



Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2022 – 10:43 pm GMT

Deposition ID : D_1292121225

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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

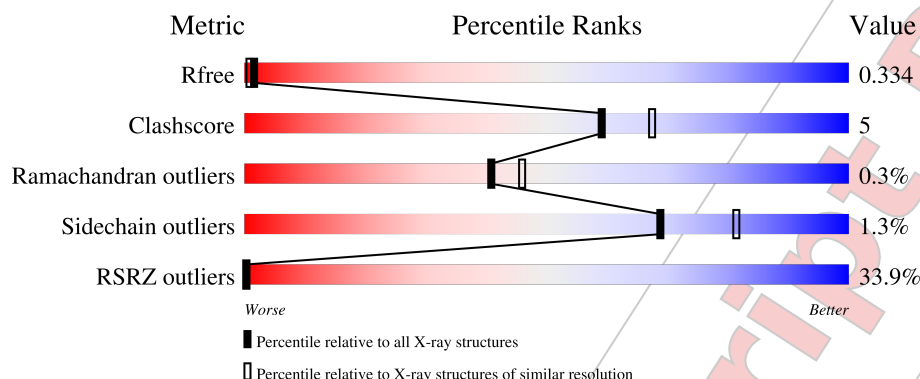
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	<div> <div>25%</div> <div>90%</div> <div>9%</div> </div>
2	B	431	<div> <div>47%</div> <div>87%</div> <div>12%</div> </div>
3	F	155	<div> <div>23%</div> <div>84%</div> <div>16%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8210 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
1	A	431	Total	C	N	O	S	2	8	0
			3406	2162	579	640	25			

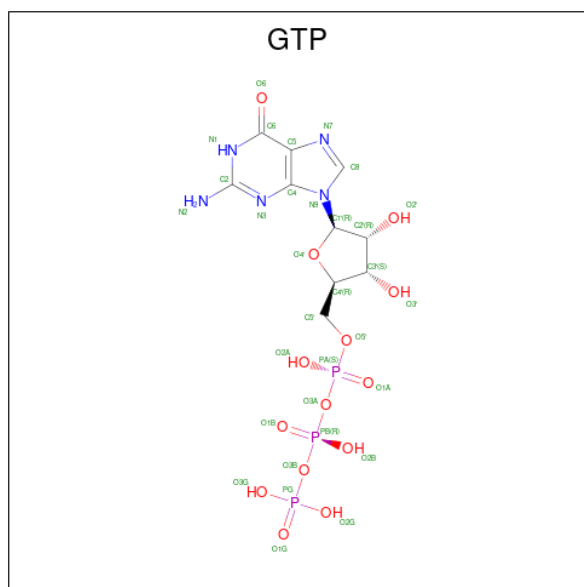
- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	5	3	0
			3371	2117	573	654	27			

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	155	Total	C	N	O	S	0	1	0
			1154	728	195	228	3			

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

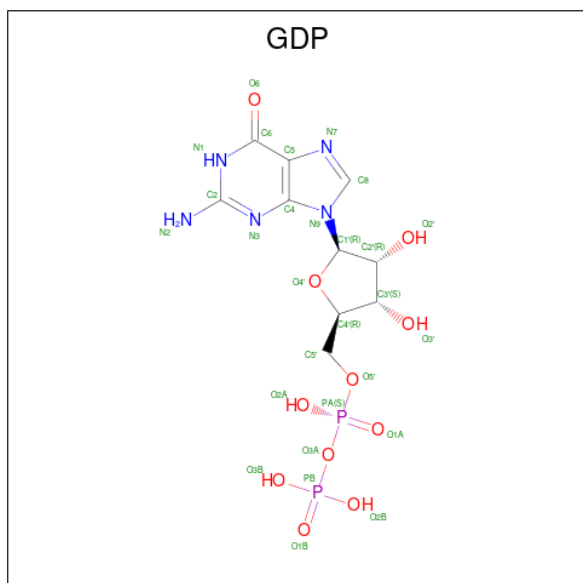


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

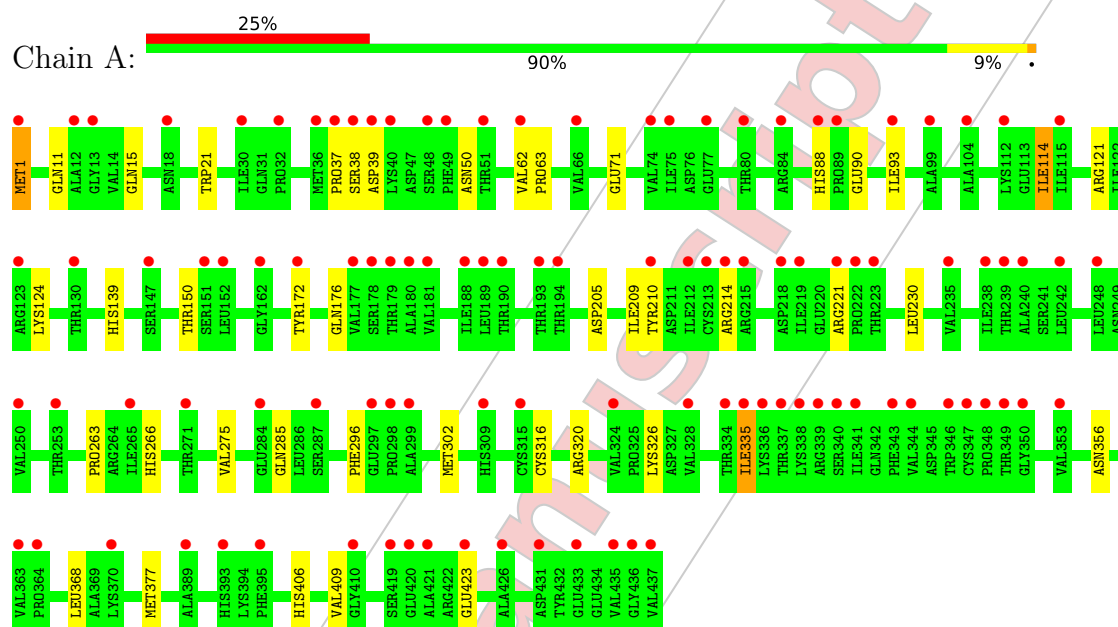
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	S	218	Total	O	0	0
			218	218		

