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

Dec 30, 2021 – 02:39 pm GMT

Deposition ID : D_1292120003

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

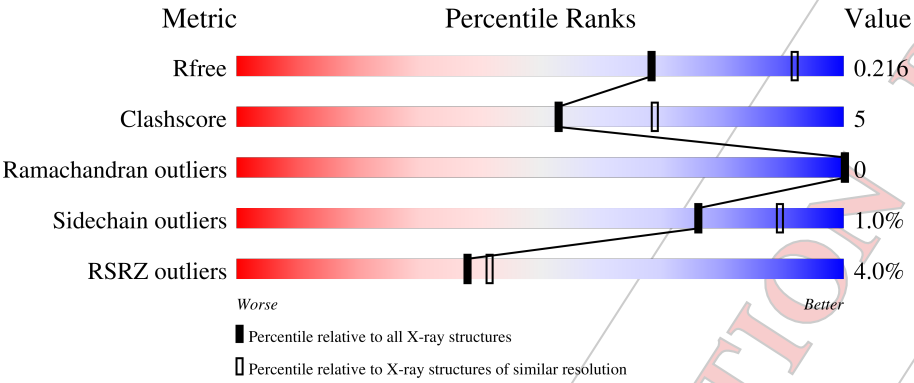
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 2.51 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	687	3% 86% 14%
2	B	687	4% 85% 15%
3	C	678	4% 88% 11%
4	D	689	5% 86% 13%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 22585 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 called SpoT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	687	5418	3419	969	1002	28	0	1	0

- Molecule 2 is a protein called SpoT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	687	5379	3395	950	1007	27	0	0	0

- Molecule 3 is a protein called SpoT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	678	5335	3369	948	991	27	0	0	0

- Molecule 4 is a protein called SpoT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	689	5374	3396	951	999	28	0	0	0

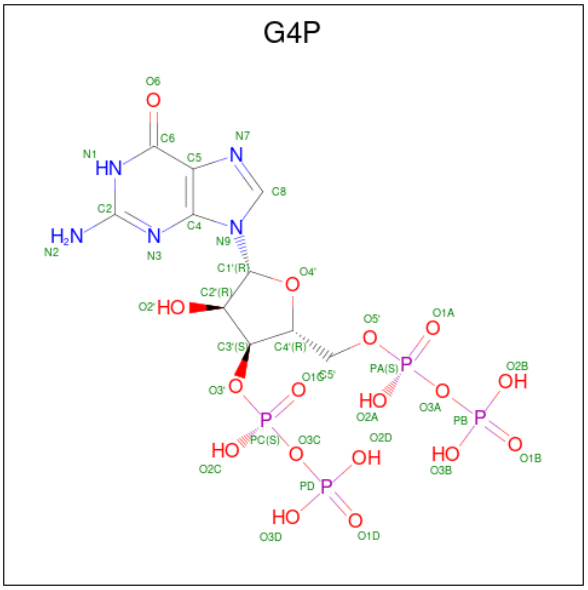
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

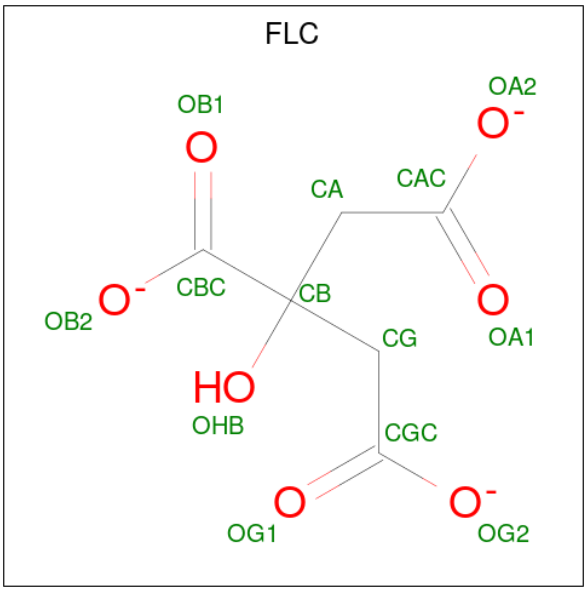
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0
6	C	1	Total Zn 1 1	0	0
6	D	1	Total Zn 1 1	0	0

