	5:E:94:ILE:HG13	2.21	0.41
3:C:46:ASP:OD1	3:C:46:ASP:N	2.53	0.41
4:D:156:LYS:HD3	4:D:156:LYS:HA	1.90	0.41
4:D:419:THR:HA	4:D:422:GLU:HB3	2.03	0.41
6:F:73:ARG:HB2	6:F:76[B]:SER:OG	2.21	0.41
1:A:47:ASP:O	1:A:50:ASN:HB2	2.21	0.40
4:D:282:GLN:O	4:D:284:ARG:N	2.54	0.40
1:A:10:GLY:O	1:A:14:VAL:HG23	2.21	0.40
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.56	0.40
2:B:145:THR:O	2:B:149:MET:HB3	2.21	0.40
2:B:320:ARG:O	2:B:373:MET:HA	2.21	0.40
2:B:56:ALA:HB3	2:B:60:LYS:HD3	2.03	0.40
2:B:192:HIS:CE1	2:B:424[A]:ASN:OD1	2.75	0.40
3:C:335:ILE:HG22	3:C:341:ILE:HD11	2.04	0.40
4:D:412:GLY:O	5:E:136:ASN:ND2	2.50	0.40
6:F:149:ALA:CB	6:F:182:ILE:HG12	2.51	0.40
3:C:195:LEU:HD12	3:C:195:LEU:HA	1.78	0.40
4:D:86:ILE:HD12	4:D:86:ILE:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:GLU:OE2	4:D:113:GLU:CA	2.68	0.40
4:D:115:VAL:O	4:D:119:LEU:HG	2.21	0.40
4:D:136:GLN:O	4:D:136:GLN:HG3	2.21	0.40
6:F:147:TRP:HB2	6:F:169:LEU:HD11	2.03	0.40
4:D:32:PRO:HA	4:D:83:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/439 (102%)	439 (98%)	8 (2%)	0	100	100
2	B	437/428 (102%)	421 (96%)	13 (3%)	3 (1%)	22	46
3	C	448/440 (102%)	433 (97%)	14 (3%)	1 (0%)	47	73
4	D	433/431 (100%)	403 (93%)	28 (6%)	2 (0%)	29	54
5	E	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
6	F	309/320 (97%)	294 (95%)	14 (4%)	1 (0%)	41	66
All	All	2193/2179 (101%)	2107 (96%)	79 (4%)	7 (0%)	41	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	283	HIS
4	D	276	THR
2	B	278	ARG
2	B	281	GLN
2	B	304	ALA
4	D	282	GLN
6	F	92	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/370 (103%)	365 (96%)	15 (4%)	32	61
2	B	380/370 (103%)	360 (95%)	20 (5%)	22	48
3	C	381/371 (103%)	368 (97%)	13 (3%)	37	66
4	D	376/372 (101%)	354 (94%)	22 (6%)	19	43
5	E	111/109 (102%)	109 (98%)	2 (2%)	59	83
6	F	293/289 (101%)	275 (94%)	18 (6%)	18	41
All	All	1921/1881 (102%)	1831 (95%)	90 (5%)	26	54

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	46	ASP
1	A	71	GLU
1	A	120	ASP
1	A	181	VAL
1	A	242	LEU
1	A	250	VAL
1	A	257	THR
1	A	284	GLU
1	A	285	GLN
1	A	302	MET
1	A	329	ASN
1	A	368	LEU
1	A	390	ARG
1	A	413	MET
2	B	55	GLU
2	B	60	LYS
2	B	79	ARG
2	B	80	SER
2	B	90	ASP
2	B	124	LYS
2	B	139	HIS

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Mol	Chain	Res	Type
2	B	147[A]	SER
2	B	147[B]	SER
2	B	155	SER
2	B	207	GLU
2	B	260	VAL
2	B	278	ARG
2	B	281	GLN
2	B	353	THR
2	B	355	VAL
2	B	357	ASP
2	B	377	PHE
2	B	387	LEU
2	B	400	ARG
3	C	18	ASN
3	C	71	GLU
3	C	124	LYS
3	C	164	LYS
3	C	170	SER
3	C	178	SER
3	C	195	LEU
3	C	221	ARG
3	C	285	GLN
3	C	338	LYS
3	C	342	GLN
3	C	347	CYS
3	C	430	LYS
4	D	50	ASN
4	D	59	ASN
4	D	68	VAL
4	D	70	LEU
4	D	71	GLU
4	D	76	ASP
4	D	94	PHE
4	D	139	HIS
4	D	172	MET
4	D	247	GLN
4	D	248	LEU
4	D	278	ARG
4	D	282	GLN
4	D	283	TYR
4	D	284	ARG
4	D	286	LEU

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Mol	Chain	Res	Type
4	D	298	SER
4	D	302	MET
4	D	323	MET
4	D	345	GLU
4	D	377	PHE
4	D	414	ASP
5	E	14	CYS
5	E	103	GLN
6	F	19	ARG
6	F	33	ASP
6	F	89	GLU
6	F	90	SER
6	F	91	CYS
6	F	131	PHE
6	F	162	ILE
6	F	192	LEU
6	F	196	HIS
6	F	197	ARG
6	F	211	TYR
6	F	240	LEU
6	F	272	MET
6	F	284[A]	LEU
6	F	284[B]	LEU
6	F	296	MET
6	F	311	SER
6	F	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	283	HIS
1	A	285	GLN
2	B	136	GLN
2	B	385	GLN
2	B	433	GLN
4	D	133	GLN
4	D	281	GLN
4	D	300	ASN
6	F	239	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic and 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GTP	X	507	-	26,34,34	1.01	2 (7%)	32,54,54	0.69	1 (3%)
10	GDP	X	509	8	24,30,30	0.98	3 (12%)	30,47,47	0.67	1 (3%)
12	ACP	X	511	-	27,33,33	0.92	1 (3%)	32,52,52	0.85	2 (6%)
10	GDP	X	504	8	24,30,30	1.00	2 (8%)	30,47,47	0.65	1 (3%)
7	GTP	X	501	8	26,34,34	1.00	2 (7%)	32,54,54	0.69	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GTP	X	507	-	-	5/18/38/38	0/3/3/3
10	GDP	X	509	8	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ACP	X	511	-	-	8/15/38/38	0/3/3/3
10	GDP	X	504	8	-	4/12/32/32	0/3/3/3
7	GTP	X	501	8	-	4/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	504	GDP	C5-C6	-2.73	1.41	1.47
10	X	509	GDP	C5-C6	-2.69	1.41	1.47
7	X	507	GTP	C5-C6	-2.69	1.42	1.47
7	X	501	GTP	C5-C6	-2.67	1.42	1.47
12	X	511	ACP	PB-O2B	-2.51	1.50	1.56
7	X	507	GTP	C8-N7	-2.14	1.31	1.35
10	X	509	GDP	C8-N7	-2.09	1.31	1.35
10	X	504	GDP	C8-N7	-2.09	1.31	1.35
7	X	501	GTP	C8-N7	-2.09	1.31	1.35
10	X	509	GDP	C5-C4	-2.00	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	X	511	ACP	O1G-PG-C3B	-2.33	106.22	111.24
12	X	511	ACP	C5-C6-N6	2.28	123.82	120.35
7	X	507	GTP	O6-C6-C5	2.07	128.41	124.37
7	X	501	GTP	O6-C6-C5	2.04	128.37	124.37
10	X	509	GDP	O6-C6-C5	2.04	128.35	124.37
10	X	504	GDP	O6-C6-C5	2.03	128.34	124.37

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	501	GTP	C5'-O5'-PA-O1A
7	X	507	GTP	C5'-O5'-PA-O1A
10	X	504	GDP	C5'-O5'-PA-O1A
10	X	509	GDP	C5'-O5'-PA-O1A
12	X	511	ACP	PG-C3B-PB-O1B
12	X	511	ACP	PG-C3B-PB-O2B
12	X	511	ACP	PG-C3B-PB-O3A
12	X	511	ACP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
12	X	511	ACP	C3'-C4'-C5'-O5'
10	X	509	GDP	PB-O3A-PA-O1A
7	X	501	GTP	C5'-O5'-PA-O3A
10	X	509	GDP	C5'-O5'-PA-O3A
7	X	507	GTP	PB-O3A-PA-O2A
7	X	501	GTP	C5'-O5'-PA-O2A
7	X	507	GTP	C5'-O5'-PA-O2A
10	X	504	GDP	C5'-O5'-PA-O2A
10	X	509	GDP	C5'-O5'-PA-O2A
10	X	504	GDP	PB-O3A-PA-O2A
10	X	509	GDP	PB-O3A-PA-O2A
7	X	507	GTP	C5'-O5'-PA-O3A
10	X	504	GDP	C5'-O5'-PA-O3A
12	X	511	ACP	C5'-O5'-PA-O3A
7	X	501	GTP	PB-O3A-PA-O2A
7	X	507	GTP	PB-O3A-PA-O1A
12	X	511	ACP	C5'-O5'-PA-O1A
12	X	511	ACP	C5'-O5'-PA-O2A

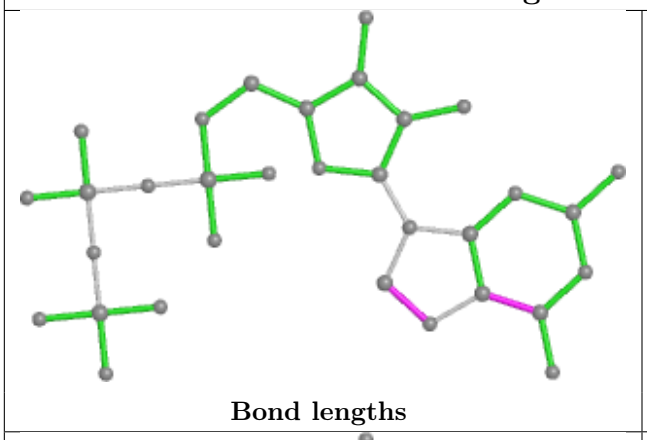
There are no ring outliers.

4 monomers are involved in 5 short contacts:

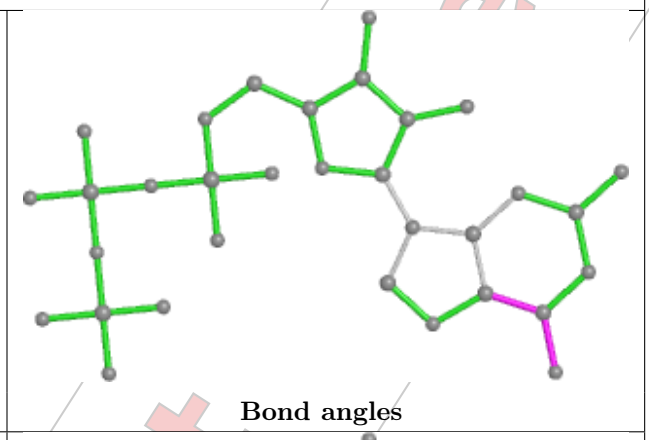
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	X	507	GTP	1	0
10	X	509	GDP	1	0
12	X	511	ACP	2	0
7	X	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

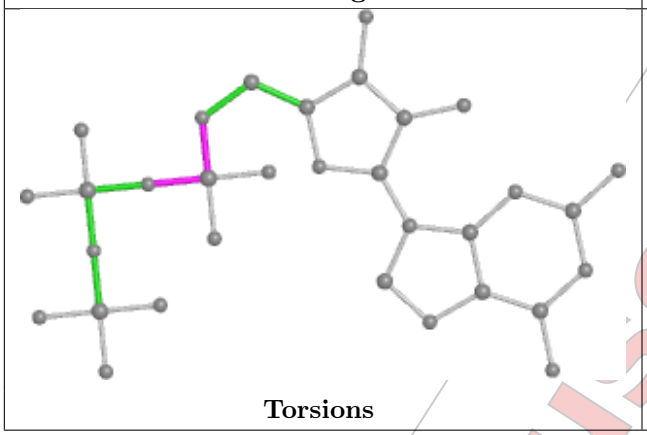
Ligand GTP X 507



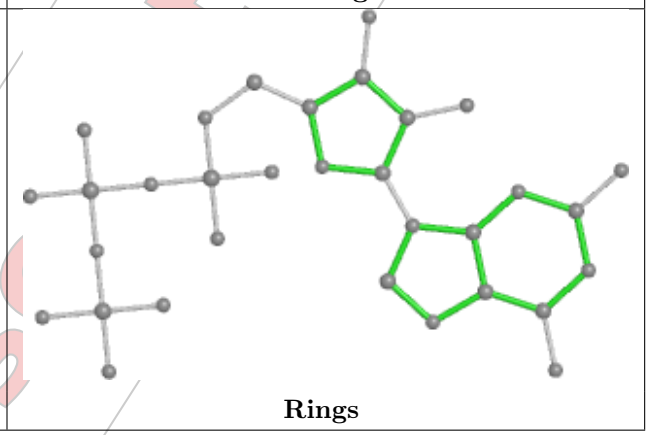
Bond lengths



Bond angles

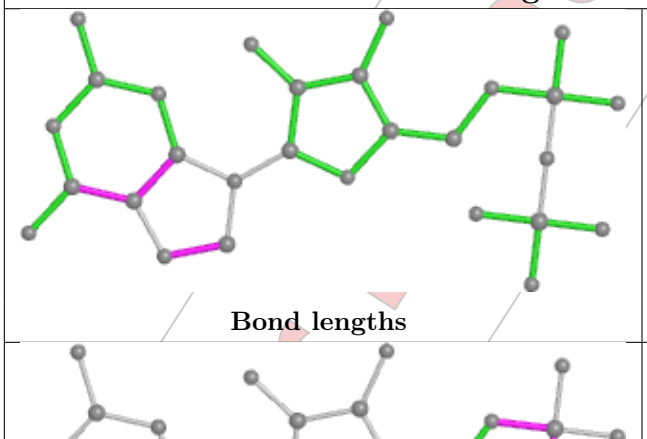


Torsions

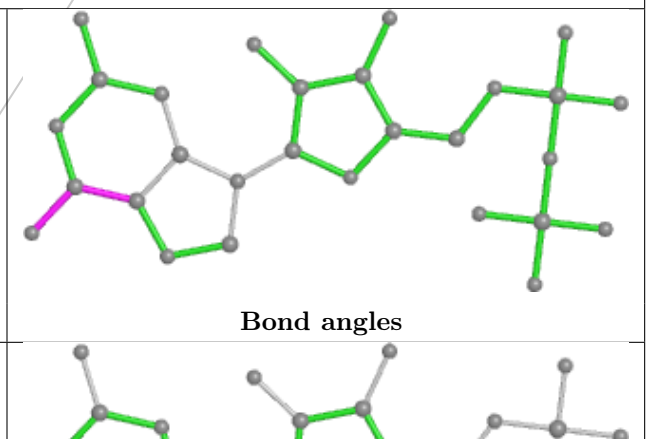


Rings

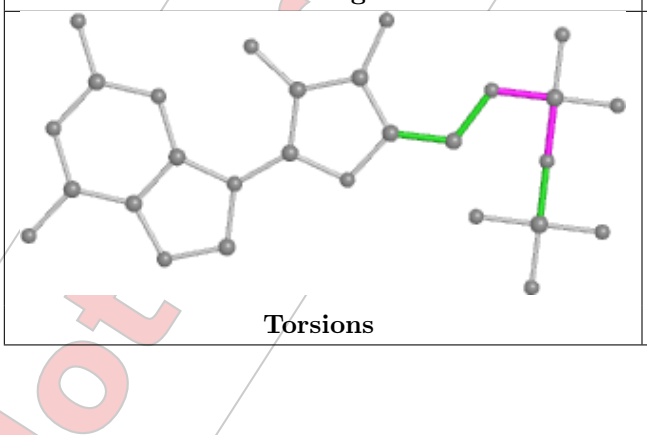
Ligand GDP X 509



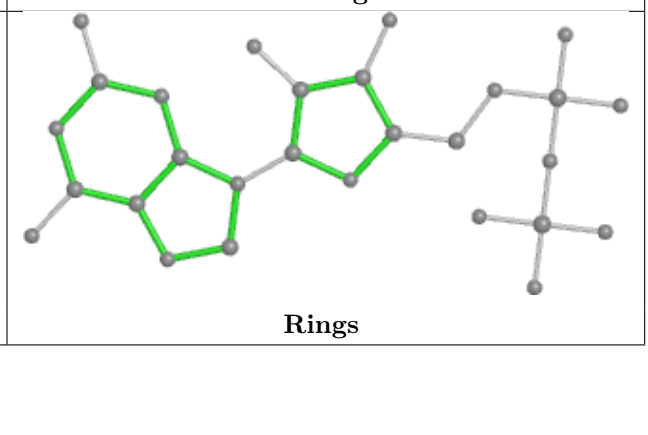
Bond lengths



Bond angles

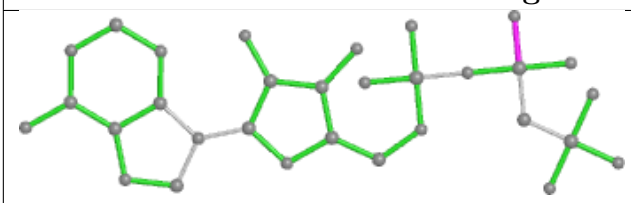


Torsions

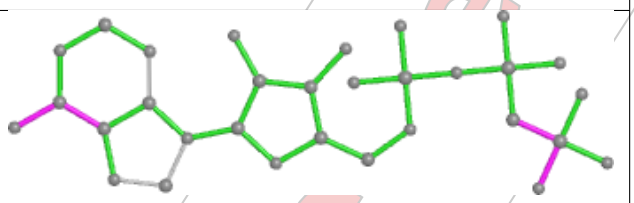


Rings

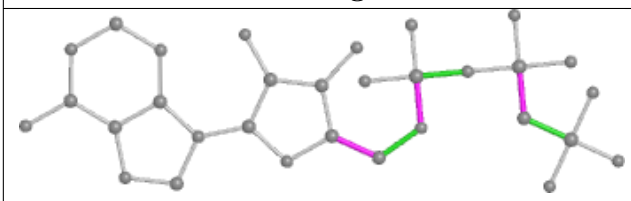
Ligand ACP X 511



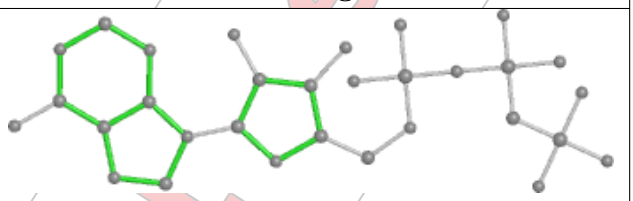
Bond lengths



Bond angles

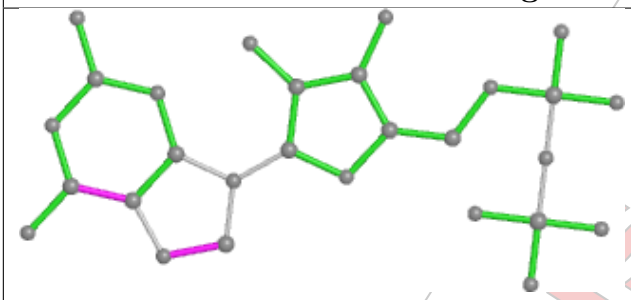


Torsions

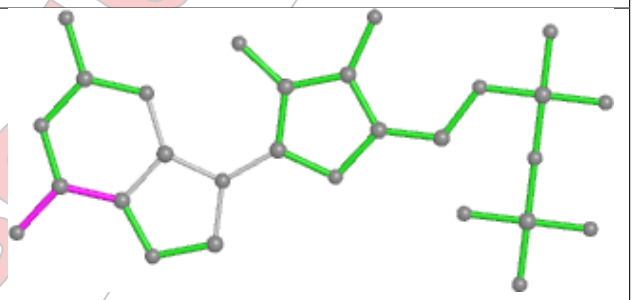


Rings

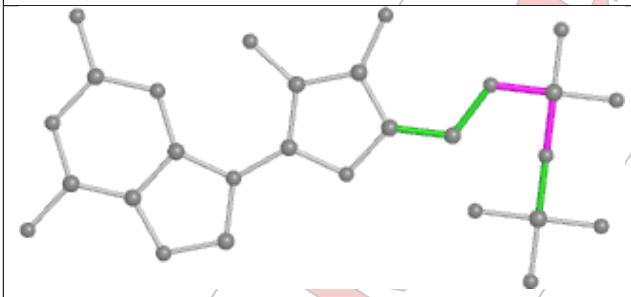
Ligand GDP X 504



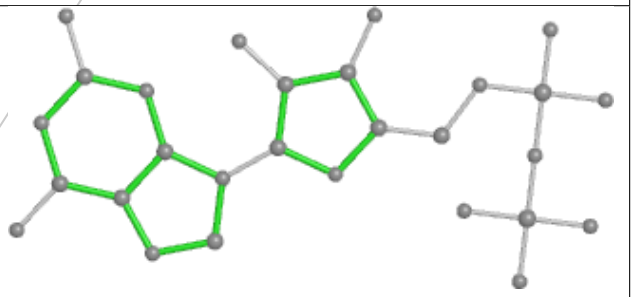
Bond lengths



Bond angles

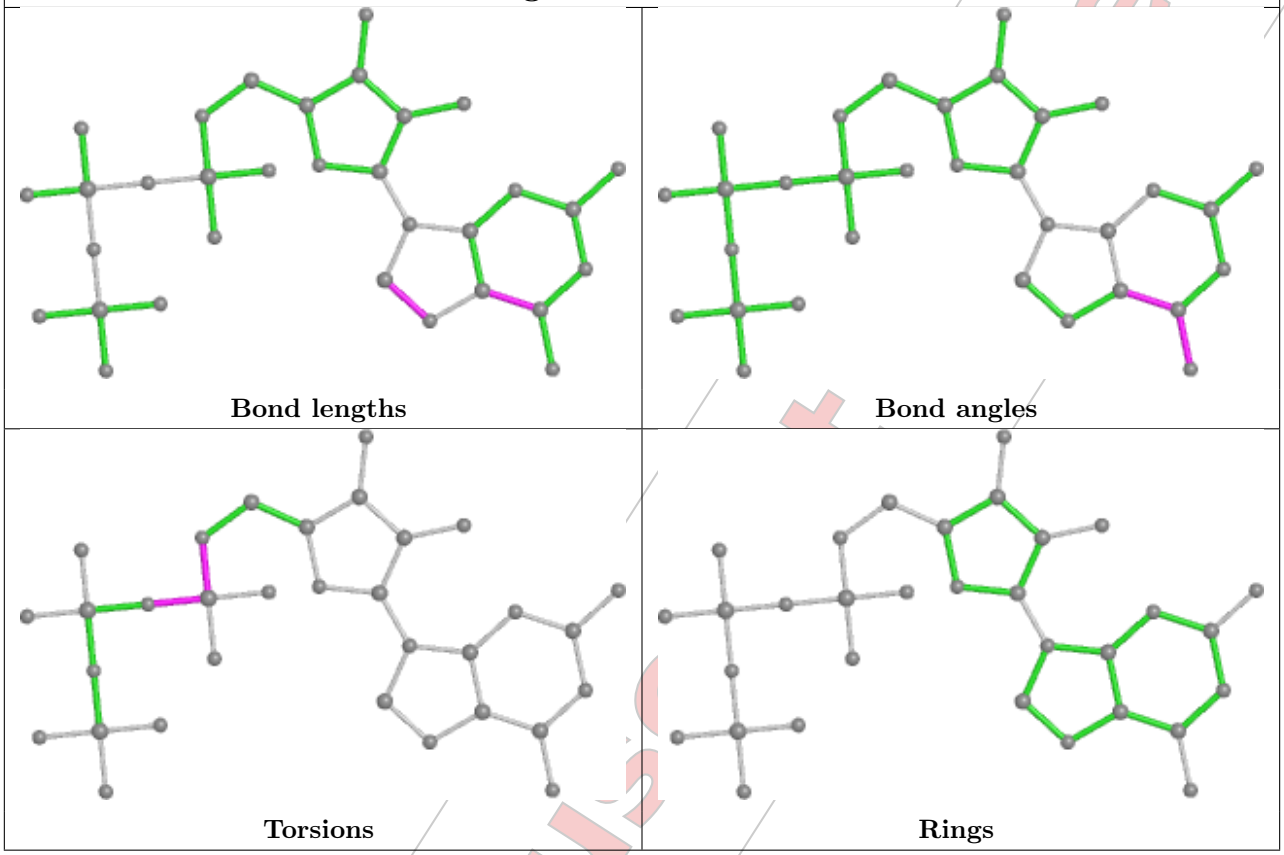


Torsions



Rings

Ligand GTP X 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	6
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	31.51
1	F	362:ALA	C	373:SER	N	19.14
1	F	102:PRO	C	125:THR	N	12.94
1	F	151:SER	C	162:ILE	N	12.03
1	F	136:ASN	C	144:GLY	N	10.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	173:ILE	C	179:VAL	N	8.39
1	F	231:ALA	C	235:ASP	N	6.80

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

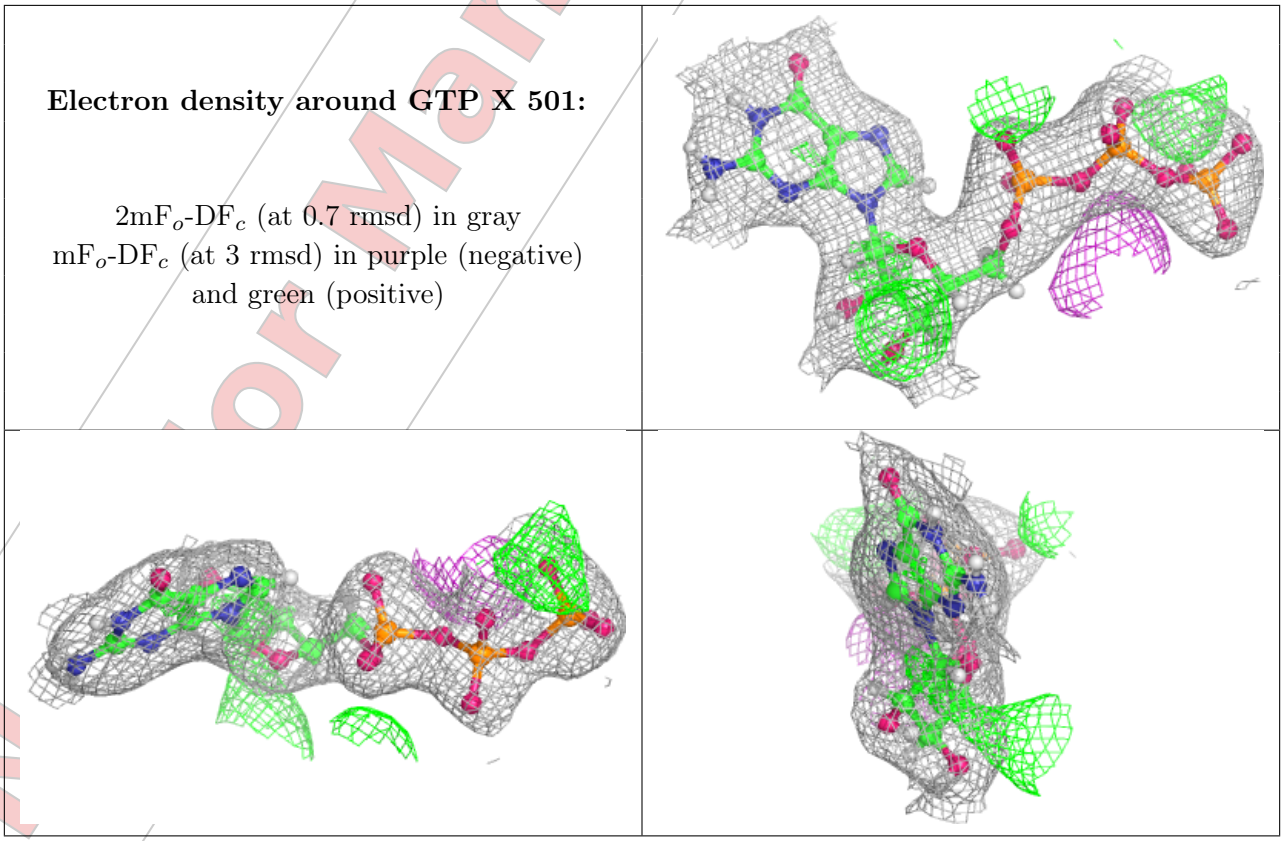
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

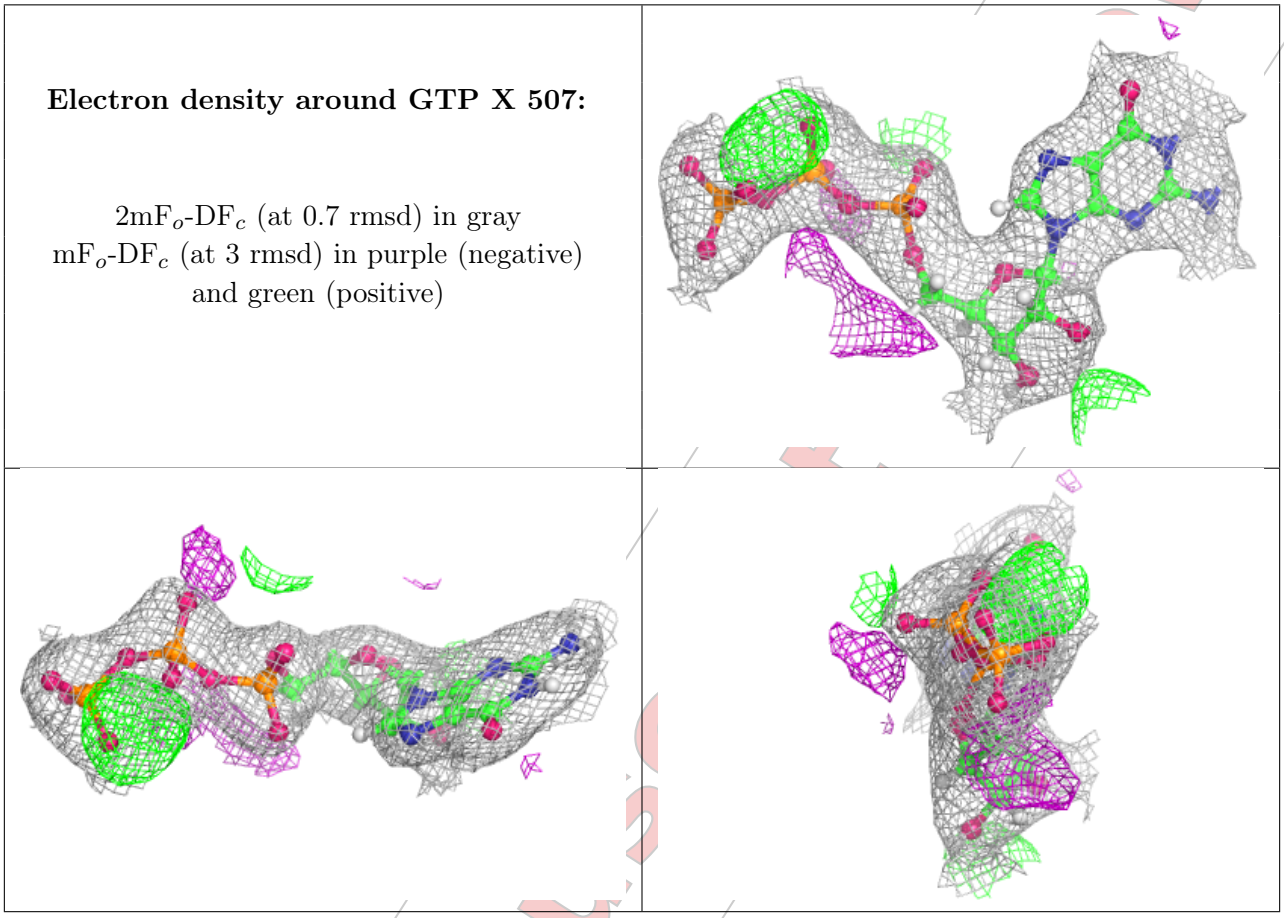
Electron density around GTP X 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



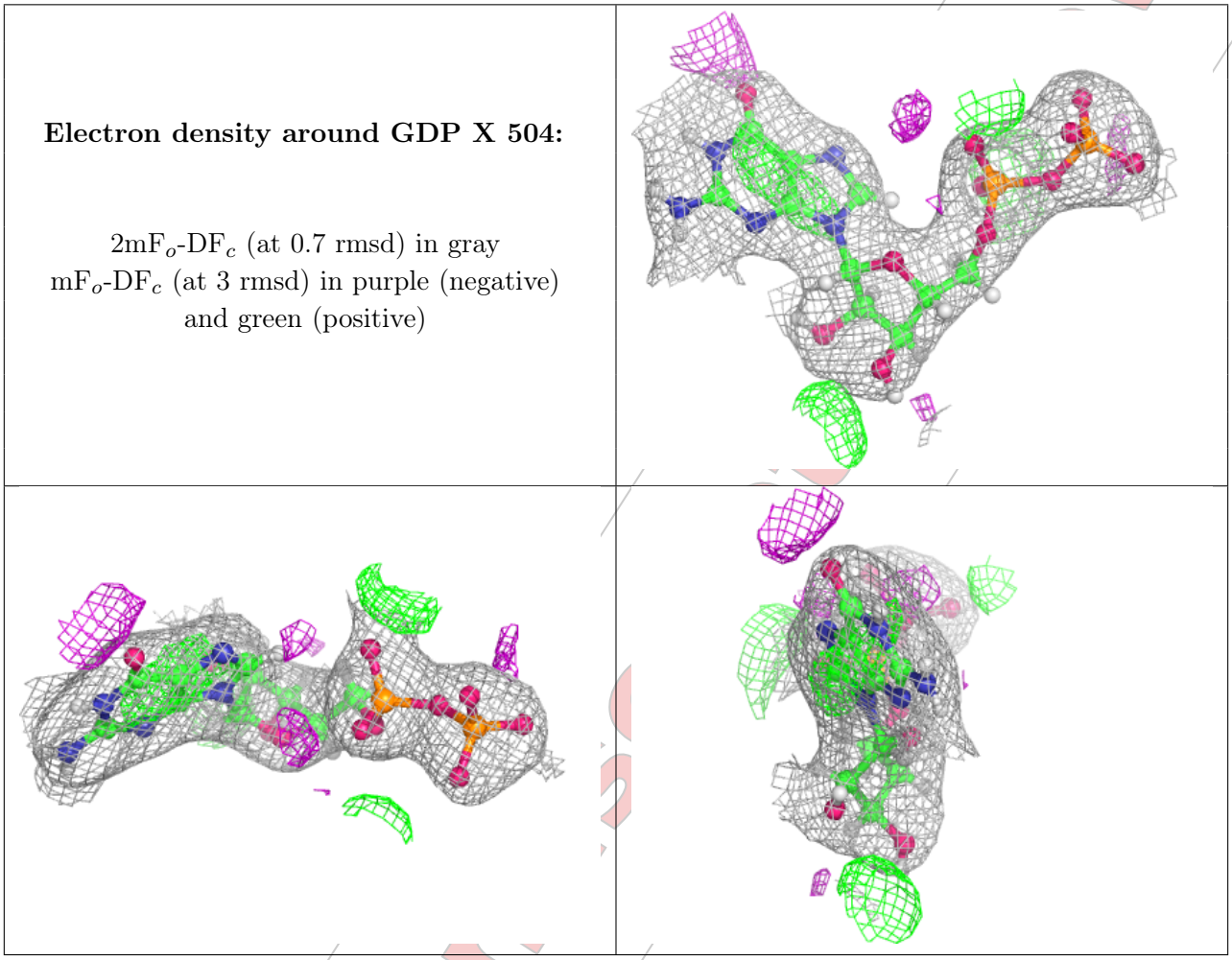
Electron density around GTP X 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



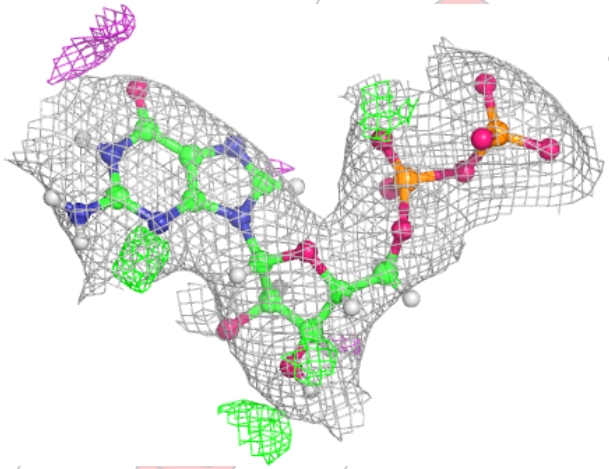
Electron density around GDP X 504:

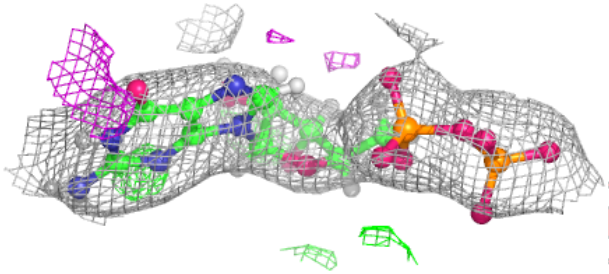
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

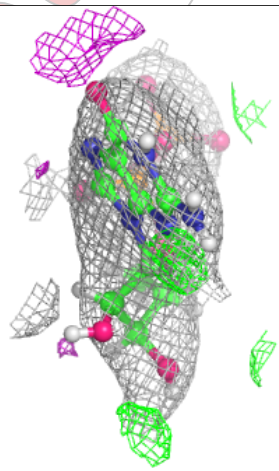


Electron density around GDP X 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

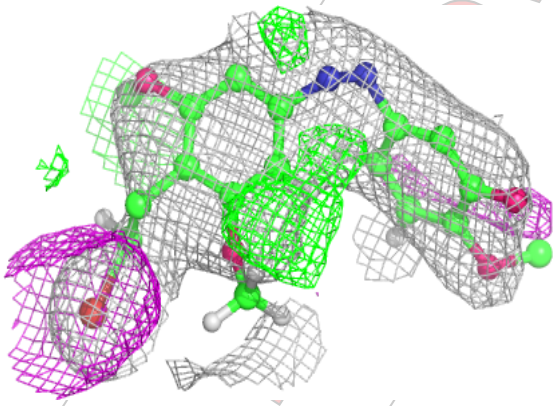


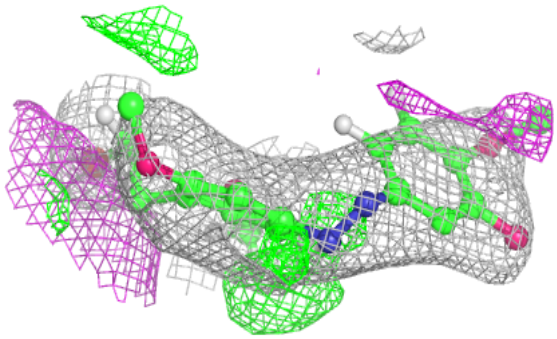


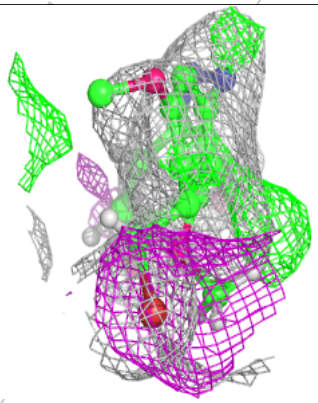


Electron density around SQB X 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

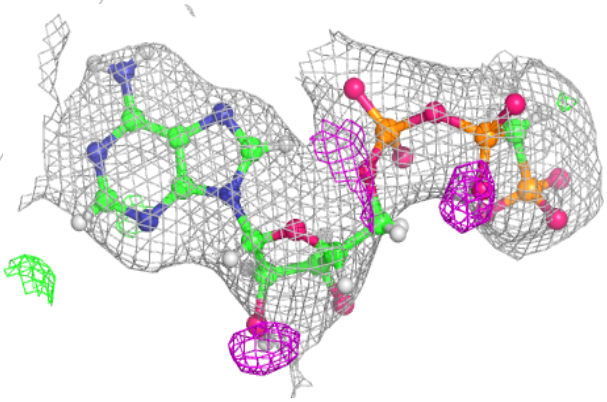


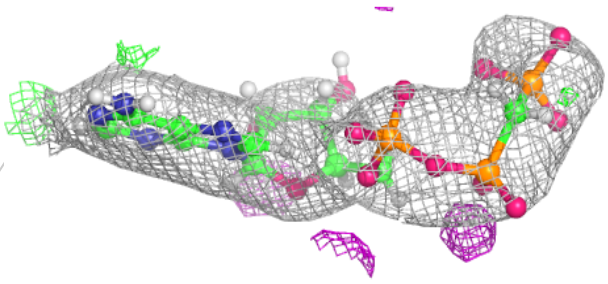


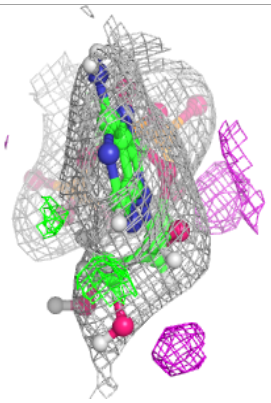


Electron density around ACP X 511:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2023 – 09:21 pm GMT

Deposition ID : D_1292128627

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

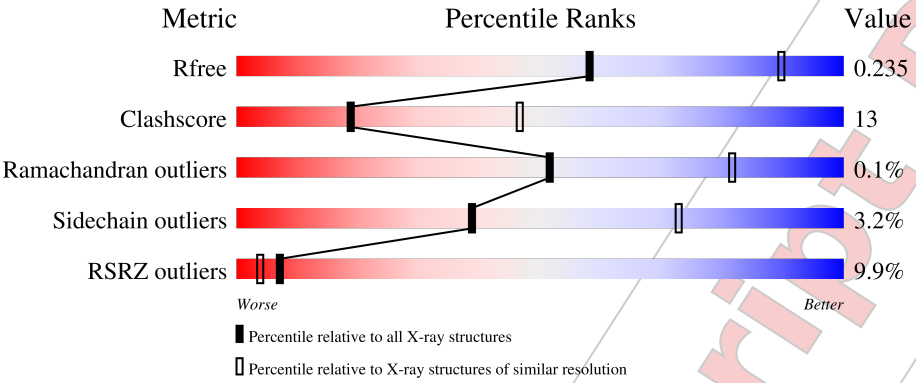
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	4% 83% 17%
2	B	428	8% 72% 27%
3	C	440	3% 84% 16%
4	D	431	7% 76% 23%

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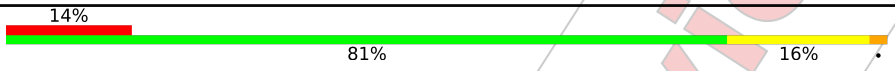
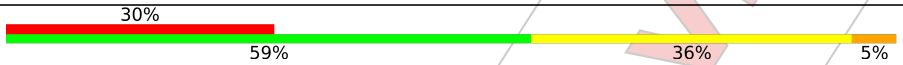
Mol	Chain	Length	Quality of chain
5	E	123	
6	F	351	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 18186 atoms, of which 103 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3480	2211	584	661	24	0	12	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3441	2167	581	664	29	7	15	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	440	3519	2231	588	674	26	0	18	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	431	3411	2143	580	660	28	0	6	0

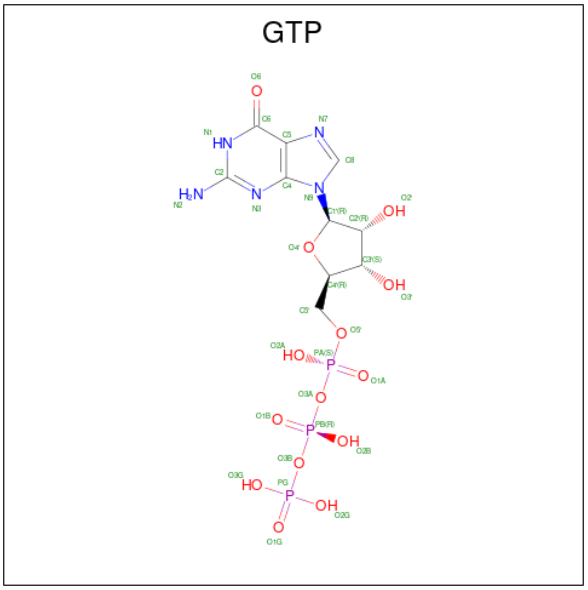
- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	123	1042	644	188	204	6	0	5	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	351	2890	1861	488	527	14	18	8	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	X	1	Total C N O P 32 10 5 14 3	0	0
7	X	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	X	1	Total Mg 1 1	0	0
8	X	1	Total Mg 1 1	0	0
8	X	1	Total Mg 1 1	0	0
8	X	1	Total Mg 1 1	1	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	X	1	Total Ca 1 1	0	0
9	X	1	Total Ca 1 1	1	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	X	1	Total Ca 1 1	1	0
9	X	1	Total Ca 1 1	0	0

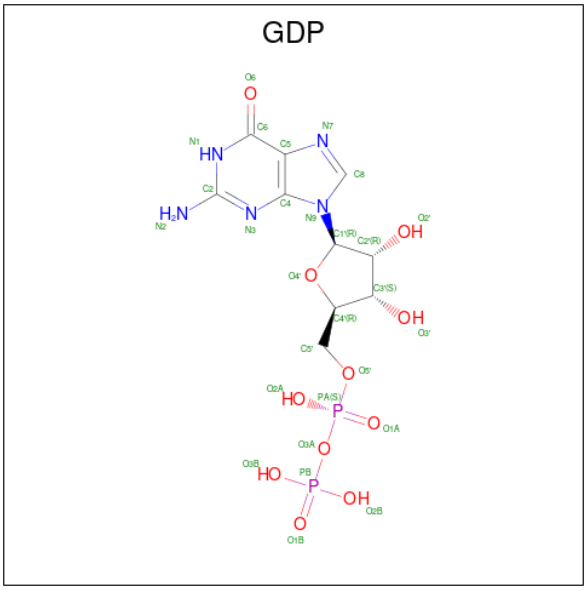
- Molecule 10 is a ligand with the chemical component id EPA but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for EPA. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	X	1	Total C H N O S 73 26 39 1 6 1	0	0
10	X	1	Total C H N O S 73 26 39 1 6 1	0	0

- Molecule 11 is a ligand with the chemical component id COL but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for COL. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

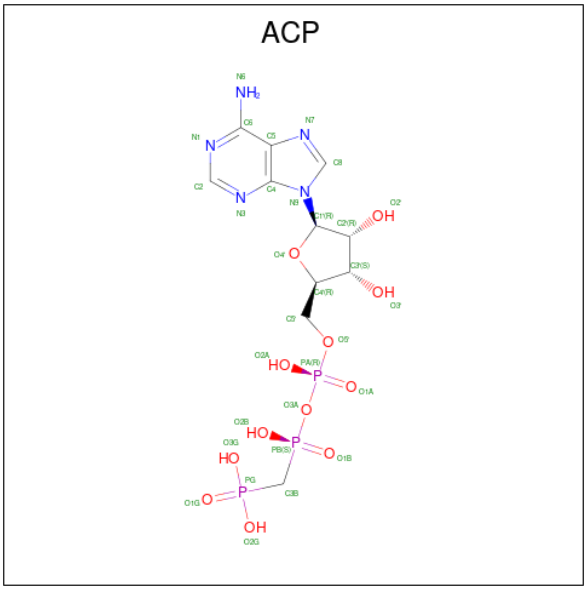
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	X	1	Total C H N O 54 22 25 1 6	0	0

- Molecule 12 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	X	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
12	X	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	X	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 14 is water.