3 Residue-property plots

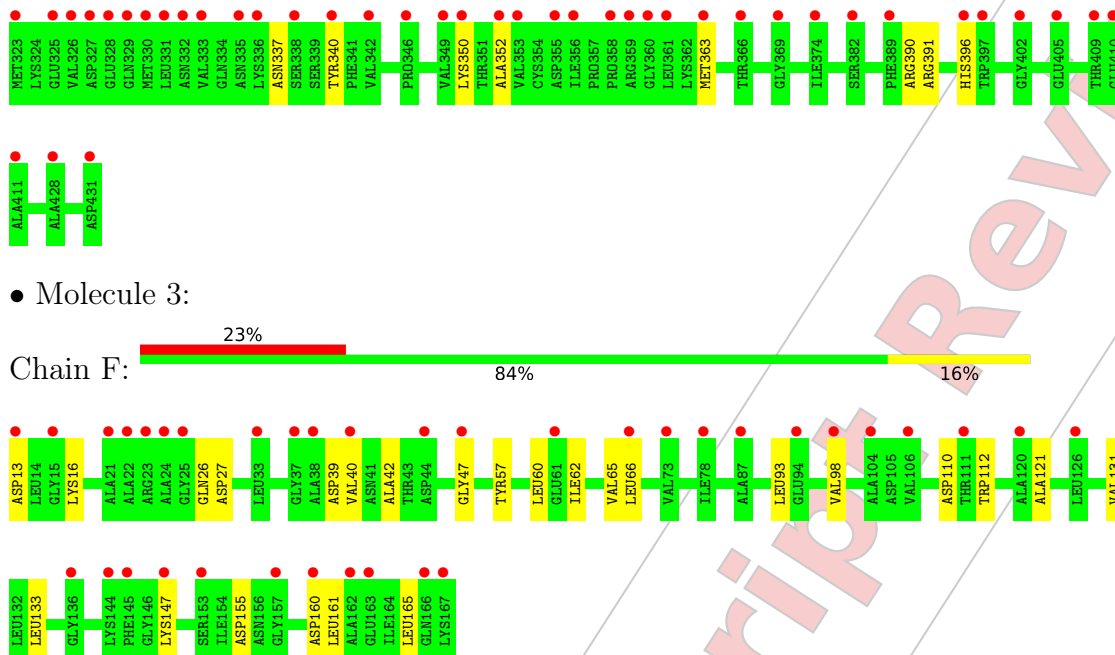
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:



• Molecule 2:





• 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	74.53Å 92.58Å 83.99Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	9.49 – 2.20 9.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (9.49-2.20) 93.6 (9.49-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 2.21Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.285 , 0.334 0.285 , 0.334	Depositor DCC
R_{free} test set	1854 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, 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	0.24	0/3504	0.45	0/4756
2	B	0.24	0/3451	0.45	0/4677
3	F	0.22	0/1173	0.40	0/1595
All	All	0.24	0/8128	0.44	0/11028

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 [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	3406	0	3326	25	0
2	B	3371	0	3226	36	0
3	F	1154	0	1151	17	0
4	A	32	0	12	1	0
5	A	1	0	0	0	0
6	B	28	0	12	1	0
7	S	218	0	0	13	0
All	All	8210	0	7727	74	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 5.