- Molecule 7 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



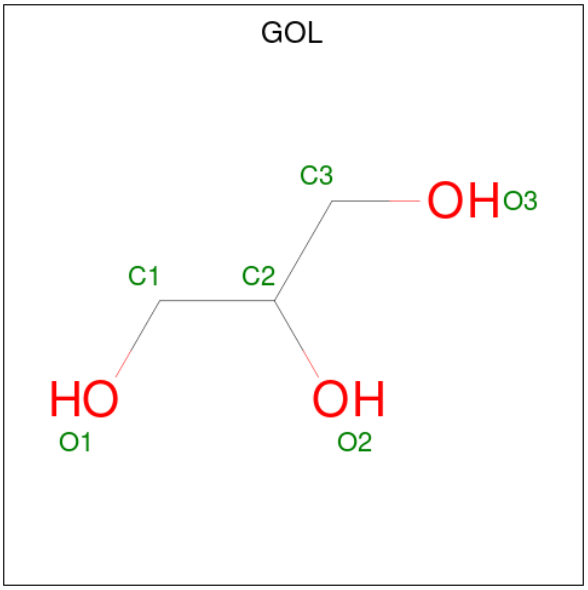
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 36 10 5 17 4	0	0
7	B	1	Total C N O P 36 10 5 17 4	0	0
7	C	1	Total C N O P 36 10 5 17 4	0	0
7	D	1	Total C N O P 36 10 5 17 4	0	0

- Molecule 8 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 13 6 7	0	0
8	C	1	Total C O 13 6 7	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 6 3 3	0	0
9	C	1	Total C O 6 3 3	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total Mg 1 1	0	0
10	E	1	Total Mg 1 1	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	Total Cl 1 1	0	0
11	F	1	Total Cl 1 1	0	0
11	F	1	Total Cl 1 1	0	0

- Molecule 12 is water.

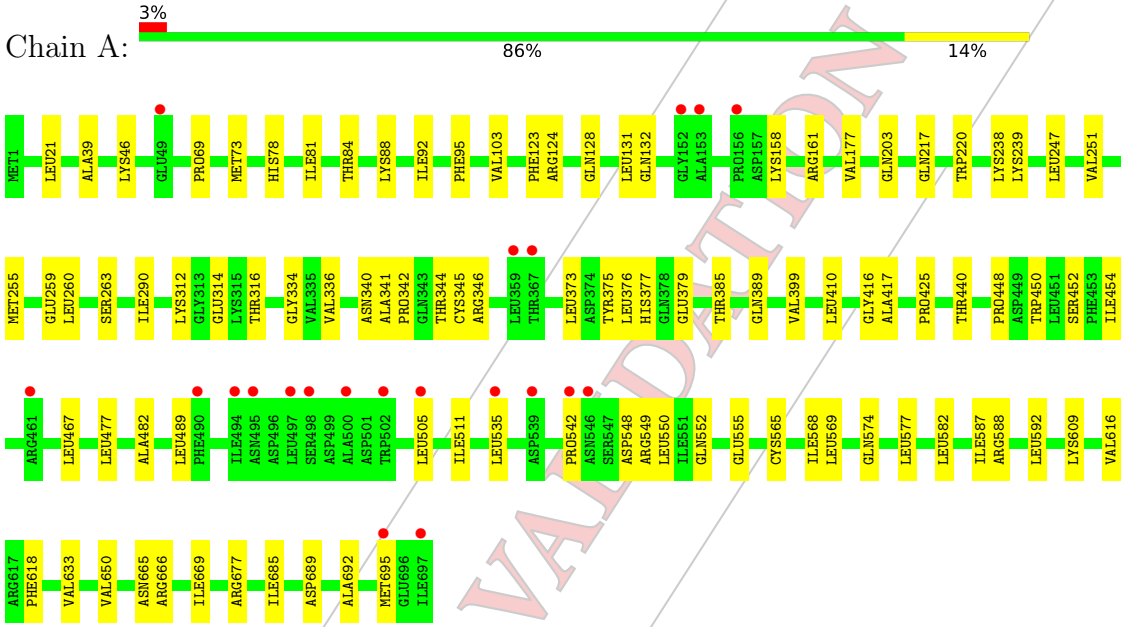
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	W	872	Total O 872 872	0	0

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.