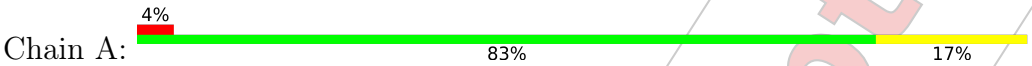
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	S	44	Total	O	0	0
			44	44		

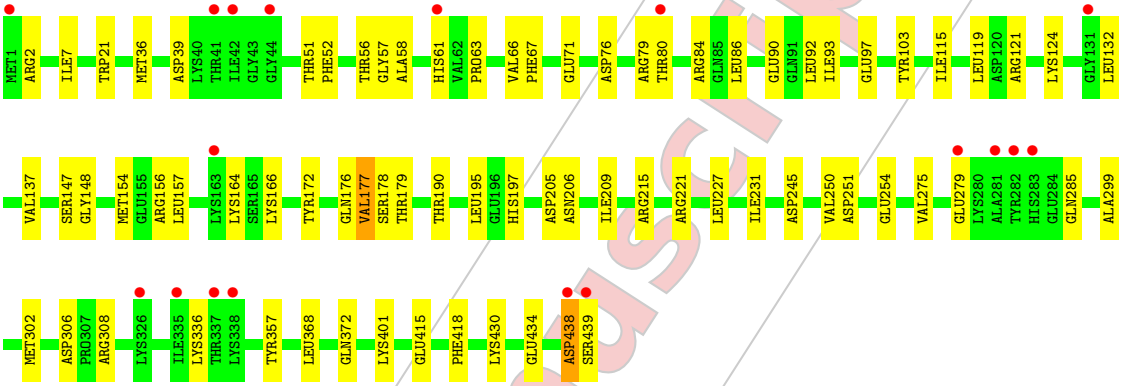
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1:

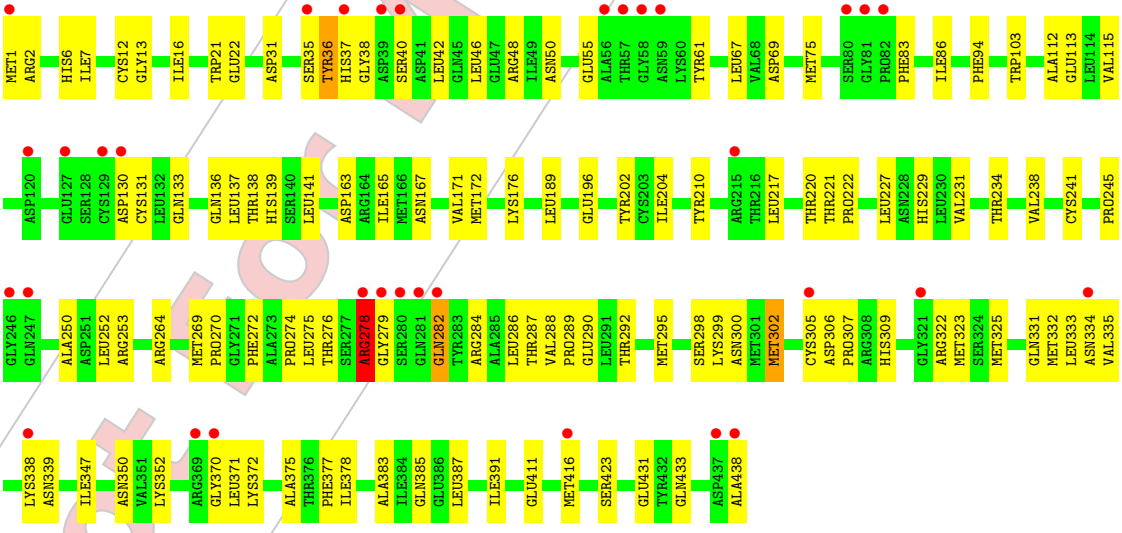
Chain A:





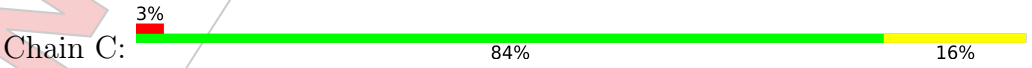
• Molecule 2:

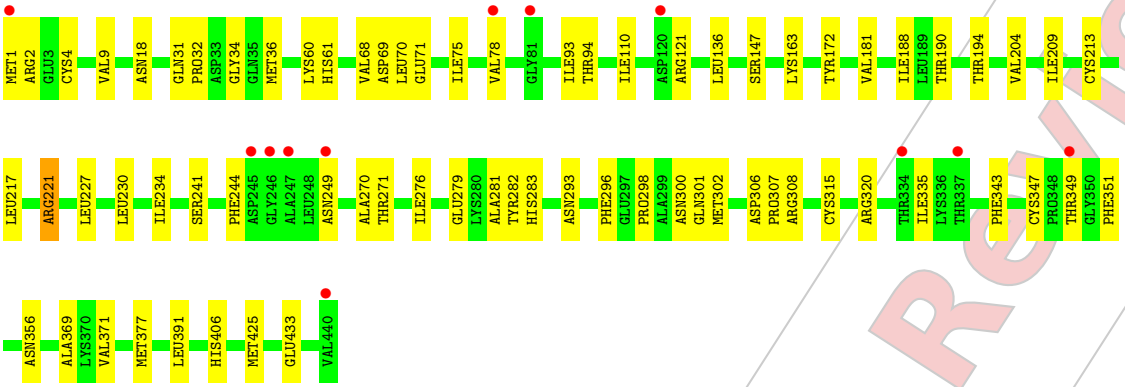
Chain B:



• Molecule 3:

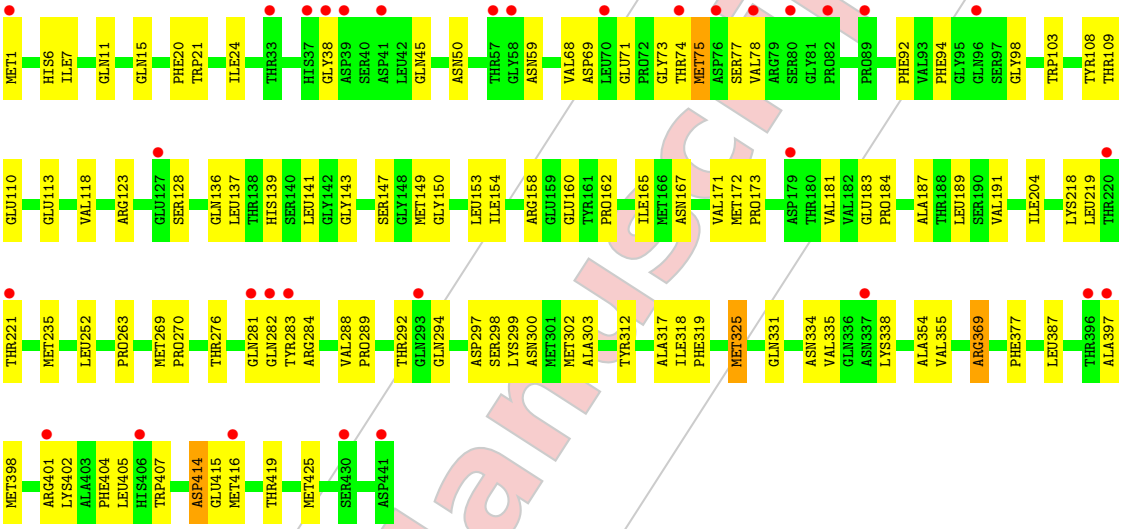
Chain C:





• Molecule 4:

Chain D:

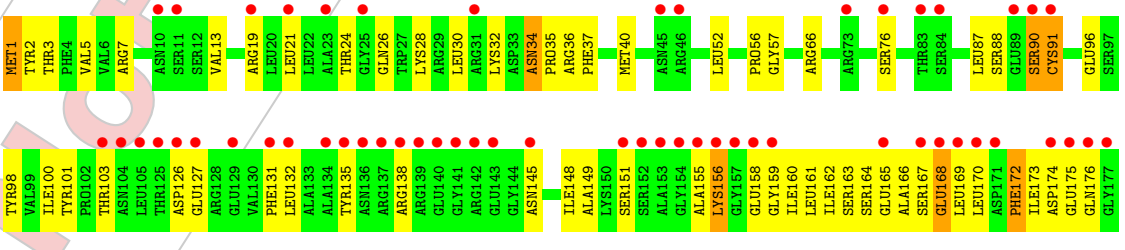


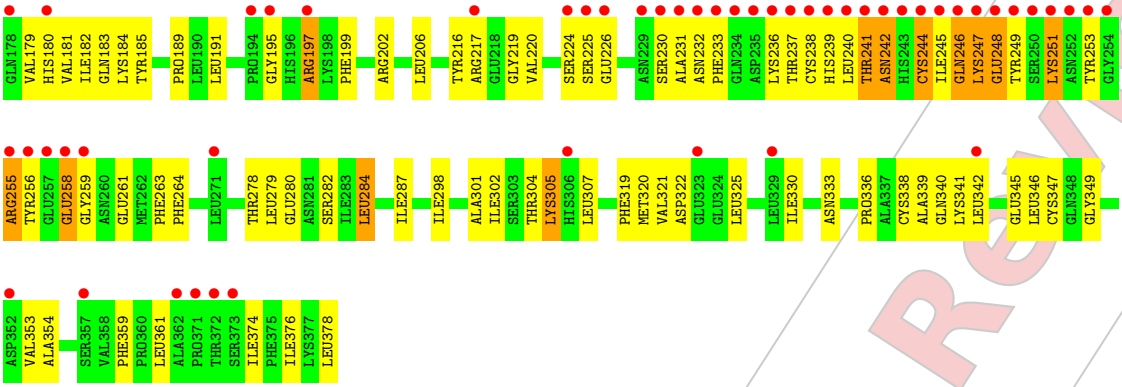
• Molecule 5:

Chain E:

• Molecule 6:

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.76Å 160.76Å 180.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.26 – 2.80 15.26 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.26-2.80) 99.9 (15.26-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.51Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.178 , 0.227 0.193 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18186	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, EPA, ACP, CA, MG, COL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	0/3594	0.73	0/4881
2	B	0.50	0/3555	0.78	2/4813 (0.0%)
3	C	0.55	0/3648	0.73	1/4955 (0.0%)
4	D	0.48	0/3504	0.74	1/4748 (0.0%)
5	E	0.54	0/1066	0.81	2/1415 (0.1%)
6	F	0.46	0/2975	0.77	1/4022 (0.0%)
All	All	0.50	0/18342	0.75	7/24834 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
6	F	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	264	ARG	CD-NE-CZ	5.74	131.63	123.60
6	F	181	VAL	CG1-CB-CG2	5.35	119.46	110.90
2	B	264	ARG	NE-CZ-NH2	-5.28	117.66	120.30
4	D	158	ARG	CA-CB-CG	5.26	124.97	113.40
3	C	433	GLU	CA-CB-CG	5.13	124.68	113.40
5	E	119	MET	CA-CB-CG	5.10	121.97	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	119	MET	CB-CG-SD	-5.06	97.23	112.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
2	B	278	ARG	Sidechain
4	D	369	ARG	Sidechain
6	F	255	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3480	0	3427	68	0
2	B	3441	0	3356	119	2
3	C	3519	0	3458	60	2
4	D	3411	0	3306	79	0
5	E	1042	0	1065	15	0
6	F	2890	0	2894	144	0
7	X	64	0	24	0	0
8	X	4	0	0	0	0
9	X	4	0	0	0	0
10	X	68	78	30	8	0
11	X	29	25	0	3	0
12	X	56	0	24	3	0
13	X	31	0	14	4	0
14	S	44	0	0	1	0
All	All	18083	103	17598	465	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HH21	2:B:325:MET:HE2	1.12	1.07
1:A:176:GLN:HG3	6:F:56:PRO:HB3	1.33	1.06
2:B:338:LYS:O	2:B:338:LYS:NZ	1.90	1.02
4:D:284:ARG:HH22	4:D:294:GLN:HE22	1.05	0.96
4:D:318:ILE:HD12	4:D:354:ALA:HB3	1.49	0.92
2:B:75:MET:HE1	2:B:94:PHE:HB3	1.51	0.91
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.51	0.90
6:F:167:SER:HA	6:F:170:LEU:HG	1.50	0.90
3:C:279:GLU:N	3:C:279:GLU:OE2	2.05	0.90
6:F:155:ALA:H	6:F:158:GLU:HB3	1.36	0.90
1:A:221:ARG:HH21	2:B:325:MET:CE	1.84	0.90
6:F:131:PHE:CE1	6:F:182:ILE:HG21	2.06	0.90
1:A:306:ASP:OD1	1:A:308:ARG:HD3	1.74	0.88
6:F:135:TYR:CZ	6:F:166:ALA:HB2	2.08	0.88
3:C:204:VAL:HG22	3:C:302[B]:MET:CE	2.06	0.86
6:F:161:LEU:HD23	6:F:169:LEU:HD23	1.56	0.85
4:D:1:MET:HG3	4:D:50:ASN:HD22	1.41	0.85
2:B:238[B]:VAL:HG22	2:B:378:ILE:HD11	1.60	0.83
6:F:3:THR:HB	6:F:30:LEU:HD11	1.61	0.83
3:C:204:VAL:HG22	3:C:302[B]:MET:HE3	1.61	0.82
6:F:263:PHE:HE1	6:F:341:LYS:HD3	1.44	0.82
10:X:506:EPA:O5	10:X:506:EPA:O3	1.91	0.81
4:D:317:ALA:O	4:D:318:ILE:HD13	1.79	0.81
2:B:278:ARG:HD2	2:B:279:GLY:HA2	1.63	0.81
3:C:18:ASN:HD21	3:C:78:VAL:HG22	1.44	0.81
2:B:331:GLN:HA	2:B:334:ASN:HD21	1.45	0.80
6:F:217:ARG:HD3	6:F:376:ILE:HG13	1.64	0.80
1:A:154:MET:HE2	1:A:154:MET:HA	1.65	0.79
4:D:334:ASN:OD1	4:D:338:LYS:HE3	1.83	0.79
2:B:305:CYS:HB3	2:B:383:ALA:O	1.82	0.79
2:B:331:GLN:HA	2:B:334:ASN:ND2	1.98	0.78
2:B:332:MET:O	2:B:335:VAL:HG12	1.84	0.77
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.20	0.77
6:F:3:THR:HB	6:F:30:LEU:CD1	2.14	0.77
4:D:292:THR:HG22	4:D:335:VAL:HG21	1.66	0.76
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	1.68	0.76
4:D:1:MET:HG3	4:D:50:ASN:ND2	2.01	0.76
2:B:288:VAL:HG22	2:B:323:MET:HE2	1.67	0.76
4:D:284:ARG:HH22	4:D:294:GLN:NE2	1.82	0.75
3:C:209:ILE:HG22	3:C:227:LEU:HD22	1.67	0.74
6:F:3:THR:OG1	6:F:37:PHE:HA	1.87	0.74
4:D:1:MET:CG	4:D:50:ASN:HD22	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:CG	6:F:56:PRO:HB3	2.14	0.73
6:F:173:ILE:HD13	6:F:180:HIS:HB2	1.69	0.73
6:F:184:LYS:HD2	6:F:185:TYR:N	2.02	0.72
1:A:179:THR:O	2:B:352:LYS:HE2	1.88	0.72
2:B:370:GLY:O	2:B:371:LEU:HD13	1.89	0.72
6:F:32:LYS:HD3	6:F:32:LYS:N	2.04	0.71
3:C:4[A]:CYS:SG	3:C:136:LEU:HG	2.31	0.71
6:F:167:SER:HA	6:F:170:LEU:CG	2.20	0.71
1:A:56:THR:HG22	1:A:58:ALA:H	1.53	0.71
2:B:75:MET:HE1	2:B:94:PHE:CB	2.19	0.71
6:F:131:PHE:HE1	6:F:182:ILE:HG21	1.52	0.71
3:C:249:ASN:OD1	3:C:356[A]:ASN:ND2	2.24	0.70
6:F:135:TYR:CE2	6:F:166:ALA:HB2	2.25	0.70
2:B:75:MET:CE	2:B:94:PHE:HB3	2.21	0.70
2:B:274:PRO:HG2	10:X:506:EPA:C25	2.22	0.70
4:D:1:MET:HG3	4:D:50:ASN:CB	2.22	0.70
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.69
1:A:97:GLU:OE1	2:B:1:MET:HE2	1.92	0.69
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.27	0.69
2:B:75:MET:HE1	2:B:94:PHE:CG	2.28	0.69
4:D:59:ASN:OD1	4:D:59:ASN:O	2.11	0.69
6:F:7:ARG:HD3	6:F:40:MET:HE3	1.74	0.69
2:B:2:ARG:HB2	2:B:2:ARG:CZ	2.22	0.69
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.08	0.69
2:B:279:GLY:O	2:B:282:GLN:HB3	1.92	0.68
6:F:195:GLY:HA3	6:F:197:ARG:HD2	1.74	0.68
2:B:36:TYR:CD2	2:B:46:LEU:HD21	2.28	0.68
3:C:234:ILE:HG21	3:C:302[B]:MET:SD	2.34	0.68
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.09	0.68
3:C:18:ASN:ND2	3:C:78:VAL:HG22	2.09	0.67
6:F:34:ASN:HD22	6:F:35:PRO:HD2	1.59	0.67
2:B:295[A]:MET:HE2	2:B:377:PHE:HB2	1.76	0.67
4:D:103:TRP:CE3	4:D:189:LEU:HD13	2.31	0.66
1:A:401:LYS:HE2	2:B:438:ALA:HB1	1.77	0.66
3:C:270:ALA:O	3:C:302[B]:MET:HG3	1.95	0.66
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.26	0.66
2:B:217:LEU:HD22	10:X:506:EPA:H141	1.77	0.66
2:B:287:THR:OG1	2:B:289:PRO:HD2	1.96	0.65
2:B:385:GLN:HE22	2:B:433:GLN:NE2	1.94	0.65
4:D:416:MET:HA	4:D:419:THR:OG1	1.97	0.65
6:F:330:ILE:HG21	13:X:515:ACP:H5'2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:HIS:CD2	4:D:21:TRP:HE1	2.14	0.65
4:D:141:LEU:HD12	4:D:172:MET:SD	2.36	0.65
1:A:166:LYS:HE2	1:A:197:HIS:O	1.97	0.64
6:F:30:LEU:HD22	6:F:34:ASN:OD1	1.98	0.64
5:E:44:ASP:HB3	5:E:45:PRO:HD3	1.79	0.64
2:B:238[B]:VAL:HG22	2:B:378:ILE:CD1	2.26	0.64
3:C:244:PHE:HB2	3:C:356[B]:ASN:HD21	1.61	0.64
4:D:317:ALA:C	4:D:318:ILE:HD13	2.19	0.63
6:F:132:LEU:HD21	6:F:170:LEU:HD23	1.80	0.63
3:C:276:ILE:CD1	3:C:369:ALA:HB3	2.28	0.63
4:D:276:THR:HB	4:D:281:GLN:HG3	1.79	0.63
1:A:285:GLN:HA	1:A:285:GLN:OE1	1.99	0.63
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.33	0.63
1:A:250:VAL:HG12	1:A:254:GLU:OE1	1.97	0.63
1:A:285:GLN:HG3	1:A:372[B]:GLN:NE2	2.14	0.63
2:B:241[B]:CYS:HB2	11:X:507:COL:C14	2.29	0.62
6:F:172:PHE:O	6:F:172:PHE:CD1	2.52	0.62
6:F:202:ARG:HB3	6:F:220[B]:VAL:HG12	1.82	0.62
1:A:336:LYS:HG3	5:E:24:LEU:HD13	1.81	0.62
6:F:258:GLU:N	6:F:258:GLU:OE1	2.33	0.62
2:B:221:THR:HG22	2:B:221:THR:O	1.99	0.61
6:F:1:MET:HE3	6:F:28:LYS:HG2	1.82	0.61
6:F:349:GLY:O	6:F:353[B]:VAL:HG12	1.99	0.61
2:B:136:GLN:HA	2:B:167:ASN:O	2.00	0.61
6:F:172:PHE:O	6:F:172:PHE:HD1	1.84	0.61
1:A:79:ARG:O	1:A:84:ARG:HB2	2.01	0.60
2:B:75:MET:HE1	2:B:94:PHE:CD2	2.37	0.60
3:C:276:ILE:HD12	3:C:276:ILE:O	2.02	0.60
2:B:338:LYS:HG3	2:B:339:ASN:OD1	2.01	0.60
6:F:151:SER:HG	6:F:180:HIS:CE1	2.20	0.60
6:F:172:PHE:O	6:F:175:GLU:HB3	2.02	0.59
6:F:225:SER:H	6:F:246:GLN:HE22	1.50	0.59
3:C:276:ILE:HD13	3:C:281:ALA:HB2	1.83	0.59
4:D:11:GLN:HB3	12:X:513:GDP:O2A	2.02	0.59
1:A:357:TYR:CE2	5:E:17:GLY:HA2	2.36	0.59
4:D:294:GLN:HG2	4:D:300:ASN:ND2	2.17	0.59
2:B:141:LEU:HD12	2:B:172:MET:SD	2.42	0.59
2:B:36:TYR:HE1	2:B:38:GLY:HA3	1.68	0.58
3:C:296:PHE:HZ	3:C:351:PHE:HE2	1.50	0.58
4:D:183:GLU:N	4:D:184:PRO:HD2	2.18	0.58
2:B:36:TYR:CE2	2:B:46:LEU:CD1	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HD3	1:A:336:LYS:O	2.02	0.58
2:B:2:ARG:NH2	2:B:131:CYS:SG	2.76	0.58
6:F:135:TYR:CE1	6:F:166:ALA:HB2	2.38	0.58
6:F:219:GLY:HA3	6:F:264:PHE:CZ	2.38	0.58
2:B:46:LEU:N	2:B:46:LEU:HD12	2.19	0.58
2:B:278:ARG:HE	2:B:282:GLN:HE21	1.50	0.58
2:B:333:LEU:HD13	6:F:57:GLY:HA3	1.85	0.58
6:F:339:ALA:HB3	6:F:342:LEU:HD12	1.85	0.58
10:X:512:EPA:C13	10:X:512:EPA:C25	2.82	0.58
3:C:293[B]:ASN:OD1	3:C:335:ILE:HD11	2.04	0.58
6:F:34:ASN:HD22	6:F:35:PRO:CD	2.16	0.58
6:F:132:LEU:HD21	6:F:170:LEU:CD2	2.34	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.57
4:D:404:PHE:O	4:D:407:TRP:HB2	2.03	0.57
1:A:90:GLU:HG2	1:A:124:LYS:NZ	2.20	0.57
6:F:225:SER:O	6:F:253:TYR:HB3	2.04	0.57
3:C:271:THR:HG23	3:C:300:ASN:O	2.04	0.57
2:B:292:THR:O	2:B:295[A]:MET:HG2	2.04	0.57
4:D:162:PRO:HB2	5:E:119:MET:HE1	1.86	0.57
2:B:202:TYR:CZ	2:B:238[B]:VAL:HG11	2.40	0.57
3:C:70:LEU:HD13	3:C:110:ILE:CG2	2.35	0.57
6:F:162:ILE:HG13	6:F:236:LYS:HE3	1.87	0.56
3:C:270:ALA:HB3	3:C:302[B]:MET:HG3	1.88	0.56
3:C:315[B]:CYS:SG	3:C:377:MET:SD	3.03	0.56
6:F:96:GLU:OE2	6:F:98:TYR:OH	2.20	0.56
6:F:131:PHE:HE1	6:F:182:ILE:CG2	2.18	0.56
6:F:165:GLU:HB2	6:F:168:GLU:HB3	1.87	0.56
4:D:191:VAL:HG11	4:D:425:MET:HE3	1.88	0.56
6:F:161:LEU:HD23	6:F:169:LEU:CD2	2.32	0.56
2:B:288:VAL:HG22	2:B:323:MET:CE	2.35	0.56
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.86	0.56
2:B:295[B]:MET:SD	2:B:375:ALA:HB1	2.46	0.56
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.87	0.56
3:C:301:GLN:NE2	3:C:307:PRO:HG2	2.21	0.56
6:F:5:VAL:HG13	6:F:32:LYS:HA	1.88	0.56
6:F:330:ILE:N	6:F:330:ILE:HD13	2.21	0.56
1:A:176:GLN:HG3	6:F:56:PRO:CB	2.22	0.55
2:B:36:TYR:CE1	2:B:38:GLY:N	2.74	0.55
4:D:123:ARG:NH1	4:D:160:GLU:OE1	2.38	0.55
4:D:171:VAL:HA	4:D:204:ILE:O	2.06	0.55
6:F:131:PHE:O	6:F:135:TYR:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:343:PHE:HB2	3:C:349:THR:HG22	1.88	0.55
6:F:345:GLU:O	6:F:347:CYS:N	2.39	0.55
2:B:176:LYS:HD3	2:B:210:TYR:CD2	2.42	0.55
2:B:250:ALA:HB3	11:X:507:COL:C14	2.37	0.55
2:B:370:GLY:C	2:B:371:LEU:HD22	2.27	0.55
6:F:263:PHE:HE1	6:F:341:LYS:CD	2.18	0.55
6:F:320:MET:HB2	6:F:330:ILE:HD11	1.89	0.55
2:B:227:LEU:O	2:B:231:VAL:HG23	2.05	0.55
2:B:234:THR:O	2:B:238[A]:VAL:HG13	2.07	0.55
4:D:270:PRO:HG2	4:D:302:MET:HB2	1.89	0.55
2:B:288:VAL:CG2	2:B:323:MET:HE2	2.35	0.54
4:D:136:GLN:HA	4:D:167:ASN:O	2.06	0.54
6:F:161:LEU:HB2	6:F:172:PHE:CD2	2.41	0.54
6:F:233:PHE:O	6:F:236:LYS:HG3	2.07	0.54
6:F:191:LEU:HD12	6:F:197:ARG:O	2.06	0.54
6:F:253:TYR:HB2	6:F:256:TYR:CZ	2.43	0.54
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.08	0.54
4:D:74:THR:O	4:D:78:VAL:HG23	2.07	0.54
4:D:276:THR:H	10:X:512:EPA:C25	2.20	0.54
4:D:297:ASP:OD2	4:D:299:LYS:HG2	2.08	0.54
6:F:135:TYR:OH	6:F:164:SER:O	2.24	0.54
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.40	0.54
2:B:295[B]:MET:CG	2:B:377:PHE:HB2	2.38	0.54
2:B:298:SER:HB2	2:B:307:PRO:HD2	1.88	0.54
4:D:414:ASP:OD2	4:D:414:ASP:N	2.41	0.54
1:A:36:MET:HB3	1:A:61:HIS:NE2	2.23	0.53
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.08	0.53
1:A:221:ARG:NH2	2:B:325:MET:HE2	1.98	0.53
3:C:1:MET:HG2	3:C:2:ARG:CZ	2.37	0.53
2:B:269:MET:CE	2:B:305:CYS:HB2	2.39	0.53
6:F:131:PHE:CE1	6:F:182:ILE:CG2	2.87	0.53
3:C:209:ILE:HD11	3:C:302[A]:MET:SD	2.48	0.53
6:F:225:SER:H	6:F:246:GLN:NE2	2.06	0.53
3:C:31:GLN:HB3	3:C:32:PRO:HD2	1.90	0.53
1:A:221:ARG:NH2	2:B:325:MET:CE	2.64	0.53
6:F:224:SER:OG	6:F:238:CYS:HA	2.08	0.53
3:C:234:ILE:HG12	3:C:302[B]:MET:SD	2.49	0.53
6:F:138:ARG:C	6:F:145:ASN:HD21	2.11	0.53
1:A:97:GLU:OE1	2:B:1:MET:CE	2.57	0.53
6:F:278:THR:O	6:F:282:SER:OG	2.26	0.53
1:A:154:MET:HE2	1:A:154:MET:CA	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:NH1	2:B:278:ARG:HG3	2.25	0.52
2:B:1:MET:SD	2:B:133:GLN:HG3	2.49	0.52
6:F:160:ILE:HD12	6:F:160:ILE:N	2.24	0.52
6:F:259:GLY:O	6:F:261:GLU:HG3	2.09	0.52
1:A:209[A]:ILE:HG22	1:A:227:LEU:CD2	2.38	0.52
6:F:191:LEU:HA	6:F:197:ARG:O	2.10	0.52
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.92	0.52
6:F:161:LEU:HB2	6:F:172:PHE:CE2	2.45	0.52
2:B:286:LEU:HD11	10:X:506:EPA:S	2.50	0.51
6:F:199:PHE:O	6:F:320:MET:HE3	2.10	0.51
6:F:206:LEU:HD21	6:F:354:ALA:HB2	1.93	0.51
2:B:55:GLU:HG2	2:B:61:TYR:CE1	2.45	0.51
3:C:301:GLN:HE22	3:C:307:PRO:HG2	1.75	0.51
4:D:143:GLY:O	4:D:147[B]:SER:OG	2.28	0.51
4:D:181:VAL:HB	4:D:398:MET:HE1	1.92	0.51
6:F:173:ILE:HD13	6:F:180:HIS:CB	2.40	0.51
3:C:1:MET:HG2	3:C:2:ARG:NH2	2.26	0.51
3:C:75:ILE:HD12	3:C:94:THR:CG2	2.40	0.51
4:D:165:ILE:HG21	4:D:252:LEU:HB3	1.91	0.51
6:F:32:LYS:HD3	6:F:32:LYS:H	1.74	0.51
6:F:280:GLU:HG2	6:F:284[B]:LEU:HD12	1.93	0.51
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.94	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.93	0.51
6:F:245:ILE:HA	6:F:248:GLU:HB3	1.93	0.51
6:F:21:LEU:O	6:F:24:THR:HG23	2.10	0.51
3:C:343:PHE:CG	3:C:349:THR:HG22	2.46	0.51
4:D:319:PHE:HB2	4:D:355:VAL:HG22	1.93	0.51
2:B:220:THR:O	2:B:222:PRO:HD3	2.11	0.50
6:F:220[B]:VAL:HG23	6:F:263:PHE:CE2	2.46	0.50
3:C:9:VAL:HG22	3:C:68[B]:VAL:CG1	2.41	0.50
4:D:191:VAL:CG1	4:D:425:MET:HE3	2.41	0.50
3:C:34:GLY:HA3	3:C:60:LYS:HG3	1.92	0.50
5:E:111:ASN:N	5:E:111:ASN:HD22	2.09	0.50
2:B:250:ALA:HB1	11:X:507:COL:C12	2.41	0.50
6:F:241:THR:N	13:X:515:ACP:O3'	2.45	0.50
1:A:245:ASP:O	5:E:16:SER:HB2	2.11	0.49
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.32	0.49
2:B:171:VAL:HA	2:B:204:ILE:O	2.12	0.49
3:C:241:SER:HA	3:C:249:ASN:HD21	1.77	0.49
4:D:143:GLY:HA3	12:X:513:GDP:O3A	2.12	0.49
4:D:191:VAL:HG11	4:D:425:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:284:ARG:NH2	4:D:294:GLN:HE22	1.90	0.49
6:F:244:CYS:O	6:F:246:GLN:N	2.45	0.49
2:B:387:LEU:O	2:B:391:ILE:HD12	2.12	0.49
3:C:351:PHE:CD1	3:C:351:PHE:N	2.81	0.49
4:D:74:THR:O	4:D:75:MET:C	2.50	0.49
2:B:1:MET:HE3	2:B:253:ARG:HH11	1.78	0.49
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.95	0.49
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG23	1.94	0.49
1:A:67:PHE:HB2	1:A:92:LEU:HD23	1.95	0.49
3:C:221:ARG:HG3	4:D:325:MET:HB3	1.94	0.49
6:F:1:MET:CE	6:F:28:LYS:HG2	2.42	0.49
6:F:287:ILE:HG23	6:F:319:PHE:CZ	2.48	0.49
2:B:305:CYS:O	2:B:306:ASP:C	2.51	0.48
6:F:189:PRO:O	6:F:191:LEU:HD22	2.13	0.48
2:B:1:MET:CE	2:B:253:ARG:NH1	2.76	0.48
2:B:36:TYR:CD1	2:B:37:HIS:N	2.81	0.48
3:C:172:TYR:CE2	3:C:391:LEU:HD22	2.48	0.48
6:F:172:PHE:CD1	6:F:172:PHE:C	2.87	0.48
3:C:75:ILE:HD12	3:C:94:THR:HG22	1.94	0.48
4:D:74:THR:HA	4:D:77:SER:OG	2.13	0.48
6:F:172:PHE:HE1	6:F:176:GLN:OE1	1.95	0.48
3:C:270:ALA:C	3:C:302[B]:MET:HG3	2.34	0.48
6:F:163:SER:OG	6:F:169:LEU:HG	2.13	0.48
3:C:1:MET:CG	3:C:2:ARG:CZ	2.91	0.48
4:D:11:GLN:O	4:D:15:GLN:HG2	2.13	0.48
4:D:75:MET:HG3	4:D:92:PHE:HD2	1.78	0.48
6:F:216:TYR:CE1	6:F:374:ILE:HD13	2.49	0.48
6:F:226:GLU:HG3	6:F:237:THR:HG21	1.95	0.48
2:B:36:TYR:HE1	2:B:38:GLY:CA	2.27	0.48
6:F:40:MET:SD	6:F:52:LEU:HD21	2.53	0.48
2:B:36:TYR:HD1	2:B:37:HIS:N	2.12	0.48
6:F:3:THR:HB	6:F:30:LEU:HD12	1.94	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
6:F:90:SER:O	6:F:91:CYS:C	2.52	0.47
6:F:162:ILE:HB	6:F:233:PHE:HD2	1.78	0.47
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.95	0.47
3:C:93:ILE:HD11	3:C:121:ARG:HG3	1.96	0.47
6:F:226:GLU:HG3	6:F:237:THR:CG2	2.44	0.47
6:F:263:PHE:CE1	6:F:341:LYS:HE3	2.50	0.47
4:D:149:MET:HB3	4:D:149:MET:HE2	1.74	0.47
4:D:402:LYS:CE	4:D:415:GLU:OE2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:199:PHE:O	6:F:320:MET:CE	2.62	0.47
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.95	0.47
6:F:34:ASN:HD22	6:F:35:PRO:N	2.12	0.47
2:B:1:MET:HE1	2:B:253:ARG:HH12	1.79	0.47
2:B:322:ARG:HH11	2:B:322:ARG:HB2	1.80	0.47
6:F:126:ASP:OD1	6:F:127:GLU:N	2.47	0.47
1:A:51[B]:THR:HG22	1:A:52:PHE:CD1	2.49	0.47
6:F:32:LYS:H	6:F:32:LYS:CD	2.27	0.47
6:F:148:ILE:HG12	6:F:149:ALA:N	2.29	0.47
6:F:333:ASN:HB3	14:S:40:HOH:O	2.15	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.47
3:C:190:THR:O	3:C:194[B]:THR:HG23	2.15	0.47
5:E:138:GLU:O	5:E:139:LEU:HD23	2.15	0.47
6:F:138:ARG:HB2	6:F:145:ASN:OD1	2.14	0.47
2:B:306:ASP:HB3	2:B:309:HIS:CE1	2.50	0.46
2:B:7:ILE:O	2:B:137:LEU:HA	2.16	0.46
3:C:276:ILE:HD13	3:C:369:ALA:HB3	1.97	0.46
5:E:9:ILE:HG12	5:E:21:GLU:HB3	1.97	0.46
1:A:132:LEU:O	1:A:164:LYS:NZ	2.32	0.46
2:B:42:LEU:HD22	2:B:245:PRO:HD2	1.97	0.46
3:C:204:VAL:HG22	3:C:302[B]:MET:HE1	1.91	0.46
4:D:141:LEU:HA	4:D:147[B]:SER:HB3	1.97	0.46
6:F:258:GLU:H	6:F:258:GLU:CD	2.17	0.46
1:A:56:THR:HG22	1:A:57:GLY:N	2.30	0.46
2:B:163:ASP:O	2:B:253:ARG:NH2	2.46	0.46
4:D:269:MET:HG3	4:D:303:ALA:HB3	1.97	0.46
1:A:438:ASP:O	1:A:439:SER:C	2.54	0.46
2:B:302:MET:HE3	2:B:302:MET:HB3	1.86	0.46
4:D:288:VAL:HB	4:D:289:PRO:HD3	1.97	0.46
6:F:100:ILE:HD13	6:F:126:ASP:OD1	2.15	0.46
2:B:275:LEU:HA	10:X:506:EPA:O4	2.15	0.46
4:D:20:PHE:CZ	4:D:24:ILE:HD13	2.51	0.46
3:C:343:PHE:CB	3:C:349:THR:HG22	2.46	0.46
6:F:237:THR:HG21	6:F:251:LYS:HD3	1.98	0.46
6:F:148:ILE:HG13	6:F:160:ILE:HG23	1.97	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.51	0.46
1:A:156:ARG:HD2	1:A:156:ARG:HA	1.78	0.45
2:B:272:PHE:O	2:B:300:ASN:OD1	2.35	0.45
4:D:404:PHE:O	4:D:405:LEU:C	2.54	0.45
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.99	0.45
4:D:172:MET:HA	4:D:173:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.97	0.45
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.16	0.45
4:D:68:VAL:HG12	4:D:149:MET:HE1	1.99	0.45
5:E:81:GLU:O	5:E:84[B]:GLN:HG2	2.16	0.45
6:F:13:VAL:HG21	6:F:336:PRO:O	2.16	0.45
6:F:34:ASN:HD22	6:F:34:ASN:C	2.20	0.45
2:B:269:MET:HE3	2:B:305:CYS:HB2	1.98	0.45
3:C:69:ASP:O	3:C:94:THR:HA	2.17	0.45
6:F:148:ILE:CG1	6:F:149:ALA:N	2.80	0.45
6:F:284[A]:LEU:HD12	6:F:284[A]:LEU:HA	1.76	0.45
3:C:213:CYS:O	3:C:217:LEU:HB2	2.17	0.45
4:D:69:ASP:O	4:D:94:PHE:HA	2.17	0.45
6:F:103:THR:HG23	6:F:174:ASP:OD2	2.17	0.45
4:D:172:MET:HG3	4:D:387:LEU:HD21	1.99	0.45
6:F:148:ILE:HG22	6:F:183:GLN:O	2.15	0.45
6:F:2:TYR:CE1	6:F:359:PHE:HB3	2.52	0.44
4:D:1:MET:HG3	4:D:50:ASN:HB2	1.96	0.44
4:D:123:ARG:NH1	4:D:160:GLU:OE2	2.50	0.44
2:B:2:ARG:HG2	2:B:50[B]:ASN:OD1	2.16	0.44
4:D:312:TYR:CE1	4:D:377:PHE:HZ	2.35	0.44
4:D:288:VAL:HG12	4:D:331:GLN:HG3	1.98	0.44
6:F:184:LYS:HD2	6:F:184:LYS:C	2.37	0.44
1:A:137:VAL:HG21	1:A:154:MET:CE	2.47	0.44
1:A:308:ARG:HH21	6:F:301:ALA:C	2.21	0.44
4:D:294:GLN:CG	4:D:300:ASN:ND2	2.80	0.44
1:A:115:ILE:O	1:A:119:LEU:HD22	2.17	0.44
3:C:406:HIS:CG	4:D:263:PRO:HD3	2.52	0.44
6:F:159:GLY:C	6:F:160:ILE:HD12	2.37	0.44
6:F:338:CYS:SG	6:F:339:ALA:N	2.90	0.44
3:C:147:SER:HB2	3:C:190:THR:HB	1.99	0.44
6:F:131:PHE:C	6:F:131:PHE:CD2	2.91	0.44
1:A:154:MET:CE	1:A:157:LEU:HD12	2.48	0.44
1:A:415:GLU:O	1:A:418:PHE:HB2	2.17	0.44
2:B:36:TYR:CZ	2:B:46:LEU:CD1	2.99	0.44
3:C:306:ASP:OD1	3:C:308:ARG:HG3	2.18	0.43
6:F:100:ILE:HD13	6:F:100:ILE:HA	1.83	0.43
6:F:101:TYR:HD1	6:F:179:VAL:HG22	1.82	0.43
1:A:430:LYS:HD3	1:A:434:GLU:OE1	2.18	0.43
5:E:75:LYS:HE3	5:E:75:LYS:HB3	1.42	0.43
1:A:115:ILE:HG13	1:A:119:LEU:CD2	2.48	0.43
2:B:295[B]:MET:HG2	2:B:377:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:26:GLN:HB2	6:F:361:LEU:HD12	2.00	0.43
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.18	0.43
6:F:298[B]:ILE:HG12	6:F:298[B]:ILE:O	2.17	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.01	0.43
2:B:40:SER:OG	2:B:42:LEU:HB2	2.19	0.43
2:B:141:LEU:CD1	2:B:172:MET:CE	2.97	0.43
4:D:397:ALA:O	4:D:401:ARG:NH1	2.51	0.43
1:A:336:LYS:HG3	5:E:24:LEU:CD1	2.48	0.43
2:B:75:MET:HE2	2:B:75:MET:HB2	1.81	0.43
2:B:385:GLN:HE22	2:B:433:GLN:HE22	1.65	0.43
3:C:298:PRO:HA	3:C:301:GLN:NE2	2.33	0.43
4:D:294:GLN:CG	4:D:300:ASN:HD22	2.32	0.43
6:F:280:GLU:HA	6:F:284[B]:LEU:HB2	1.99	0.43
6:F:325:LEU:HD23	6:F:325:LEU:HA	1.67	0.43
2:B:31:ASP:OD1	2:B:35:SER:O	2.36	0.43
2:B:1:MET:HE1	2:B:253:ARG:NH1	2.34	0.43
4:D:103:TRP:HD1	4:D:147[A]:SER:OG	2.02	0.43
6:F:226:GLU:CG	6:F:237:THR:HG23	2.49	0.43
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.54	0.43
2:B:141:LEU:HD12	2:B:172:MET:CE	2.49	0.43
6:F:247:LYS:HZ1	6:F:259:GLY:HA2	1.84	0.43
3:C:230:LEU:O	3:C:234:ILE:HD12	2.19	0.42
3:C:209:ILE:HD11	3:C:302[A]:MET:HG3	2.02	0.42
4:D:38:GLY:HA3	4:D:45:GLN:OE1	2.19	0.42
6:F:279:LEU:HG	6:F:284[B]:LEU:HG	2.00	0.42
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.42
4:D:20:PHE:CD1	4:D:235:MET:HE2	2.54	0.42
6:F:263:PHE:CE1	6:F:341:LYS:HD3	2.36	0.42
2:B:1:MET:HE3	2:B:253:ARG:NH1	2.34	0.42
4:D:7:ILE:O	4:D:137:LEU:HA	2.19	0.42
6:F:184:LYS:HD2	6:F:185:TYR:H	1.79	0.42
1:A:63:PRO:CD	1:A:86:LEU:HG	2.50	0.42
5:E:47:LEU:HD23	5:E:47:LEU:O	2.20	0.42
6:F:239:HIS:O	6:F:240:LEU:C	2.58	0.42
2:B:48:ARG:HH21	2:B:245:PRO:HA	1.84	0.42
2:B:229:HIS:ND1	10:X:506:EPA:C6	2.83	0.42
4:D:71:GLU:HG2	4:D:98:GLY:HA2	2.00	0.42
6:F:376:ILE:HG22	6:F:378:LEU:CD1	2.50	0.42
4:D:218:LYS:O	4:D:219:LEU:HD23	2.20	0.42
6:F:5:VAL:HG12	6:F:7:ARG:HG3	2.02	0.42
6:F:304:THR:HG22	6:F:307:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:279:LEU:O	6:F:284[B]:LEU:HG	2.20	0.42
6:F:340:GLN:CD	6:F:340:GLN:H	2.23	0.42
2:B:287:THR:HG22	2:B:290:GLU:OE1	2.20	0.42
3:C:276:ILE:HD11	3:C:371:VAL:CG1	2.49	0.42
4:D:123:ARG:NH1	4:D:160:GLU:CD	2.73	0.42
4:D:282:GLN:HG3	4:D:283:TYR:CG	2.55	0.42
1:A:7:ILE:HA	1:A:66[B]:VAL:HG23	2.02	0.42
2:B:13:GLY:CA	2:B:138[B]:THR:HG22	2.35	0.42
2:B:270:PRO:HG2	2:B:302:MET:HB2	2.02	0.42
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.60	0.42
6:F:101:TYR:CD1	6:F:179:VAL:HG22	2.54	0.42
2:B:112:ALA:O	2:B:115:VAL:HG12	2.20	0.41
1:A:56:THR:CG2	1:A:57:GLY:N	2.83	0.41
1:A:177:VAL:HG12	1:A:178:SER:N	2.35	0.41
1:A:357:TYR:CD2	5:E:17:GLY:HA2	2.55	0.41
4:D:109:THR:O	4:D:113:GLU:HG3	2.20	0.41
4:D:110:GLU:O	4:D:113:GLU:HB2	2.20	0.41
6:F:195:GLY:C	6:F:197:ARG:HG3	2.40	0.41
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.41
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.35	0.41
3:C:302[B]:MET:HE3	3:C:302[B]:MET:HB3	1.94	0.41
5:E:58:GLU:HA	5:E:61:ARG:NH2	2.35	0.41
6:F:298[B]:ILE:HG12	6:F:302:ILE:HG23	2.02	0.41
1:A:51[B]:THR:HG22	1:A:52:PHE:HD1	1.86	0.41
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.79	0.41
1:A:285:GLN:OE1	1:A:285:GLN:CA	2.68	0.41
2:B:12:CYS:HB2	12:X:508:GDP:C8	2.56	0.41
6:F:305:LYS:HD3	6:F:305:LYS:HA	1.72	0.41
6:F:330:ILE:HG21	13:X:515:ACP:C5'	2.47	0.41
2:B:36:TYR:CE1	2:B:38:GLY:CA	3.03	0.41
4:D:108:TYR:O	5:E:134:ARG:HD3	2.20	0.41
4:D:173:PRO:HG2	4:D:187:ALA:HB2	2.02	0.41
4:D:150:GLY:O	4:D:154:ILE:HG13	2.21	0.41
6:F:155:ALA:O	6:F:156:LYS:C	2.59	0.41
6:F:263:PHE:CD1	6:F:341:LYS:HE3	2.55	0.41
3:C:249:ASN:CG	3:C:356[A]:ASN:ND2	2.74	0.41
6:F:88:SER:C	6:F:90:SER:N	2.74	0.41
6:F:231:ALA:O	6:F:233:PHE:HD1	2.04	0.40
2:B:36:TYR:HD1	2:B:37:HIS:H	1.68	0.40
2:B:67:LEU:N	2:B:67:LEU:HD12	2.35	0.40
3:C:36:MET:HB3	3:C:61:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:GLY:O	4:D:75:MET:N	2.53	0.40
4:D:118:VAL:HG11	4:D:153:LEU:HD21	2.02	0.40
6:F:321:VAL:HG22	6:F:322:ASP:N	2.35	0.40
3:C:188:ILE:HG13	3:C:425:MET:HG3	2.03	0.40
6:F:34:ASN:ND2	6:F:36:ARG:H	2.20	0.40
6:F:2:TYR:CZ	6:F:359:PHE:HB3	2.56	0.40
6:F:241:THR:HG23	13:X:515:ACP:O3'	2.21	0.40
6:F:242:ASN:ND2	6:F:245:ILE:HB	2.36	0.40
3:C:270:ALA:HB3	3:C:302[B]:MET:CG	2.50	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLU:OE1	3:C:283:HIS:NE2[4_555]	1.57	0.63
2:B:411:GLU:OE1	3:C:282:TYR:OH[4_555]	2.08	0.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/439 (102%)	432 (96%)	16 (4%)	1 (0%)	47	78
2	B	441/428 (103%)	429 (97%)	12 (3%)	0	100	100
3	C	456/440 (104%)	448 (98%)	8 (2%)	0	100	100
4	D	435/431 (101%)	419 (96%)	16 (4%)	0	100	100
5	E	124/123 (101%)	121 (98%)	3 (2%)	0	100	100
6	F	353/351 (101%)	322 (91%)	29 (8%)	2 (1%)	25	56
All	All	2258/2212 (102%)	2171 (96%)	84 (4%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	248	GLU
6	F	346	LEU
1	A	177	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/370 (103%)	378 (99%)	3 (1%)	81	94
2	B	385/370 (104%)	369 (96%)	16 (4%)	30	63
3	C	389/371 (105%)	384 (99%)	5 (1%)	69	91
4	D	378/372 (102%)	371 (98%)	7 (2%)	57	85
5	E	115/110 (104%)	107 (93%)	8 (7%)	15	40
6	F	319/313 (102%)	292 (92%)	27 (8%)	10	31
All	All	1967/1906 (103%)	1901 (97%)	66 (3%)	39	71