All (74) 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)
3:F:47:GLY:O	7:S:149:HOH:O	2.05	0.73
3:F:26:GLN:NE2	7:S:194:HOH:O	2.23	0.70
1:A:316[A]:CYS:SG	7:S:211:HOH:O	2.53	0.67
1:A:316[B]:CYS:SG	7:S:211:HOH:O	2.53	0.67
2:B:213:ARG:NH2	3:F:160:ASP:OD1	2.29	0.66
2:B:246:LEU:HG	2:B:247:ASN:H	1.60	0.65
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.76	0.65
2:B:289:LEU:HD11	2:B:363:MET:HB3	1.77	0.65
1:A:90:GLU:O	1:A:121:ARG:NH1	2.31	0.63
2:B:30:ILE:HD11	2:B:47:ILE:HD11	1.84	0.59
2:B:316:ILE:HA	2:B:352:ALA:HB3	1.84	0.59
2:B:245:GLN:O	2:B:247:ASN:N	2.36	0.58
2:B:31:ASP:OD1	2:B:35:SER:N	2.39	0.56
2:B:246:LEU:HD13	2:B:352:ALA:HB2	1.87	0.56
2:B:396:HIS:NE2	3:F:57:TYR:OH	2.32	0.55
1:A:37:PRO:O	1:A:39:ASP:N	2.39	0.55
3:F:13:ASP:OD2	3:F:16:LYS:NZ	2.37	0.55
3:F:40:VAL:HG13	3:F:66:LEU:HD22	1.90	0.53
1:A:209:ILE:HD11	1:A:302[A]:MET:HG3	1.91	0.53
3:F:133:LEU:HD11	3:F:165:LEU:HD23	1.91	0.53
2:B:123:GLU:O	7:S:39:HOH:O	2.19	0.53
3:F:147:LYS:NZ	3:F:155:ASP:OD2	2.36	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.91	0.52
2:B:69:GLU:HG2	2:B:71:GLY:H	1.74	0.51
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.91	0.51
2:B:239:CYS:SG	2:B:246:LEU:HD11	2.50	0.51
3:F:160:ASP:HB2	7:S:213:HOH:O	2.10	0.50
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.94	0.49
2:B:54:ALA:HB3	2:B:58:LYS:HB3	1.95	0.49
2:B:61:PRO:HD3	2:B:84:ILE:HG13	1.94	0.49
1:A:263:PRO:HA	7:S:177:HOH:O	2.11	0.49
1:A:263:PRO:O	1:A:266:HIS:ND1	2.37	0.48
2:B:337:ASN:HB3	2:B:340:TYR:HD2	1.79	0.48
1:A:406:HIS:HA	1:A:409:VAL:HG22	1.95	0.48
2:B:202:ILE:HD13	2:B:229:VAL:HG13	1.94	0.48
1:A:15:GLN:NE2	4:A:501:GTP:O6	2.47	0.47
2:B:156[A]:ARG:NH1	2:B:194:GLU:O	2.47	0.47
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.50	0.46
2:B:51:TYR:O	2:B:62:ARG:NH2	2.49	0.46
2:B:39:ASP:N	2:B:39:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLN:HB2	2:B:246:LEU:H	1.53	0.45
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.52	0.44
3:F:60:LEU:HD11	3:F:98:VAL:HG21	1.99	0.44
2:B:247:ASN:ND2	2:B:253:LEU:HD13	2.33	0.44
2:B:261:PRO:HB2	7:S:33:HOH:O	2.18	0.44
1:A:124:LYS:NZ	7:S:189:HOH:O	2.31	0.43
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.53	0.43
1:A:93:ILE:HG22	1:A:114:ILE:HD11	1.99	0.43
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.54	0.43
3:F:27:ASP:N	3:F:27:ASP:OD1	2.50	0.43
3:F:93:LEU:HD11	3:F:131:VAL:HG21	2.01	0.42
2:B:247:ASN:ND2	7:S:203:HOH:O	2.16	0.42
2:B:275:SER:HB2	2:B:278:SER:HB3	2.01	0.42
2:B:19:LYS:HD3	2:B:19:LYS:HA	1.91	0.42
1:A:296:PHE:CZ	1:A:377:MET:HE1	2.54	0.42
2:B:390:ARG:HD2	3:F:112:TRP:NE1	2.35	0.42
2:B:391:ARG:NH2	3:F:110:ASP:OD2	2.50	0.42
2:B:121:ARG:NH2	2:B:158:GLU:OE2	2.53	0.42
1:A:210:TYR:CE2	1:A:214[B]:ARG:HD2	2.55	0.42
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.55	0.41
1:A:176:GLN:OE1	1:A:176:GLN:N	2.47	0.41
1:A:320:ARG:HA	1:A:356:ASN:O	2.20	0.41
3:F:39:ASP:HB3	3:F:42:ALA:HB2	2.01	0.41
1:A:11:GLN:HB2	7:S:212:HOH:O	2.21	0.41
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.92	0.41
1:A:1:MET:HG2	1:A:50:ASN:HB2	2.02	0.41
3:F:62:ILE:HA	3:F:65:VAL:HG22	2.03	0.40
1:A:285:GLN:NE2	7:S:196:HOH:O	2.36	0.40
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.56	0.40
2:B:107:THR:OG1	2:B:108:GLU:N	2.54	0.40
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.04	0.40
2:B:156[A]:ARG:NH1	2:B:195:ASN:HA	2.37	0.40
2:B:320:ARG:HG3	7:S:147:HOH:O	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	435/431 (101%)	420 (97%)	13 (3%)	2 (0%)	29	31
2	B	432/431 (100%)	410 (95%)	21 (5%)	1 (0%)	47	55
3	F	154/155 (99%)	151 (98%)	3 (2%)	0	100	100
All	All	1021/1017 (100%)	981 (96%)	37 (4%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
2	B	246	LEU
1	A	114	ILE