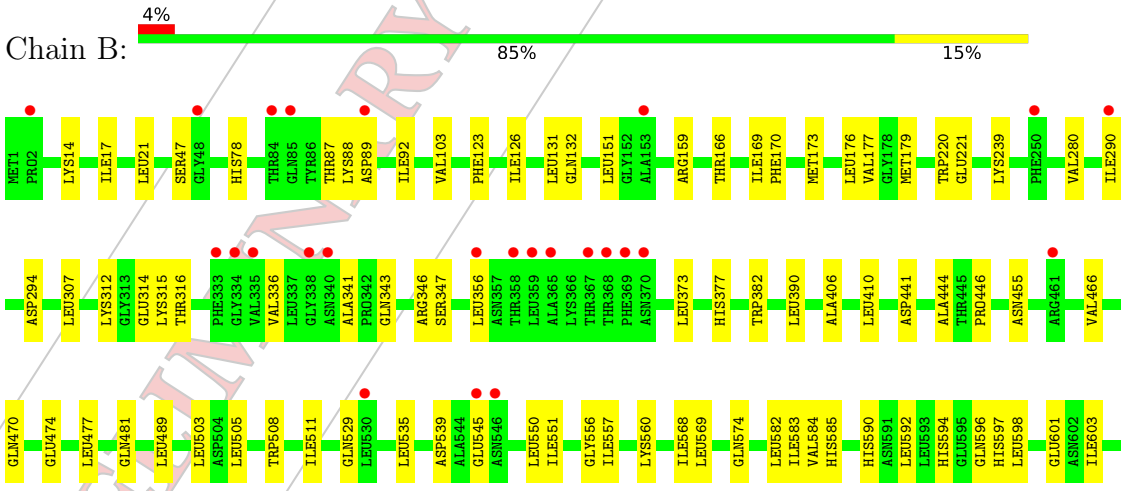
- Molecule 1: SpoT

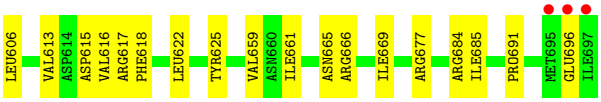
Chain A:



- Molecule 2: SpoT

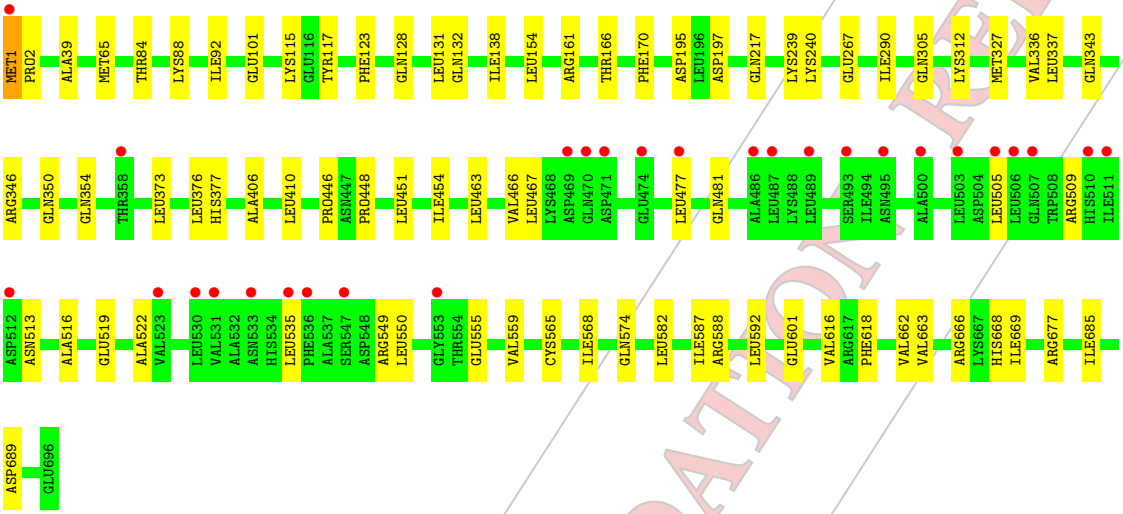
Chain B:





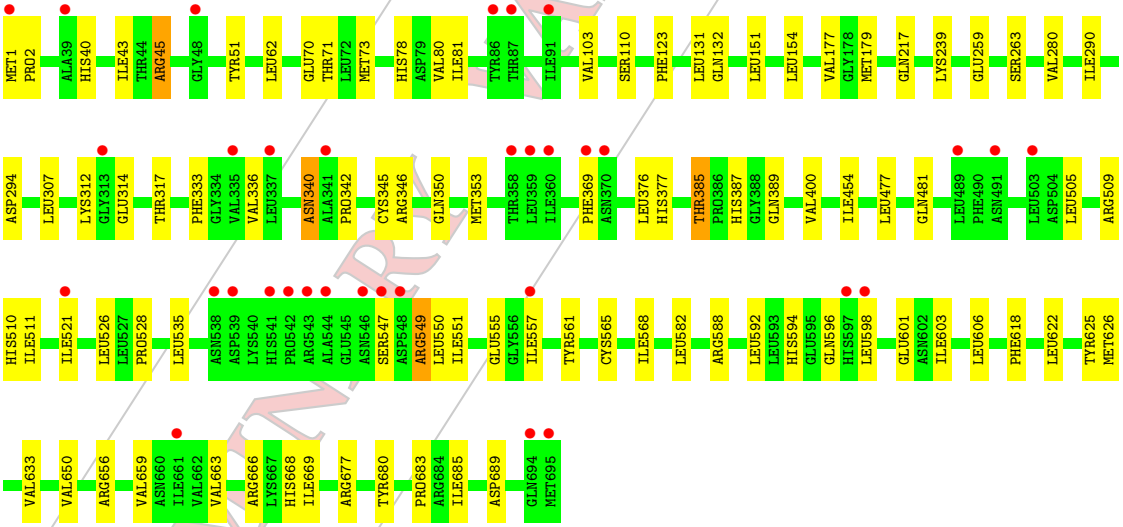
• Molecule 3: SpoT

Chain C:



• Molecule 4: SpoT

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.79Å 133.76Å 211.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.51 48.88 – 2.51	Depositor EDS
% Data completeness (in resolution range)	67.3 (48.88-2.51) 67.3 (48.88-2.51)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.221 , 0.258 0.219 , 0.216	Depositor DCC
R_{free} test set	4299 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	60.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22585	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4426e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MN, ZN, MG, CL, G4P, FLC, GOL

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	0.38	0/5522	0.57	0/7492
2	B	0.39	0/5476	0.60	0/7432
3	C	0.37	0/5434	0.55	0/7374
4	D	0.38	0/5476	0.58	0/7439
All	All	0.38	0/21908	0.57	0/29737

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	5418	0	5365	57	0
2	B	5379	0	5292	68	0
3	C	5335	0	5271	47	0
4	D	5374	0	5267	62	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	36	0	11	0	0
7	B	36	0	11	0	0
7	C	36	0	11	0	0
7	D	36	0	11	0	0
8	A	13	0	5	3	0
8	C	13	0	5	0	0
9	A	6	0	8	0	0
9	B	6	0	8	0	0
9	C	12	0	16	0	0
10	E	2	0	0	0	0
11	F	3	0	0	1	0
12	W	872	0	0	3	0
All	All	22585	0	21281	231	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 (231) 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)
4:D:626:MET:HE1	4:D:683:PRO:HG3	1.50	0.91
2:B:594:HIS:CE1	2:B:598:LEU:HD22	2.12	0.84
1:A:334:GLY:H	1:A:340:ASN:HD21	1.26	0.83
1:A:416:GLY:HA3	2:B:503:LEU:HD13	1.61	0.82
2:B:17:ILE:HD11	2:B:21:LEU:HD12	1.62	0.81
2:B:455:ASN:HB2	2:B:556:GLY:HA2	1.60	0.81
1:A:238:LYS:NZ	8:A:1002:FLC:HA2	1.97	0.79
1:A:548:ASP:OD1	1:A:549:ARG:HD2	1.87	0.75
1:A:448:PRO:HB3	1:A:467:LEU:HD11	1.69	0.74
4:D:596:GLN:HG2	4:D:603:ILE:HG13	1.69	0.73
3:C:115:LYS:O	3:C:161:ARG:NH2	2.21	0.73
2:B:446:PRO:HG2	2:B:466:VAL:HG11	1.70	0.73
2:B:550:LEU:HD11	2:B:616:VAL:HG11	1.69	0.73
4:D:626:MET:CE	4:D:683:PRO:HG3	2.19	0.73
1:A:550:LEU:HD11	1:A:616:VAL:HG11	1.71	0.72
2:B:455:ASN:HB2	2:B:556:GLY:CA	2.18	0.72
1:A:238:LYS:HZ2	8:A:1002:FLC:HA2	1.52	0.71
2:B:343:GLN:HG3	12:W:860:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:290:ILE:HD11	4:D:312:LYS:HB2	1.74	0.69
2:B:470:GLN:HG2	2:B:474:GLU:HG2	1.73	0.68
4:D:557:ILE:HD12	4:D:582:LEU:HB2	1.76	0.66
3:C:373:LEU:HD22	3:C:377:HIS:CE1	2.30	0.66
2:B:87:THR:HG22	2:B:89:ASP:H	1.61	0.66
2:B:568:ILE:HG13	2:B:618:PHE:HB3	1.77	0.65
2:B:691:PRO:HG2	2:B:696:GLU:HG2	1.78	0.65
3:C:138:ILE:HD11	3:C:336:VAL:CG1	2.27	0.65