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	251	ASP
1	A	438	ASP
2	B	36	TYR
2	B	130	ASP
2	B	139	HIS
2	B	196[A]	GLU
2	B	196[B]	GLU
2	B	276	THR
2	B	278	ARG
2	B	282	GLN
2	B	299	LYS
2	B	302	MET
2	B	372	LYS
2	B	416	MET
2	B	423[A]	SER

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Mol	Chain	Res	Type
2	B	423[B]	SER
2	B	431[A]	GLU
2	B	431[B]	GLU
3	C	71	GLU
3	C	163	LYS
3	C	181	VAL
3	C	221	ARG
3	C	347	CYS
4	D	75	MET
4	D	128	SER
4	D	139	HIS
4	D	298	SER
4	D	325	MET
4	D	369	ARG
4	D	414	ASP
5	E	6	MET
5	E	13	LYS
5	E	75	LYS
5	E	77	GLU
5	E	88	GLU
5	E	108[A]	ASN
5	E	108[B]	ASN
5	E	111	ASN
6	F	1	MET
6	F	19	ARG
6	F	34	ASN
6	F	66	ARG
6	F	76[A]	SER
6	F	76[B]	SER
6	F	87	LEU
6	F	90	SER
6	F	91	CYS
6	F	156	LYS
6	F	168	GLU
6	F	172	PHE
6	F	197	ARG
6	F	230	SER
6	F	232	ASN
6	F	241	THR
6	F	242	ASN
6	F	244	CYS
6	F	246	GLN

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Mol	Chain	Res	Type
6	F	247	LYS
6	F	249	TYR
6	F	251	LYS
6	F	255	ARG
6	F	258	GLU
6	F	284[A]	LEU
6	F	284[B]	LEU
6	F	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	283	HIS
1	A	329	ASN
1	A	342	GLN
2	B	192	HIS
2	B	282	GLN
2	B	300	ASN
2	B	334	ASN
2	B	424	ASN
2	B	433	GLN
3	C	18	ASN
3	C	256	GLN
3	C	301	GLN
4	D	50	ASN
4	D	59	ASN
4	D	294	GLN
4	D	300	ASN
5	E	92	ASN
5	E	111	ASN
5	E	124	GLN
6	F	34	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic and 3 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	GDP	X	508	8	24,30,30	0.88	0	30,47,47	1.18	4 (13%)
7	GTP	X	510	8	26,34,34	1.04	3 (11%)	32,54,54	0.70	1 (3%)
7	GTP	X	501	8	26,34,34	1.07	2 (7%)	32,54,54	1.34	6 (18%)
13	ACP	X	515	-	27,33,33	0.89	1 (3%)	32,52,52	0.85	1 (3%)
12	GDP	X	513	8	24,30,30	1.04	1 (4%)	30,47,47	1.04	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	GDP	X	508	8	-	3/12/32/32	0/3/3/3
7	GTP	X	510	8	-	6/18/38/38	0/3/3/3
7	GTP	X	501	8	-	6/18/38/38	0/3/3/3
13	ACP	X	515	-	-	7/15/38/38	0/3/3/3
12	GDP	X	513	8	-	8/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	501	GTP	C5-C6	-3.19	1.40	1.47
12	X	513	GDP	C6-N1	-3.12	1.33	1.37
7	X	510	GTP	C5-C6	-2.76	1.41	1.47
13	X	515	ACP	PB-O2B	-2.37	1.50	1.56
7	X	510	GTP	C8-N7	-2.17	1.31	1.35
7	X	501	GTP	C2-N3	2.05	1.38	1.33
7	X	510	GTP	C5-C4	-2.00	1.38	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	501	GTP	C8-N7-C5	3.18	109.05	102.99
7	X	501	GTP	C5-C6-N1	2.90	119.07	113.95
12	X	508	GDP	C8-N7-C5	2.65	108.05	102.99
7	X	501	GTP	C2-N1-C6	-2.33	120.80	125.10
7	X	501	GTP	PB-O3B-PG	-2.31	124.89	132.83
13	X	515	ACP	C5-C6-N6	2.28	123.81	120.35
12	X	508	GDP	O6-C6-C5	-2.27	119.94	124.37
12	X	508	GDP	C5-C6-N1	2.23	117.89	113.95
12	X	508	GDP	O3B-PB-O3A	2.22	112.08	104.64
7	X	501	GTP	PA-O3A-PB	-2.20	125.26	132.83
12	X	513	GDP	C8-N7-C5	2.17	107.12	102.99
7	X	501	GTP	O2G-PG-O3B	2.07	111.59	104.64
7	X	510	GTP	O6-C6-C5	2.05	128.38	124.37
12	X	513	GDP	C5-C6-N1	2.02	117.52	113.95

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	501	GTP	PB-O3B-PG-O2G
7	X	501	GTP	C5'-O5'-PA-O1A
7	X	501	GTP	C5'-O5'-PA-O2A
7	X	510	GTP	C5'-O5'-PA-O1A
12	X	508	GDP	C5'-O5'-PA-O1A
12	X	508	GDP	C5'-O5'-PA-O2A
12	X	513	GDP	C5'-O5'-PA-O1A
12	X	513	GDP	C3'-C4'-C5'-O5'
13	X	515	ACP	PG-C3B-PB-O1B
13	X	515	ACP	PG-C3B-PB-O2B
13	X	515	ACP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
12	X	513	GDP	O4'-C4'-C5'-O5'
13	X	515	ACP	O4'-C4'-C5'-O5'
12	X	513	GDP	PA-O3A-PB-O1B
13	X	515	ACP	C4'-C5'-O5'-PA
12	X	513	GDP	C5'-O5'-PA-O3A
7	X	510	GTP	C5'-O5'-PA-O2A
12	X	513	GDP	C5'-O5'-PA-O2A
13	X	515	ACP	PG-C3B-PB-O3A
7	X	501	GTP	PB-O3B-PG-O3G
7	X	510	GTP	PB-O3B-PG-O2G
12	X	513	GDP	PA-O3A-PB-O2B
12	X	513	GDP	PA-O3A-PB-O3B
7	X	501	GTP	C5'-O5'-PA-O3A
7	X	510	GTP	C5'-O5'-PA-O3A
12	X	508	GDP	C5'-O5'-PA-O3A
7	X	501	GTP	PB-O3A-PA-O2A
7	X	510	GTP	PB-O3A-PA-O1A
7	X	510	GTP	PB-O3A-PA-O2A
13	X	515	ACP	C5'-O5'-PA-O1A

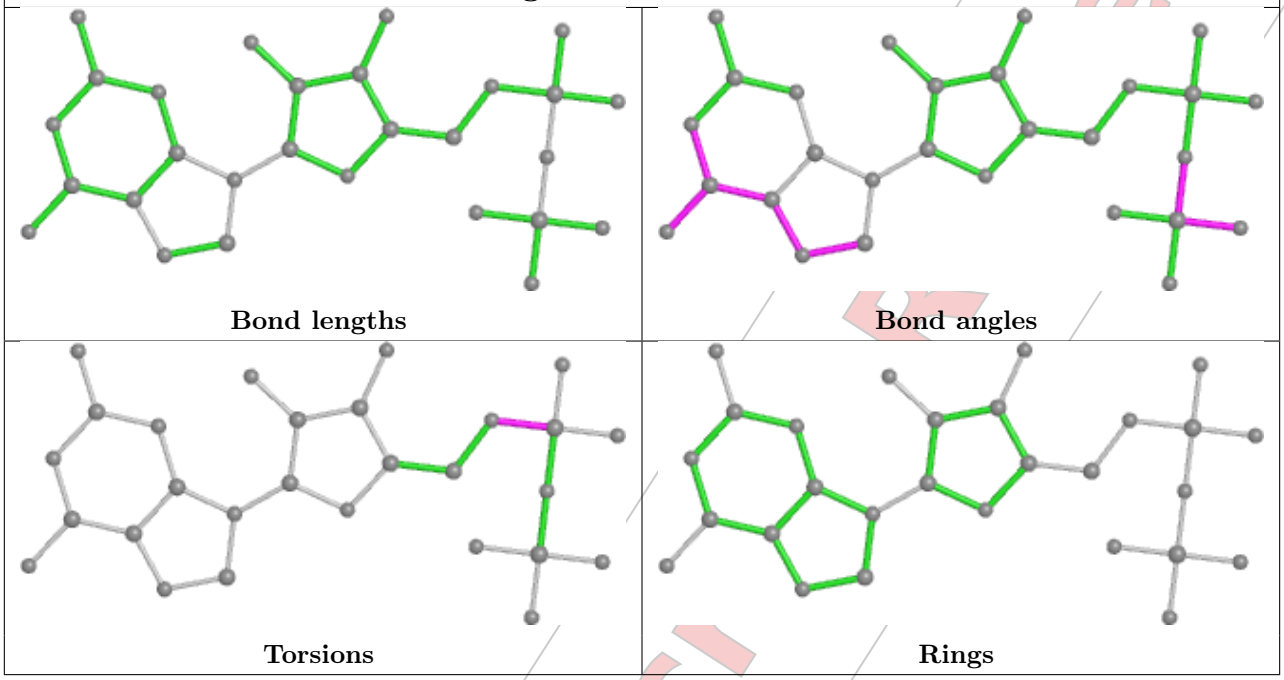
There are no ring outliers.

3 monomers are involved in 7 short contacts:

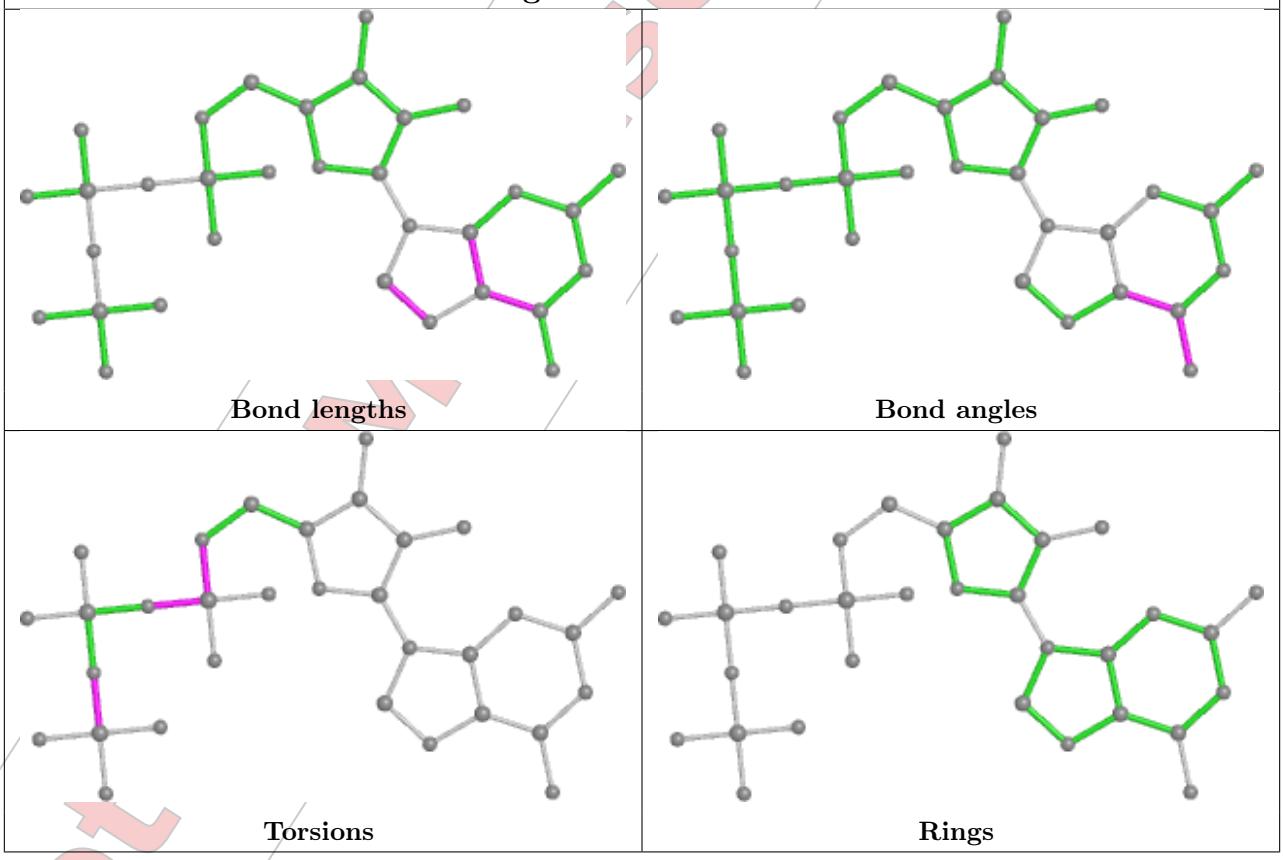
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	X	508	GDP	1	0
13	X	515	ACP	4	0
12	X	513	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

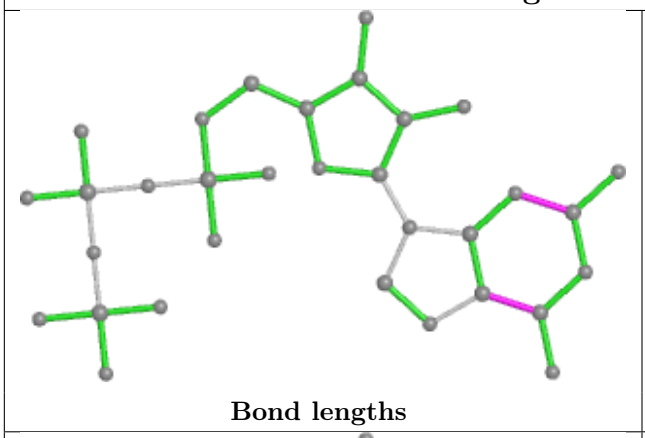
Ligand GDP X 508



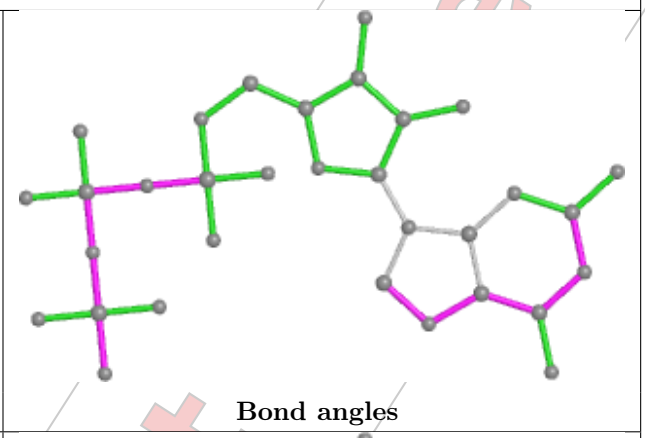
Ligand GTP X 510



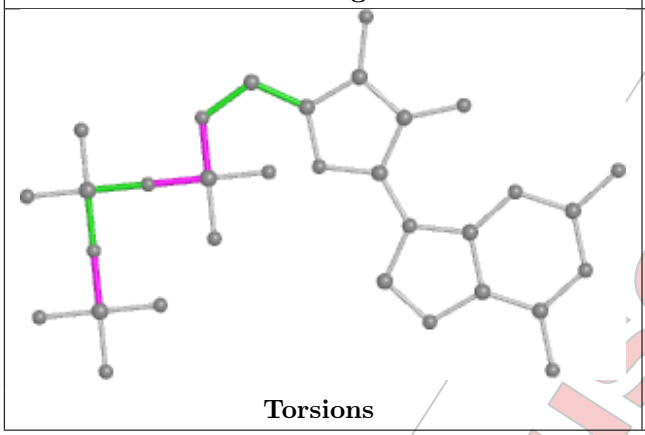
Ligand GTP X 501



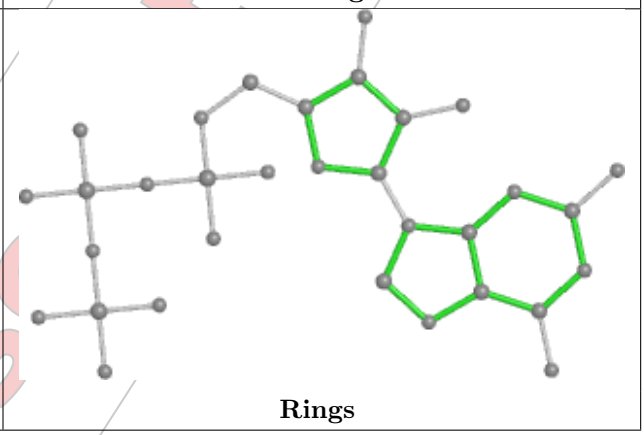
Bond lengths



Bond angles

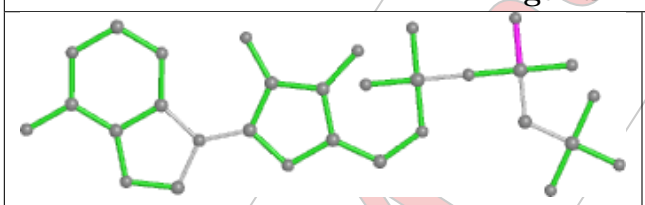


Torsions

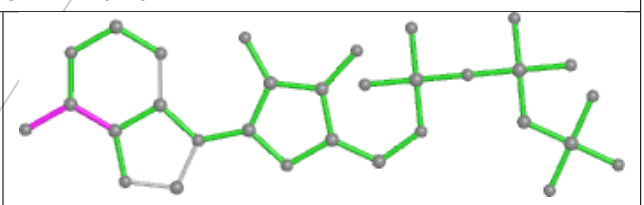


Rings

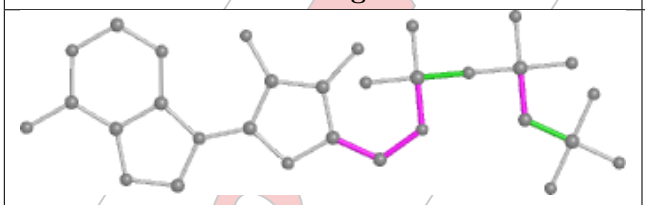
Ligand ACP X 515



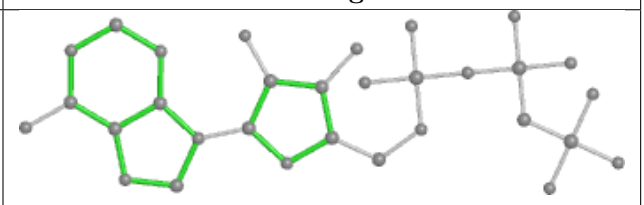
Bond lengths



Bond angles

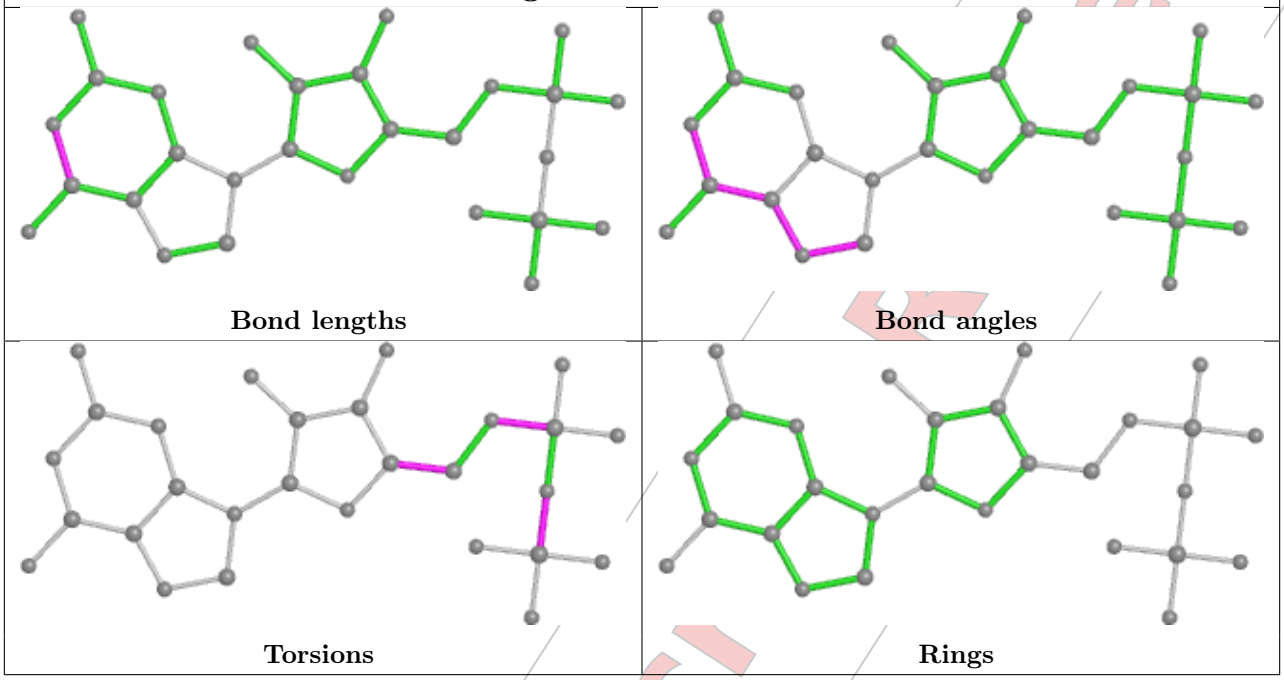


Torsions



Rings

Ligand GDP X 513



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	2
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	34.14
1	F	362:ALA	C	371:PRO	N	14.08
1	F	105:LEU	C	125:THR	N	12.54

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	439/439 (100%)	0.13	18 (4%) 37 27	35, 55, 98, 179	0
2	B	428/428 (100%)	0.33	33 (7%) 13 7	30, 53, 105, 163	4 (0%)
3	C	440/440 (100%)	-0.07	12 (2%) 54 44	26, 44, 79, 115	0
4	D	431/431 (100%)	0.29	32 (7%) 14 8	38, 64, 108, 170	3 (0%)
5	E	123/123 (100%)	0.68	17 (13%) 2 1	43, 72, 124, 184	0
6	F	351/351 (100%)	1.37	106 (30%) 0 0	48, 88, 184, 219	0
All	All	2212/2212 (100%)	0.39	218 (9%) 7 4	26, 59, 128, 219	7 (0%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	371	PRO	12.2
6	F	253	TYR	11.3
5	E	142	GLU	9.0
6	F	137	ARG	8.8
4	D	441	ASP	8.5
6	F	157	GLY	8.3
6	F	372	THR	7.9
6	F	252	ASN	7.8
6	F	254	GLY	7.7
6	F	232	ASN	7.4
6	F	167	SER	7.1
1	A	439	SER	7.0
2	B	279	GLY	6.3
6	F	155	ALA	6.0
6	F	136	ASN	6.0
6	F	125	THR	6.0
6	F	141	GLY	5.9
6	F	255	ARG	5.8
5	E	143	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	5.6
6	F	158	GLU	5.6
6	F	154	GLY	5.6
6	F	171	ASP	5.6
6	F	233	PHE	5.5
6	F	175	GLU	5.5
5	E	141	GLU	5.5
6	F	248	GLU	5.4
6	F	142	ARG	5.4
6	F	138	ARG	5.4
6	F	156	LYS	5.3
2	B	59	ASN	5.3
6	F	251	LYS	5.3
6	F	249	TYR	5.2
2	B	305	CYS	5.2
6	F	139	ARG	5.1
6	F	244	CYS	5.1
6	F	243	HIS	5.0
6	F	250	SER	5.0
6	F	165	GLU	4.8
6	F	178	GLN	4.7
6	F	258	GLU	4.7
4	D	416	MET	4.6
6	F	103	THR	4.5
6	F	259	GLY	4.5
4	D	57	THR	4.5
6	F	238	CYS	4.5
6	F	90	SER	4.4
6	F	126	ASP	4.4
4	D	283	TYR	4.4
6	F	234	GLN	4.3
3	C	337	THR	4.2
6	F	241	THR	4.2
1	A	282	TYR	4.2
6	F	91	CYS	4.2
2	B	58	GLY	4.2
6	F	104	ASN	4.1
2	B	280	SER	4.1
6	F	134	ALA	4.1
6	F	143	GLU	4.0
6	F	194	PRO	4.0
6	F	242	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
6	F	46	ARG	3.9
6	F	237	THR	3.9
2	B	438	ALA	3.9
4	D	80	SER	3.9
6	F	240	LEU	3.9
6	F	83	THR	3.9
2	B	278	ARG	3.8
2	B	80	SER	3.8
6	F	153	ALA	3.8
1	A	337	THR	3.8
2	B	281	GLN	3.8
4	D	179	ASP	3.7
6	F	235	ASP	3.7
6	F	245	ILE	3.7
2	B	321	GLY	3.7
6	F	105	LEU	3.7
6	F	11	SER	3.6
6	F	195	GLY	3.6
6	F	229	ASN	3.6
6	F	225	SER	3.5
4	D	220	THR	3.5
6	F	84	SER	3.5
2	B	1	MET	3.4
6	F	170	LEU	3.4
2	B	57	THR	3.4
6	F	159	GLY	3.4
6	F	246	GLN	3.4
2	B	369	ARG	3.4
2	B	246	GLY	3.3
2	B	370	GLY	3.3
5	E	27	PRO	3.3
2	B	82	PRO	3.3
6	F	129	GLU	3.2
6	F	76[A]	SER	3.2
4	D	76	ASP	3.2
6	F	176	GLN	3.2
4	D	37	HIS	3.2
6	F	89	GLU	3.2
2	B	215	ARG	3.1
6	F	25	GLY	3.1
6	F	168	GLU	3.1
6	F	132	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	221[A]	THR	3.1
2	B	39	ASP	3.0
6	F	236	LYS	3.0
4	D	406	HIS	3.0
6	F	256	TYR	3.0
2	B	338	LYS	3.0
5	E	44	ASP	3.0
2	B	56	ALA	3.0
1	A	335	ILE	2.9
6	F	174	ASP	2.9
1	A	131	GLY	2.9
3	C	440	VAL	2.9
2	B	129	CYS	2.9
6	F	10	ASN	2.9
1	A	80[A]	THR	2.9
6	F	271[A]	LEU	2.9
3	C	1	MET	2.9
3	C	334	THR	2.9
4	D	96	GLN	2.9
4	D	127	GLU	2.9
6	F	152	SER	2.8
4	D	89	PRO	2.8
6	F	177	GLY	2.8
4	D	82	PRO	2.8
6	F	73	ARG	2.8
6	F	180	HIS	2.8
3	C	247	ALA	2.7
6	F	373	SER	2.7
4	D	281	GLN	2.7
2	B	40	SER	2.7
1	A	44	GLY	2.7
5	E	131	GLU	2.7
6	F	257	GLU	2.7
4	D	38	GLY	2.7
6	F	21	LEU	2.7
1	A	279	GLU	2.7
2	B	247	GLN	2.7
6	F	140	GLU	2.7
5	E	6	MET	2.7
6	F	224	SER	2.6
4	D	337	ASN	2.6
1	A	163	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	128	LYS	2.6
2	B	334	ASN	2.6
5	E	48	GLU	2.6
6	F	239	HIS	2.6
5	E	140	LYS	2.6
3	C	249	ASN	2.6
4	D	397	ALA	2.6
3	C	349	THR	2.6
1	A	281	ALA	2.6
6	F	135	TYR	2.5
6	F	226	GLU	2.5
4	D	282	GLN	2.5
6	F	23	ALA	2.5
2	B	437	ASP	2.5
1	A	338	LYS	2.5
6	F	323	GLU	2.4
2	B	81	GLY	2.4
6	F	231	ALA	2.4
1	A	283	HIS	2.4
4	D	39	ASP	2.4
6	F	247	LYS	2.4
6	F	169	LEU	2.4
6	F	357	SER	2.4
2	B	37	HIS	2.4
5	E	9	ILE	2.4
6	F	217	ARG	2.4
6	F	329	LEU	2.4
4	D	33	THR	2.4
4	D	58	GLY	2.4
2	B	127	GLU	2.4
6	F	342	LEU	2.4
5	E	103	GLN	2.3
3	C	78	VAL	2.3
6	F	151	SER	2.3
1	A	326	LYS	2.3
4	D	293	GLN	2.3
6	F	197	ARG	2.3
6	F	127	GLU	2.3
6	F	362	ALA	2.3
2	B	35	SER	2.3
5	E	28	SER	2.3
5	E	106	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.3
6	F	31	ARG	2.3
3	C	246	GLY	2.3
3	C	120[A]	ASP	2.2
6	F	306	HIS	2.2
6	F	131	PHE	2.2
1	A	41	THR	2.2
6	F	45	ASN	2.2
4	D	74	THR	2.2
5	E	139	LEU	2.2
6	F	230	SER	2.2
4	D	78	VAL	2.2
5	E	122	ARG	2.2
4	D	430	SER	2.2
4	D	401	ARG	2.2
1	A	42	ILE	2.1
2	B	416	MET	2.1
2	B	282	GLN	2.1
6	F	19	ARG	2.1
1	A	61	HIS	2.1
2	B	130	ASP	2.1
6	F	145	ASN	2.1
4	D	70	LEU	2.0
5	E	138	GLU	2.0
3	C	245	ASP	2.0
4	D	41	ASP	2.0
6	F	352	ASP	2.0
3	C	81	GLY	2.0
2	B	120	ASP	2.0
4	D	396	THR	2.0
4	D	1	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

LIGAND-RSR INFOmissingINFO

6.5 Other polymers

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2023 – 08:52 pm GMT

Deposition ID : D_1292128624

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

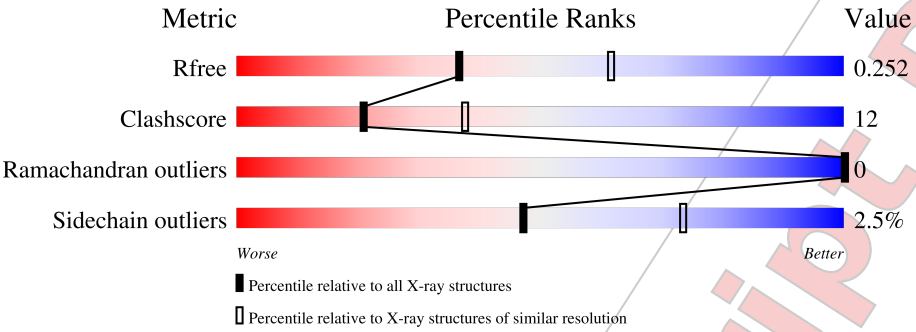
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	439	74% 25% .
2	B	429	79% 20%
3	C	440	83% 16%
4	D	430	76% 23% .
5	E	123	80% 18% .
6	F	332	64% 34% .