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	367/365 (100%)	360 (98%)	7 (2%)	57	71
2	B	366/372 (98%)	361 (99%)	5 (1%)	67	80
3	F	120/120 (100%)	120 (100%)	0	100	100
All	All	853/857 (100%)	841 (99%)	12 (1%)	69	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	71	GLU
1	A	221	ARG
1	A	326	LYS
1	A	335	ILE
1	A	423[A]	GLU
1	A	423[B]	GLU
2	B	137	HIS
2	B	245	GLN
2	B	246	LEU
2	B	284	LEU
2	B	350	LYS

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	128	GLN
2	B	195	ASN
2	B	247	ASN
2	B	337	ASN
2	B	426	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 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	A	501	5	26,34,34	0.97	1 (3%)	33,54,54	1.79	7 (21%)
6	GDP	B	501	-	24,30,30	1.19	2 (8%)	31,47,47	1.96	8 (25%)

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	A	501	5	-	6/18/38/38	0/3/3/3
6	GDP	B	501	-	-	3/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	GDP	C5-C6	4.22	1.48	1.41
4	A	501	GTP	C6-N1	3.08	1.38	1.33
6	B	501	GDP	C5-C4	2.45	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	N3-C2-N1	-5.33	120.12	127.22
6	B	501	GDP	C2-N3-C4	4.94	121.00	115.36
4	A	501	GTP	C2-N3-C4	4.28	120.24	115.36
6	B	501	GDP	C2-N1-C6	4.05	122.36	115.93
6	B	501	GDP	C5-C6-N1	-3.97	118.00	123.43
6	B	501	GDP	C4-C5-C6	-3.84	117.13	120.80
6	B	501	GDP	N3-C2-N1	-3.31	122.81	127.22
4	A	501	GTP	PB-O3B-PG	-3.24	121.70	132.83
4	A	501	GTP	PA-O3A-PB	-3.08	122.25	132.83
6	B	501	GDP	PA-O3A-PB	-3.06	122.32	132.83
4	A	501	GTP	C5-C6-N1	-2.80	119.61	123.43
6	B	501	GDP	C3'-C2'-C1'	2.78	105.16	100.98
6	B	501	GDP	C4-C5-N7	-2.74	106.54	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	C2-N1-C6	2.51	119.92	115.93
4	A	501	GTP	C3'-C2'-C1'	2.28	104.41	100.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

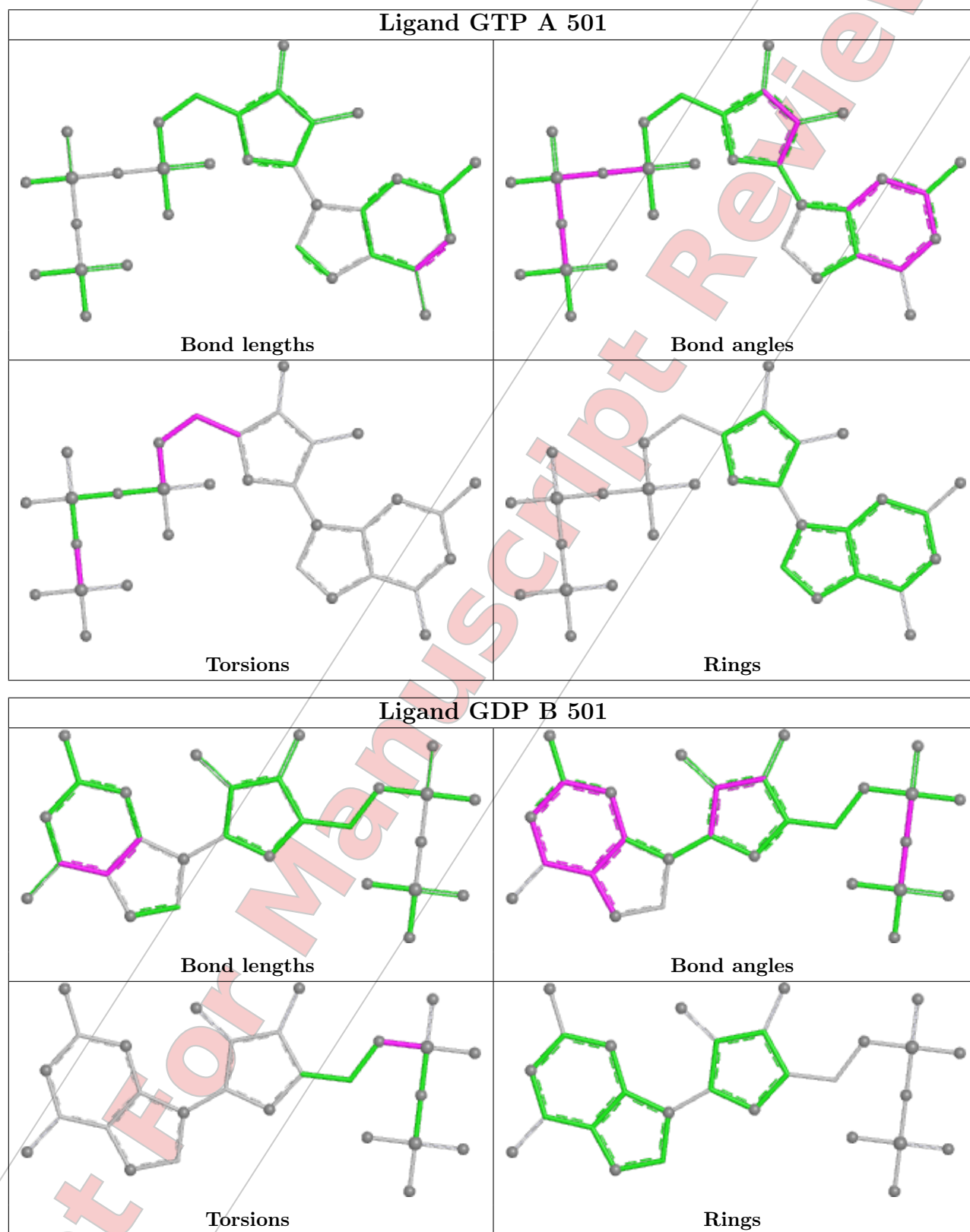
Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C4'-C5'-O5'-PA
6	B	501	GDP	C5'-O5'-PA-O3A
4	A	501	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GTP	1	0
6	B	501	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 than 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.