3:C:446:PRO:HG2	3:C:466:VAL:HG21	1.77	0.65
4:D:663:VAL:HG22	4:D:668:HIS:CG	2.32	0.65
2:B:312:LYS:NZ	2:B:315:LYS:HA	2.14	0.62
3:C:555:GLU:HB2	11:F:2:CL:CL	2.37	0.62
1:A:373:LEU:HD22	1:A:377:HIS:CE1	2.34	0.61
4:D:131:LEU:O	4:D:346:ARG:HD3	2.01	0.61
4:D:177:VAL:HG21	4:D:179:MET:HE3	1.81	0.61
2:B:569:LEU:HD22	2:B:613:VAL:HG22	1.83	0.60
1:A:290:ILE:HD11	1:A:312:LYS:HB2	1.83	0.59
4:D:557:ILE:HD12	4:D:582:LEU:CB	2.33	0.59
1:A:452:SER:HB3	1:A:482:ALA:HA	1.85	0.59
3:C:354:GLN:HB2	12:W:611:HOH:O	2.01	0.59
1:A:549:ARG:HG3	1:A:555:GLU:HG3	1.84	0.59
4:D:663:VAL:HG22	4:D:668:HIS:ND1	2.17	0.59
2:B:176:LEU:HD22	2:B:356:LEU:HD11	1.86	0.58
3:C:587:ILE:HG23	3:C:588:ARG:HG2	1.84	0.58
4:D:177:VAL:CG2	4:D:179:MET:HE3	2.34	0.57
2:B:677:ARG:HG3	2:B:685:ILE:HD12	1.86	0.57
3:C:549:ARG:HG3	3:C:555:GLU:HA	1.86	0.57
3:C:550:LEU:HD11	3:C:616:VAL:HG11	1.87	0.57
4:D:625:TYR:HA	4:D:656:ARG:HG2	1.87	0.57
3:C:663:VAL:HG13	3:C:668:HIS:HB3	1.86	0.57
2:B:14:LYS:HA	2:B:17:ILE:HG22	1.87	0.56
3:C:290:ILE:HD11	3:C:312:LYS:HB2	1.86	0.56
1:A:247:LEU:O	1:A:251:VAL:HG23	2.05	0.56
1:A:505:LEU:HD11	1:A:535:LEU:HD11	1.87	0.56
3:C:448:PRO:HB3	3:C:467:LEU:HG	1.89	0.55
3:C:559:VAL:HG12	3:C:582:LEU:HB3	1.88	0.55
4:D:312:LYS:HD3	4:D:317:THR:HG22	1.87	0.55
2:B:382:TRP:HD1	2:B:390:LEU:HD11	1.71	0.55
1:A:552:GLN:HG3	1:A:609:LYS:HA	1.88	0.55
1:A:342:PRO:O	1:A:345:CYS:HB2	2.07	0.55
1:A:73:MET:CE	1:A:95:PHE:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:OE1	1:A:379:GLU:HA	2.06	0.54
3:C:138:ILE:HD11	3:C:336:VAL:HG11	1.88	0.54
4:D:177:VAL:O	4:D:336:VAL:HB	2.07	0.54
2:B:596:GLN:HA	2:B:603:ILE:HG13	1.89	0.54
2:B:17:ILE:CD1	2:B:21:LEU:HD12	2.35	0.54
3:C:451:LEU:HA	3:C:454:ILE:HG12	1.90	0.54
4:D:400:VAL:HB	4:D:454:ILE:HD11	1.89	0.54
2:B:173:MET:O	2:B:177:VAL:HG12	2.08	0.54
4:D:40:HIS:ND1	4:D:43:ILE:HD12	2.23	0.54
4:D:626:MET:HE1	4:D:680:TYR:HB3	1.90	0.53
1:A:577:LEU:HD23	1:A:582:LEU:HD13	1.88	0.53
4:D:565:CYS:HA	4:D:689:ASP:HB3	1.90	0.53
2:B:312:LYS:O	2:B:316:THR:O	2.27	0.53
2:B:568:ILE:HG13	2:B:618:PHE:CB	2.39	0.52
3:C:565:CYS:HA	3:C:689:ASP:HB3	1.92	0.52
1:A:568:ILE:HG13	1:A:618:PHE:CB	2.40	0.52
4:D:568:ILE:HG13	4:D:618:PHE:CB	2.40	0.52
2:B:177:VAL:HG22	2:B:177:VAL:O	2.11	0.51
3:C:505:LEU:HD11	3:C:535:LEU:HD11	1.92	0.51
4:D:151:LEU:CD1	4:D:154:LEU:HD22	2.41	0.51
1:A:217:GLN:HG2	1:A:239:LYS:HD2	1.91	0.51
1:A:565:CYS:HA	1:A:689:ASP:HB3	1.93	0.50
2:B:177:VAL:HG13	2:B:179:MET:HE3	1.93	0.50
3:C:568:ILE:HG13	3:C:618:PHE:CB	2.41	0.50