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 18174 atoms, of which 252 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3441	2175	585	658	23	0	2	0

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	429	3386	2125	579	655	27	2	3	0

- Molecule 3 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	440	3464	2190	590	661	23	0	4	0

- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	430	3376	2117	577	656	26	2	1	0

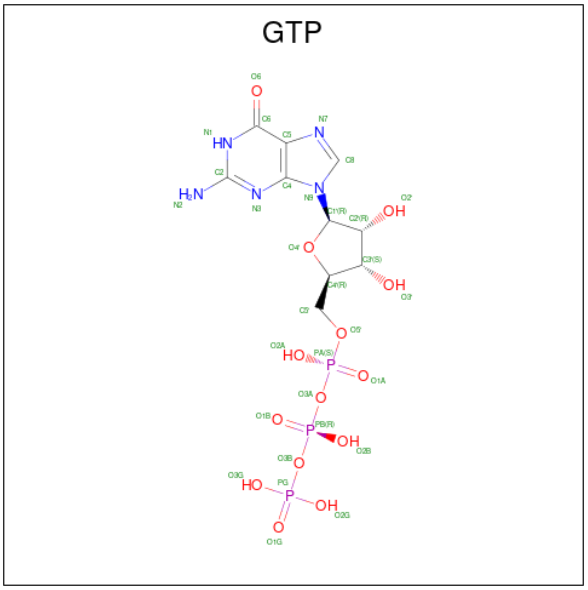
- Molecule 5 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	123	1020	628	184	202	6	0	1	0

- Molecule 6 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	332	2714	1740	464	495	15	0	1	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	X	1	Total C N O P 32 10 5 14 3	0	0
7	X	1	Total C N O P 32 10 5 14 3	0	0

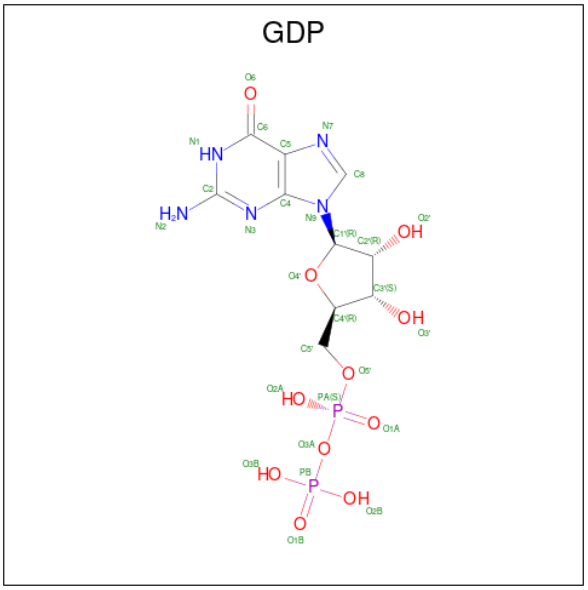
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	X	1	Total Mg 1 1	0	0
8	X	1	Total Mg 1 1	0	0
8	X	1	Total Mg 1 1	0	0
8	X	1	Total Mg 1 1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

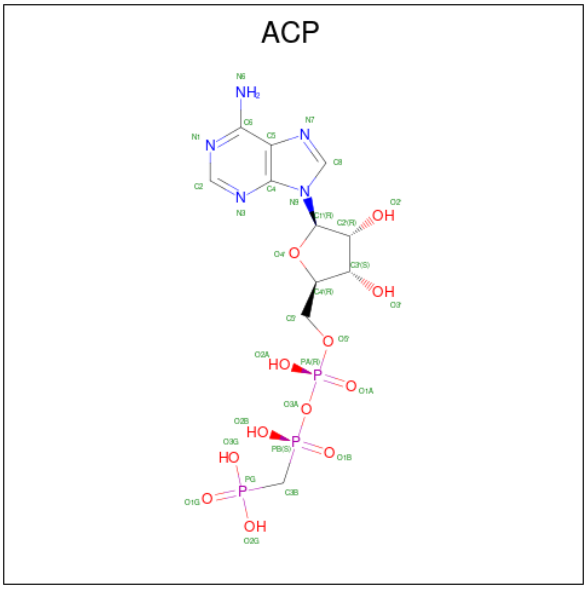
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	X	1	Total Ca 1 1	0	0
9	X	1	Total Ca 1 1	0	0

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	X	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
10	X	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	X	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

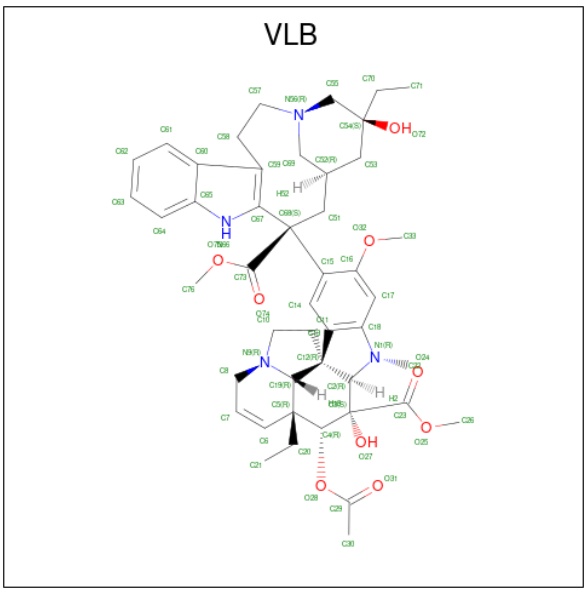
- Molecule 12 is a ligand with the chemical component id COL but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for COL. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	X	1	Total	C	H	N	O	0	0
			54	22	25	1	6		

- Molecule 13 is a ligand with the chemical component id EPA but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for EPA. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	X	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		
13	X	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		

- Molecule 14 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula: $C_{46}H_{58}N_4O_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	X	1	Total	C	H	N	O	0	0
			117	46	58	4	9		

- Molecule 15 is a ligand with the chemical component id POU but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for POU. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	X	1	Total	C	H	O	0	0
			86	27	48	11		

- Molecule 16 is a ligand with the chemical component id ANS but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for ANS. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	X	1	Total	C	Cl	H	N	O	0	0
			87	32	1	43	2	9		

- Molecule 17 is water.

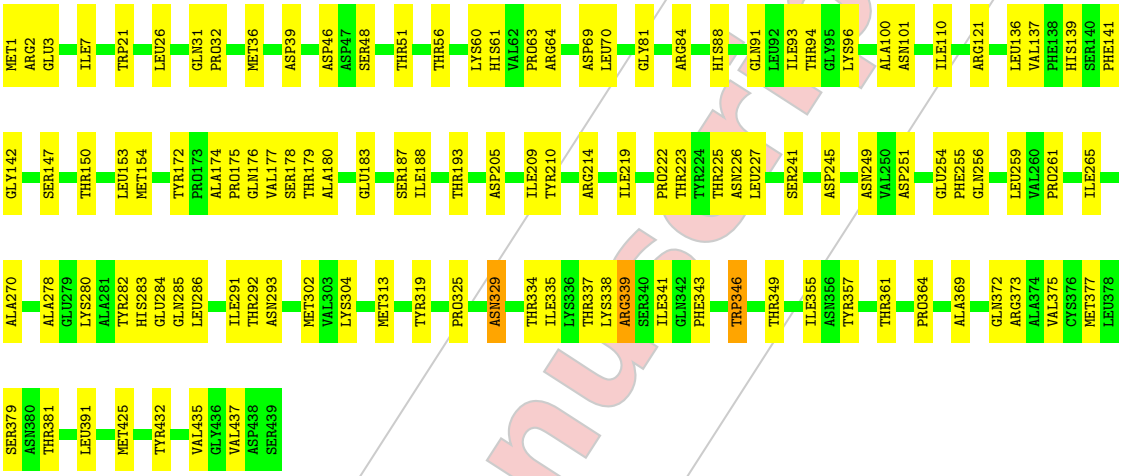
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	S	126	Total	O	0	0
			126	126		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

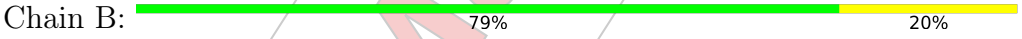
• Molecule 1: Tubulin alpha-1B chain

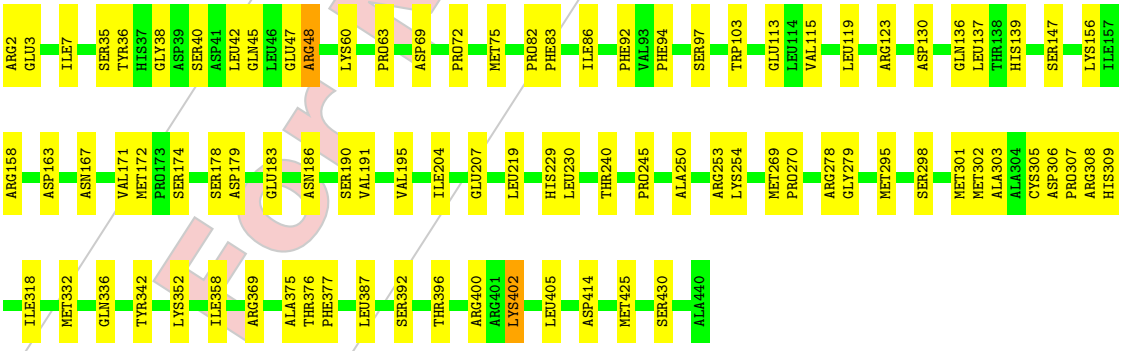
Chain A:



• Molecule 2: Tubulin beta-2B chain

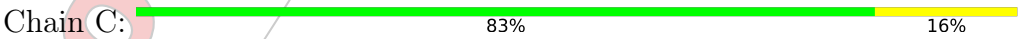
Chain B:



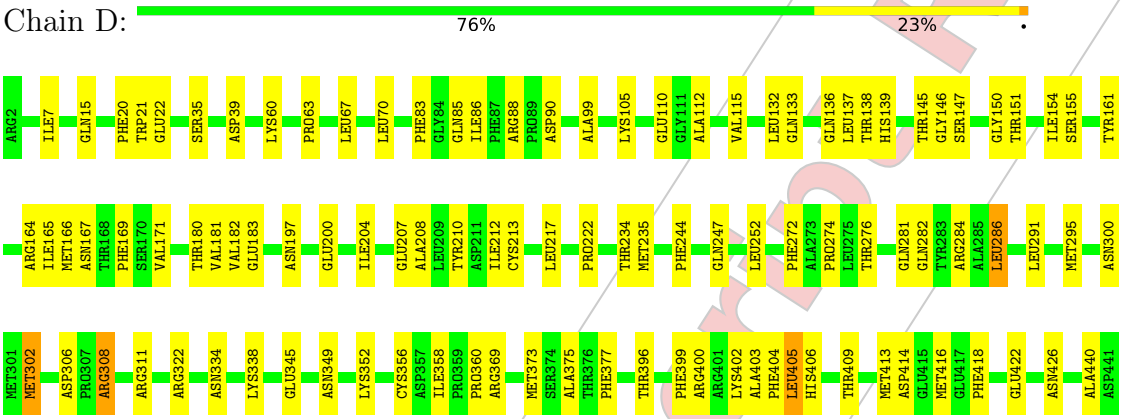


• Molecule 3: Tubulin alpha-1B chain

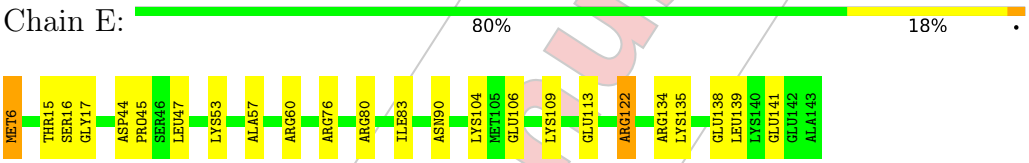
Chain C:



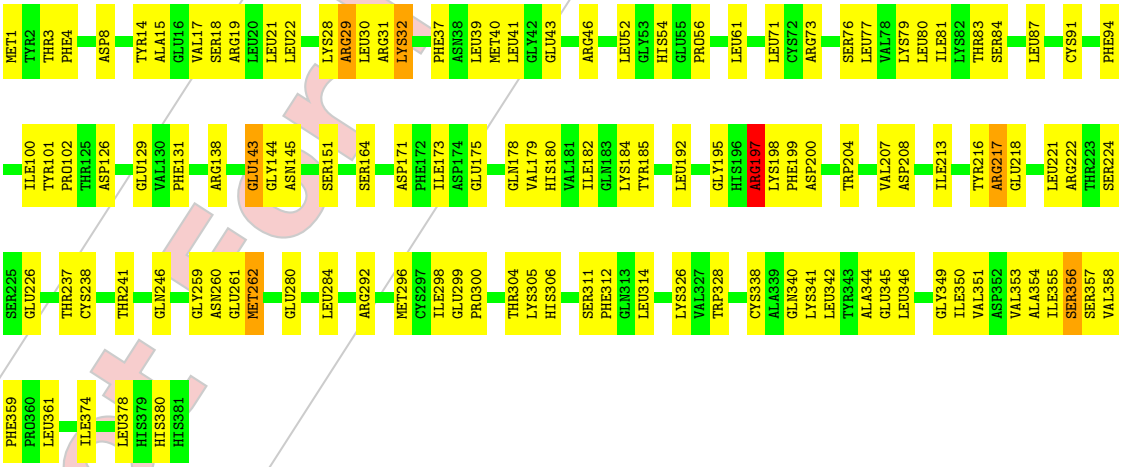
• Molecule 4: Tubulin beta-2B chain



• Molecule 5: Stathmin-4



• Molecule 6: Tubulin-Tyrosine Ligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.00Å 160.34Å 181.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.29 – 2.50 15.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.29-2.50) 74.4 (15.29-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.04 (at 1.90Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.185 , 0.239 0.199 , 0.252	Depositor DCC
R_{free} test set	1990 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	-7.5	Xtriage
Anisotropy	-0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.64	EDS
Total number of atoms	18174	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, ANS, COL, CA, EPA, VLB, GTP, MG, POU, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/3517	0.52	0/4772
2	B	0.33	0/3463	0.54	0/4690
3	C	0.33	0/3550	0.54	0/4817
4	D	0.31	0/3449	0.52	0/4671
5	E	0.28	0/1028	0.46	0/1364
6	F	0.31	0/2777	0.50	0/3750
All	All	0.31	0/17784	0.52	0/24064

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
5	E	0	1
6	F	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	311	ARG	Sidechain
5	E	122	ARG	Sidechain
6	F	197	ARG	Sidechain
6	F	29	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	F	31	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3441	0	3340	101	0
2	B	3386	0	3254	77	1
3	C	3464	0	3364	60	1
4	D	3376	0	3241	86	0
5	E	1020	0	1033	21	0
6	F	2714	0	2682	94	0
7	X	64	0	24	0	0
8	X	4	0	0	0	0
9	X	2	0	0	0	0
10	X	56	0	24	0	0
11	X	31	0	14	0	0
12	X	29	25	0	3	0
13	X	68	78	32	7	0
14	X	59	58	58	5	0
15	X	38	48	15	2	0
16	X	44	43	2	3	0
17	S	126	0	0	9	0
All	All	17922	252	17083	424	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (424) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:SER:OG	2:B:42:LEU:HD13	1.56	1.05
6:F:304:THR:HG21	6:F:311:SER:HB2	1.40	1.03
6:F:100:ILE:HG13	6:F:182:ILE:HD12	1.41	1.01
2:B:396:THR:O	2:B:400:ARG:HG3	1.58	1.01
6:F:14:TYR:HA	6:F:17:VAL:HG12	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:HE21	1:A:372:GLN:HG2	1.35	0.91
2:B:230:LEU:HD23	13:X:508:EPA:H81	1.50	0.91
4:D:137:LEU:HD23	4:D:139:HIS:CD2	2.06	0.90
2:B:40:SER:HG	2:B:42:LEU:HD13	1.36	0.88
2:B:75:MET:HG3	2:B:94:PHE:CD2	2.08	0.87
2:B:115:VAL:O	2:B:119:LEU:HD23	1.75	0.86
4:D:137:LEU:CD2	4:D:139:HIS:CD2	2.59	0.86
4:D:137:LEU:CD2	4:D:139:HIS:HD2	1.88	0.84
2:B:83:PHE:O	2:B:86:ILE:HG22	1.78	0.84
6:F:192:LEU:HD11	6:F:262:MET:HE1	1.59	0.83
5:E:104:LYS:HE2	17:S:197:HOH:O	1.78	0.83
3:C:293:ASN:ND2	3:C:339:ARG:HH12	1.78	0.81
2:B:240:THR:HB	2:B:318:ILE:CD1	2.11	0.80
1:A:285:GLN:NE2	1:A:372:GLN:HG2	1.96	0.80
4:D:137:LEU:HD23	4:D:139:HIS:HD2	1.48	0.77
3:C:271:THR:HG23	3:C:300:ASN:O	1.86	0.75
4:D:83:PHE:O	4:D:86:ILE:HG22	1.86	0.75
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.67	0.74
4:D:358:ILE:O	4:D:358:ILE:HD12	1.88	0.72
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.70	0.72
4:D:208:ALA:O	4:D:212:ILE:HG12	1.88	0.72
6:F:131:PHE:CE2	6:F:182:ILE:HG21	2.25	0.72
1:A:372:GLN:HA	1:A:372:GLN:NE2	2.05	0.71
6:F:340:GLN:CD	6:F:340:GLN:H	1.93	0.71
6:F:39:LEU:HD23	6:F:40:MET:N	2.06	0.71
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.73	0.71
6:F:280:GLU:HA	6:F:284:LEU:HB2	1.73	0.71
6:F:171:ASP:O	6:F:175:GLU:HG2	1.89	0.71
2:B:392:SER:O	2:B:396:THR:HG23	1.90	0.70
4:D:406:HIS:HA	4:D:409:THR:CG2	2.21	0.70
6:F:39:LEU:HD21	6:F:41:LEU:HD23	1.73	0.70
4:D:406:HIS:HA	4:D:409:THR:HG22	1.72	0.70
2:B:219:LEU:HD21	13:X:508:EPA:H21	1.74	0.70
4:D:35:SER:OG	4:D:60:LYS:HE3	1.92	0.70
6:F:226:GLU:HB2	6:F:238:CYS:HB3	1.73	0.69
1:A:339:ARG:HB3	1:A:341:ILE:CD1	2.22	0.69
2:B:240:THR:HB	2:B:318:ILE:HD11	1.74	0.69
2:B:352:LYS:HG3	12:X:507:COL:C4	2.23	0.69
4:D:402:LYS:CA	4:D:405:LEU:HD11	2.23	0.68
2:B:308:ARG:HG2	15:X:510:POU:H47	1.74	0.68
4:D:136:GLN:HA	4:D:167:ASN:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:143:GLU:HG3	6:F:144:GLY:N	2.07	0.68
4:D:180:THR:O	4:D:183:GLU:HG3	1.94	0.68
3:C:209:ILE:HD11	3:C:302:MET:SD	2.34	0.68
1:A:223:THR:HG22	1:A:226:ASN:OD1	1.94	0.67
6:F:304:THR:CG2	6:F:311:SER:HB2	2.21	0.66
3:C:177:VAL:HG12	3:C:177:VAL:O	1.95	0.66
6:F:138:ARG:HB2	6:F:145:ASN:HD21	1.61	0.65
1:A:339:ARG:HB3	1:A:341:ILE:HD12	1.78	0.65
2:B:156:LYS:HE2	5:E:76:ARG:NE	2.10	0.65
6:F:195:GLY:HA3	6:F:197:ARG:HD3	1.79	0.65
6:F:341:LYS:HD2	6:F:341:LYS:O	1.96	0.65
2:B:179:ASP:HB3	3:C:352:LYS:HG3	1.79	0.64
1:A:334:THR:O	1:A:337:THR:HG22	1.96	0.64
2:B:136:GLN:HA	2:B:167:ASN:O	1.97	0.64
14:X:509:VLB:H511	14:X:509:VLB:H763	1.79	0.64
3:C:4[B]:CYS:SG	3:C:136:LEU:HG	2.37	0.64
2:B:158:ARG:HD3	17:S:105:HOH:O	1.97	0.63
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.33	0.63
1:A:251:ASP:OD1	1:A:254:GLU:HG3	1.97	0.63
4:D:244:PHE:CD2	4:D:358:ILE:HD11	2.34	0.63
4:D:402:LYS:HB3	4:D:405:LEU:HD11	1.81	0.63
6:F:178:GLN:HA	6:F:178:GLN:OE1	1.98	0.63
1:A:372:GLN:HA	1:A:372:GLN:HE21	1.63	0.62
6:F:138:ARG:HD2	6:F:145:ASN:OD1	1.99	0.62
6:F:151:SER:HB2	6:F:179:VAL:O	2.00	0.62
4:D:295:MET:HG3	4:D:377:PHE:HB2	1.80	0.62
1:A:223:THR:HG23	1:A:225:THR:N	2.14	0.62
2:B:298:SER:HB2	2:B:307:PRO:HD2	1.81	0.61
1:A:223:THR:HG23	1:A:225:THR:H	1.64	0.61
6:F:1:MET:CE	6:F:28:LYS:HB2	2.30	0.61
4:D:334:ASN:OD1	4:D:338:LYS:HE2	2.00	0.61
6:F:87:LEU:O	6:F:91:CYS:HB2	1.99	0.61
6:F:14:TYR:CA	6:F:17:VAL:HG12	2.27	0.61
6:F:192:LEU:HD11	6:F:262:MET:CE	2.29	0.61
2:B:369:ARG:HG3	2:B:369:ARG:HH11	1.66	0.60
1:A:335:ILE:O	1:A:339:ARG:HB2	2.01	0.60
2:B:69:ASP:O	2:B:94:PHE:HA	2.02	0.60
1:A:261:PRO:HD2	17:S:194:HOH:O	2.02	0.60
5:E:44:ASP:HB3	5:E:45:PRO:HD2	1.84	0.59
4:D:286:LEU:HD12	4:D:286:LEU:O	2.01	0.59
6:F:101:TYR:HD2	6:F:126:ASP:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:405:LEU:HD12	4:D:405:LEU:H	1.66	0.59
3:C:320:ARG:HA	3:C:356:ASN:O	2.03	0.59
3:C:177:VAL:HG11	3:C:224:TYR:CE1	2.38	0.59
4:D:402:LYS:HB3	4:D:405:LEU:CD1	2.33	0.59
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.84	0.58
2:B:40:SER:OG	2:B:42:LEU:CD1	2.42	0.58
4:D:132:LEU:O	4:D:164:ARG:NH1	2.36	0.58
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.85	0.58
4:D:63:PRO:HD3	4:D:86:ILE:HG12	1.86	0.58
2:B:191:VAL:O	2:B:195:VAL:HG13	2.04	0.58
3:C:1:MET:HG2	3:C:2:ARG:H	1.68	0.58
6:F:345:GLU:CG	6:F:374:ILE:HG21	2.33	0.58
1:A:293:ASN:OD1	1:A:339:ARG:NH1	2.37	0.58
6:F:217:ARG:HG3	6:F:218:GLU:HG2	1.84	0.58
1:A:174:ALA:HB3	1:A:177:VAL:HG23	1.86	0.57
3:C:229[B]:ARG:HD3	3:C:363:VAL:HG21	1.86	0.57
3:C:248:LEU:HD12	3:C:357:TYR:OH	2.04	0.57
4:D:154:ILE:HG23	4:D:166:MET:HG2	1.85	0.57
2:B:295:MET:SD	2:B:375:ALA:HB1	2.44	0.57
3:C:48:SER:HB3	3:C:243:ARG:O	2.04	0.57
6:F:14:TYR:HA	6:F:17:VAL:CG1	2.30	0.57
1:A:209:ILE:HD11	1:A:302:MET:SD	2.45	0.57
6:F:131:PHE:HE2	6:F:182:ILE:HG21	1.67	0.57
1:A:1:MET:HA	1:A:1:MET:CE	2.34	0.57
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.87	0.56
1:A:175:PRO:HA	1:A:179:THR:HG22	1.87	0.56
3:C:27:GLU:HG2	3:C:361:THR:CG2	2.35	0.56
3:C:224:TYR:HE2	4:D:247[A]:GLN:HE22	1.52	0.56
3:C:244:PHE:CZ	3:C:358:GLN:HG2	2.40	0.56
4:D:171:VAL:HA	4:D:204:ILE:O	2.06	0.56
4:D:244:PHE:CE2	4:D:358:ILE:HD11	2.40	0.56
1:A:26:LEU:HD21	1:A:364:PRO:HD3	1.86	0.56
6:F:184:LYS:HD2	6:F:185:TYR:N	2.20	0.56
6:F:19:ARG:HD3	6:F:19:ARG:N	2.20	0.56
4:D:137:LEU:HD21	4:D:139:HIS:CD2	2.40	0.55
1:A:255:PHE:O	1:A:259:LEU:HB2	2.06	0.55
2:B:278:ARG:HG3	2:B:279:GLY:HA3	1.89	0.55
3:C:93:ILE:HD11	3:C:121:ARG:HG3	1.88	0.55
6:F:296[A]:MET:SD	6:F:380:HIS:ND1	2.80	0.55
1:A:214:ARG:HG2	1:A:219:ILE:O	2.07	0.55
3:C:70:LEU:HD13	3:C:110:ILE:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:CD1	1:A:375:VAL:HG22	2.42	0.55
3:C:167:LEU:HD22	3:C:200:CYS:HB3	1.88	0.55
6:F:14:TYR:HD1	6:F:17:VAL:HG11	1.72	0.55
4:D:402:LYS:CB	4:D:405:LEU:HD11	2.37	0.55
6:F:200:ASP:OD1	6:F:222:ARG:HB2	2.07	0.55
5:E:6:MET:O	5:E:6:MET:HG3	2.06	0.55
6:F:358:VAL:HG23	6:F:359:PHE:CD2	2.41	0.55
1:A:48:SER:O	1:A:51:THR:HG23	2.06	0.55
6:F:39:LEU:CD2	6:F:41:LEU:HD23	2.37	0.54
6:F:39:LEU:HD21	6:F:41:LEU:CD2	2.37	0.54
1:A:177:VAL:O	1:A:177:VAL:HG22	2.08	0.54
2:B:171:VAL:HA	2:B:204:ILE:O	2.08	0.54
2:B:240:THR:CB	2:B:318:ILE:HD11	2.37	0.54
6:F:259:GLY:O	6:F:261:GLU:HG3	2.08	0.54
4:D:70:LEU:HG	4:D:145:THR:HG23	1.89	0.54
6:F:213:ILE:HG22	6:F:378:LEU:HD12	1.88	0.54
1:A:26:LEU:HD21	1:A:364:PRO:CD	2.38	0.53
1:A:338:LYS:O	1:A:338:LYS:HG2	2.09	0.53
1:A:56:THR:HG21	1:A:60:LYS:HB3	1.91	0.53
2:B:48:ARG:HH21	2:B:245:PRO:HA	1.72	0.53
6:F:292:ARG:O	6:F:296[B]:MET:HB2	2.08	0.53
1:A:293:ASN:HD21	1:A:339:ARG:HH12	1.55	0.53
3:C:209:ILE:HG22	3:C:227:LEU:HD22	1.91	0.53
4:D:405:LEU:O	4:D:409:THR:HG22	2.07	0.53
14:X:509:VLB:H262	14:X:509:VLB:N1	2.24	0.53
6:F:102:PRO:HB3	6:F:173:ILE:O	2.09	0.53
1:A:377:MET:HE3	1:A:379:SER:HB3	1.90	0.53
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.24	0.53
3:C:7:ILE:HG21	3:C:153:LEU:HD21	1.91	0.53
3:C:27:GLU:HG2	3:C:361:THR:HG22	1.91	0.53
3:C:417:GLU:HB3	17:S:35:HOH:O	2.08	0.53
1:A:56:THR:CG2	1:A:60:LYS:HB3	2.39	0.53
3:C:293:ASN:HD21	3:C:339:ARG:HH12	1.53	0.52
4:D:67:LEU:N	4:D:67:LEU:HD12	2.24	0.52
3:C:251:ASP:OD1	3:C:252:LEU:N	2.42	0.52
4:D:276:THR:OG1	4:D:281:GLN:HG2	2.09	0.52
1:A:180:ALA:O	1:A:183:GLU:HG3	2.10	0.52
2:B:369:ARG:HG3	2:B:369:ARG:NH1	2.21	0.52
3:C:71:GLU:HG2	3:C:98:ASP:HB3	1.92	0.52
4:D:360:PRO:C	4:D:369:ARG:HA	2.30	0.52
5:E:109:LYS:HE2	5:E:113:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.44	0.52
2:B:219:LEU:HD21	13:X:508:EPA:C2	2.39	0.52
2:B:318:ILE:HG23	2:B:376:THR:HB	1.90	0.52
6:F:73:ARG:HB2	6:F:76:SER:OG	2.09	0.52
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.45	0.51
4:D:295:MET:CG	4:D:377:PHE:HB2	2.39	0.51
4:D:396:THR:O	4:D:400:ARG:HB2	2.10	0.51
6:F:213:ILE:CG2	6:F:378:LEU:HD12	2.40	0.51
3:C:244:PHE:CE1	3:C:358:GLN:HG2	2.45	0.51
4:D:403:ALA:O	4:D:404:PHE:HB2	2.09	0.51
4:D:404:PHE:HE2	16:X:517:ANS:C3	2.24	0.51
2:B:156:LYS:HE2	5:E:76:ARG:CZ	2.40	0.51
6:F:129:GLU:OE1	6:F:129:GLU:HA	2.10	0.51
1:A:101:ASN:ND2	2:B:254:LYS:HE2	2.25	0.51
3:C:271:THR:HG22	3:C:272:TYR:N	2.25	0.51
4:D:402:LYS:HA	4:D:405:LEU:HD11	1.93	0.51
6:F:222:ARG:O	6:F:241:THR:HB	2.10	0.51
3:C:177:VAL:CG1	3:C:224:TYR:CE1	2.94	0.51
6:F:346:LEU:O	6:F:350:ILE:HG13	2.11	0.50
2:B:82:PRO:O	2:B:83:PHE:HB2	2.11	0.50
14:X:509:VLB:C73	14:X:509:VLB:O32	2.59	0.50
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.93	0.50
4:D:213:CYS:HA	4:D:217:LEU:HB2	1.93	0.50
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.94	0.50
6:F:3:THR:OG1	6:F:37:PHE:HA	2.11	0.50
4:D:165:ILE:HG21	4:D:252:LEU:HB3	1.93	0.50
1:A:282:TYR:O	1:A:283:HIS:HB2	2.11	0.50
3:C:60:LYS:HB2	3:C:60:LYS:NZ	2.25	0.50
4:D:360:PRO:C	4:D:369:ARG:CA	2.80	0.50
1:A:56:THR:CG2	1:A:60:LYS:H	2.23	0.50
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.50
1:A:136:LEU:HD12	1:A:136:LEU:N	2.27	0.50
1:A:175:PRO:HA	1:A:179:THR:CG2	2.42	0.49
3:C:271:THR:HG22	3:C:272:TYR:H	1.76	0.49
4:D:7:ILE:O	4:D:137:LEU:HA	2.11	0.49
2:B:97:SER:O	3:C:2:ARG:NH2	2.46	0.49
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.95	0.49
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.48	0.49
2:B:42:LEU:C	2:B:45:GLN:N	2.66	0.49
5:E:80:ARG:HA	5:E:83:ILE:HG22	1.94	0.49
4:D:181:VAL:HG22	16:X:517:ANS:O2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:4:PHE:O	6:F:29:ARG:HA	2.13	0.49
6:F:18:SER:HA	6:F:21:LEU:HD12	1.94	0.49
6:F:71:LEU:HD22	6:F:298:ILE:HD13	1.94	0.49
14:X:509:VLB:H763	14:X:509:VLB:C51	2.42	0.49
2:B:229:HIS:CE1	13:X:508:EPA:C9	2.96	0.49
4:D:306:ASP:OD1	4:D:308:ARG:HB2	2.13	0.49
6:F:344:ALA:O	6:F:346:LEU:N	2.42	0.49
1:A:154:MET:HE2	1:A:154:MET:HA	1.94	0.48
2:B:270:PRO:O	2:B:302:MET:HB2	2.13	0.48
2:B:332:MET:O	2:B:336:GLN:HG3	2.13	0.48
3:C:177:VAL:O	3:C:177:VAL:CG1	2.61	0.48
4:D:21:TRP:CZ3	4:D:63:PRO:HB3	2.48	0.48
6:F:61:LEU:HD22	6:F:358:VAL:HG21	1.95	0.48
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.95	0.48
1:A:338:LYS:O	1:A:339:ARG:HD2	2.13	0.48
2:B:305[B]:CYS:O	2:B:307:PRO:HD3	2.13	0.48
1:A:245:ASP:O	5:E:16:SER:HB2	2.13	0.48
6:F:198:LYS:HG2	6:F:199:PHE:H	1.79	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.28	0.48
4:D:112:ALA:HB1	5:E:134:ARG:HH21	1.77	0.48
6:F:350:ILE:O	6:F:354:ALA:HB3	2.14	0.48
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.43	0.48
1:A:286:LEU:N	1:A:286:LEU:HD22	2.27	0.48
1:A:36:MET:HG2	1:A:61:HIS:CE1	2.48	0.48
3:C:325:PRO:HB3	14:X:509:VLB:C65	2.43	0.48
6:F:79:LYS:O	6:F:83:THR:OG1	2.22	0.48
1:A:56:THR:HG22	1:A:60:LYS:O	2.14	0.48
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.48
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.79	0.48
3:C:298:PRO:HD2	17:S:136:HOH:O	2.13	0.48
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.14	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
1:A:291:ILE:CD1	1:A:375:VAL:HG23	2.42	0.47
2:B:269:MET:HE3	2:B:301:MET:HG3	1.95	0.47
2:B:278:ARG:HG3	2:B:279:GLY:CA	2.44	0.47
3:C:298:PRO:O	3:C:301:GLN:HG2	2.14	0.47
4:D:356:CYS:SG	4:D:358:ILE:CD1	3.02	0.47
2:B:42:LEU:HD22	2:B:358:ILE:HD11	1.96	0.47
1:A:319:TYR:CE1	1:A:375:VAL:HG22	2.50	0.47
4:D:146:GLY:O	4:D:150:GLY:HA3	2.15	0.47
4:D:402:LYS:C	4:D:405:LEU:HD11	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.97	0.47
6:F:246:GLN:HG2	6:F:260:ASN:OD1	2.14	0.47
4:D:86:ILE:HG12	4:D:86:ILE:O	2.14	0.47
6:F:17:VAL:HG23	6:F:351:VAL:HG13	1.95	0.47
2:B:119:LEU:HB3	2:B:123:ARG:NH1	2.29	0.47
6:F:351:VAL:O	6:F:356:SER:HB2	2.15	0.46
1:A:81:GLY:O	1:A:84:ARG:HD3	2.15	0.46
6:F:32:LYS:HB2	6:F:32:LYS:HE3	1.72	0.46
1:A:357:TYR:CE2	5:E:17:GLY:HA2	2.50	0.46
4:D:70:LEU:H	4:D:145:THR:HG21	1.81	0.46
6:F:19:ARG:N	6:F:19:ARG:CD	2.79	0.46
2:B:35:SER:OG	2:B:60:LYS:HE2	2.15	0.46
2:B:178:SER:OG	2:B:183:GLU:OE2	2.21	0.46
4:D:105:LYS:HB3	4:D:110:GLU:HG3	1.98	0.46
1:A:284:GLU:CD	1:A:284:GLU:H	2.20	0.46
1:A:286:LEU:O	1:A:373:ARG:NH1	2.47	0.46
2:B:72:PRO:O	2:B:75:MET:HB2	2.16	0.46
2:B:352:LYS:HG3	12:X:507:COL:C5	2.46	0.46
6:F:15:ALA:O	6:F:19:ARG:HD3	2.16	0.46
6:F:19:ARG:HA	6:F:22:LEU:HD12	1.97	0.46
4:D:413:MET:HE2	4:D:418:PHE:CE1	2.52	0.45
6:F:28:LYS:HD3	6:F:30:LEU:HD21	1.96	0.45
6:F:216:TYR:OH	6:F:342:LEU:HD22	2.17	0.45
5:E:57:ALA:HA	5:E:60:ARG:NH1	2.32	0.45
5:E:134:ARG:NH1	5:E:134:ARG:HG3	2.31	0.45
5:E:135:LYS:O	5:E:139:LEU:HG	2.16	0.45
6:F:262:MET:HB3	6:F:262:MET:HE3	1.64	0.45
4:D:234:THR:OG1	4:D:302:MET:CE	2.64	0.45
4:D:413:MET:CE	4:D:418:PHE:CE1	2.99	0.45
1:A:137:VAL:HG21	1:A:154:MET:CE	2.46	0.45
1:A:304:LYS:HB3	6:F:54:HIS:HE1	1.80	0.45
4:D:70:LEU:HD12	4:D:99:ALA:HB2	1.98	0.45
4:D:182:VAL:HG11	16:X:517:ANS:O6	2.17	0.45
6:F:351:VAL:HG12	6:F:355:ILE:HD12	1.99	0.45
2:B:42:LEU:O	2:B:45:GLN:N	2.50	0.45
4:D:274:PRO:HB2	13:X:516:EPA:C24	2.46	0.45
6:F:204:TRP:CZ2	6:F:338:CYS:HA	2.51	0.45
2:B:250:ALA:HB1	12:X:507:COL:C12	2.46	0.45
4:D:88:ARG:HD2	4:D:90:ASP:OD1	2.17	0.45
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.98	0.45
6:F:173:ILE:HD13	6:F:180:HIS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:CD2	1:A:364:PRO:HD3	2.47	0.45
6:F:40:MET:CE	6:F:52:LEU:HD11	2.47	0.45
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.47	0.45
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.47	0.45
2:B:278:ARG:HA	2:B:279:GLY:HA2	1.64	0.45
2:B:400:ARG:HD2	17:S:148:HOH:O	2.17	0.45
4:D:413:MET:HE2	4:D:418:PHE:HE1	1.82	0.45
2:B:303:ALA:O	2:B:305[A]:CYS:N	2.47	0.44
2:B:342:TYR:CE2	15:X:510:POU:H45	2.52	0.44
4:D:167:ASN:HD22	4:D:200:GLU:HB2	1.82	0.44
3:C:141:PHE:HB3	3:C:187:SER:OG	2.17	0.44
1:A:355:ILE:O	5:E:17:GLY:HA3	2.18	0.44
1:A:337:THR:HG23	1:A:338:LYS:N	2.33	0.44
3:C:250:VAL:HG23	3:C:255:PHE:CE2	2.53	0.44
4:D:345:GLU:HG2	4:D:440:ALA:HB2	1.99	0.44
1:A:176[B]:GLN:HB2	1:A:177:VAL:HG21	1.99	0.44
3:C:344:VAL:HG21	3:C:346:TRP:CE2	2.53	0.44
4:D:147:SER:O	4:D:151:THR:HG23	2.18	0.44
4:D:276:THR:OG1	13:X:516:EPA:C24	2.66	0.44
4:D:234:THR:OG1	4:D:302:MET:HE2	2.18	0.44
4:D:244:PHE:CE2	4:D:358:ILE:CD1	3.01	0.44
6:F:200:ASP:OD1	6:F:222:ARG:HD2	2.17	0.44
1:A:292:THR:HG22	1:A:335:ILE:HG13	2.00	0.43
3:C:224:TYR:HE2	4:D:247[A]:GLN:NE2	2.16	0.43
4:D:138:THR:HG22	4:D:169:PHE:HB2	1.99	0.43
2:B:119:LEU:HB3	2:B:123:ARG:HH12	1.83	0.43
3:C:1:MET:CG	3:C:131:GLY:HA3	2.48	0.43
3:C:85:GLN:HB2	17:S:182:HOH:O	2.18	0.43
6:F:39:LEU:CD2	6:F:41:LEU:CD2	2.96	0.43
6:F:326:LYS:HE2	6:F:328:TRP:CZ2	2.54	0.43
1:A:325:PRO:O	1:A:329:ASN:OD1	2.36	0.43
2:B:179:ASP:HB2	3:C:352:LYS:HZ2	1.83	0.43
3:C:1:MET:HB2	3:C:1:MET:HE2	1.72	0.43
3:C:47:ASP:O	3:C:50:ASN:HB2	2.18	0.43
4:D:22:GLU:HG3	4:D:83:PHE:CD1	2.53	0.43
6:F:226:GLU:HG3	6:F:237:THR:CG2	2.48	0.43
3:C:251:ASP:HB3	17:S:34:HOH:O	2.18	0.43
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.45	0.43
3:C:217:LEU:HD21	3:C:368:LEU:HD23	2.01	0.43
4:D:399:PHE:CE1	4:D:405:LEU:HD21	2.53	0.43
6:F:221:LEU:O	6:F:261:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.01	0.43
6:F:71:LEU:HD22	6:F:298:ILE:CD1	2.49	0.43
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.52	0.43
4:D:83:PHE:O	4:D:86:ILE:CG2	2.61	0.43
1:A:293:ASN:ND2	1:A:339:ARG:HH12	2.17	0.43
6:F:8:ASP:HB2	6:F:43:GLU:HA	2.01	0.43
1:A:26:LEU:HB3	1:A:361:THR:HG21	2.01	0.42
1:A:176[A]:GLN:C	1:A:177:VAL:HG22	2.39	0.42
1:A:241:SER:HB2	1:A:249:ASN:O	2.19	0.42
4:D:291:LEU:HD11	4:D:373:MET:HB3	2.01	0.42
1:A:339:ARG:HB3	1:A:341:ILE:HD11	1.98	0.42
1:A:176[A]:GLN:HG2	6:F:56:PRO:HB3	2.00	0.42
1:A:285:GLN:HA	1:A:285:GLN:OE1	2.19	0.42
6:F:14:TYR:CD1	6:F:17:VAL:HG11	2.52	0.42
2:B:75:MET:SD	2:B:92:PHE:HD2	2.41	0.42
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.19	0.42
4:D:272:PHE:O	4:D:300:ASN:ND2	2.44	0.42
6:F:81:ILE:HD12	6:F:94:PHE:CD2	2.54	0.42
6:F:314:LEU:HD22	6:F:350:ILE:HD11	2.01	0.42
2:B:3:GLU:OE1	2:B:130:ASP:N	2.52	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.42
3:C:217:LEU:O	3:C:218:ASP:HB2	2.19	0.42
4:D:360:PRO:C	4:D:369:ARG:N	2.73	0.42
6:F:299:GLU:N	6:F:300:PRO:HD2	2.35	0.42
1:A:176[B]:GLN:O	1:A:177:VAL:HG13	2.20	0.42
1:A:179:THR:O	2:B:352:LYS:NZ	2.52	0.42
1:A:245:ASP:OD2	5:E:15:THR:OG1	2.37	0.42
2:B:358:ILE:N	2:B:358:ILE:HD12	2.35	0.42
2:B:405:LEU:HD12	2:B:405:LEU:HA	1.80	0.42
3:C:68:VAL:HG21	3:C:118:VAL:HG21	2.02	0.42
6:F:305:LYS:O	6:F:306:HIS:HB2	2.19	0.42
3:C:27:GLU:HG2	3:C:361:THR:HG21	2.02	0.42
13:X:508:EPA:C25	13:X:508:EPA:C13	2.98	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.19	0.42
2:B:402:LYS:HG3	2:B:405:LEU:CD2	2.49	0.42
6:F:208:ASP:HB2	17:S:160:HOH:O	2.19	0.42
6:F:345:GLU:O	6:F:349:GLY:N	2.47	0.42
3:C:119:LEU:HD11	3:C:156:ARG:HB3	2.02	0.41
3:C:156:ARG:HD2	3:C:156:ARG:HA	1.83	0.41
1:A:36:MET:CG	1:A:36:MET:O	2.68	0.41
3:C:250:VAL:CG2	3:C:255:PHE:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.41
2:B:147:SER:OG	2:B:190:SER:OG	2.24	0.41
6:F:15:ALA:O	6:F:19:ARG:NE	2.53	0.41
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.03	0.41
2:B:392:SER:HB2	2:B:425:MET:HE2	2.03	0.41
3:C:255:PHE:CE2	3:C:318:LEU:HD11	2.55	0.41
4:D:197:ASN:OD1	5:E:122:ARG:NH2	2.52	0.41
5:E:106:GLU:HA	5:E:106:GLU:OE1	2.20	0.41
6:F:284:LEU:HA	6:F:284:LEU:HD23	1.80	0.41
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.55	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.20	0.41
3:C:99:ALA:HB3	3:C:144:GLY:HA3	2.03	0.41
6:F:80:LEU:O	6:F:84:SER:OG	2.22	0.41
1:A:2:ARG:HG3	1:A:2:ARG:HH11	1.85	0.41
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.56	0.41
2:B:2:ARG:HH21	2:B:130:ASP:HB2	1.85	0.41
4:D:414:ASP:OD1	4:D:416:MET:HG2	2.21	0.41
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.03	0.41
1:A:88:HIS:N	1:A:91:GLN:OE1	2.37	0.41
1:A:179:THR:HG23	2:B:352:LYS:HZ2	1.86	0.41
1:A:283:HIS:NE2	1:A:369:ALA:HB1	2.36	0.41
3:C:168:GLU:OE2	3:C:194:THR:HG21	2.21	0.41
3:C:209:ILE:CD1	3:C:302:MET:SD	3.07	0.41
4:D:39:ASP:OD1	4:D:39:ASP:N	2.53	0.41
4:D:112:ALA:O	4:D:115:VAL:HG12	2.20	0.41
4:D:295:MET:SD	4:D:375:ALA:HB1	2.61	0.41
1:A:36:MET:CG	1:A:39:ASP:HB2	2.51	0.41
3:C:225:THR:O	3:C:229[A]:ARG:HG3	2.21	0.41
4:D:161:TYR:HB3	4:D:164:ARG:HG3	2.02	0.41
6:F:77:LEU:O	6:F:81:ILE:HG13	2.21	0.41
6:F:178:GLN:OE1	6:F:178:GLN:CA	2.68	0.41
4:D:349:ASN:O	4:D:352:LYS:HE2	2.21	0.40
5:E:138:GLU:HA	5:E:141:GLU:HB2	2.02	0.40
6:F:40:MET:HE3	6:F:52:LEU:HD11	2.03	0.40
6:F:173:ILE:CD1	6:F:180:HIS:HB2	2.52	0.40
6:F:207:VAL:O	6:F:312:PHE:HB2	2.22	0.40
6:F:226:GLU:HG3	6:F:237:THR:HG22	2.01	0.40
3:C:55:GLU:HA	3:C:60:LYS:O	2.21	0.40
5:E:47:LEU:HD23	5:E:47:LEU:O	2.22	0.40
2:B:179:ASP:CB	3:C:352:LYS:HG3	2.49	0.40
3:C:392:ASP:OD2	3:C:429:GLU:OE2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:PRO:CD	4:D:86:ILE:HG12	2.51	0.40
6:F:226:GLU:CG	6:F:237:THR:HG22	2.51	0.40
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.86	0.40
4:D:20:PHE:CD1	4:D:235:MET:HE2	2.57	0.40
4:D:60:LYS:HD2	4:D:60:LYS:HA	1.78	0.40
4:D:210:TYR:CD1	4:D:222:PRO:HG2	2.57	0.40
4:D:345:GLU:CD	4:D:345:GLU:H	2.25	0.40
5:E:53:LYS:HE2	5:E:53:LYS:HB3	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLU:OE2	3:C:283:HIS:NE2[4_555]	1.62	0.58