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
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	10.27

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	1.49	107 (24%) 0 0	24, 35, 54, 85	2 (0%)
2	B	431/431 (100%)	2.34	202 (46%) 0 0	29, 45, 73, 124	0
3	F	155/155 (100%)	1.50	36 (23%) 0 0	25, 35, 48, 73	0
All	All	1017/1017 (100%)	1.85	345 (33%) 0 0	24, 38, 67, 124	2 (0%)

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	282	ARG	13.9
2	B	283	ALA	13.3
2	B	280	GLN	11.4
2	B	281	TYR	11.2
2	B	42	LEU	11.2
1	A	437	VAL	9.7
2	B	41	ASP	9.1
2	B	80	PRO	8.3
2	B	431	ASP	8.1
1	A	335	ILE	8.0
2	B	248	ALA	7.7
2	B	275	SER	7.5
2	B	277	GLY	7.5
2	B	243	PRO	7.2
1	A	436	GLY	7.1
2	B	95	SER	7.1
2	B	93	GLY	6.7
1	A	38	SER	6.6
2	B	56	GLY	6.4
2	B	92	PHE	6.3
2	B	57	ASN	6.2
2	B	130	LEU	6.2
1	A	339	ARG	6.1

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Mol	Chain	Res	Type	RSRZ
2	B	36	TYR	6.1
2	B	128	ASP	6.0
2	B	284	LEU	6.0
2	B	87	PRO	6.0
2	B	73	MET	5.9
1	A	39	ASP	5.9
2	B	247	ASN	5.9
2	B	39	ASP	5.7
2	B	322	SER	5.6
2	B	279	GLN	5.5
2	B	54	ALA	5.3
2	B	72	THR	5.3
2	B	75	SER	5.2
2	B	63	ALA	5.1
2	B	37	HIS	5.1
1	A	324	VAL	5.1
2	B	246	LEU	5.0
3	F	167	LYS	5.0
2	B	127	CYS	4.9
2	B	193	VAL	4.9
1	A	178	SER	4.8
2	B	332	ASN	4.8
1	A	338	LYS	4.8
2	B	58	LYS	4.8
3	F	163	GLU	4.7
2	B	79	GLY	4.7
1	A	37	PRO	4.7
2	B	286	VAL	4.7
2	B	38	GLY	4.6
2	B	46	ARG	4.6
1	A	349	THR	4.5
2	B	333	VAL	4.4
2	B	78	SER	4.4
3	F	73	VAL	4.3
3	F	22	ALA	4.3
1	A	177	VAL	4.3
1	A	350	GLY	4.3
2	B	1	MET	4.2
2	B	363	MET	4.2
2	B	44	LEU	4.1
2	B	172	SER	4.1
2	B	121	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	109	GLY	4.0
1	A	340	SER	4.0
2	B	212	PHE	4.0
2	B	402	GLY	4.0
1	A	435	VAL	4.0
2	B	361	LEU	3.9
1	A	75	ILE	3.9
2	B	31	ASP	3.9
1	A	364	PRO	3.9
2	B	55	THR	3.8
2	B	74	ASP	3.8
1	A	40	LYS	3.8
3	F	145	PHE	3.8
2	B	82	GLY	3.8
2	B	352	ALA	3.8
2	B	34	GLY	3.8
2	B	43	GLN	3.7
2	B	215	LEU	3.7
2	B	81	PHE	3.7
1	A	218	ASP	3.7
3	F	104	ALA	3.7
1	A	298	PRO	3.7
1	A	336	LYS	3.7
1	A	299	ALA	3.7
2	B	221	THR	3.7
2	B	30	ILE	3.7
2	B	200	TYR	3.6
2	B	245	GLN	3.6
3	F	147	LYS	3.6
2	B	411	ALA	3.6
3	F	23	ARG	3.6
2	B	49	VAL	3.6
2	B	244	GLY	3.6
2	B	89	ASN	3.6
2	B	69	GLU	3.5
2	B	163	ILE	3.5
2	B	331	LEU	3.5
2	B	177[A]	ASP	3.5
2	B	315	ALA	3.5
1	A	284	GLU	3.5
3	F	120	ALA	3.5
3	F	166	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	278	SER	3.4
3	F	13	ASP	3.4
1	A	222	PRO	3.4
2	B	222	TYR	3.4
2	B	237	THR	3.4
2	B	249	ASP	3.4
2	B	326	VAL	3.4
2	B	323	MET	3.4
2	B	409	THR	3.4
2	B	129	CYS	3.4
2	B	303	CYS	3.4
2	B	397	TRP	3.3
1	A	151	SER	3.3
2	B	285	THR	3.3
1	A	426	ALA	3.3
2	B	24	ILE	3.3
1	A	18	ASN	3.3
3	F	37	GLY	3.2
2	B	287	PRO	3.2
2	B	359	ARG	3.2
1	A	363	VAL	3.2
1	A	36	MET	3.2
2	B	157	GLU	3.2
2	B	238	THR	3.2
3	F	25	GLY	3.2
2	B	273	LEU	3.2
2	B	108	GLU	3.2
2	B	125	GLU	3.2
2	B	184	ASN	3.2
2	B	325	GLU	3.2
2	B	114	ASP	3.2
1	A	337	THR	3.2
1	A	80	THR	3.2
2	B	291	GLN	3.2
2	B	26	ASP	3.2
2	B	335	ASN	3.2
1	A	30	ILE	3.1
2	B	199	THR	3.1
2	B	265	PHE	3.1
2	B	320	ARG	3.1
1	A	1	MET	3.1
2	B	84	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	274	THR	3.1
1	A	423[A]	GLU	3.1
2	B	70	PRO	3.1
2	B	83	GLN	3.1
2	B	328	GLU	3.1
2	B	102	ALA	3.1
2	B	349	VAL	3.1
2	B	210	ILE	3.1
2	B	239	CYS	3.1
2	B	113	VAL	3.0