3:C:343:GLN:HB3	3:C:346:ARG:HH21	1.77	0.50
3:C:509:ARG:HA	3:C:601:GLU:HB2	1.93	0.50
4:D:594:HIS:CE1	4:D:598:LEU:HD11	2.46	0.50
2:B:529:GLN:HB2	2:B:557:ILE:HD11	1.93	0.50
3:C:240:LYS:HE2	3:C:267:GLU:HG3	1.93	0.50
3:C:350:GLN:HB3	3:C:662:VAL:HG11	1.93	0.50
2:B:441:ASP:HB3	2:B:444:ALA:HB2	1.94	0.49
2:B:560:LYS:HD2	2:B:583:ILE:HD12	1.94	0.49
2:B:87:THR:HG22	2:B:89:ASP:N	2.27	0.49
3:C:132:GLN:O	3:C:346:ARG:NH1	2.46	0.49
1:A:677:ARG:HG3	1:A:685:ILE:HD12	1.94	0.49
1:A:39:ALA:HB1	1:A:84:THR:HG21	1.95	0.49
3:C:677:ARG:HG3	3:C:685:ILE:HD12	1.94	0.49
2:B:88:LYS:O	2:B:92:ILE:HG13	2.13	0.49
3:C:574:GLN:HB3	3:C:592:LEU:HD21	1.94	0.49
4:D:509:ARG:HD2	4:D:526:LEU:HD13	1.94	0.49
3:C:663:VAL:HG11	3:C:669:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:TRP:NE1	2:B:316:THR:HG21	2.27	0.48
4:D:385:THR:HB	4:D:389:GLN:HB3	1.95	0.48
2:B:505:LEU:HD11	2:B:535:LEU:HD11	1.96	0.48
2:B:131:LEU:O	2:B:346:ARG:HD3	2.14	0.48
4:D:45:ARG:HG2	4:D:51:TYR:HD1	1.77	0.48
2:B:290:ILE:HD11	2:B:312:LYS:HD3	1.95	0.48
4:D:582:LEU:HD21	4:D:606:LEU:HD11	1.95	0.48
4:D:663:VAL:CG2	4:D:668:HIS:CG	2.97	0.48
2:B:625:TYR:HB2	2:B:684:ARG:HB3	1.94	0.48
2:B:622:LEU:HD21	2:B:669:ILE:HD11	1.95	0.47
1:A:574:GLN:HB3	1:A:592:LEU:HD21	1.97	0.47
1:A:131:LEU:O	1:A:346:ARG:HD3	2.13	0.47
4:D:477:LEU:O	4:D:481:GLN:HG3	2.15	0.47
4:D:505:LEU:HD11	4:D:535:LEU:HD11	1.96	0.47
2:B:382:TRP:CD1	2:B:390:LEU:HD11	2.48	0.47
4:D:350:GLN:HA	4:D:353:MET:HE3	1.95	0.47
1:A:587:ILE:HG23	1:A:588:ARG:HG2	1.96	0.47
2:B:551:ILE:HG21	2:B:606:LEU:HD13	1.96	0.47
2:B:585:HIS:HB2	2:B:592:LEU:HD13	1.97	0.47
3:C:101:GLU:HG3	12:W:680:HOH:O	2.15	0.47
4:D:677:ARG:HG3	4:D:685:ILE:HD12	1.96	0.47
2:B:508:TRP:NE1	2:B:601:GLU:HA	2.30	0.47
1:A:81:ILE:HD12	1:A:103:VAL:HG12	1.97	0.46
2:B:17:ILE:CG1	2:B:21:LEU:HD12	2.46	0.46
1:A:425:PRO:HG3	2:B:511:ILE:O	2.14	0.46
4:D:333:PHE:HA	4:D:340:ASN:HD21	1.80	0.46
1:A:124:ARG:HB3	1:A:375:TYR:CE2	2.51	0.46
1:A:489:LEU:HG	1:A:542:PRO:HG2	1.98	0.46
2:B:177:VAL:CG1	2:B:179:MET:HE3	2.46	0.46
2:B:294:ASP:HA	2:B:307:LEU:HD23	1.98	0.46
3:C:195:ASP:OD1	3:C:197:ASP:OD1	2.34	0.46
1:A:78:HIS:HA	1:A:103:VAL:HG13	1.97	0.46
3:C:217:GLN:HG2	3:C:239:LYS:HD2	1.97	0.45
3:C:568:ILE:HG13	3:C:618:PHE:HB2	1.98	0.45
4:D:132:GLN:O	4:D:346:ARG:NH1	2.50	0.45
4:D:217:GLN:HG2	4:D:239:LYS:HD2	1.98	0.45
4:D:280:VAL:HG21	4:D:307:LEU:HD13	1.98	0.45
4:D:568:ILE:HG13	4:D:618:PHE:HB2	1.99	0.45
4:D:633:VAL:HG13	4:D:650:VAL:HG11	1.98	0.45
1:A:385:THR:HB	1:A:389:GLN:HB3	1.97	0.45