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/439 (99%)	420 (96%)	16 (4%)	0	100	100
2	B	428/429 (100%)	413 (96%)	15 (4%)	0	100	100
3	C	442/440 (100%)	426 (96%)	16 (4%)	0	100	100
4	D	427/430 (99%)	414 (97%)	13 (3%)	0	100	100
5	E	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
6	F	321/332 (97%)	304 (95%)	17 (5%)	0	100	100
All	All	2174/2193 (99%)	2096 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/370 (100%)	360 (97%)	11 (3%)	41	68
2	B	371/370 (100%)	366 (99%)	5 (1%)	69	87
3	C	375/371 (101%)	370 (99%)	5 (1%)	69	87
4	D	369/371 (100%)	355 (96%)	14 (4%)	33	58
5	E	111/110 (101%)	110 (99%)	1 (1%)	78	92
6	F	298/297 (100%)	286 (96%)	12 (4%)	31	56
All	All	1895/1889 (100%)	1847 (98%)	48 (2%)	47	73

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	96	LYS
1	A	178	SER
1	A	193	THR
1	A	256	GLN
1	A	280	LYS
1	A	329	ASN
1	A	339	ARG
1	A	346	TRP
1	A	381	THR
1	A	437	VAL
2	B	48	ARG
2	B	139	HIS
2	B	402	LYS
2	B	414	ASP
2	B	430	SER
3	C	46	ASP
3	C	120	ASP
3	C	283	HIS
3	C	339	ARG
3	C	430	LYS
4	D	15	GLN

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Mol	Chain	Res	Type
4	D	85	GLN
4	D	133	GLN
4	D	155	SER
4	D	207	GLU
4	D	282	GLN
4	D	284	ARG
4	D	286	LEU
4	D	302	MET
4	D	308	ARG
4	D	322	ARG
4	D	405	LEU
4	D	422	GLU
4	D	426	ASN
5	E	6	MET
6	F	32	LYS
6	F	46	ARG
6	F	143	GLU
6	F	164	SER
6	F	197	ARG
6	F	217	ARG
6	F	224	SER
6	F	262	MET
6	F	353	VAL
6	F	356	SER
6	F	357	SER
6	F	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	285	GLN
1	A	372	GLN
3	C	293	ASN
4	D	139	HIS
6	F	260	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 6 are monoatomic and 5 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	ACP	X	506	-	27,33,33	0.89	1 (3%)	32,52,52	0.80	2 (6%)
14	VLB	X	509	-	63,67,67	1.76	16 (25%)	79,108,108	2.38	26 (32%)
7	GTP	X	511	8	26,34,34	1.02	3 (11%)	32,54,54	0.69	1 (3%)
10	GDP	X	504	8	24,30,30	1.02	3 (12%)	30,47,47	0.67	1 (3%)
7	GTP	X	501	8	26,34,34	0.99	2 (7%)	32,54,54	0.69	1 (3%)
10	GDP	X	514	8	24,30,30	0.99	2 (8%)	30,47,47	0.66	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	X	506	-	-	0/15/38/38	0/3/3/3
14	VLB	X	509	-	-	15/38/131/131	0/7/9/9
7	GTP	X	511	8	-	6/18/38/38	0/3/3/3
10	GDP	X	504	8	-	4/12/32/32	0/3/3/3
7	GTP	X	501	8	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GDP	X	514	8	-	4/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	509	VLB	C57-N56	5.12	1.59	1.47
14	X	509	VLB	C68-C73	-3.87	1.50	1.53
14	X	509	VLB	C58-C59	-3.84	1.45	1.52
14	X	509	VLB	C19-N9	3.18	1.52	1.47
14	X	509	VLB	O75-C76	-3.02	1.38	1.45
14	X	509	VLB	C5-C6	-2.82	1.45	1.51
14	X	509	VLB	O27-C3	-2.75	1.37	1.42
10	X	504	GDP	C5-C6	-2.73	1.41	1.47
7	X	511	GTP	C5-C6	-2.69	1.41	1.47
7	X	501	GTP	C5-C6	-2.68	1.42	1.47
10	X	514	GDP	C5-C6	-2.66	1.42	1.47
14	X	509	VLB	C70-C54	2.53	1.57	1.53
14	X	509	VLB	O25-C26	-2.50	1.39	1.45
14	X	509	VLB	O32-C16	2.49	1.41	1.37
14	X	509	VLB	C57-C58	-2.42	1.45	1.52
11	X	506	ACP	PB-O2B	-2.42	1.50	1.56
14	X	509	VLB	C68-C67	-2.31	1.51	1.53
14	X	509	VLB	O32-C33	-2.23	1.36	1.42
14	X	509	VLB	C69-C52	2.19	1.55	1.52
14	X	509	VLB	C5-C19	-2.16	1.48	1.53
7	X	511	GTP	C8-N7	-2.16	1.31	1.35
10	X	504	GDP	C8-N7	-2.15	1.31	1.35
10	X	514	GDP	C8-N7	-2.13	1.31	1.35
14	X	509	VLB	C59-C67	-2.11	1.36	1.39
7	X	501	GTP	C8-N7	-2.09	1.31	1.35
7	X	511	GTP	C5-C4	-2.02	1.37	1.43
10	X	504	GDP	C5-C4	-2.02	1.37	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	X	509	VLB	O25-C23-C3	6.46	123.08	112.22
14	X	509	VLB	C52-C69-N56	6.24	121.05	111.28
14	X	509	VLB	C57-C58-C59	5.63	124.94	114.30
14	X	509	VLB	C58-C57-N56	5.43	125.56	113.44
14	X	509	VLB	O72-C54-C70	-4.87	100.35	108.75
14	X	509	VLB	O75-C73-C68	4.34	117.84	111.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	X	509	VLB	C19-C5-C6	4.30	112.68	108.28
14	X	509	VLB	O75-C73-O74	-4.27	116.44	123.93
14	X	509	VLB	C13-C18-N1	3.85	115.35	110.98
14	X	509	VLB	C63-C64-C65	-3.85	114.55	120.08
14	X	509	VLB	C22-N1-C18	-3.67	109.10	120.84
14	X	509	VLB	O25-C23-O24	-3.62	117.59	123.93
14	X	509	VLB	O32-C16-C15	3.55	120.21	116.58
14	X	509	VLB	C22-N1-C2	-3.38	110.96	119.21
14	X	509	VLB	C17-C18-N1	-3.27	123.05	127.61
14	X	509	VLB	O32-C16-C17	-3.21	118.59	124.12
14	X	509	VLB	C62-C61-C60	-3.00	116.73	120.89
14	X	509	VLB	O24-C23-C3	-2.99	119.29	123.94
14	X	509	VLB	C3-C2-N1	-2.92	108.79	112.81
14	X	509	VLB	C18-N1-C2	-2.75	105.33	109.03
14	X	509	VLB	C53-C52-C69	2.73	111.91	108.72
14	X	509	VLB	O28-C29-C30	2.34	115.39	111.09
14	X	509	VLB	C61-C60-C65	2.33	121.25	118.17
11	X	506	ACP	C5-C6-N6	2.28	123.82	120.35
11	X	506	ACP	O1G-PG-C3B	-2.18	106.53	111.24
14	X	509	VLB	C33-O32-C16	-2.08	114.38	117.53
14	X	509	VLB	C2-C12-C19	2.08	117.58	114.07
14	X	509	VLB	C21-C20-C5	-2.06	111.82	115.79
10	X	504	GDP	O6-C6-C5	2.03	128.34	124.37
7	X	511	GTP	O6-C6-C5	2.03	128.33	124.37
10	X	514	GDP	O6-C6-C5	2.03	128.33	124.37
7	X	501	GTP	O6-C6-C5	2.00	128.29	124.37

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	501	GTP	PB-O3B-PG-O2G
7	X	501	GTP	PB-O3B-PG-O3G
7	X	501	GTP	C5'-O5'-PA-O1A
7	X	511	GTP	PB-O3B-PG-O3G
7	X	511	GTP	C5'-O5'-PA-O1A
7	X	511	GTP	C5'-O5'-PA-O2A
10	X	504	GDP	C5'-O5'-PA-O1A
10	X	514	GDP	C5'-O5'-PA-O1A
14	X	509	VLB	O72-C54-C70-C71
14	X	509	VLB	C55-C54-C70-C71
14	X	509	VLB	C53-C54-C70-C71

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Mol	Chain	Res	Type	Atoms
14	X	509	VLB	C58-C57-N56-C69
14	X	509	VLB	C51-C68-C73-O75
14	X	509	VLB	C15-C68-C73-O74
14	X	509	VLB	C15-C68-C73-O75
14	X	509	VLB	C68-C73-O75-C76
14	X	509	VLB	O74-C73-O75-C76
14	X	509	VLB	C3-C23-O25-C26
14	X	509	VLB	O24-C23-O25-C26
10	X	514	GDP	C5'-O5'-PA-O3A
7	X	501	GTP	C5'-O5'-PA-O2A
10	X	504	GDP	C5'-O5'-PA-O2A
10	X	514	GDP	C5'-O5'-PA-O2A
10	X	514	GDP	PB-O3A-PA-O2A
14	X	509	VLB	O25-C23-C3-C4
14	X	509	VLB	C67-C68-C73-O75
7	X	501	GTP	PB-O3A-PA-O2A
14	X	509	VLB	C67-C68-C73-O74
7	X	501	GTP	C5'-O5'-PA-O3A
7	X	511	GTP	C5'-O5'-PA-O3A
10	X	504	GDP	C5'-O5'-PA-O3A
7	X	501	GTP	PB-O3A-PA-O1A
7	X	511	GTP	PB-O3A-PA-O1A
7	X	511	GTP	PB-O3A-PA-O2A
10	X	504	GDP	PB-O3A-PA-O2A
7	X	501	GTP	PB-O3B-PG-O1G
14	X	509	VLB	C58-C57-N56-C55

There are no ring outliers.

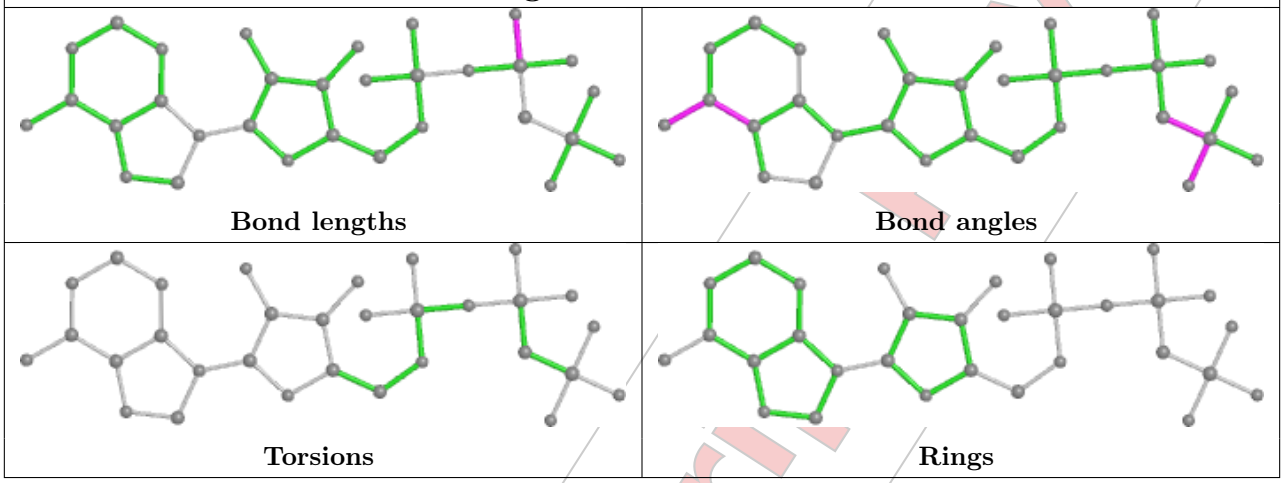
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	X	509	VLB	5	0

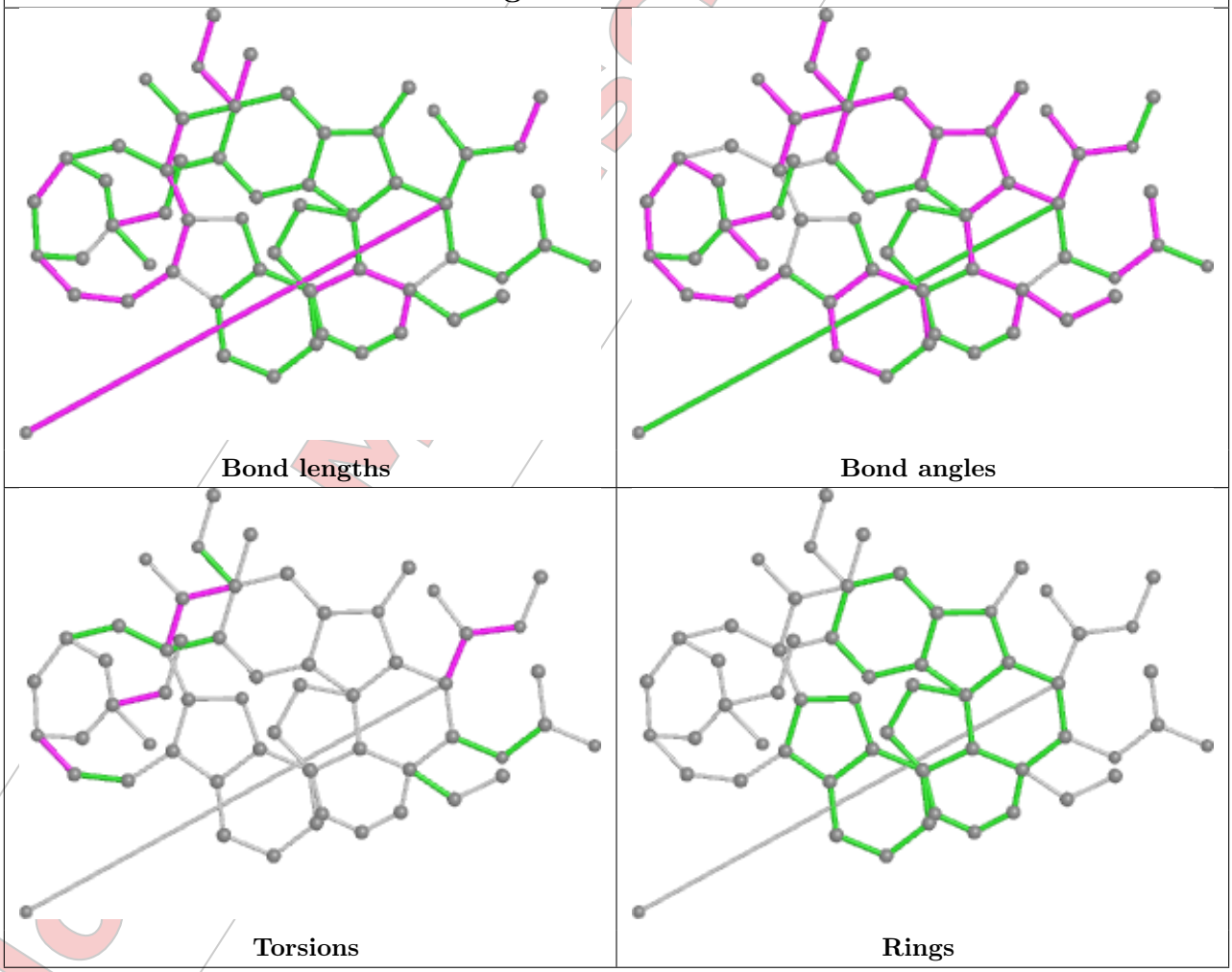
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

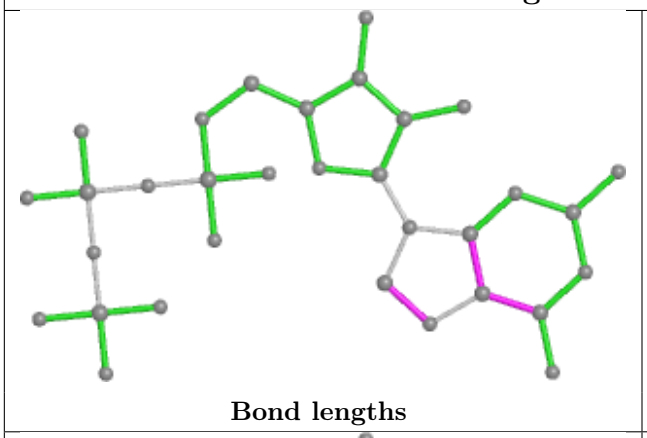
Ligand ACP X 506



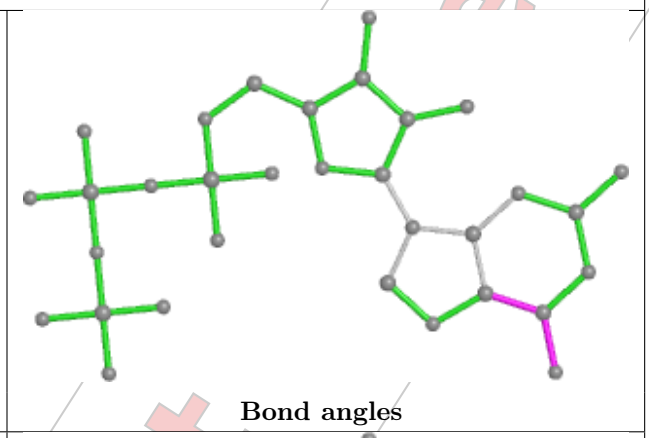
Ligand VLB X 509



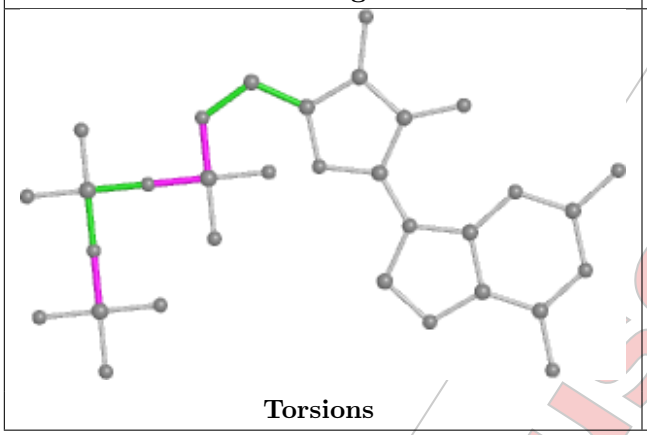
Ligand GTP X 511



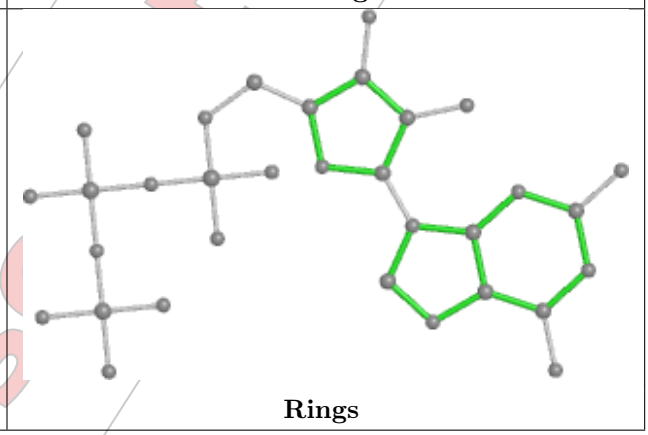
Bond lengths



Bond angles

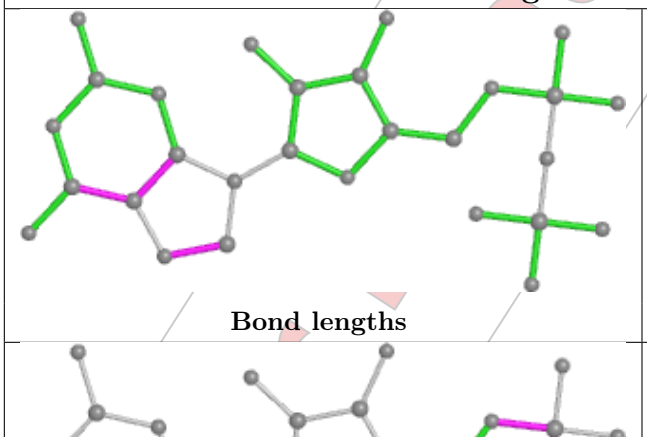


Torsions

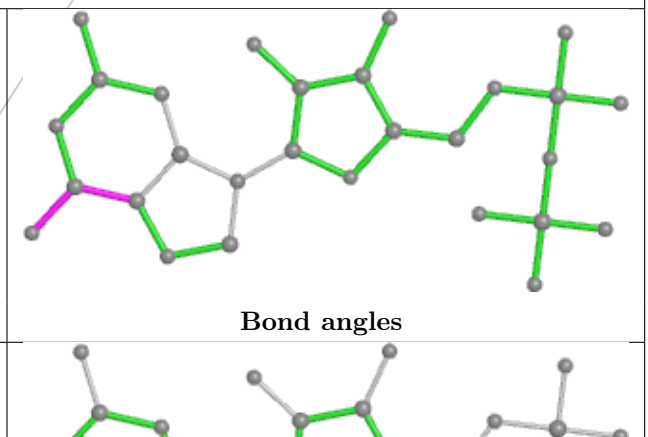


Rings

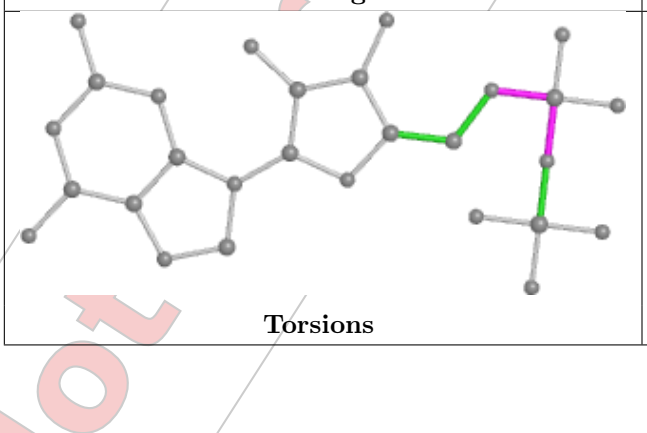
Ligand GDP X 504



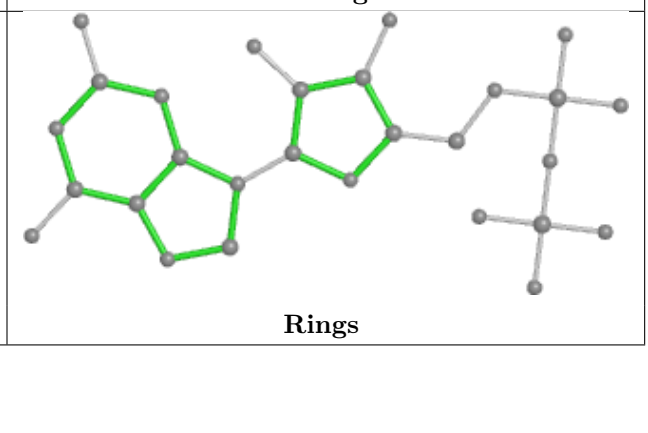
Bond lengths



Bond angles

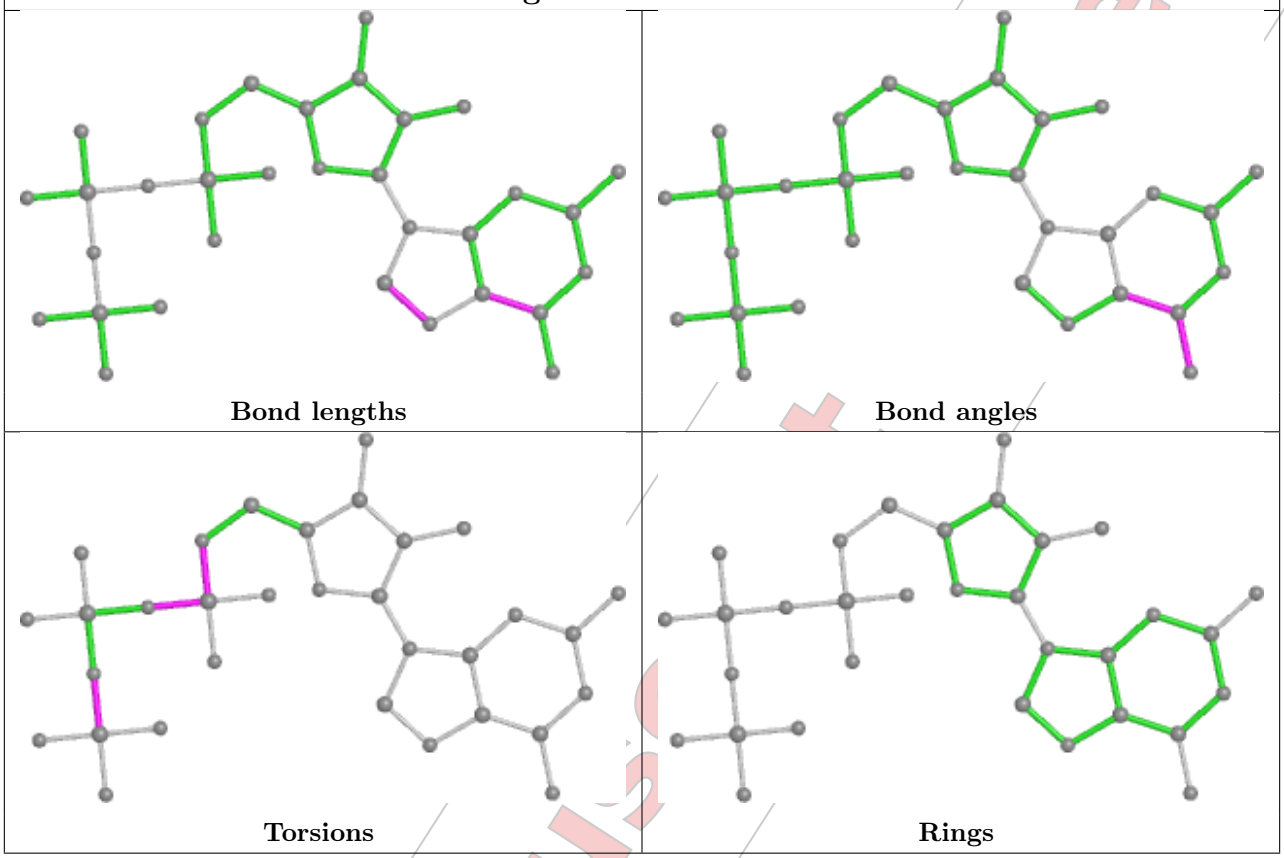


Torsions

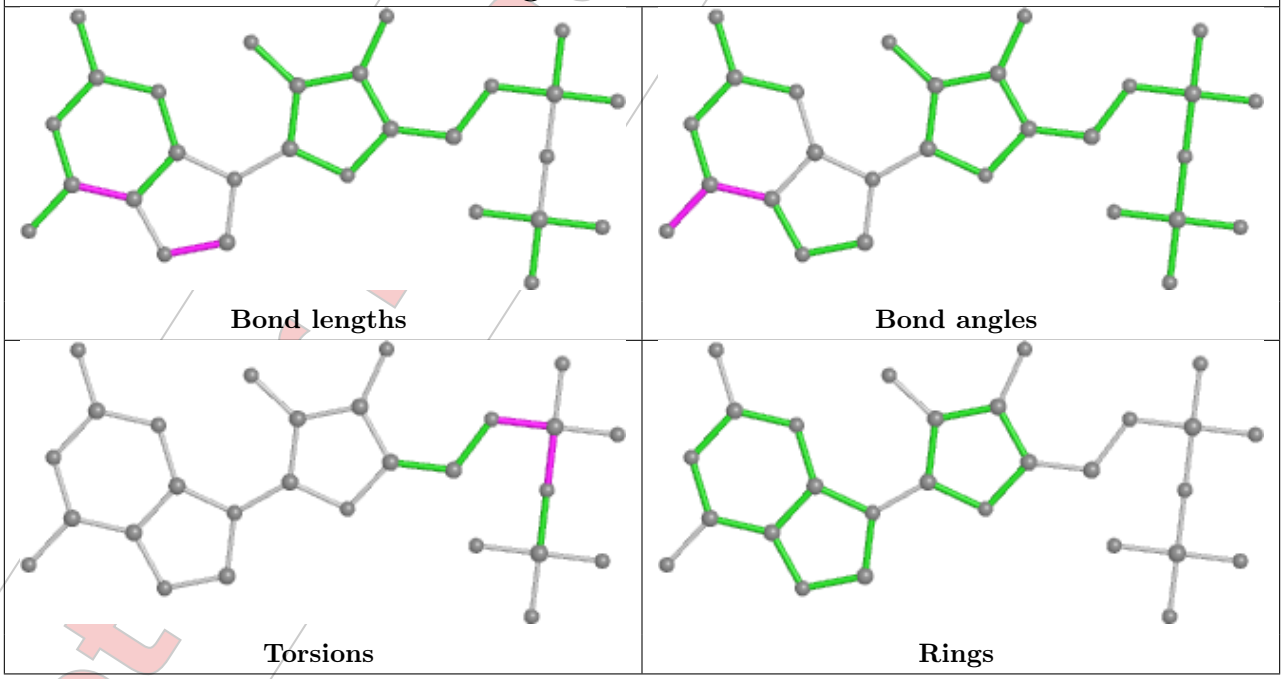


Rings

Ligand GTP X 501



Ligand GDP X 514



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	5
1	A	2
5	E	1
4	D	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	31.73
1	F	362:ALA	C	372:THR	N	16.08
1	F	155:ALA	C	162:ILE	N	13.76
1	F	246:GLN	C	256:TYR	N	12.22
1	F	102:PRO	C	125:THR	N	12.20
1	F	231:ALA	C	235:ASP	N	7.76
1	A	176[A]:GLN	C	177:VAL	N	5.41
1	A	176[B]:GLN	C	177:VAL	N	5.38
1	D	360:PRO	C	369:ARG	N	2.73
1	B	42:LEU	C	45:GLN	N	2.66

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

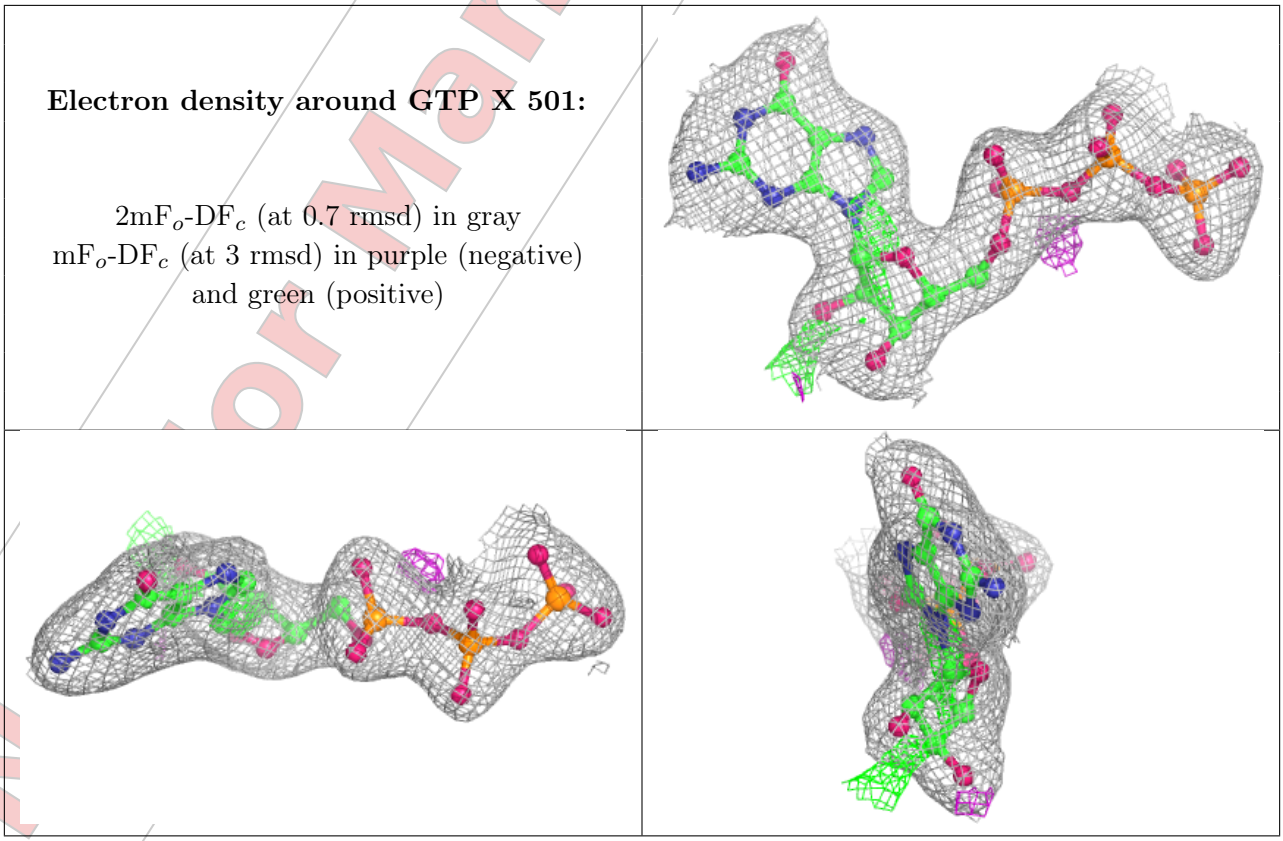
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

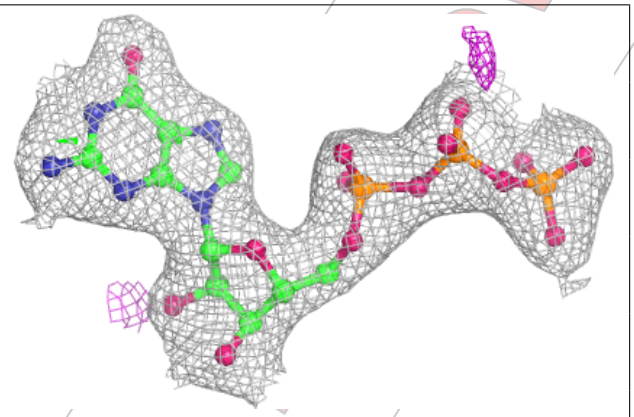
Electron density around GTP X 501:

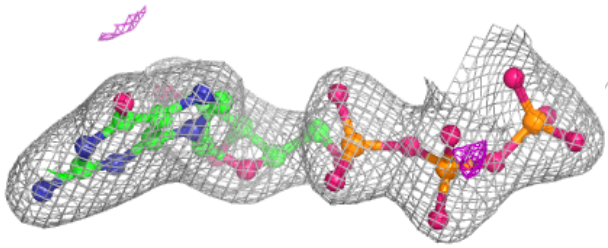
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

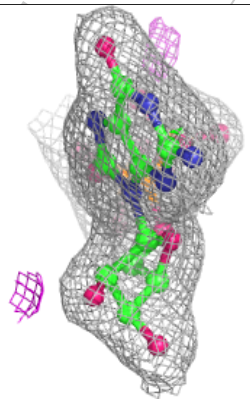


Electron density around GTP X 511:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

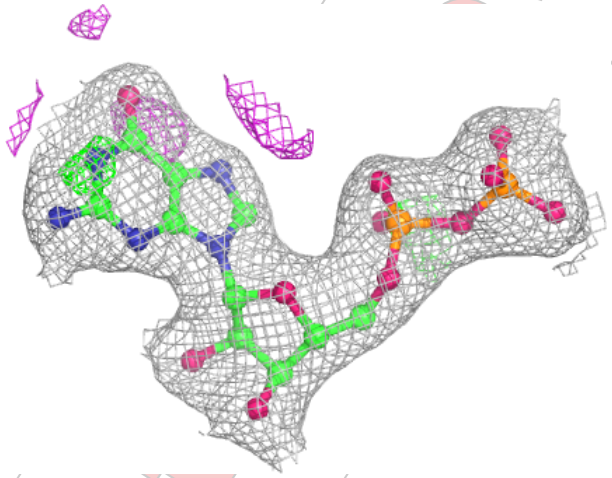


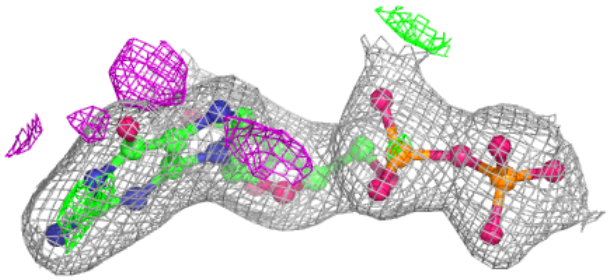


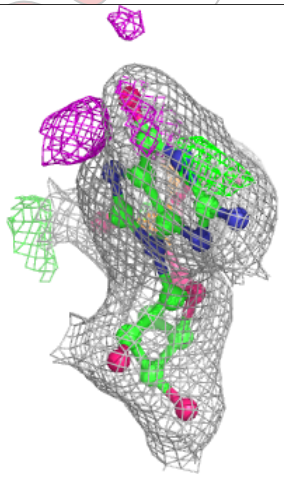


Electron density around GDP X 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