3	F	144	LYS	3.0
2	B	120	VAL	3.0
1	A	215	ARG	3.0
2	B	176	SER	3.0
2	B	160	PRO	3.0
2	B	50	TYR	3.0
2	B	289	LEU	3.0
1	A	104	ALA	3.0
1	A	212	ILE	3.0
2	B	59	TYR	2.9
2	B	360	GLY	2.9
2	B	294	PHE	2.9
2	B	48	ASN	2.9
2	B	396	HIS	2.9
3	F	98	VAL	2.9
2	B	340	TYR	2.9
1	A	393	HIS	2.9
1	A	214[A]	ARG	2.9
1	A	239	THR	2.9
2	B	366	THR	2.9
2	B	155	ILE	2.9
2	B	353	VAL	2.9
1	A	190	THR	2.8
2	B	142	GLY	2.8
2	B	206	ALA	2.8
2	B	342	VAL	2.8
2	B	85	PHE	2.8
2	B	115	SER	2.8
2	B	327	ASP	2.8
1	A	344	VAL	2.8
1	A	219	ILE	2.8
2	B	35	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	405	GLU	2.8
2	B	336	LYS	2.8
1	A	180	ALA	2.7
1	A	235	VAL	2.7
2	B	389	PHE	2.7
2	B	40	SER	2.7
1	A	99	ALA	2.7
3	F	38	ALA	2.7
2	B	175	VAL	2.7
3	F	106	VAL	2.7
1	A	410	GLY	2.7
2	B	253	LEU	2.7
2	B	47	ILE	2.7
2	B	356	ILE	2.7
1	A	348	PRO	2.7
1	A	248	LEU	2.7
2	B	67	ASP	2.7
2	B	410	GLU	2.7
2	B	179	VAL	2.7
1	A	271	THR	2.7
1	A	346	TRP	2.7
2	B	29	GLY	2.7
3	F	78	ILE	2.7
2	B	64	ILE	2.6
2	B	90	PHE	2.6
1	A	93	ILE	2.6
2	B	166	THR	2.6
2	B	98	GLY	2.6
1	A	62	VAL	2.6
2	B	313	VAL	2.6
1	A	297	GLU	2.6
3	F	87	ALA	2.6
1	A	347	CYS	2.6
1	A	179	THR	2.6
1	A	223	THR	2.6
1	A	433	GLU	2.6
2	B	12	CYS	2.6
2	B	156[A]	ARG	2.6
3	F	126	LEU	2.6
1	A	250	VAL	2.6
2	B	227	HIS	2.6
1	A	89	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	242	PHE	2.5
2	B	111	GLU	2.5
3	F	136	GLY	2.5
1	A	334	THR	2.5
1	A	341	ILE	2.5
1	A	242	LEU	2.5
1	A	343	PHE	2.5
2	B	99	ASN	2.5
1	A	421	ALA	2.5
2	B	126	SER	2.5
3	F	21	ALA	2.5
3	F	153	SER	2.5
3	F	94	GLU	2.5
2	B	68	LEU	2.5
2	B	355	ASP	2.5
1	A	221	ARG	2.5
2	B	159	TYR	2.5
2	B	428	ALA	2.4
1	A	112	LYS	2.4
1	A	193	THR	2.4
1	A	188	ILE	2.4
3	F	15	GLY	2.4
1	A	152	LEU	2.4
1	A	12	ALA	2.4
1	A	420	GLU	2.4
2	B	230	SER	2.4
2	B	329	GLN	2.4
1	A	315	CYS	2.4
1	A	13	GLY	2.4
3	F	24	ALA	2.4
1	A	74	VAL	2.4
2	B	151	LEU	2.4
2	B	91	VAL	2.4
2	B	382	SER	2.4
2	B	143	THR	2.3
3	F	157	GLY	2.3
1	A	147	SER	2.3
2	B	101	TRP	2.3
2	B	224	ASP	2.3
1	A	419	SER	2.3
2	B	187	LEU	2.3
2	B	201	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	123[A]	ARG	2.3
2	B	236	VAL	2.3
1	A	287	SER	2.3
1	A	130	THR	2.2
2	B	350	LYS	2.2
1	A	353	VAL	2.2
3	F	40	VAL	2.2
2	B	358	PRO	2.2
1	A	77	GLU	2.2
1	A	51	THR	2.2
1	A	253	THR	2.2
2	B	71	GLY	2.2
2	B	255	VAL	2.2
2	B	338	SER	2.2
1	A	115	ILE	2.2
2	B	52	ASN	2.2
2	B	139	LEU	2.2
3	F	33	LEU	2.2
1	A	181	VAL	2.2
1	A	328	VAL	2.2
1	A	162	GLY	2.2
2	B	196	THR	2.2
2	B	214	THR	2.2
2	B	23	VAL	2.2
2	B	234	SER	2.2
1	A	240	ALA	2.2
2	B	171	PRO	2.2
1	A	48	SER	2.2
1	A	49	PHE	2.2
1	A	88	HIS	2.2
1	A	370	LYS	2.2
2	B	219	THR	2.2
3	F	111	THR	2.2
1	A	189	LEU	2.2
1	A	66	VAL	2.1
2	B	232	THR	2.1
3	F	162	ALA	2.1
3	F	61	GLU	2.1
1	A	32	PRO	2.1
2	B	188	SER	2.1
2	B	330	MET	2.1
2	B	110	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	194	THR	2.1
2	B	235	GLY	2.1
2	B	117	LEU	2.1
3	F	160	ASP	2.1
2	B	77	ARG	2.1
1	A	389	ALA	2.1
2	B	5	VAL	2.1
2	B	374	ILE	2.1
1	A	309	HIS	2.1
1	A	172	TYR	2.1
2	B	346	PRO	2.1
2	B	22	GLU	2.0
2	B	217	LEU	2.0
2	B	107	THR	2.0
2	B	369	GLY	2.0
3	F	47	GLY	2.0
1	A	213	CYS	2.0
1	A	431	ASP	2.0
2	B	307	HIS	2.0
1	A	238	ILE	2.0
1	A	265	ILE	2.0
3	F	66	LEU	2.0
3	F	44	ASP	2.0
1	A	395	PHE	2.0
1	A	210	TYR	2.0
2	B	21	TRP	2.0
2	B	158	GLU	2.0
1	A	84	ARG	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.