1:A:410:LEU:HD23	1:A:440:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:626:MET:CE	4:D:680:TYR:HB3	2.46	0.45
2:B:280:VAL:HG21	2:B:307:LEU:HD13	1.99	0.45
2:B:582:LEU:HD21	2:B:606:LEU:HD11	1.98	0.45
3:C:65:MET:SD	3:C:337:LEU:HD11	2.56	0.45
4:D:70:GLU:HA	4:D:73:MET:HE2	1.98	0.45
1:A:341:ALA:HB3	1:A:344:THR:HG23	1.99	0.45
4:D:81:ILE:HD12	4:D:103:VAL:HG12	1.99	0.45
2:B:221:GLU:OE1	2:B:239:LYS:HE3	2.16	0.44
3:C:88:LYS:O	3:C:92:ILE:HG13	2.17	0.44
4:D:294:ASP:HA	4:D:307:LEU:HD23	2.00	0.44
4:D:400:VAL:CG1	4:D:454:ILE:HD11	2.48	0.44
2:B:78:HIS:HA	2:B:103:VAL:HG13	2.00	0.44
3:C:166:THR:HA	3:C:170:PHE:HD2	1.83	0.44
1:A:128:GLN:NE2	1:A:375:TYR:CE2	2.86	0.44
1:A:158:LYS:O	1:A:161:ARG:HG2	2.18	0.44
1:A:177:VAL:O	1:A:336:VAL:HG22	2.17	0.44
1:A:568:ILE:HG13	1:A:618:PHE:HB2	1.99	0.44
3:C:516:ALA:HA	3:C:519:GLU:HG2	2.00	0.44
4:D:259:GLU:O	4:D:263:SER:HB2	2.17	0.44
2:B:551:ILE:HD13	2:B:584:VAL:HG21	1.99	0.44
4:D:1:MET:HG2	4:D:2:PRO:HD2	2.00	0.44
1:A:203:GLN:HE21	1:A:247:LEU:HD13	1.83	0.44
4:D:78:HIS:HA	4:D:103:VAL:HG13	2.00	0.44
1:A:132:GLN:O	1:A:346:ARG:NH1	2.51	0.43
1:A:238:LYS:HZ1	8:A:1002:FLC:HA2	1.79	0.43
2:B:166:THR:HA	2:B:170:PHE:HD2	1.83	0.43
3:C:343:GLN:HB3	3:C:346:ARG:NH2	2.33	0.43
1:A:255:MET:HE1	1:A:260:LEU:HD22	2.00	0.43
2:B:574:GLN:HB3	2:B:592:LEU:HD21	2.00	0.43
3:C:666:ARG:HA	3:C:669:ILE:HG22	2.00	0.43
4:D:62:LEU:HD13	4:D:71:THR:HG22	2.00	0.43
2:B:659:VAL:HG22	2:B:661:ILE:HG23	2.00	0.43
3:C:477:LEU:O	3:C:481:GLN:HG3	2.18	0.43
4:D:551:ILE:HG21	4:D:606:LEU:HD13	2.00	0.43
2:B:446:PRO:CG	2:B:466:VAL:HG11	2.46	0.43
2:B:569:LEU:HD23	2:B:665:ASN:HB3	2.00	0.43
1:A:692:ALA:O	1:A:695:MET:O	2.37	0.42
2:B:477:LEU:O	2:B:481:GLN:HG3	2.19	0.42
3:C:117:TYR:N	3:C:161:ARG:HH21	2.17	0.42
3:C:305:GLN:HB2	3:C:327:MET:HG2	2.01	0.42
4:D:666:ARG:HA	4:D:669:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:663:VAL:CG2	4:D:668:HIS:ND1	2.81	0.42
2:B:373:LEU:HD22	2:B:377:HIS:CE1	2.54	0.42
2:B:489:LEU:HA	2:B:545:GLU:HB2	2.01	0.42
3:C:128:GLN:HG3	3:C:376:LEU:HA	2.00	0.42
4:D:40:HIS:NE2	4:D:80:VAL:HG12	2.34	0.42
1:A:450:TRP:O	1:A:454:ILE:HG12	2.19	0.42
2:B:312:LYS:HZ1	2:B:315:LYS:HA	1.83	0.42
2:B:126:ILE:HD12	2:B:169:ILE:HG21	2.00	0.42
4:D:385:THR:HG22	4:D:387:HIS:H	1.84	0.42
4:D:510:HIS:HB2	4:D:601:GLU:HB3	2.01	0.42
2:B:594:HIS:CE1	2:B:598:LEU:CD2	2.96	0.42
4:D:622:LEU:HB2	4:D:659:VAL:HG13	2.02	0.42
4:D:342:PRO:O	4:D:345:CYS:HB2	2.18	0.42
3:C:454:ILE:HD13	3:C:463:LEU:HD12	2.00	0.42
4:D:511:ILE:HD12	4:D:511:ILE:HA	1.96	0.42
1:A:21:LEU:HD22	1:A:69:PRO:HG3	2.02	0.41