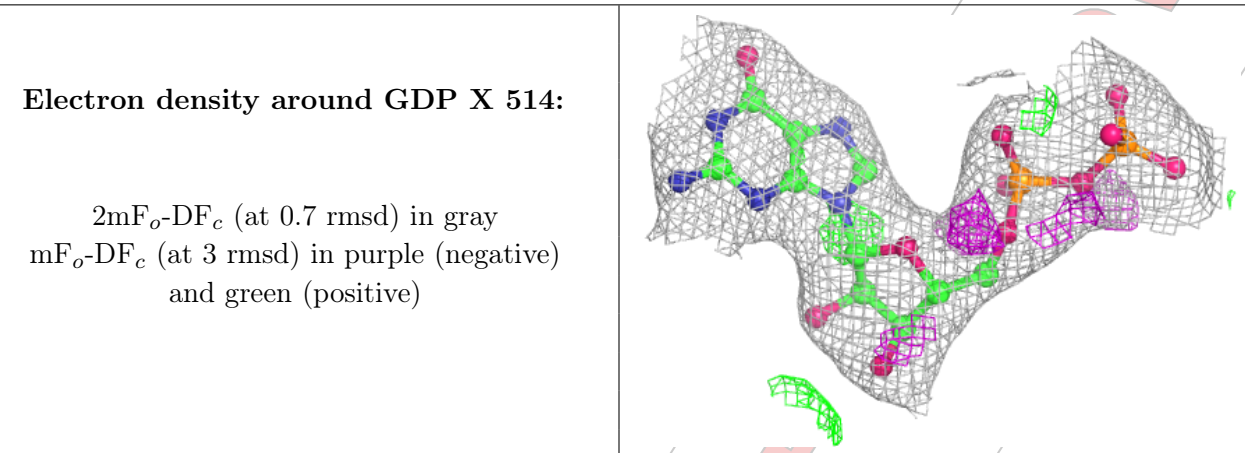






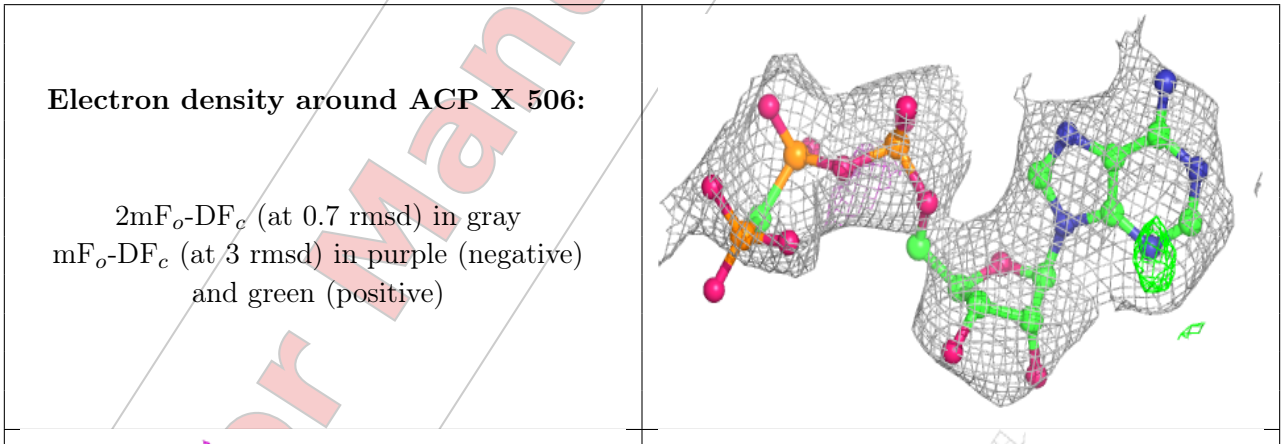
Electron density around GDP X 514:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



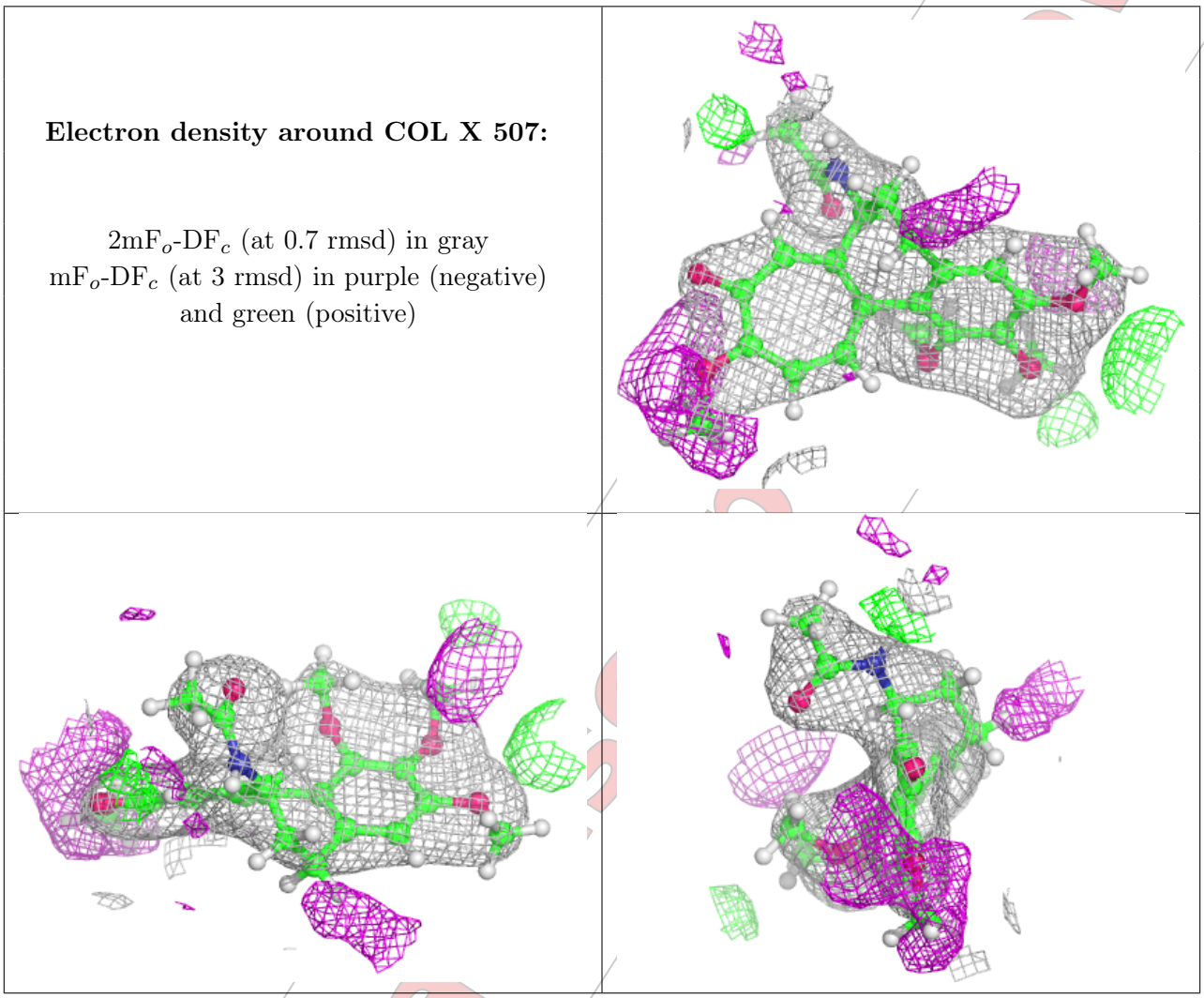
Electron density around ACP X 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



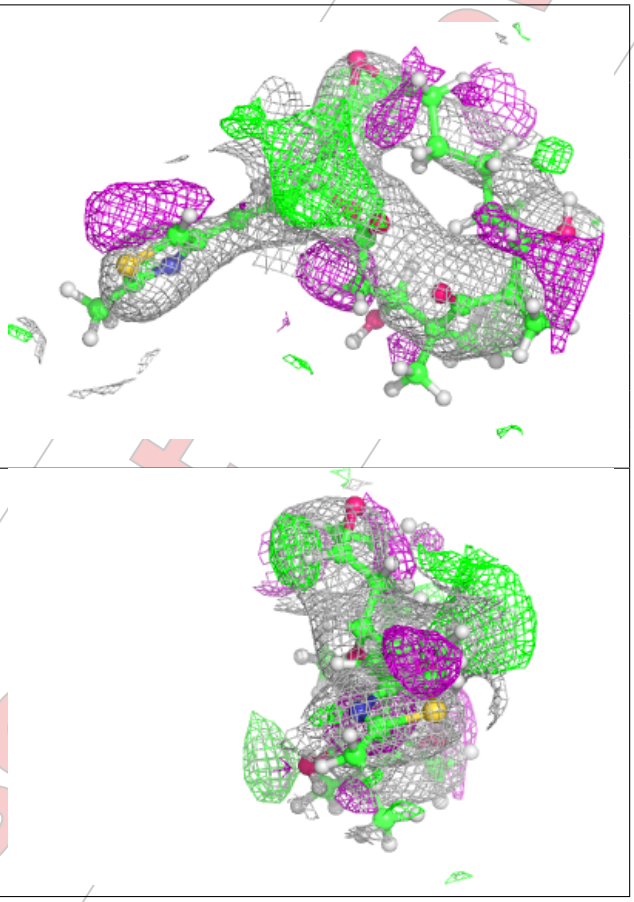
Electron density around COL X 507:

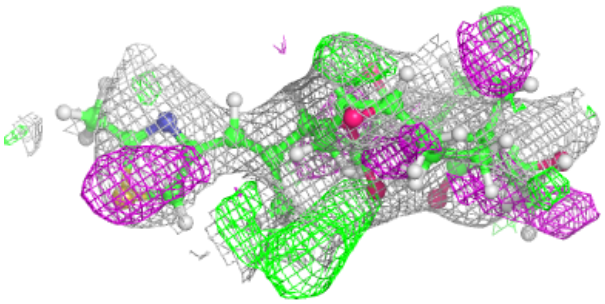
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EPA X 508:

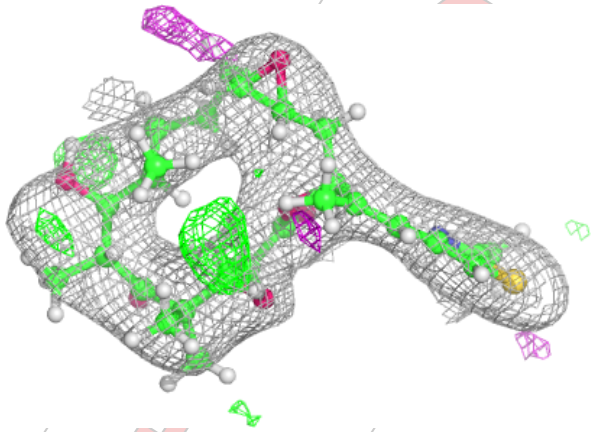
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

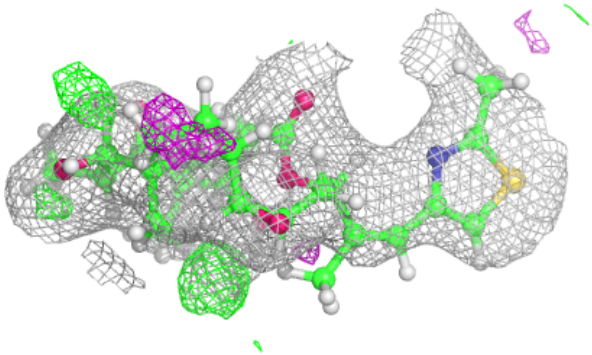


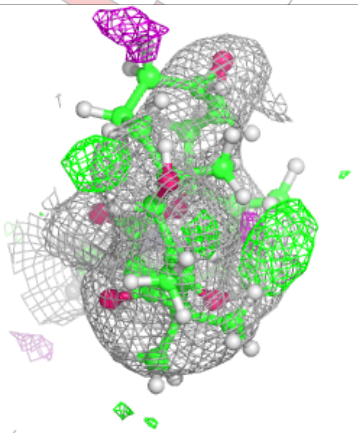


Electron density around EPA X 516:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

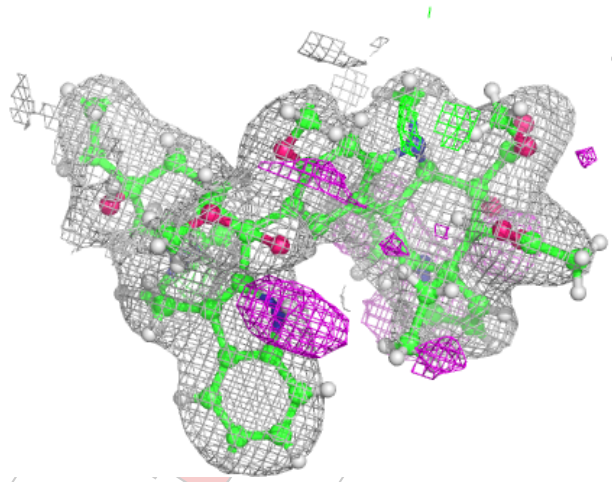


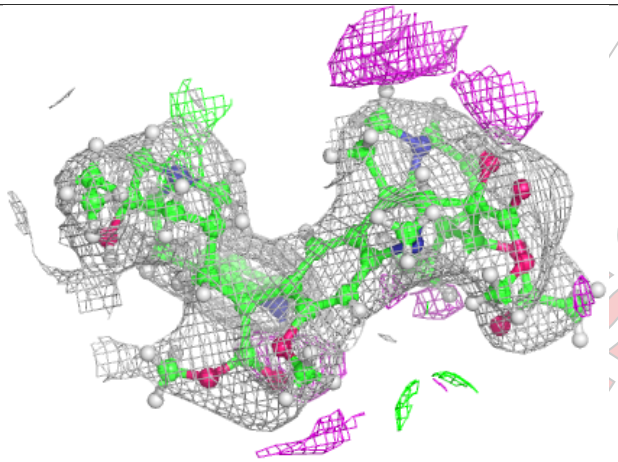


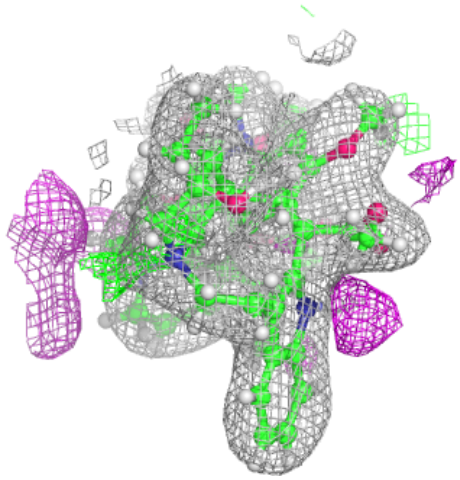


Electron density around VLB X 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

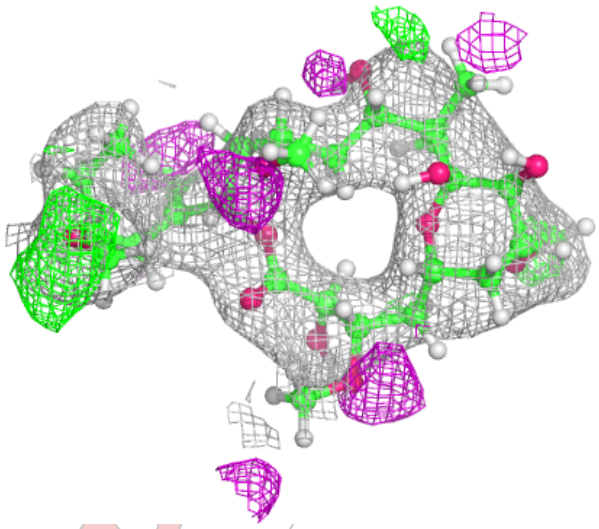


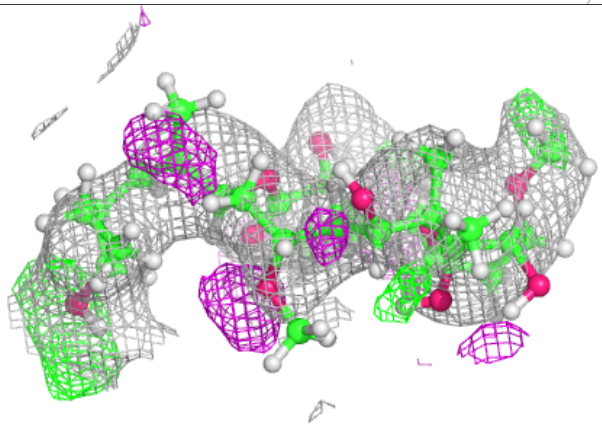


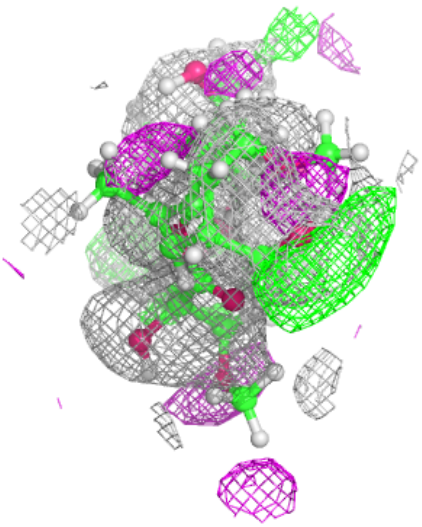


Electron density around POU X 510:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

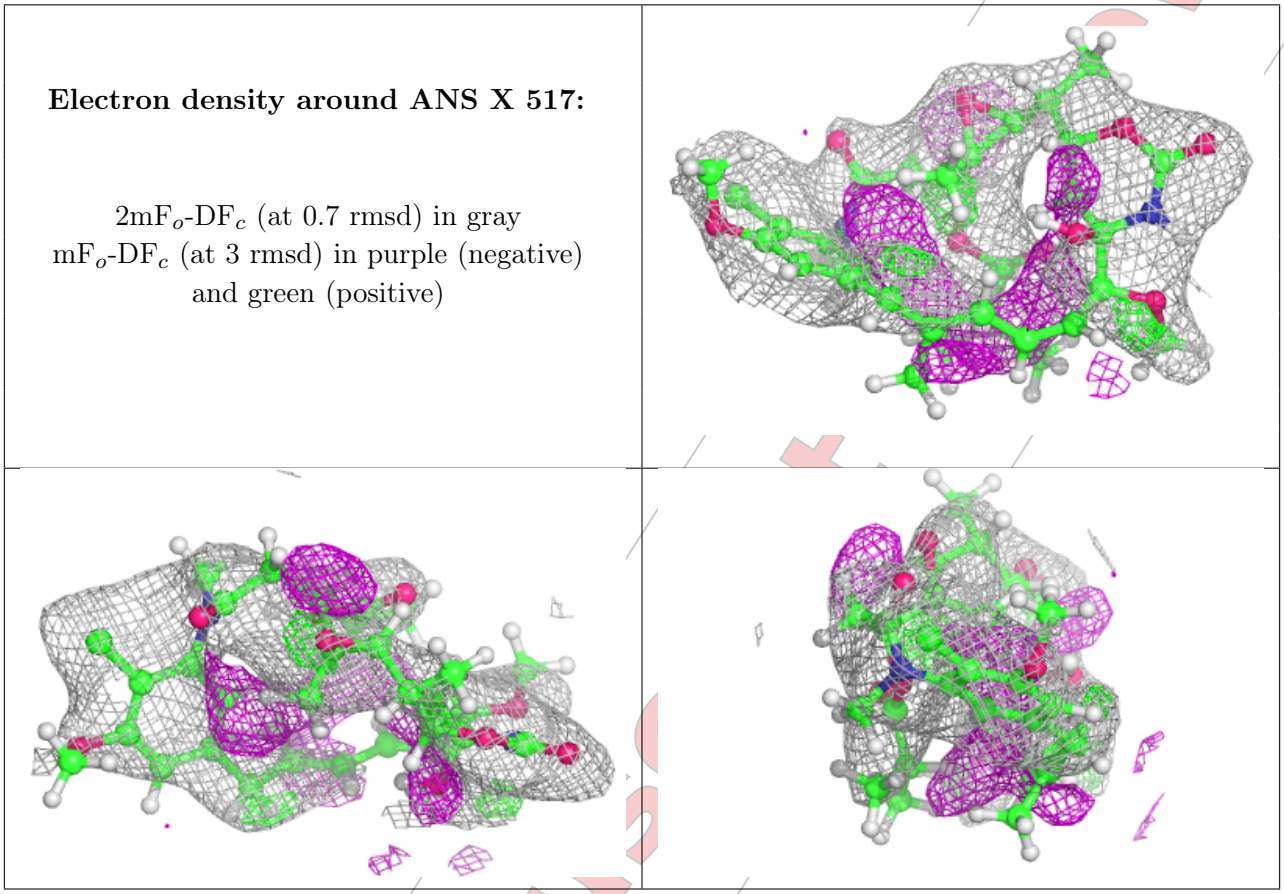






Electron density around ANS X 517:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2023 – 02:27 pm GMT

Deposition ID : D_1292128494

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

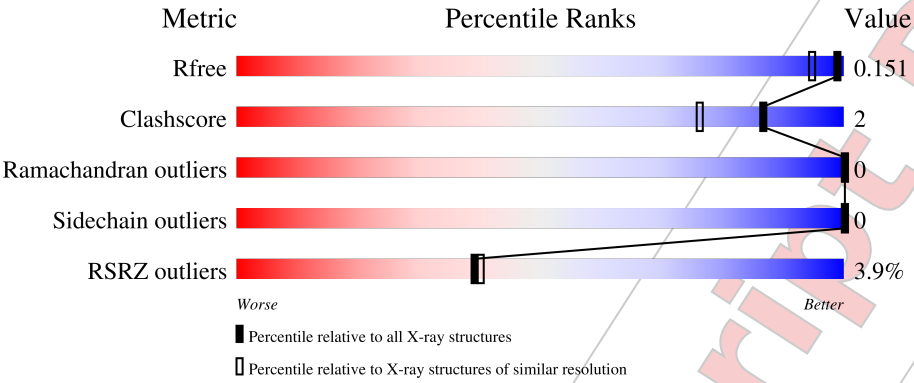
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	129	4% 91% 9%

2 Entry composition

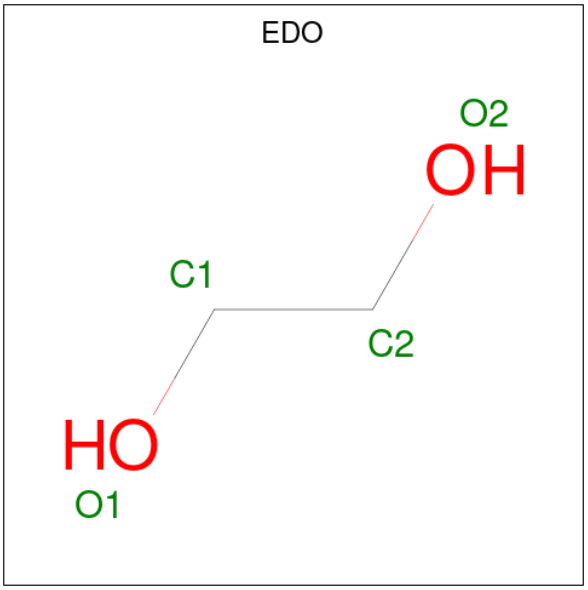
There are 6 unique types of molecules in this entry. The entry contains 1329 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1199	726	247	216	10	1	19	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

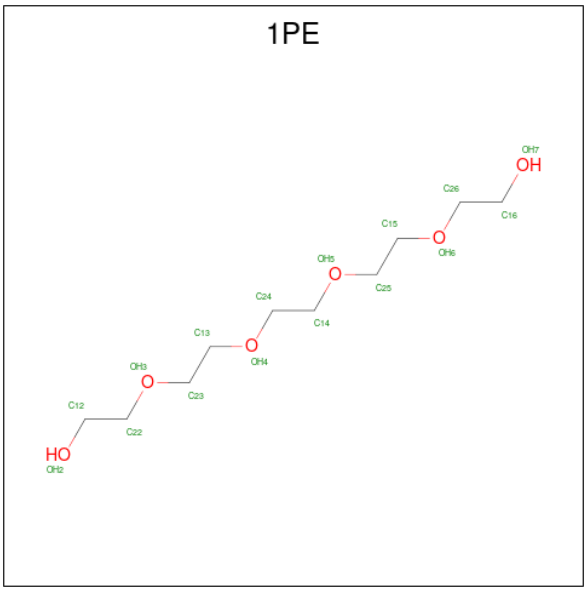
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
			Total	Cl		
3	A	1	1	1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 5 3	0	0

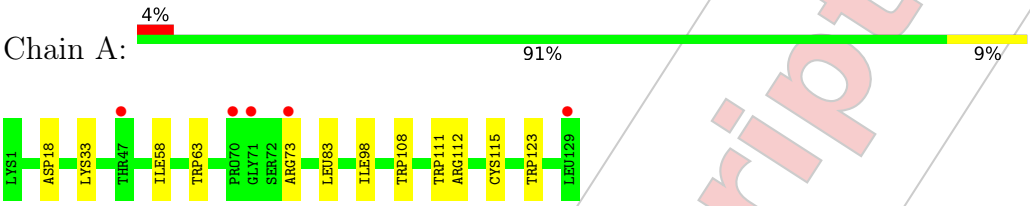
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	114	Total O 114 114	0	3

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.92Å 77.92Å 37.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.47 – 1.31 14.96 – 1.31	Depositor EDS
% Data completeness (in resolution range)	92.4 (14.47-1.31) 92.4 (14.96-1.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.31Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.125 , 0.148 0.132 , 0.151	Depositor DCC
R_{free} test set	2000 reflections (7.54%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 68.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	1329	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, CL, EDO, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.73	0/1221	0.90	1/1642 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	TRP	O-C-N	5.47	131.46	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112[A]	ARG	Sidechain
1	A	73[A]	ARG	Mainchain
1	A	73[B]	ARG	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1199	0	1151	5	0
2	A	4	0	6	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	8	0	9	0	0
6	S	114	0	0	0	0
All	All	1329	0	1166	5	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TRP:CE2	1:A:98:ILE:HG12	2.54	0.43
1:A:18[B]:ASP:OD1	1:A:18[B]:ASP:N	2.52	0.42
1:A:111:TRP:CD1	1:A:115:CYS:HB2	2.55	0.41
1:A:33:LYS:HG2	1:A:123:TRP:CH2	2.56	0.41
1:A:58:ILE:HB	1:A:83:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	147/129 (114%)	144 (98%)	3 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/105 (120%)	126 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1PE	A	1147	-	7,7,15	0.24	0	6,6,14	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	A	1136	-	3,3,3	0.47	0	2,2,2	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	A	1147	-	-	3/5/5/13	-
2	EDO	A	1136	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1136	EDO	O1-C1-C2-O2
5	A	1147	1PE	C23-C13-OH4-C24
5	A	1147	1PE	OH2-C12-C22-OH3
5	A	1147	1PE	OH4-C13-C23-OH3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	129/129 (100%)	-0.02	5 (3%) 39 40	14, 19, 31, 44	2 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	GLY	4.0
1	A	47	THR	3.1
1	A	70	PRO	2.9
1	A	129	LEU	2.5
1	A	73[A]	ARG	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1PE	A	1147	8/?	0.78	0.13	63,63,64,64	0
2	EDO	A	1136	4/?	0.94	0.06	53,53,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	A	1146	1/?	0.99	0.04	23,23,23,23	0
4	NA	A	1145	1/?	0.99	0.05	23,23,23,23	0
3	CL	A	1139	1/?	1.00	0.04	28,28,28,28	1
3	CL	A	1137	1/?	1.00	0.14	21,21,21,21	1

6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2023 – 10:43 am GMT

Deposition ID : D_1292128476

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

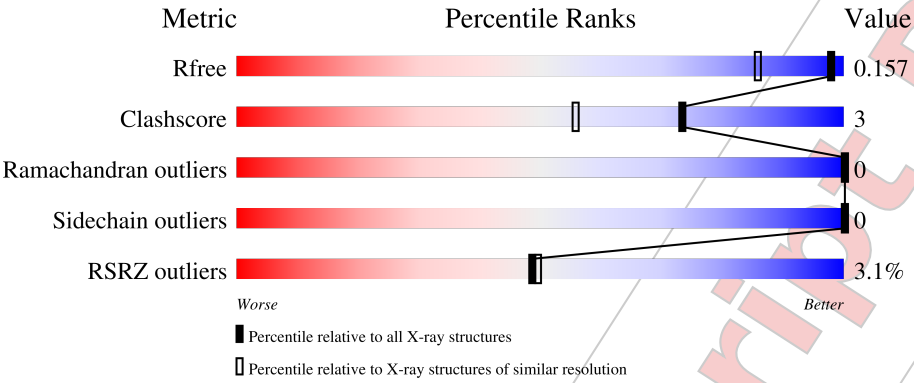
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	129	3% 89% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 1343 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1190	722	244	214	10	2	19	0

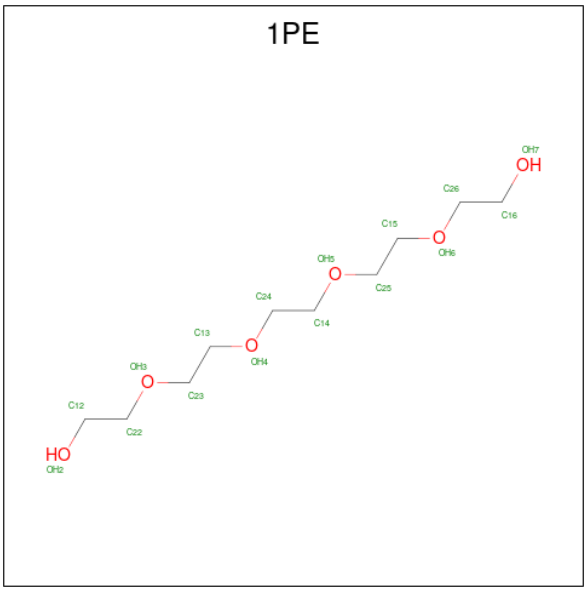
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0
2	A	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

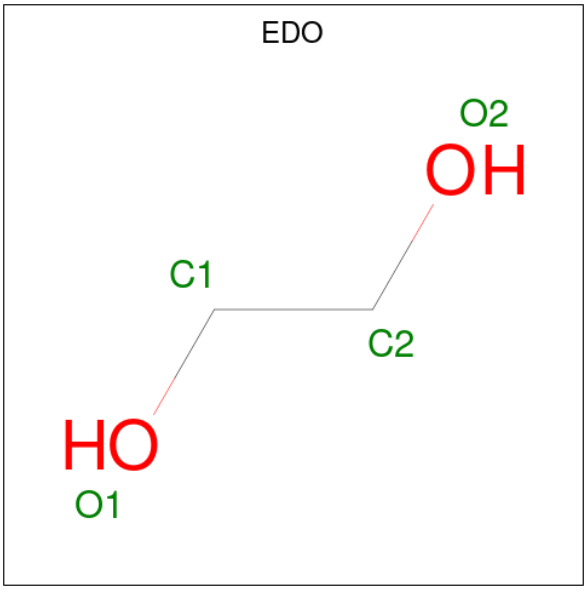
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
3	A	1	1	1	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 5 3	0	0
4	A	1	Total C O 7 4 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0

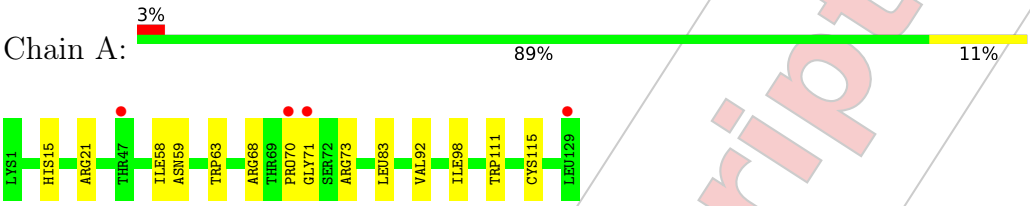
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	129	Total O 129 129	0	3

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.90Å 77.90Å 37.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.54 – 1.32 14.97 – 1.32	Depositor EDS
% Data completeness (in resolution range)	93.0 (13.54-1.32) 93.1 (14.97-1.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.32Å)	Xtriage
Refinement program	.	Depositor
R, R_{free}	0.121 , 0.156 0.125 , 0.157	Depositor DCC
R_{free} test set	2000 reflections (7.79%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	1343	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, CL, EDO, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.73	0/1212	0.85	0/1630

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1190	0	1144	8	0
2	A	3	0	0	0	0
3	A	2	0	0	0	0
4	A	15	0	18	0	0
5	A	4	0	6	0	0
6	S	129	0	0	2	0
All	All	1343	0	1168	8	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21[A]:ARG:NH1	6:S:98:HOH:O	2.29	0.63
1:A:59[B]:ASN:ND2	6:S:19:HOH:O	2.43	0.51
1:A:68[A]:ARG:O	1:A:70:PRO:HD3	2.11	0.50
1:A:15:HIS:HB3	1:A:92:VAL:HG11	1.95	0.49
1:A:63:TRP:CE2	1:A:98:ILE:HG12	2.51	0.46
1:A:71:GLY:O	1:A:73[B]:ARG:NH1	2.50	0.45
1:A:58:ILE:HB	1:A:83:LEU:HD13	2.01	0.42
1:A:111:TRP:CD1	1:A:115:CYS:HB2	2.56	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/129 (113%)	145 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/105 (119%)	125 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	1PE	A	1148	-	6,6,15	0.07	0	5,5,14	0.33	0
4	1PE	A	1147	-	7,7,15	0.17	0	6,6,14	0.28	0
5	EDO	A	1149	-	3,3,3	0.43	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	A	1148	-	-	0/4/4/13	-
4	1PE	A	1147	-	-	2/5/5/13	-
5	EDO	A	1149	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1147	1PE	C23-C13-OH4-C24
5	A	1149	EDO	O1-C1-C2-O2
4	A	1147	1PE	OH4-C13-C23-OH3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	129/129 (100%)	-0.09	4 (3%) 49 49	14, 19, 29, 49	2 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47[A]	THR	3.4
1	A	129	LEU	3.1
1	A	71	GLY	2.7
1	A	70	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1149	4/?	0.57	0.20	75,76,76,76	0
4	1PE	A	1147	8/?	0.68	0.12	56,57,57,58	0
4	1PE	A	1148	7/?	0.88	0.12	55,55,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	1138	1/?	0.99	0.03	26,26,26,26	1
3	NA	A	1146	1/?	1.00	0.03	23,23,23,23	0
2	CL	A	1137	1/?	1.00	0.12	20,20,20,20	1
2	CL	A	1139	1/?	1.00	0.02	25,25,25,25	1
3	NA	A	1145	1/?	1.00	0.03	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2023 – 04:35 pm GMT

Deposition ID : D_1292128510

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

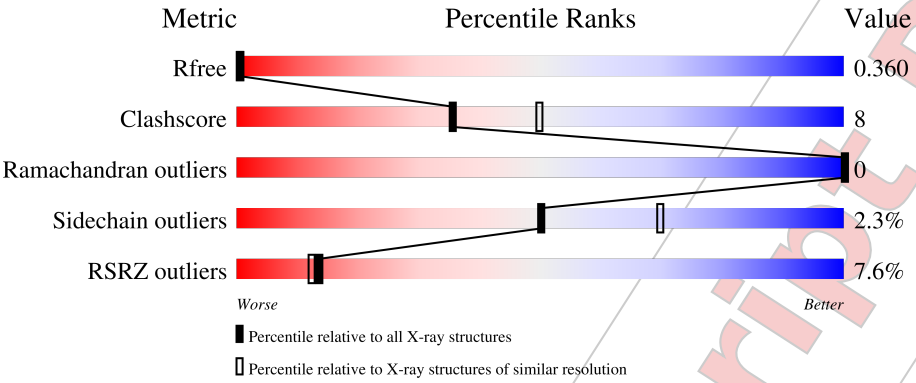
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	265	8% 80% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LFA	A	403	-	-	-	X
2	LFA	A	410	-	-	-	X
2	LFA	A	411	-	-	-	X
2	LFA	A	412	-	-	-	X
2	LFA	A	414	-	-	-	X
2	LFA	A	415	-	-	-	X
2	LFA	A	416	-	-	-	X
2	LFA	A	417	-	-	-	X
2	LFA	A	419	-	-	-	X
2	LFA	A	422	-	-	-	X
2	LFA	A	423	-	-	-	X
2	LFA	A	425	-	-	-	X
2	LFA	A	427	-	-	-	X

2 Entry composition

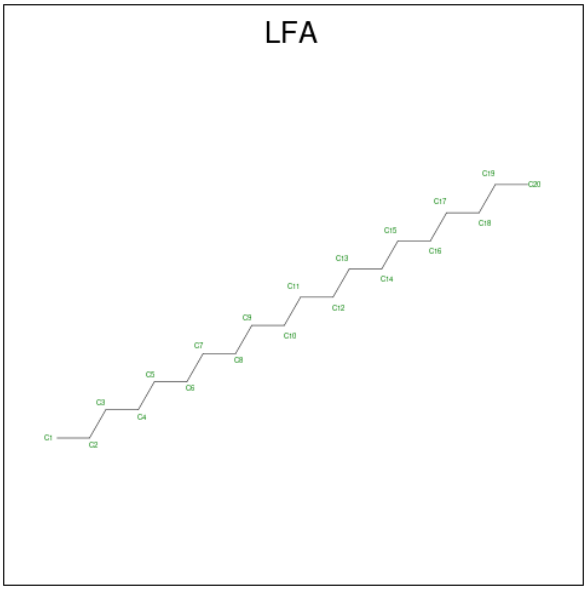
There are 3 unique types of molecules in this entry. The entry contains 2448 atoms, of which 55 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Krokinobacter eikastus rhodopsin 2 (KR2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	265	2143	1419	28	318	369	9	0	3	0

- Molecule 2 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
2	A	1	16	16	0	0
2	A	1	Total 8	C 8	0	0
2	A	1	Total 6	C 6	0	0
2	A	1	Total 6	C 6	0	0
2	A	1	Total 13	C 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C H 40 13 27	0	0

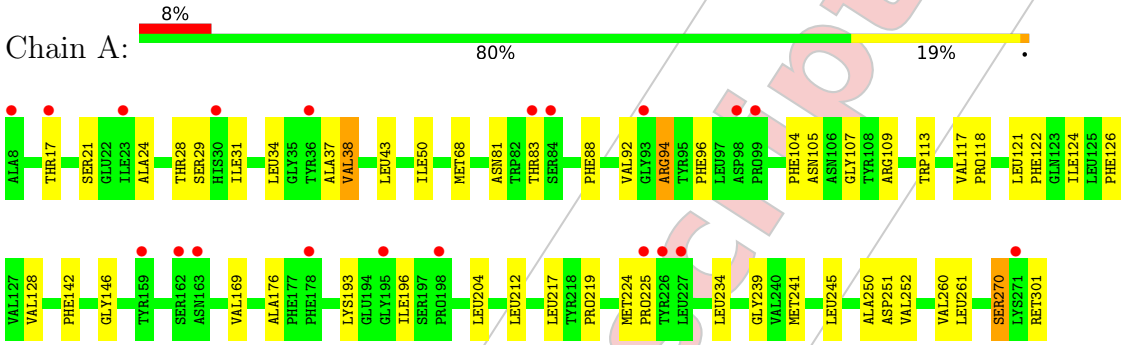
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	62	Total O 62 62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Krokinobacter eikastus rhodopsin 2 (KR2)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	41.46Å 84.89Å 234.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.83 – 2.40 14.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (14.83-2.40) 94.0 (14.83-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.327 , 0.358 0.327 , 0.360	Depositor DCC
R_{free} test set	780 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 93.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	2448	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, LFA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	1/2159 (0.0%)	0.52	0/2940

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	SER	CA-CB	-5.59	1.44	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2115	28	2092	36	1
2	A	216	27	389	13	1
3	S	62	0	0	0	0
All	All	2393	55	2481	39	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:407:LFA:H13	2:A:407:LFA:H51	1.71	0.72
1:A:34:LEU:O	1:A:38:VAL:HG13	1.93	0.67
2:A:423:LFA:H42	2:A:423:LFA:H82	1.83	0.60
1:A:301:RET:H161	1:A:301:RET:C8	2.34	0.57
1:A:301:RET:H161	1:A:301:RET:H8	1.86	0.56
1:A:81:ASN:HD21	1:A:105:ASN:H	1.58	0.52
1:A:81:ASN:ND2	1:A:105:ASN:H	2.07	0.52
1:A:117:VAL:N	1:A:118:PRO:HD2	2.24	0.52
1:A:212:LEU:HD22	2:A:425:LFA:H31	1.91	0.52
1:A:21:SER:HB3	1:A:94:ARG:NH2	2.27	0.50
1:A:252:VAL:HG11	2:A:405:LFA:H51	1.94	0.48
1:A:17:THR:HG22	2:A:428:LFA:H171	1.95	0.47
1:A:24:ALA:HA	1:A:241:MET:SD	2.55	0.46
1:A:126:PHE:HE1	2:A:418:LFA:H51	1.80	0.46
1:A:81:ASN:HD21	1:A:104:PHE:HA	1.81	0.46
1:A:117:VAL:HG11	1:A:146:GLY:HA3	1.98	0.46
1:A:113:TRP:O	1:A:117:VAL:HG23	2.15	0.45
1:A:128:VAL:HG11	1:A:204:LEU:HD21	1.98	0.45
1:A:92:VAL:HG11	1:A:96:PHE:HZ	1.82	0.45
1:A:118:PRO:O	1:A:122:PHE:HB2	2.17	0.45
1:A:217:LEU:HB2	1:A:250:ALA:HB2	1.98	0.45
1:A:261:LEU:HD21	2:A:423:LFA:H62	1.99	0.45
1:A:224:MET:N	1:A:225:PRO:HD2	2.32	0.44
1:A:37:ALA:HB1	2:A:415:LFA:H51	1.99	0.44
1:A:107:GLY:HA3	2:A:407:LFA:H81	2.00	0.44
1:A:301:RET:H7	1:A:301:RET:H181	1.87	0.44
1:A:234:LEU:O	1:A:239:GLY:HA3	2.19	0.43
1:A:31:ILE:HG12	1:A:245:LEU:HD23	2.01	0.42
1:A:121:LEU:O	1:A:124:ILE:HG22	2.19	0.41
1:A:260:VAL:HG21	2:A:402:LFA:H51	2.03	0.41
1:A:29:SER:HB3	1:A:83:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:NH1	1:A:251:ASP:OD2	2.54	0.41
1:A:28:THR:O	1:A:31:ILE:HG22	2.21	0.41
1:A:193:LYS:O	1:A:196:ILE:HG12	2.21	0.41
1:A:219:PRO:HB3	1:A:301:RET:H183	2.02	0.41
1:A:176:ALA:HB1	2:A:419:LFA:H52	2.03	0.40
2:A:423:LFA:H42	2:A:423:LFA:C8	2.51	0.40
1:A:43:LEU:N	1:A:68:MET:HG3	2.36	0.40
1:A:169:VAL:HG11	2:A:404:LFA:H31	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:CG2	2:A:428:LFA:H131[3_857]	1.41	0.19

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/265 (100%)	256 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	221/226 (98%)	216 (98%)	5 (2%)	50 70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	50	ILE
1	A	88	PHE
1	A	142	PHE
1	A	270	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LFA	A	425	-	8,8,19	0.32	0	7,7,18	0.73	0
2	LFA	A	426	-	9,9,19	0.30	0	8,8,18	0.79	0
2	LFA	A	415	-	4,4,19	0.33	0	3,3,18	0.54	0
2	LFA	A	405	-	5,5,19	0.32	0	4,4,18	0.57	0
2	LFA	A	421	-	3,3,19	0.41	0	2,2,18	0.74	0
2	LFA	A	413	-	4,4,19	0.33	0	3,3,18	0.53	0
2	LFA	A	411	-	11,11,19	0.30	0	10,10,18	0.83	0
2	LFA	A	414	-	9,9,19	0.31	0	8,8,18	0.78	0
2	LFA	A	427	-	11,11,19	0.30	0	10,10,18	0.83	0
2	LFA	A	402	-	15,15,19	0.30	0	14,14,18	0.87	0
2	LFA	A	422	-	5,5,19	0.32	0	4,4,18	0.54	0
2	LFA	A	408	-	9,9,19	0.30	0	8,8,18	0.81	0
2	LFA	A	404	-	5,5,19	0.31	0	4,4,18	0.57	0
2	LFA	A	403	-	7,7,19	0.30	0	6,6,18	0.74	0
2	LFA	A	410	-	7,7,19	0.32	0	6,6,18	0.68	0
2	LFA	A	412	-	10,10,19	0.30	0	9,9,18	0.81	0
2	LFA	A	419	-	5,5,19	0.32	0	4,4,18	0.57	0
2	LFA	A	418	-	8,8,19	0.31	0	7,7,18	0.74	0
2	LFA	A	416	-	9,9,19	0.30	0	8,8,18	0.78	0
2	LFA	A	407	-	12,12,19	0.31	0	11,11,18	0.81	0
2	LFA	A	428	-	12,12,19	0.30	0	11,11,18	0.91	0
2	LFA	A	424	-	2,2,19	0.34	0	0,1,18	-	-
2	LFA	A	423	-	9,9,19	0.32	0	8,8,18	0.75	0
2	LFA	A	417	-	8,8,19	0.31	0	7,7,18	0.74	0
2	LFA	A	420	-	4,4,19	0.32	0	3,3,18	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	425	-	-	0/6/6/17	-
2	LFA	A	426	-	-	2/7/7/17	-
2	LFA	A	415	-	-	0/2/2/17	-
2	LFA	A	405	-	-	0/3/3/17	-
2	LFA	A	421	-	-	1/1/1/17	-
2	LFA	A	413	-	-	0/2/2/17	-
2	LFA	A	411	-	-	1/9/9/17	-
2	LFA	A	414	-	-	0/7/7/17	-
2	LFA	A	427	-	-	0/9/9/17	-
2	LFA	A	402	-	-	1/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	422	-	-	0/3/3/17	-
2	LFA	A	408	-	-	0/7/7/17	-
2	LFA	A	404	-	-	0/3/3/17	-
2	LFA	A	403	-	-	0/5/5/17	-
2	LFA	A	410	-	-	1/5/5/17	-
2	LFA	A	412	-	-	1/8/8/17	-
2	LFA	A	419	-	-	0/3/3/17	-
2	LFA	A	418	-	-	3/6/6/17	-
2	LFA	A	416	-	-	1/7/7/17	-
2	LFA	A	407	-	-	3/10/10/17	-
2	LFA	A	428	-	-	7/10/10/17	-
2	LFA	A	423	-	-	2/7/7/17	-
2	LFA	A	417	-	-	1/6/6/17	-
2	LFA	A	420	-	-	0/2/2/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	421	LFA	C3-C4-C5-C6
2	A	428	LFA	C12-C13-C14-C15
2	A	428	LFA	C14-C15-C16-C17
2	A	417	LFA	C6-C7-C8-C9
2	A	407	LFA	C9-C10-C11-C12
2	A	418	LFA	C3-C4-C5-C6
2	A	423	LFA	C5-C6-C7-C8
2	A	423	LFA	C3-C4-C5-C6
2	A	407	LFA	C4-C5-C6-C7
2	A	428	LFA	C11-C12-C13-C14
2	A	428	LFA	C17-C18-C19-C20
2	A	428	LFA	C11-C10-C9-C8
2	A	407	LFA	C1-C2-C3-C4
2	A	402	LFA	C11-C12-C13-C14
2	A	428	LFA	C10-C11-C12-C13
2	A	418	LFA	C1-C2-C3-C4
2	A	426	LFA	C6-C7-C8-C9
2	A	416	LFA	C5-C6-C7-C8
2	A	410	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	418	LFA	C4-C5-C6-C7
2	A	411	LFA	C6-C7-C8-C9
2	A	428	LFA	C9-C10-C11-C12
2	A	426	LFA	C3-C4-C5-C6
2	A	412	LFA	C11-C10-C9-C8

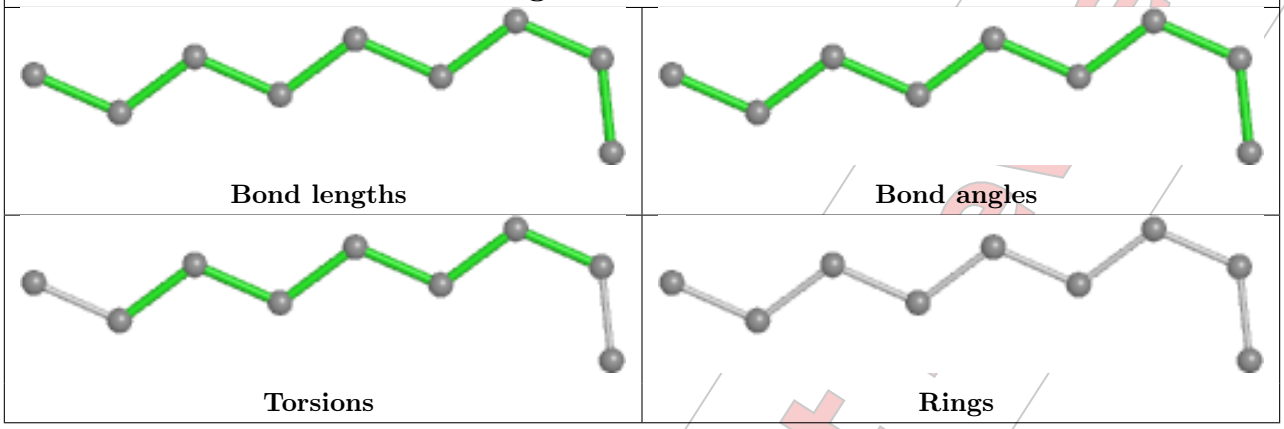
There are no ring outliers.