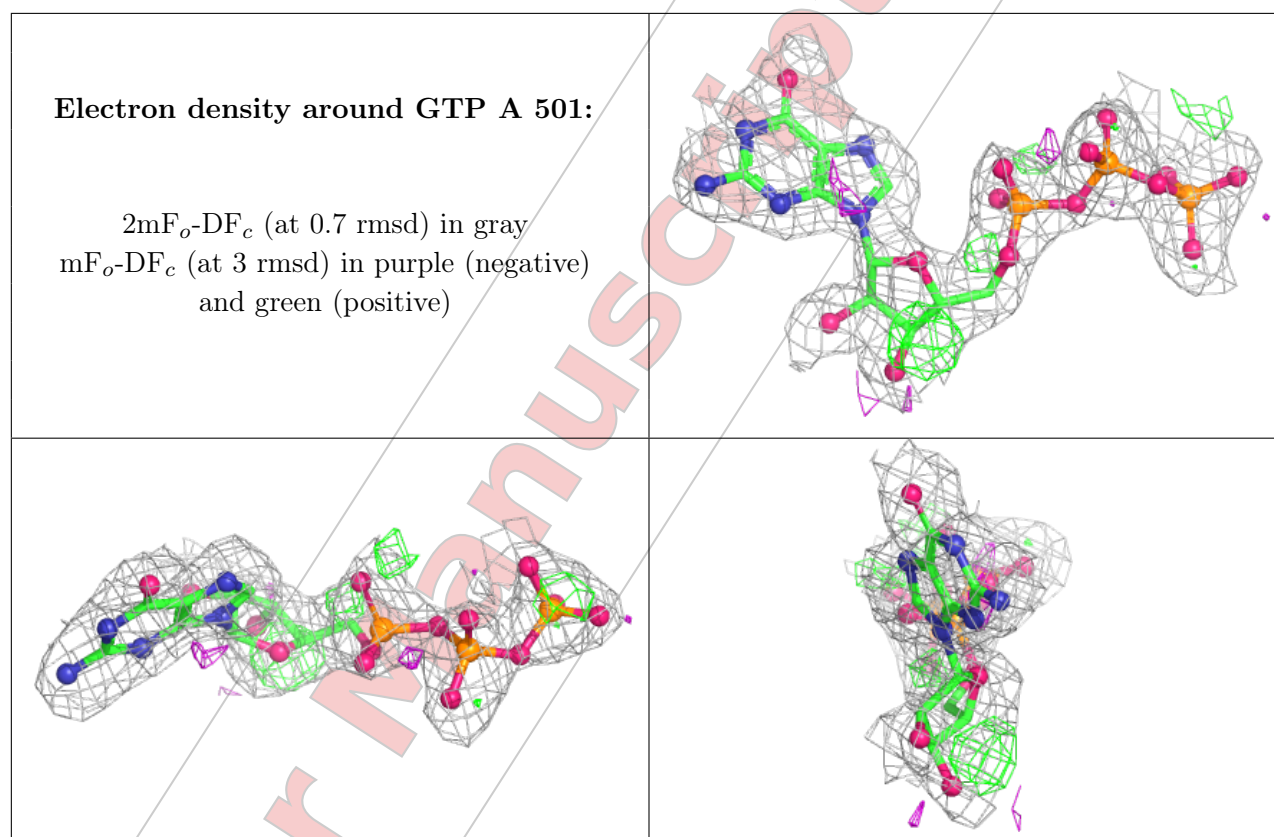
6.4 Ligands [i](#)