10 monomers are involved in 14 short contacts:

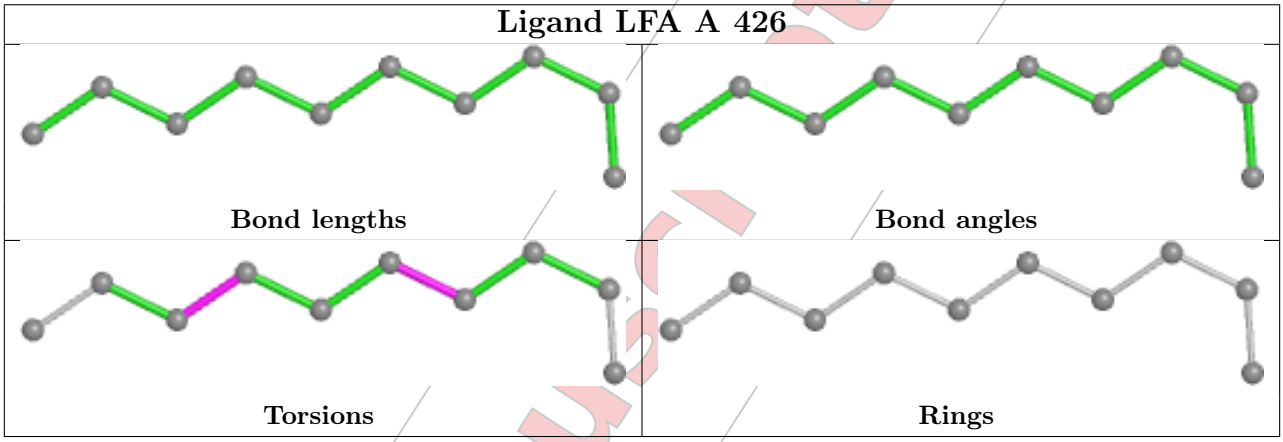
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	425	LFA	1	0
2	A	415	LFA	1	0
2	A	405	LFA	1	0
2	A	402	LFA	1	0
2	A	404	LFA	1	0
2	A	419	LFA	1	0
2	A	418	LFA	1	0
2	A	407	LFA	2	0
2	A	428	LFA	1	1
2	A	423	LFA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

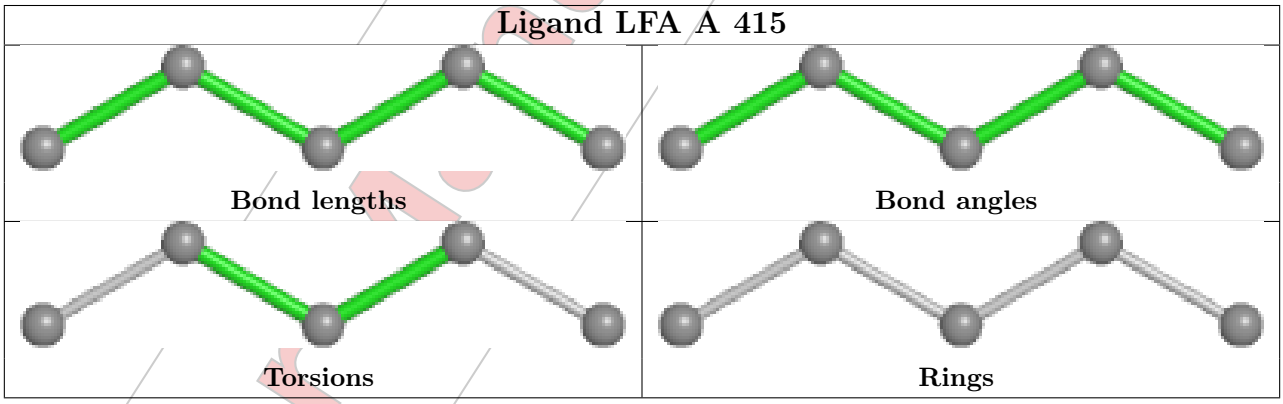
Ligand LFA A 425



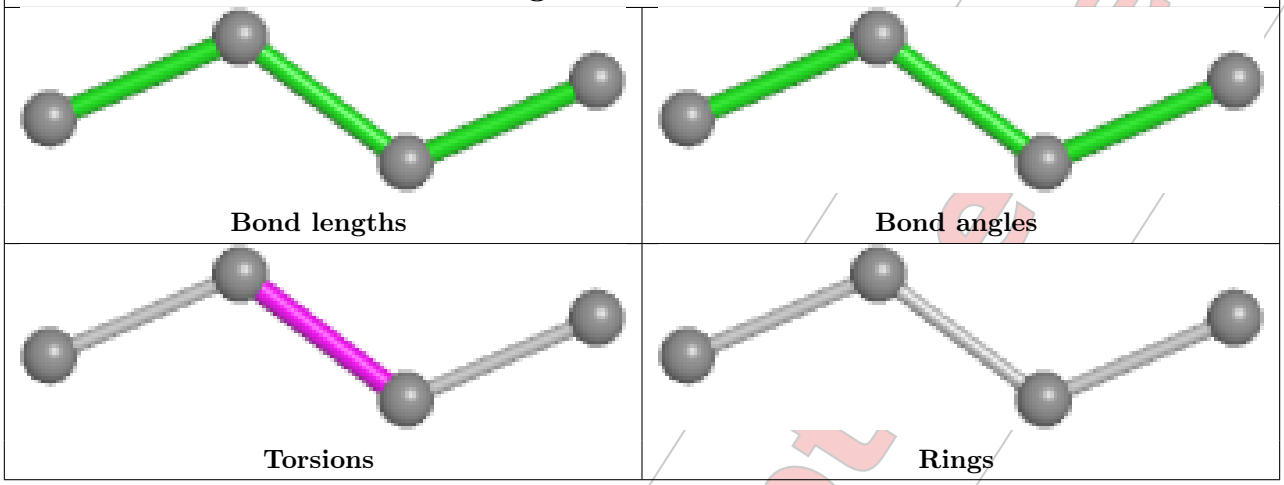
Ligand LFA A 426



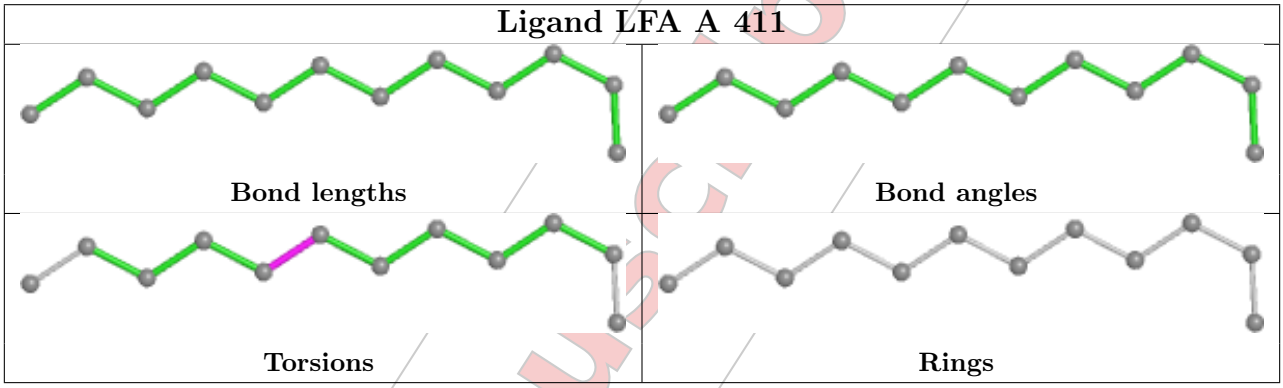
Ligand LFA A 415



Ligand LFA A 421



Ligand LFA A 411



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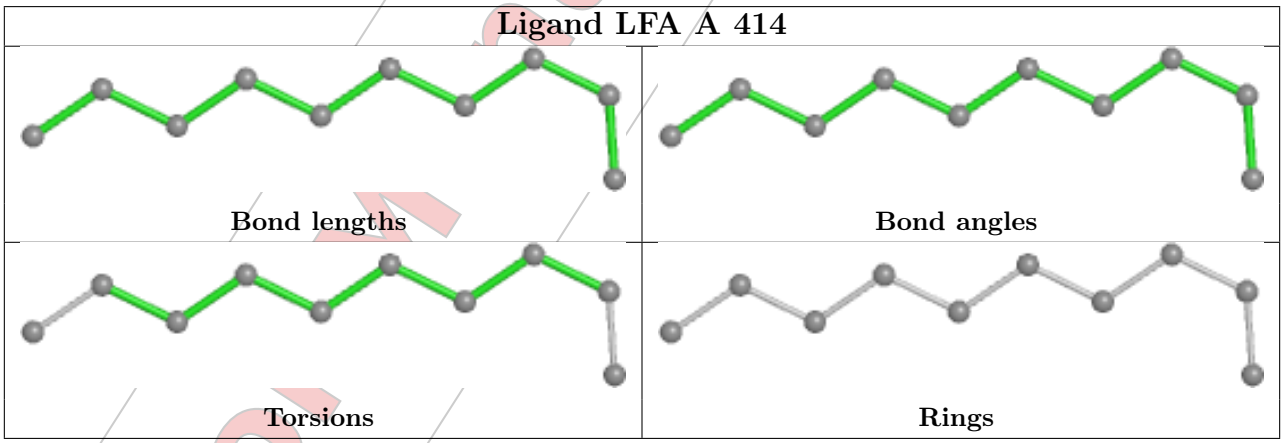
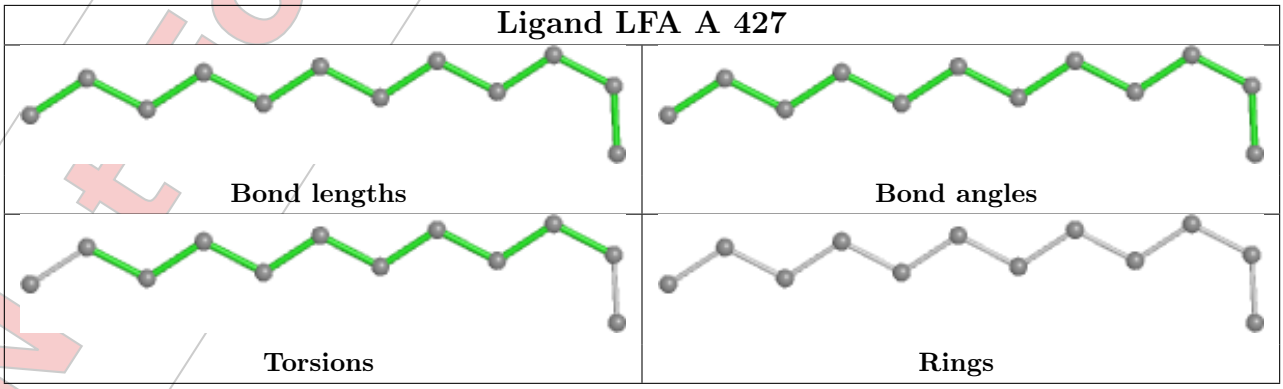


Ligand LFA A 427



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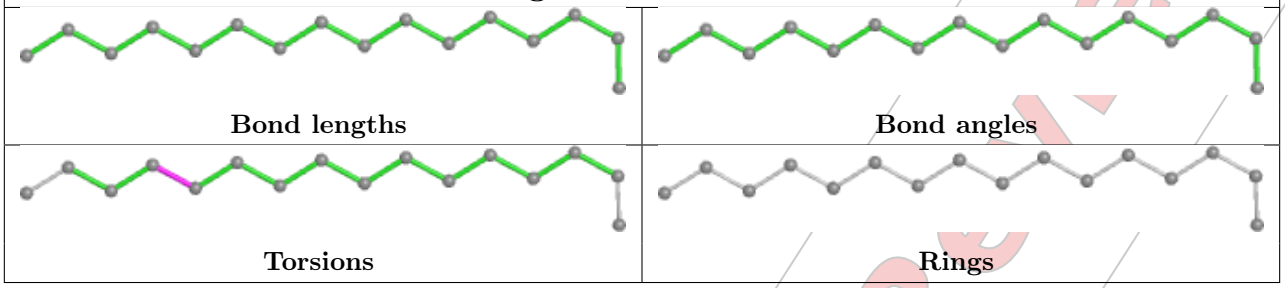

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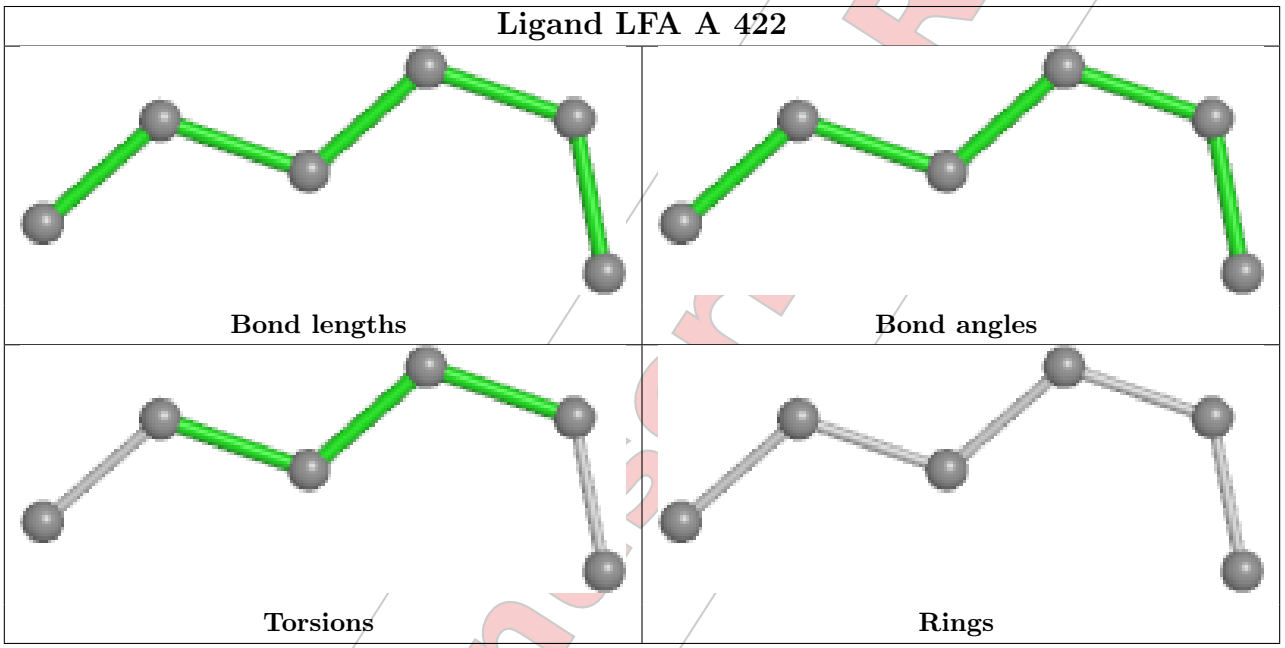
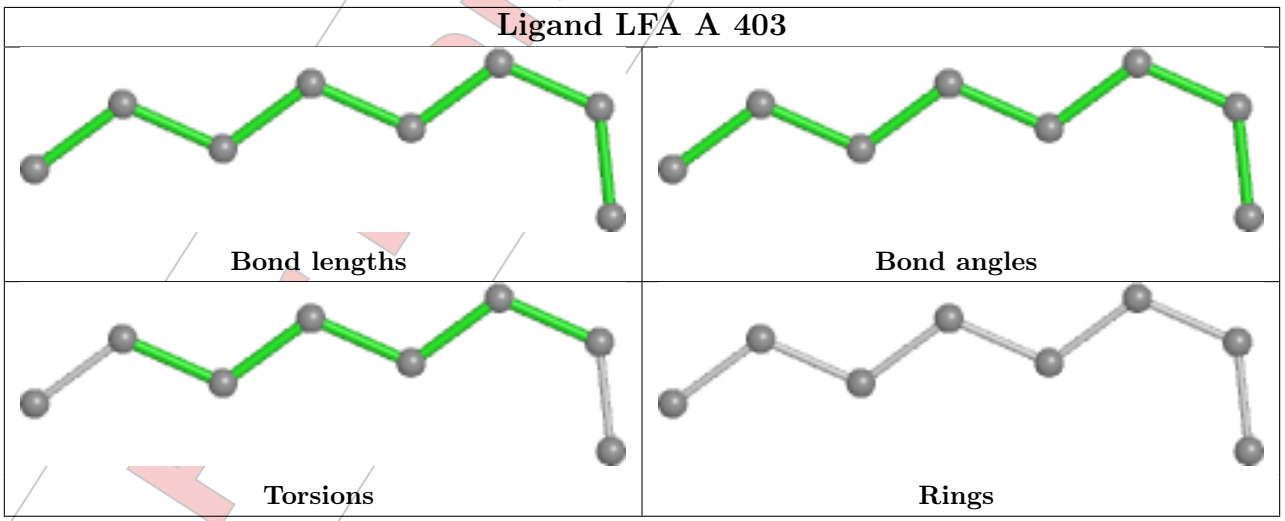
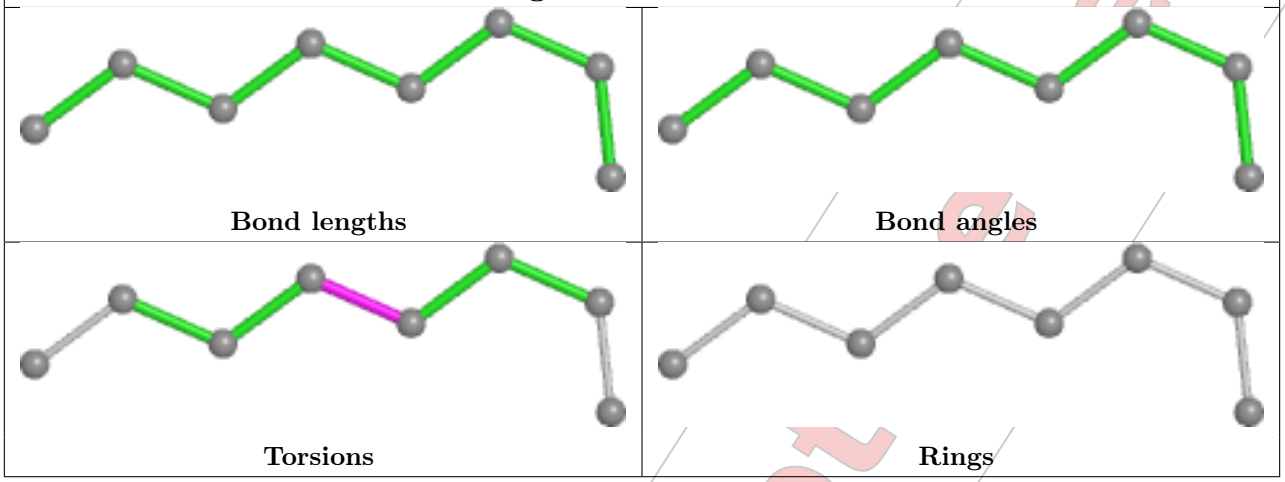


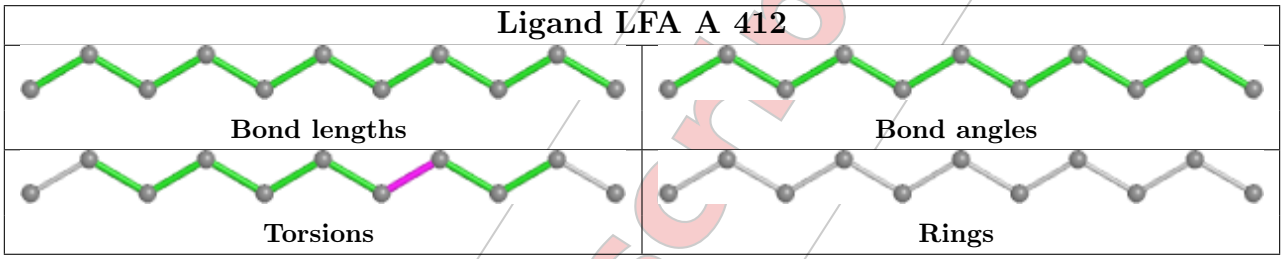
Ligand LFA A 403



Ligand LFA A 410



Ligand LFA A 412



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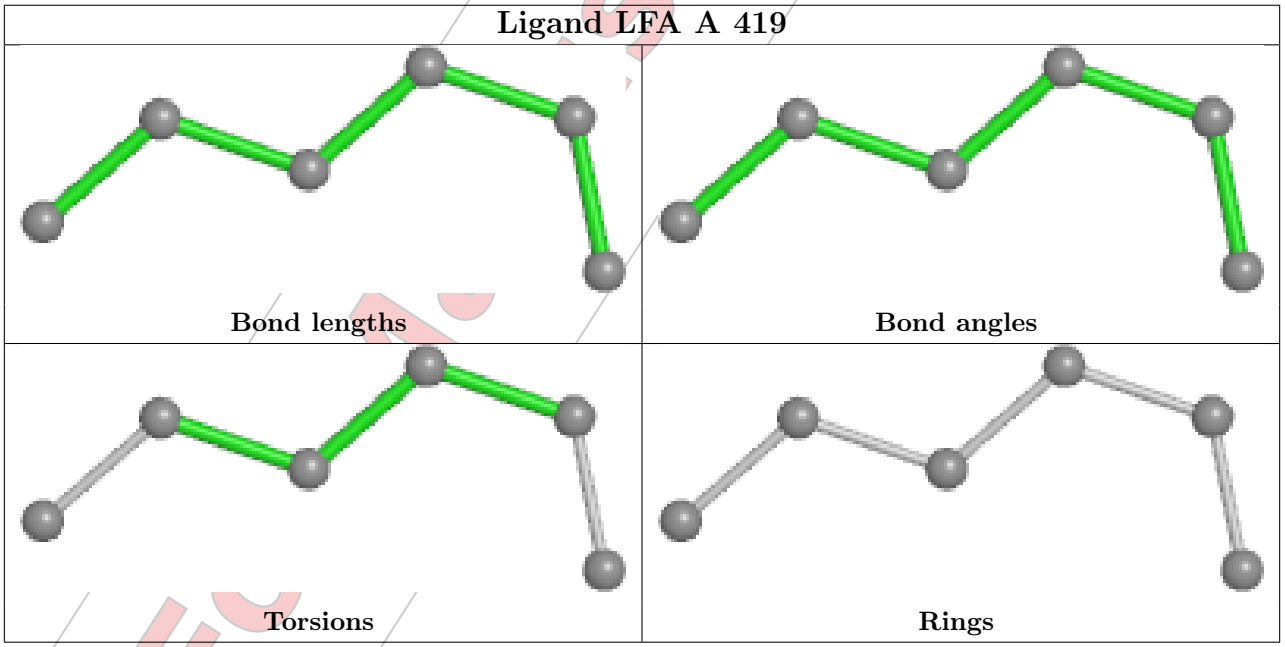

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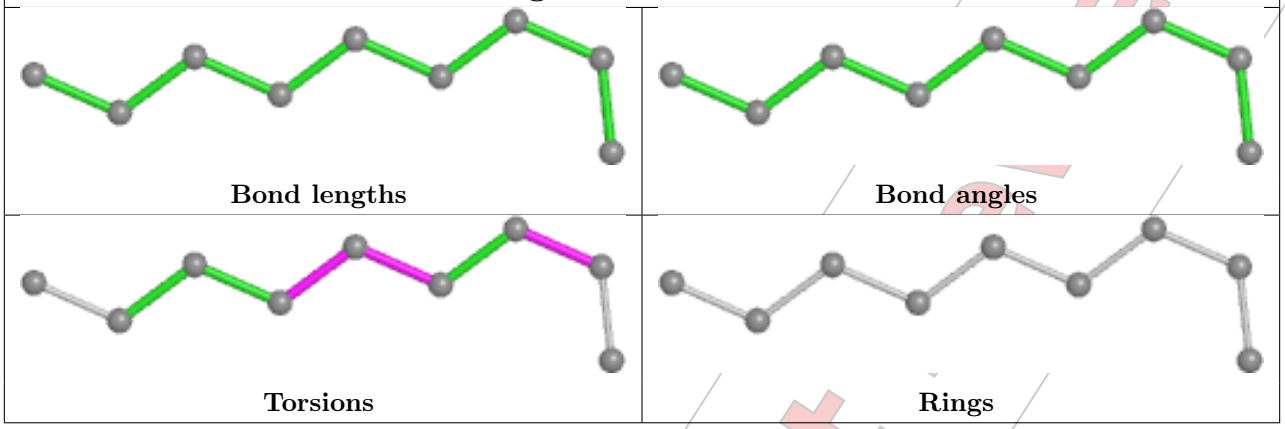

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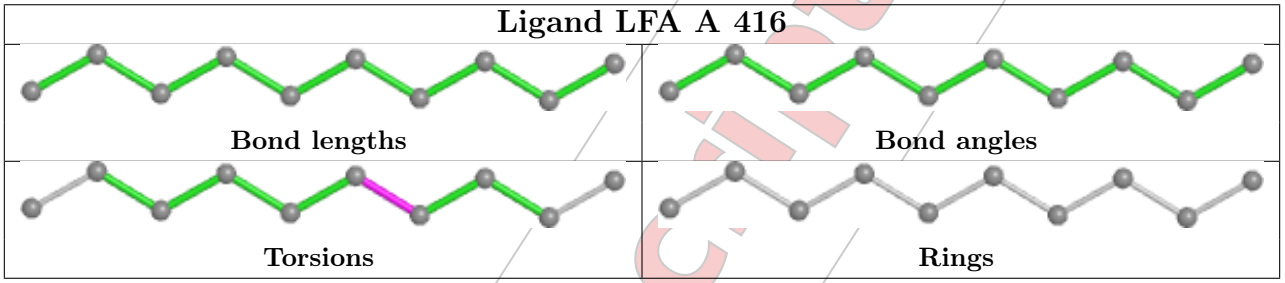
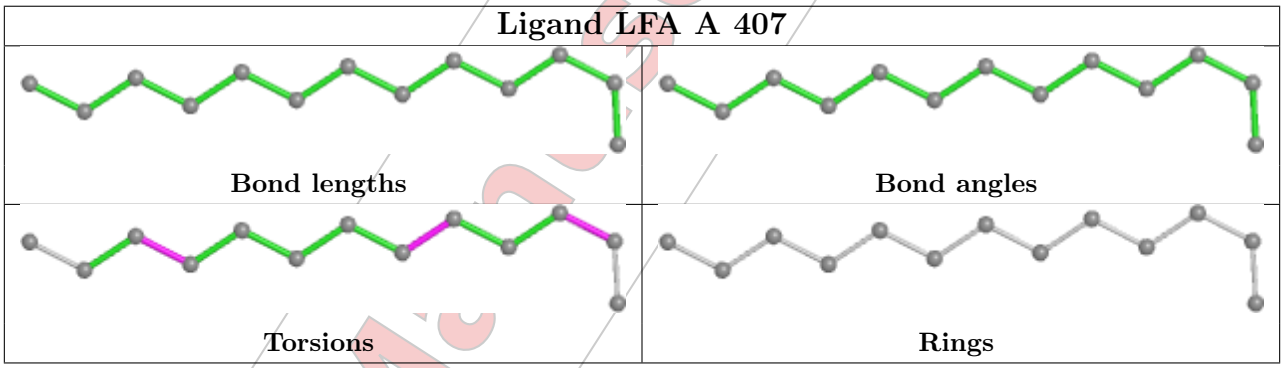
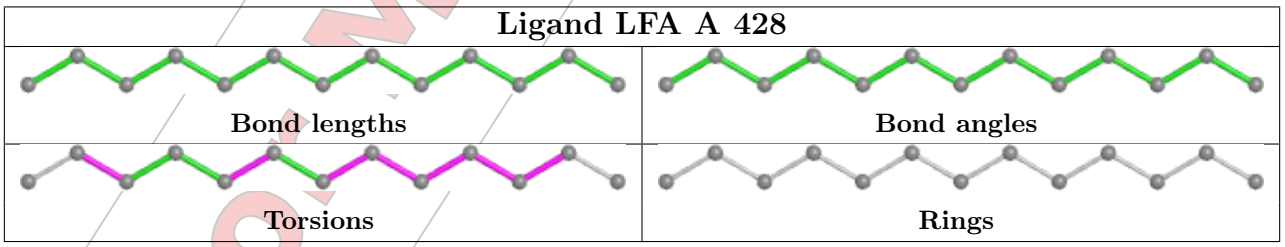
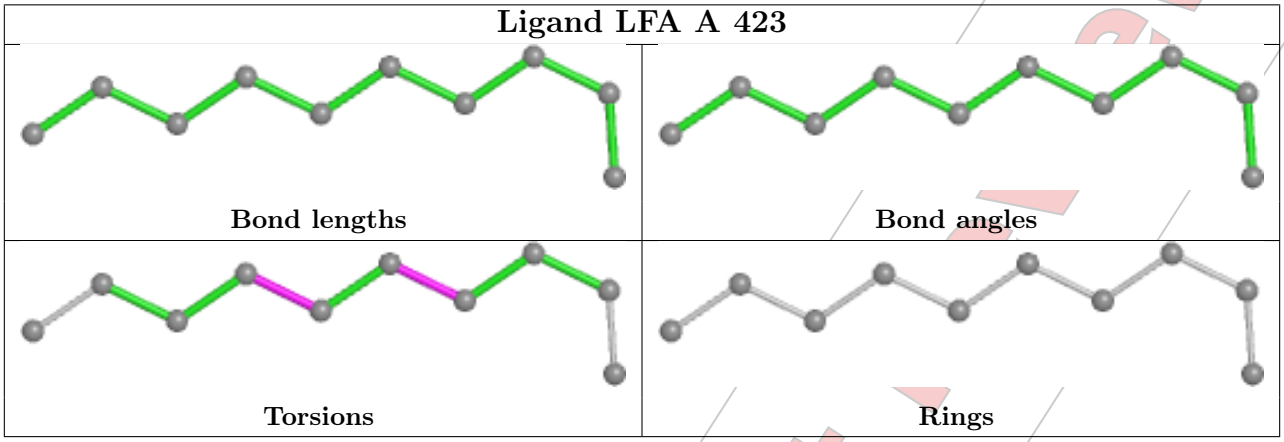


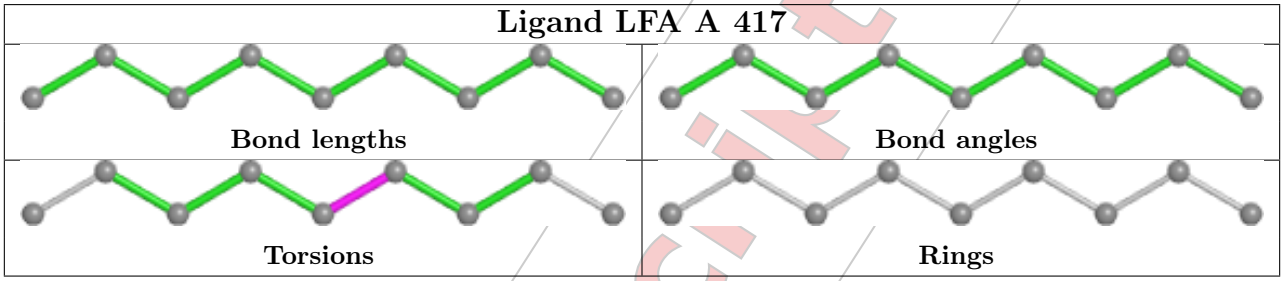
Ligand LFA A 407



Ligand LFA A 428







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	264/265 (99%)	0.40	20 (7%)	13	12	15, 33, 69, 89	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ASP	3.2
1	A	8	ALA	3.1
1	A	163	ASN	3.1
1	A	99	PRO	3.0
1	A	23	ILE	2.9
1	A	227	LEU	2.9
1	A	36	TYR	2.8
1	A	93	GLY	2.7
1	A	159	TYR	2.5
1	A	17	THR	2.4
1	A	225	PRO	2.4
1	A	195	GLY	2.3
1	A	84	SER	2.3
1	A	271	LYS	2.2
1	A	83	THR	2.2
1	A	30	HIS	2.1
1	A	198	PRO	2.1
1	A	162	SER	2.0
1	A	226	TYR	2.0
1	A	178	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

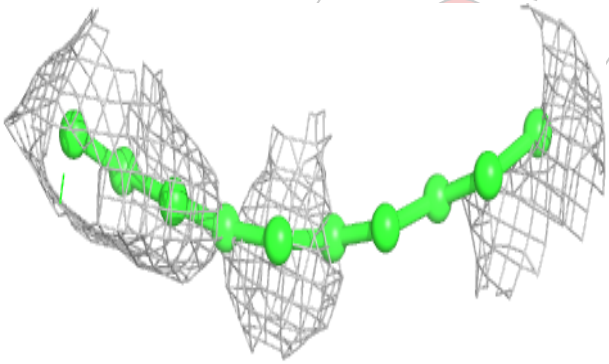
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

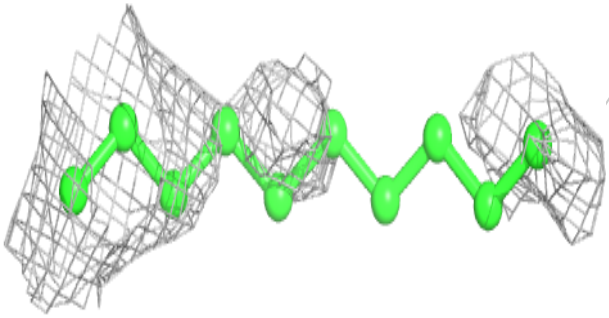
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	A	414	10/?	0.17	0.54	53,76,95,100	0
2	LFA	A	412	11/?	0.24	0.50	53,61,70,73	0
2	LFA	A	424	3/?	0.25	0.35	57,57,57,68	0
2	LFA	A	422	6/?	0.26	0.55	50,66,73,78	0
2	LFA	A	427	12/?	0.36	0.48	36,56,64,66	0
2	LFA	A	403	8/?	0.48	0.48	34,35,39,39	8
2	LFA	A	417	9/?	0.51	0.55	57,71,77,83	0
2	LFA	A	415	5/?	0.53	0.42	34,36,47,51	0
2	LFA	A	416	10/?	0.53	0.40	48,50,57,58	0
2	LFA	A	413	5/?	0.55	0.40	46,49,58,61	0
2	LFA	A	410	8/?	0.56	0.43	40,43,48,56	0
2	LFA	A	411	12/?	0.59	0.49	52,58,60,70	0
2	LFA	A	423	10/?	0.59	0.40	41,46,53,56	0
2	LFA	A	418	9/?	0.60	0.26	37,47,50,51	0
2	LFA	A	407	13/?	0.63	0.28	36,42,52,53	0
2	LFA	A	428	13/?	0.64	0.26	65,79,82,83	40
2	LFA	A	420	5/?	0.66	0.23	39,44,51,55	0
2	LFA	A	426	10/?	0.66	0.32	44,48,57,58	0
2	LFA	A	425	9/?	0.67	0.56	41,54,76,79	0
2	LFA	A	405	6/?	0.70	0.24	47,52,56,58	0
2	LFA	A	419	6/?	0.73	0.47	38,45,57,58	0
2	LFA	A	404	6/?	0.75	0.20	41,45,51,51	0
2	LFA	A	421	4/?	0.76	0.36	35,36,44,49	0
2	LFA	A	408	10/?	0.79	0.31	32,37,44,46	0
2	LFA	A	402	16/?	0.80	0.18	30,39,46,46	0

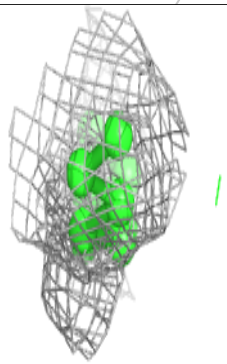
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LFA A 414:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

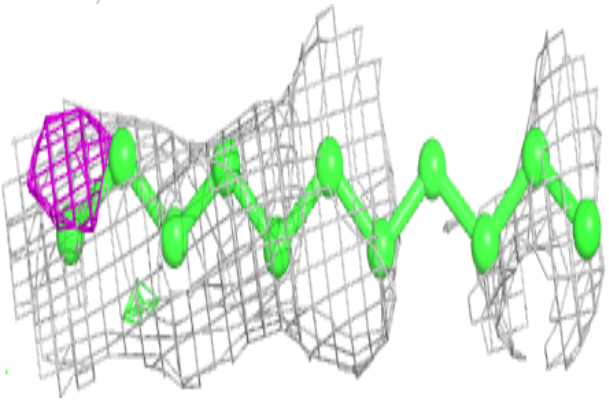


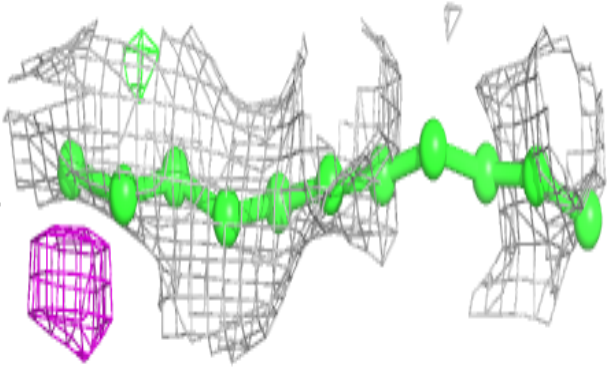


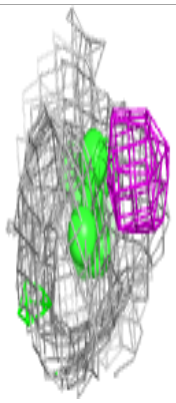


Electron density around LFA A 412:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

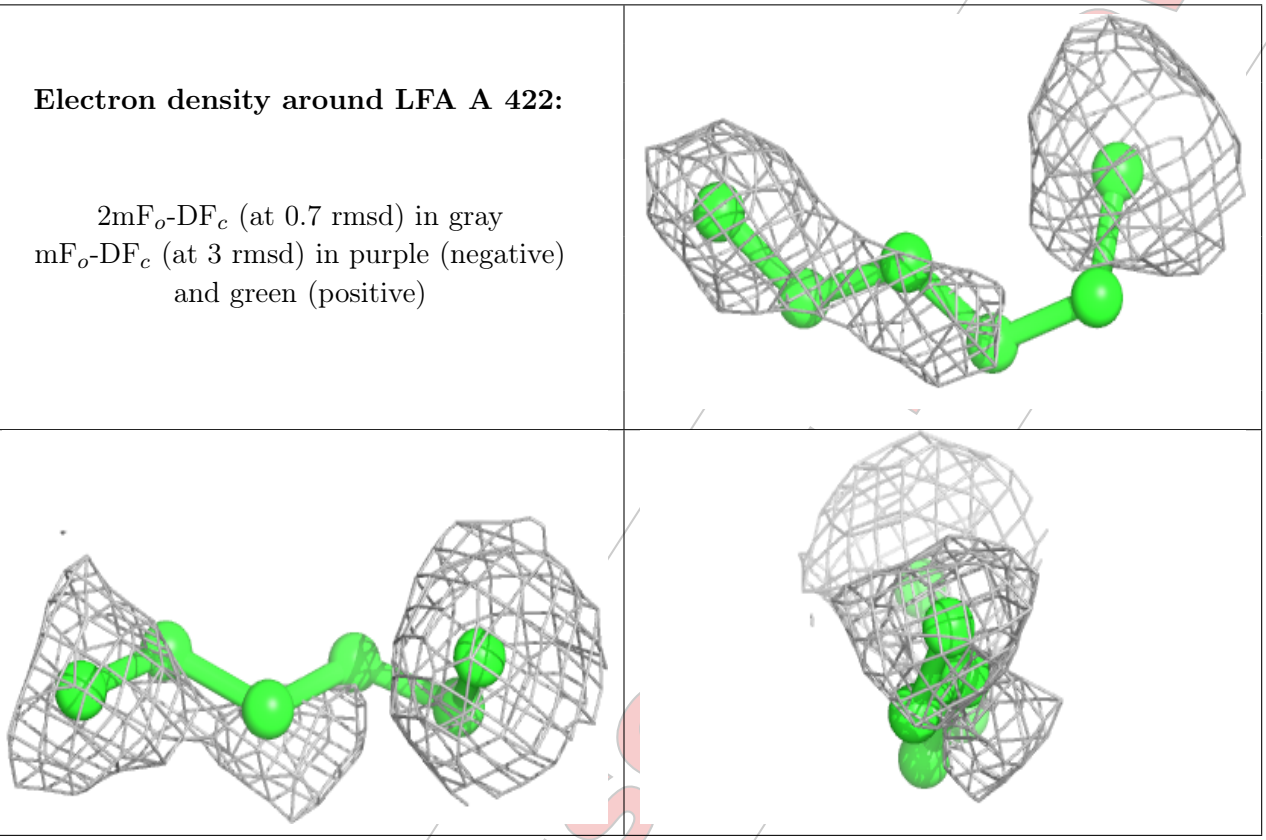






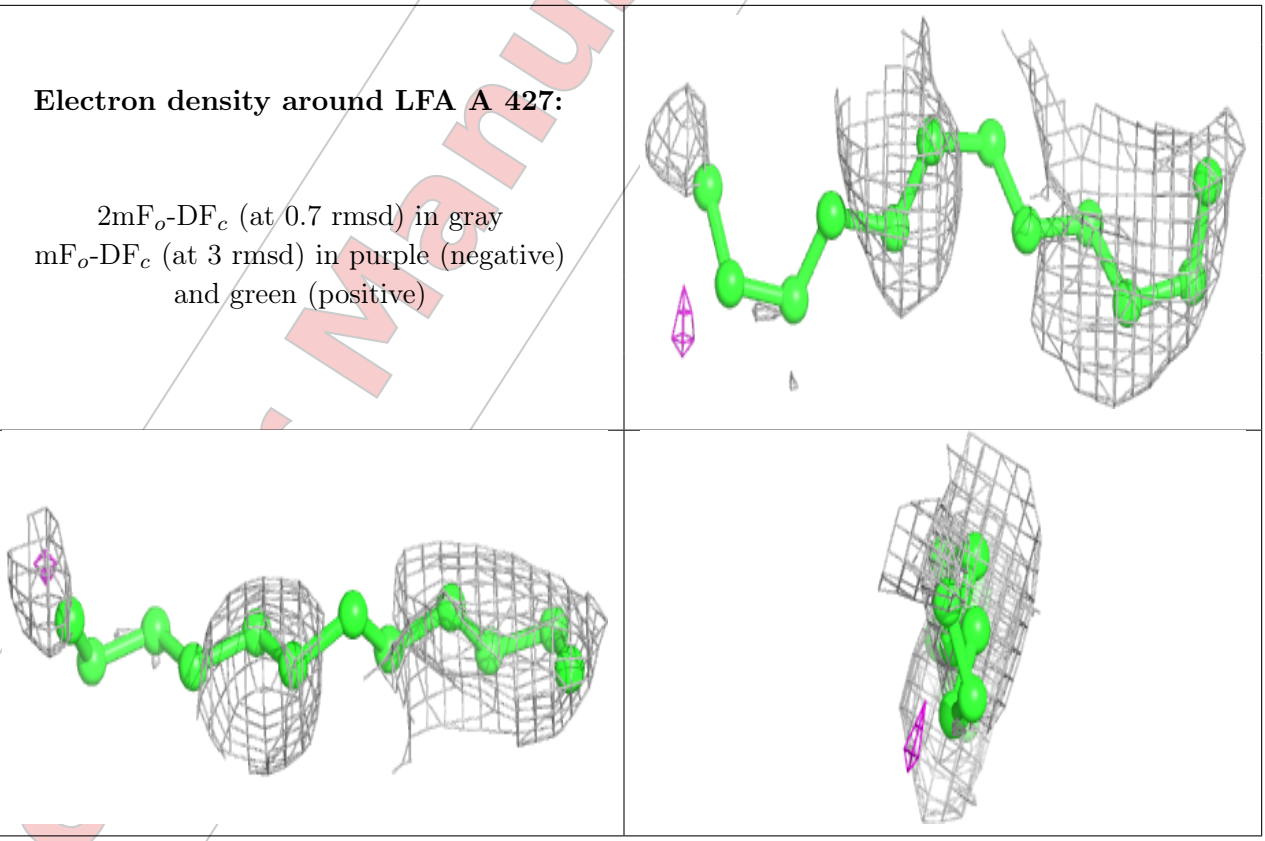
Electron density around LFA A 422:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



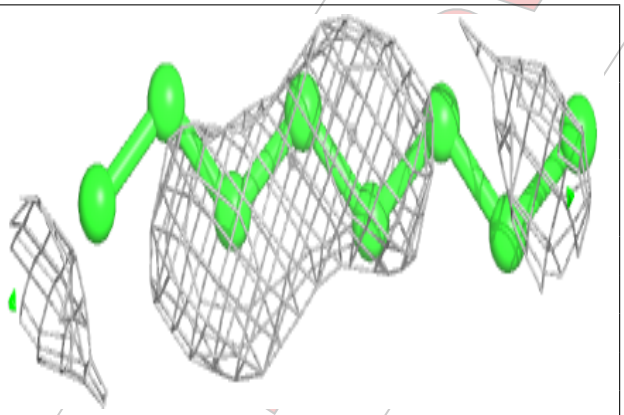
Electron density around LFA A 427:

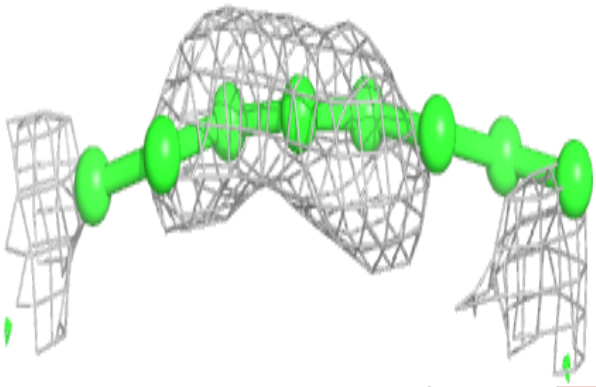
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

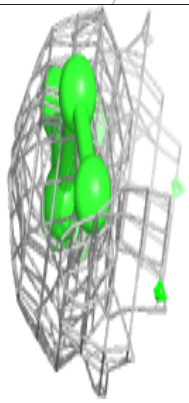


Electron density around LFA A 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

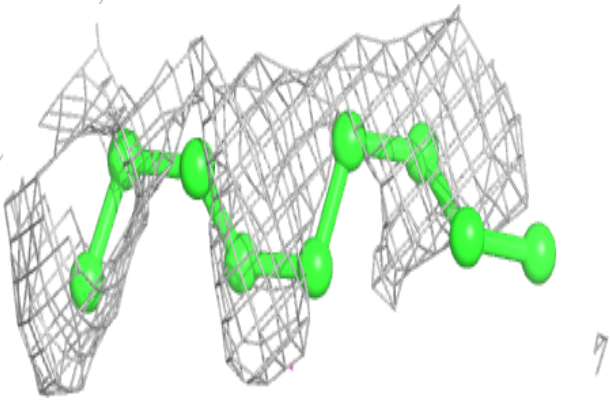


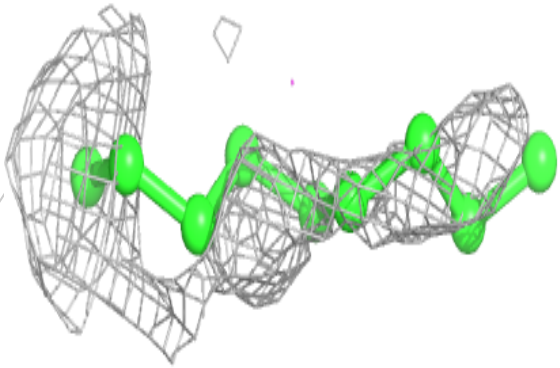


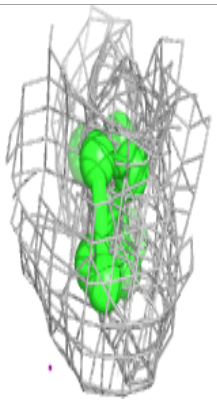


Electron density around LFA A 417:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

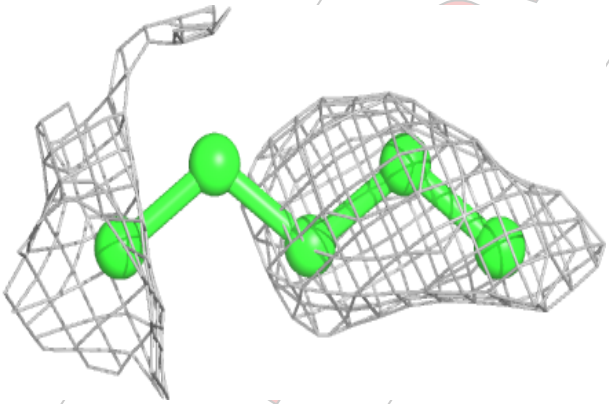


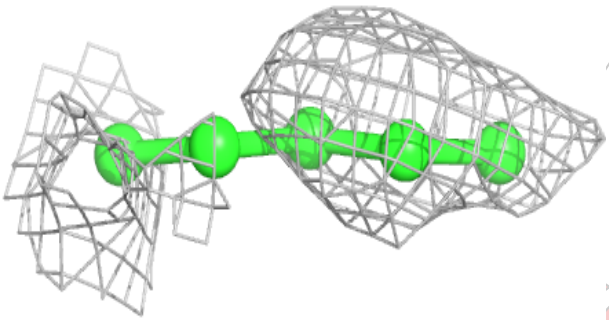


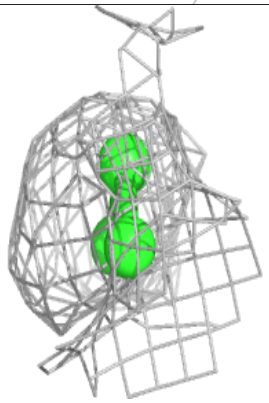


Electron density around LFA A 415:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

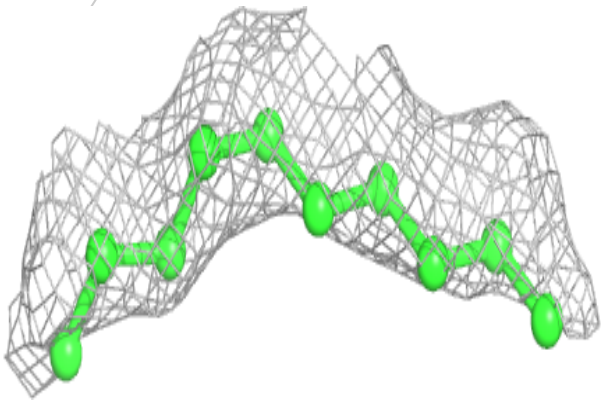


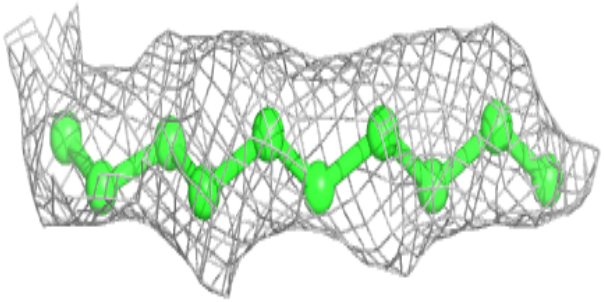


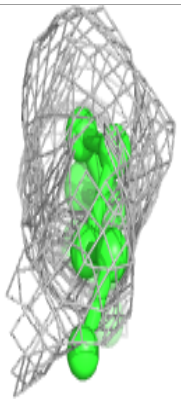


Electron density around LFA A 416:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

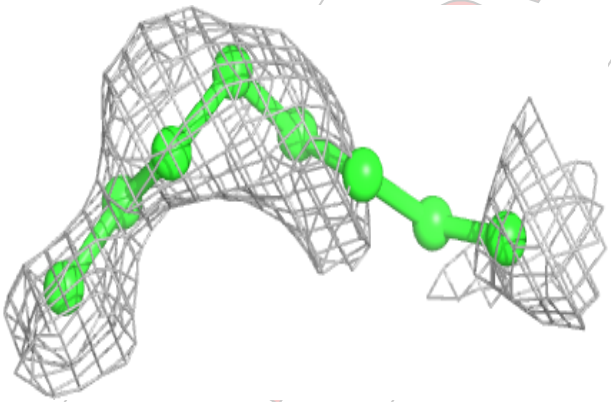


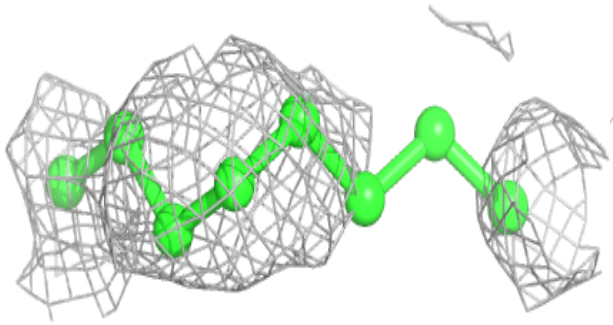


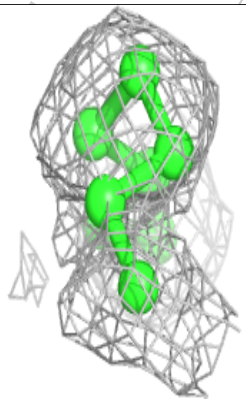


Electron density around LFA A 410:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

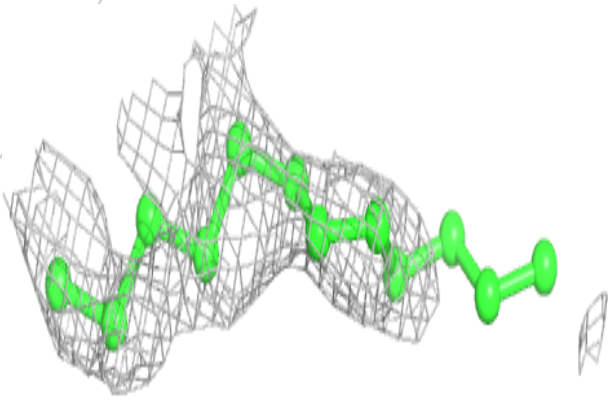


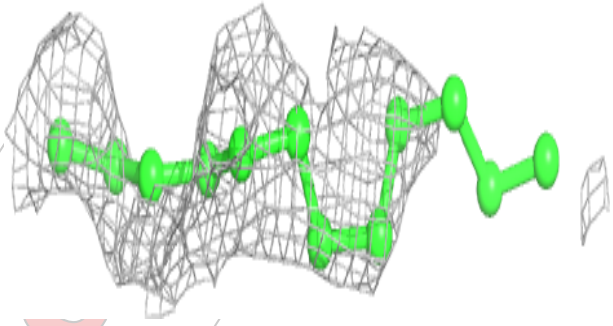


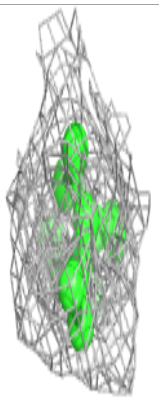


Electron density around LFA A 411:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

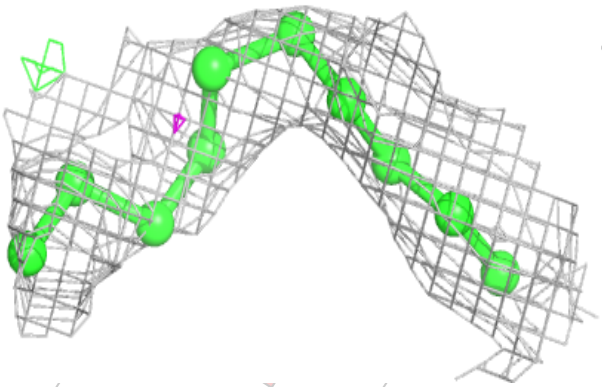


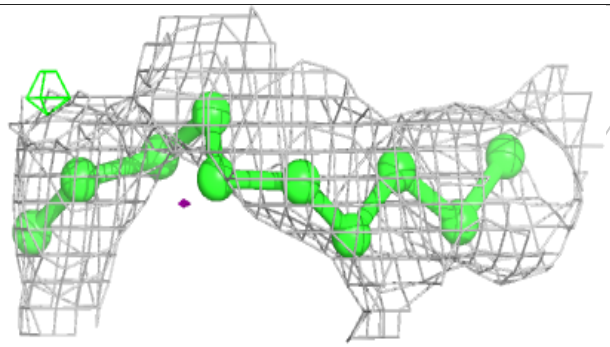


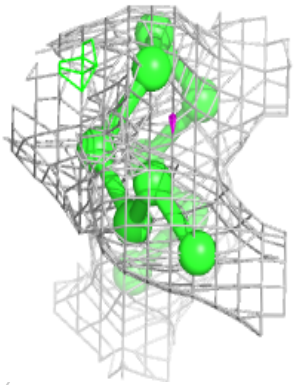


Electron density around LFA A 423:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

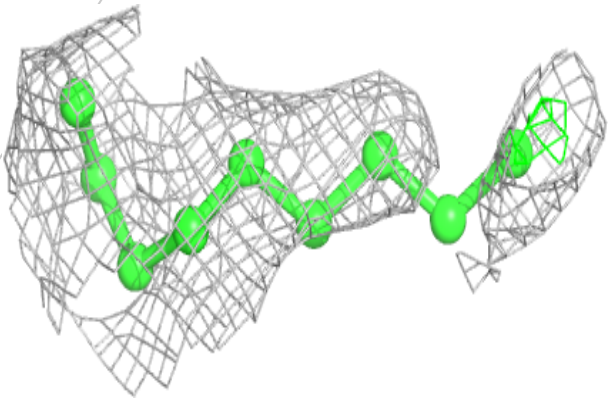


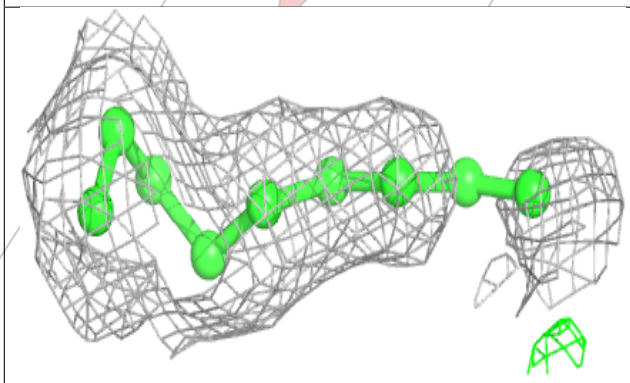


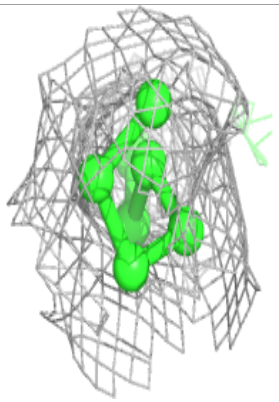


Electron density around LFA A 418:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

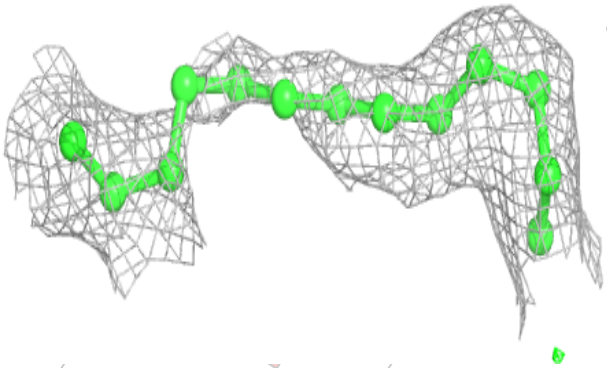


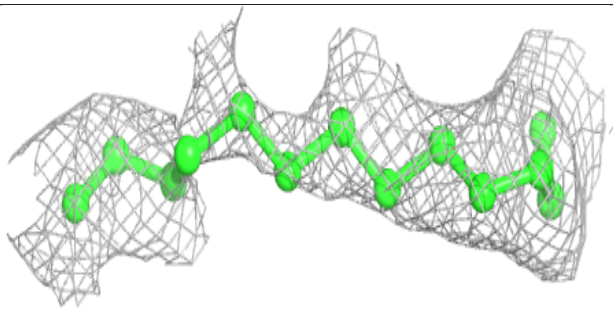


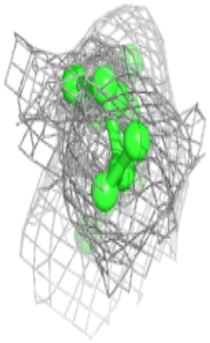


Electron density around LFA A 407:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

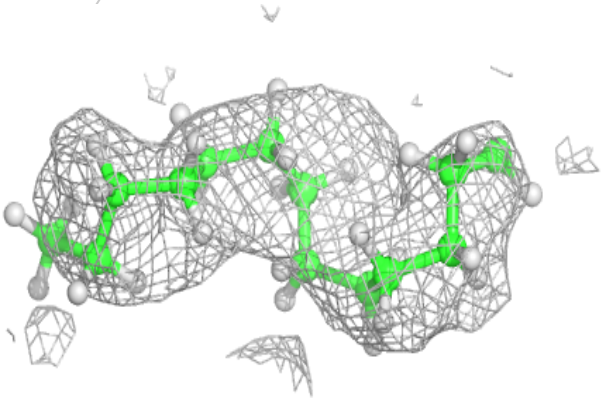


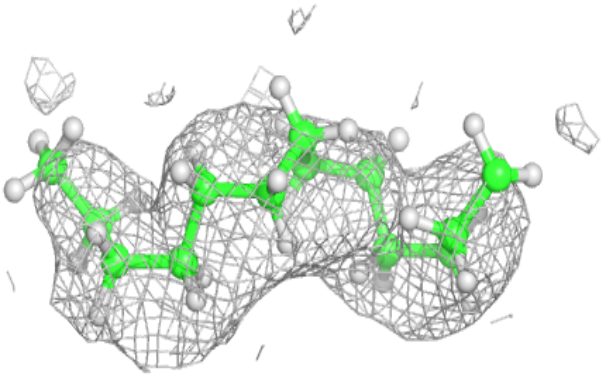


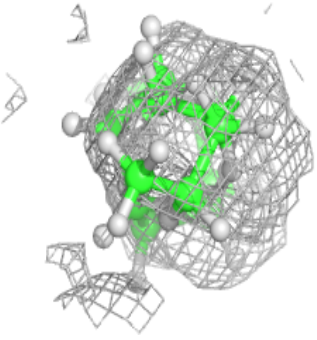


Electron density around LFA A 428:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

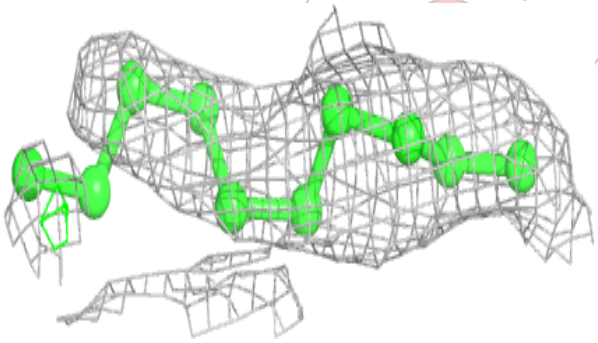


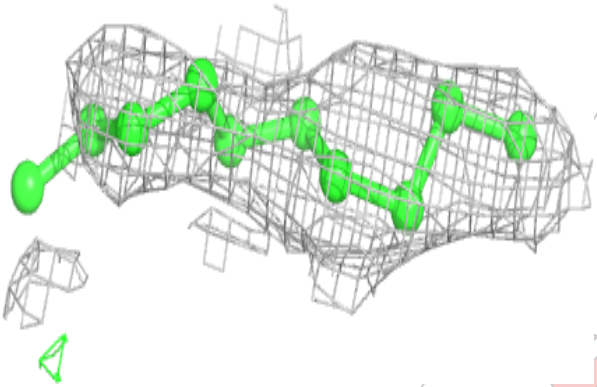


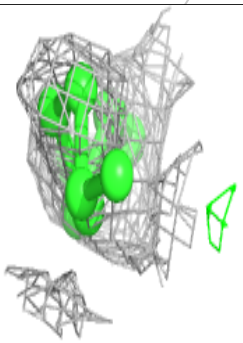


Electron density around LFA A 426:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

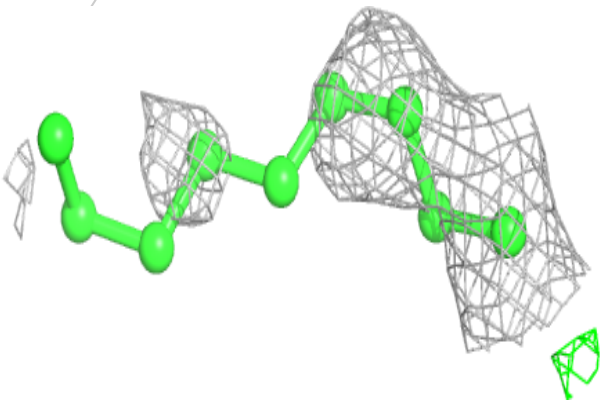


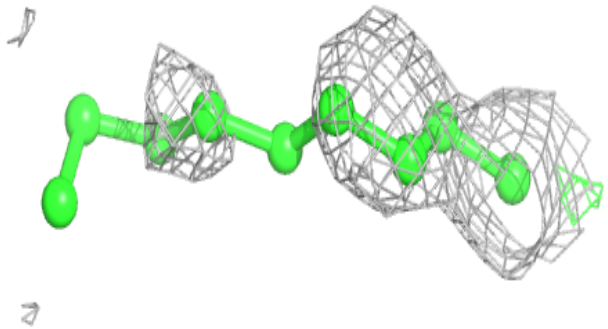


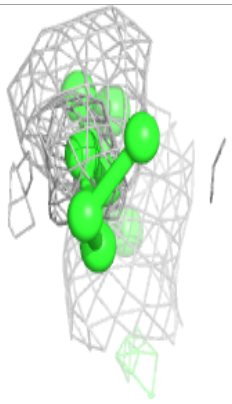


Electron density around LFA A 425:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

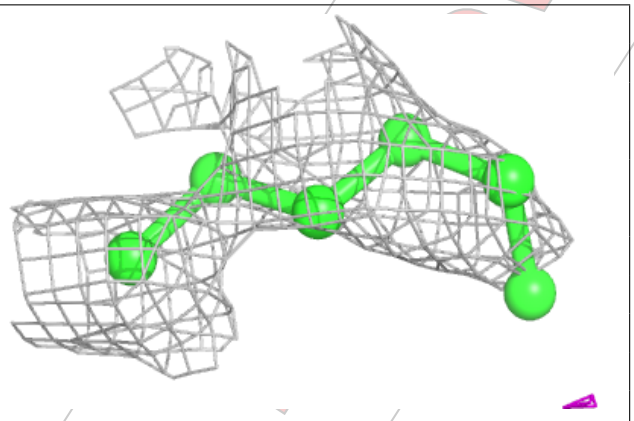


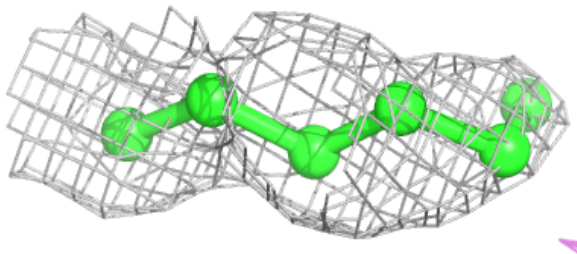


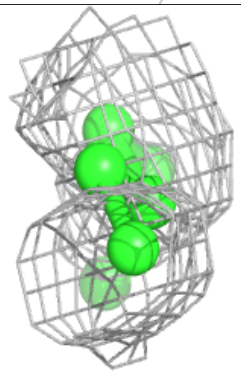


Electron density around LFA A 419:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

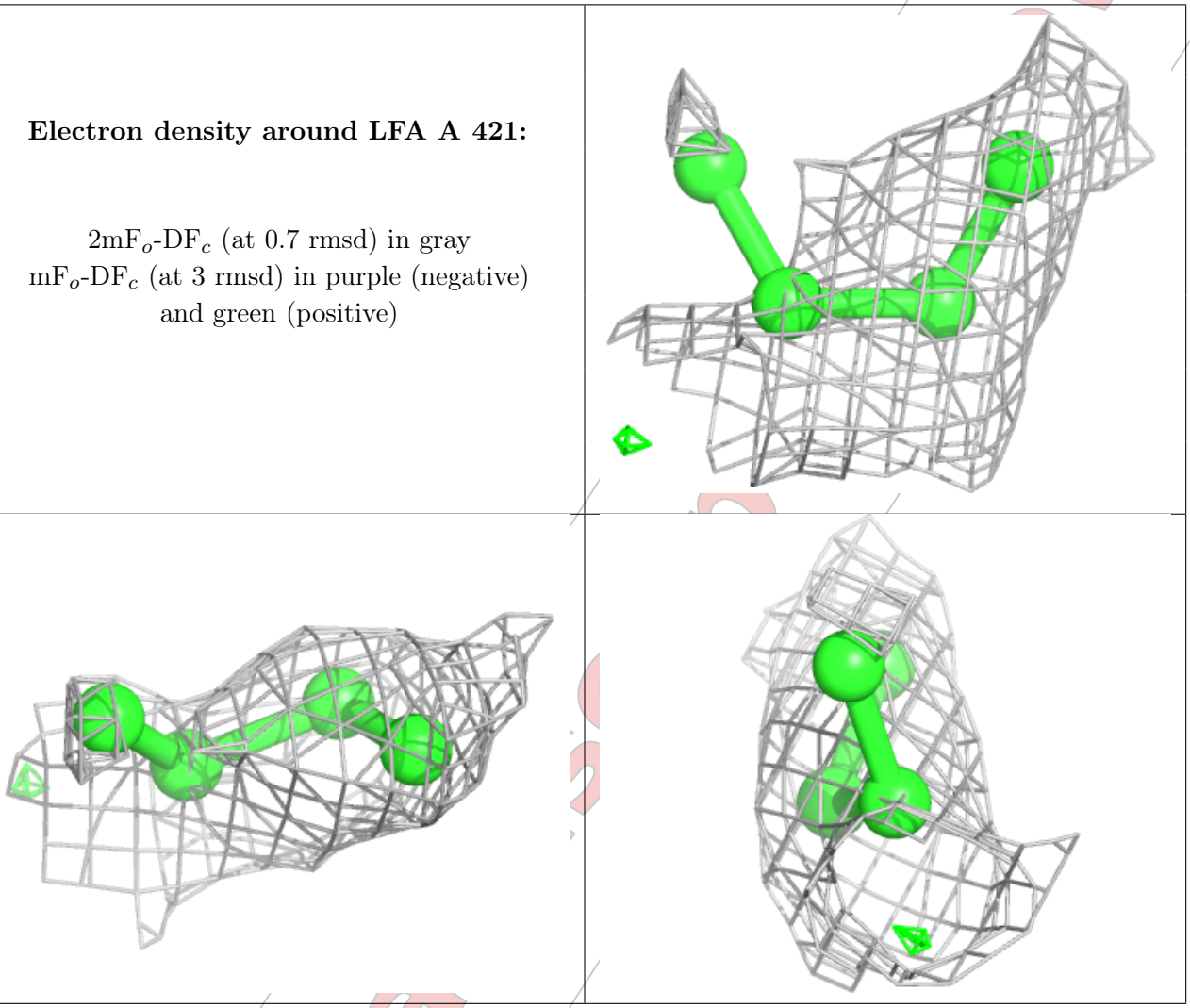






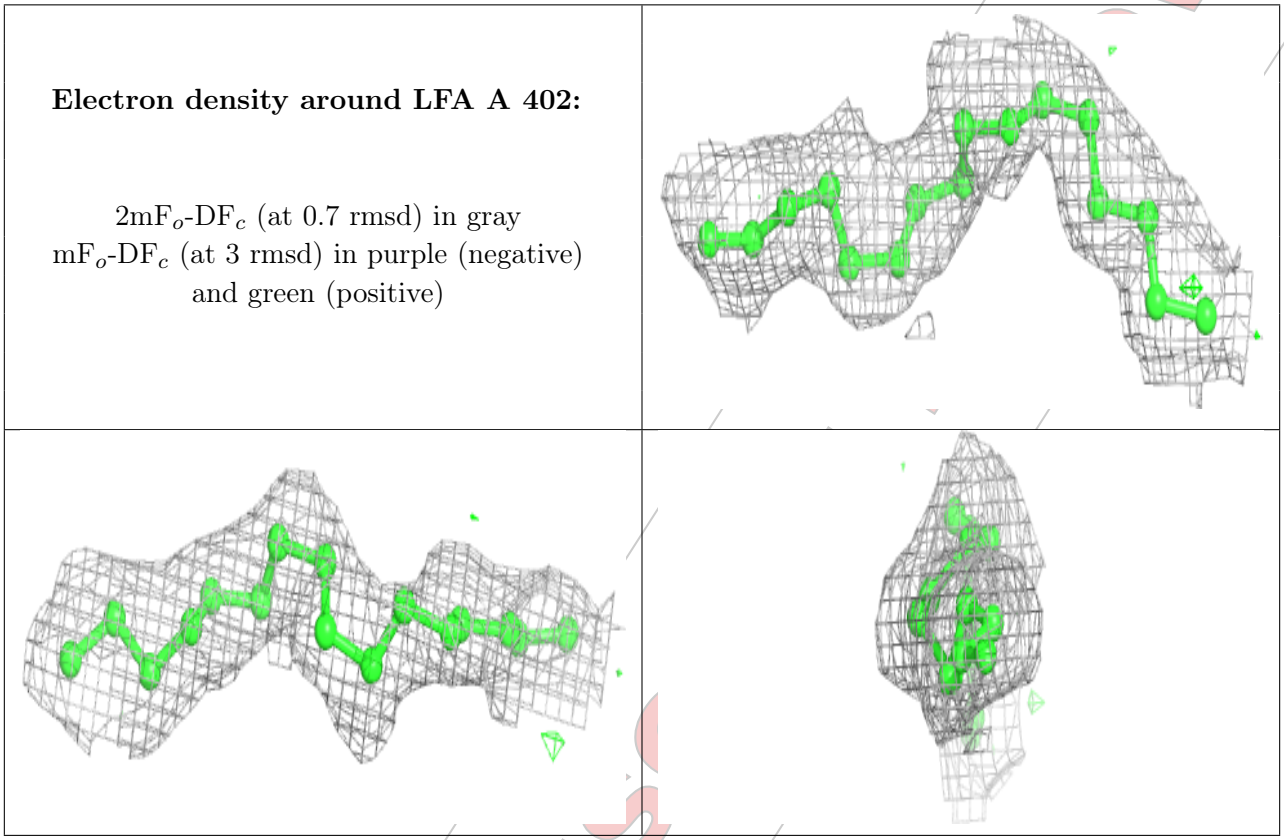
Electron density around LFA A 421:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LFA A 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Feb 7, 2023 – 01:55 pm GMT

Deposition ID : D_1292128496

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

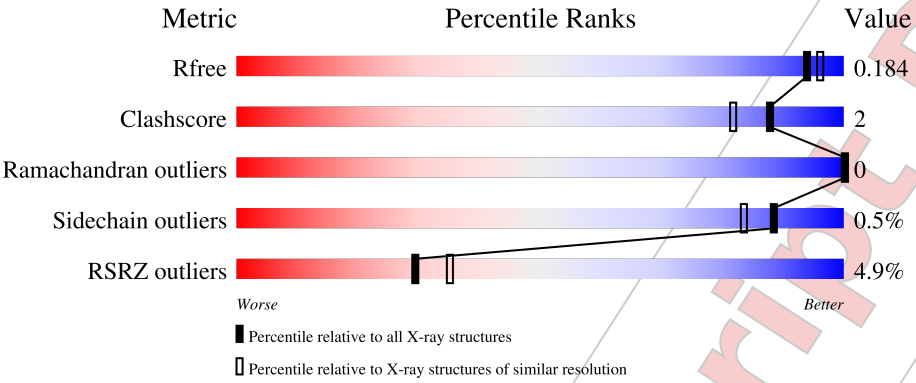
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	5% 94% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5038 atoms, of which 2547 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Krokinobacter eikastus rhodopsin 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	288	4928	1659	2547	329	383	10	0	12	0

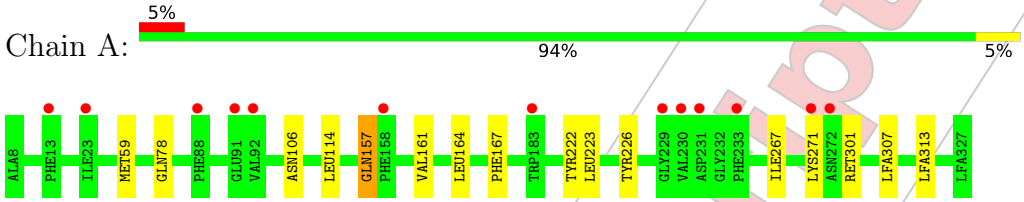
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	S	109	110	110	0	4

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Krokinobacter eikastus rhodopsin 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	41.46Å 84.89Å 234.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.97 – 1.76 15.97 – 1.76	Depositor EDS
% Data completeness (in resolution range)	68.8 (15.97-1.76) 68.7 (15.97-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.155 , 0.184 0.155 , 0.184	Depositor DCC
R_{free} test set	2000 reflections (6.97%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 97.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5038	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, LFA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.50	0/2239	0.62	0/3046

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2381	2547	2514	10	0
2	S	110	0	0	2	0
All	All	2491	2547	2514	10	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:RET:H8	1:A:301:RET:H161	1.70	0.72
1:A:161:VAL:HG22	2:S:56:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD22	1:A:307:LFA:H31	1.98	0.46
1:A:106[A]:ASN:ND2	1:A:157:GLN:OE1	2.48	0.43
1:A:167:PHE:CE1	1:A:222:TYR:CZ	3.06	0.43
1:A:164:LEU:HD13	1:A:226:TYR:CE2	2.53	0.43
1:A:78[A]:GLN:NE2	2:S:58[A]:HOH:O	2.52	0.42
1:A:223:LEU:HD11	1:A:313:LFA:C1	2.51	0.41
1:A:59:MET:HE2	1:A:59:MET:HA	2.03	0.41
1:A:267:ILE:HG22	1:A:271:LYS:NZ	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	275/288 (96%)	269 (98%)	6 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	230/227 (101%)	229 (100%)	1 (0%)	91 87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	265/288 (92%)	-0.08	13 (4%) 29 35	14, 31, 66, 108	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	PHE	6.9
1	A	272	ASN	5.6
1	A	23	ILE	4.4
1	A	230	VAL	4.4
1	A	231	ASP	3.2
1	A	158	PHE	3.0
1	A	271	LYS	2.9
1	A	229	GLY	2.8
1	A	13	PHE	2.7
1	A	92	VAL	2.6
1	A	88	PHE	2.3
1	A	91	GLU	2.1
1	A	183	TRP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.