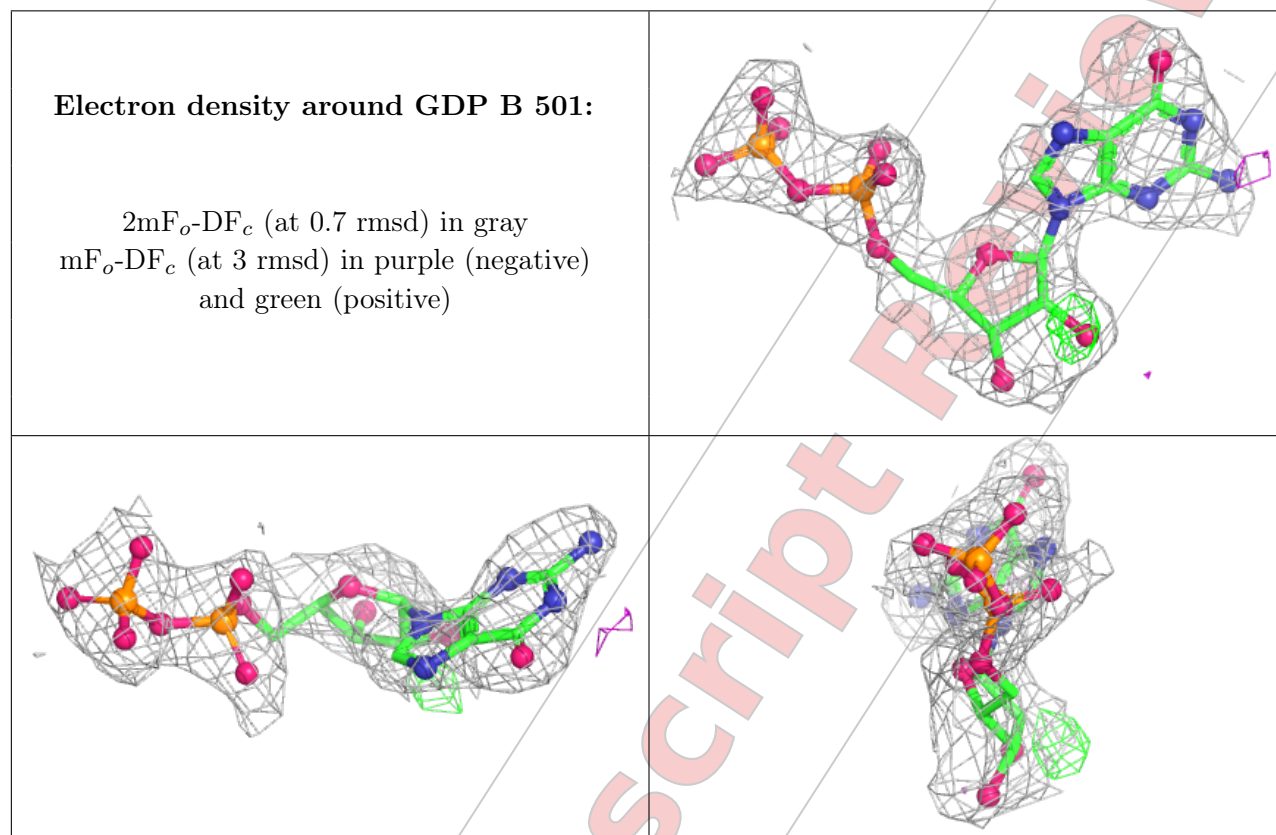
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th 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	A	502	1/?	0.54	0.37	33,33,33,33	0
4	GTP	A	501	32/?	0.82	0.24	22,27,32,36	0
6	GDP	B	501	28/?	0.84	0.21	33,39,46,54	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.