1:A:131:LEU:HD12	1:A:376:LEU:HD22	2.01	0.41
1:A:511:ILE:HD12	1:A:511:ILE:HA	1.97	0.41
4:D:81:ILE:HD12	4:D:103:VAL:CG1	2.50	0.41
1:A:259:GLU:O	1:A:263:SER:HB2	2.20	0.41
4:D:336:VAL:HG22	4:D:342:PRO:HA	2.02	0.41
2:B:151:LEU:HG	2:B:159:ARG:HG2	2.02	0.41
2:B:406:ALA:HB3	2:B:410:LEU:HD12	2.03	0.41
4:D:549:ARG:HE	4:D:555:GLU:HA	1.85	0.41
1:A:477:LEU:HD12	2:B:597:HIS:HB2	2.02	0.41
4:D:131:LEU:HD12	4:D:376:LEU:HD22	2.01	0.41
4:D:521:ILE:HG23	4:D:528:PRO:HD3	2.02	0.41
1:A:399:VAL:HG11	1:A:417:ALA:HB2	2.02	0.41
1:A:569:LEU:HD23	1:A:665:ASN:HB3	2.02	0.41
2:B:132:GLN:O	2:B:346:ARG:NH1	2.54	0.41
2:B:347:SER:OG	2:B:617:ARG:HD2	2.21	0.41
1:A:633:VAL:HG13	1:A:650:VAL:HG11	2.03	0.41
1:A:666:ARG:HA	1:A:669:ILE:HG22	2.02	0.41
2:B:336:VAL:HG13	2:B:341:ALA:HB1	2.03	0.41
2:B:550:LEU:HD21	2:B:613:VAL:HG21	2.03	0.41
2:B:666:ARG:HA	2:B:669:ILE:HG22	2.03	0.41
3:C:406:ALA:HB3	3:C:410:LEU:HD12	2.03	0.41
3:C:1:MET:N	3:C:2:PRO:HD2	2.36	0.41
3:C:138:ILE:HD11	3:C:336:VAL:HG13	2.02	0.41
4:D:377:HIS:HD2	4:D:561:TYR:HE2	1.69	0.41
1:A:46:LYS:NZ	1:A:158:LYS:NZ	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:O	1:A:92:ILE:HG13	2.22	0.40
1:A:220:TRP:CE2	1:A:316:THR:HG21	2.55	0.40
1:A:399:VAL:HG11	1:A:417:ALA:CB	2.51	0.40
3:C:467:LEU:HD13	3:C:522:ALA:HB1	2.02	0.40
4:D:45:ARG:HG2	4:D:51:TYR:CD1	2.56	0.40
4:D:588:ARG:HA	4:D:588:ARG:HD3	1.87	0.40
3:C:131:LEU:O	3:C:346:ARG:HD3	2.22	0.40
3:C:39:ALA:HB1	3:C:84:THR:HG21	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	682/687 (99%)	665 (98%)	17 (2%)	0	100	100
2	B	679/687 (99%)	656 (97%)	23 (3%)	0	100	100
3	C	672/678 (99%)	655 (98%)	17 (2%)	0	100	100
4	D	685/689 (99%)	662 (97%)	23 (3%)	0	100	100
All	All	2718/2741 (99%)	2638 (97%)	80 (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	582/604 (96%)	580 (100%)	2 (0%)	92 97
2	B	574/602 (95%)	568 (99%)	6 (1%)	76 89
3	C	571/595 (96%)	567 (99%)	4 (1%)	84 93
4	D	568/605 (94%)	557 (98%)	11 (2%)	57 79
All	All	2295/2406 (95%)	2272 (99%)	23 (1%)	76 89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	PHE
1	A	314	GLU
2	B	47	SER
2	B	123	PHE
2	B	314	GLU
2	B	539	ASP
2	B	590	HIS
2	B	615	ASP
3	C	1	MET
3	C	123	PHE
3	C	154	LEU
3	C	513	ASN
4	D	45	ARG
4	D	110	SER
4	D	123	PHE
4	D	314	GLU
4	D	340	ASN
4	D	369	PHE
4	D	385	THR
4	D	547	SER
4	D	549	ARG
4	D	550	LEU
4	D	592	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	203	GLN
1	A	204	ASN
1	A	340	ASN
1	A	563	HIS

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Mol	Chain	Res	Type
1	A	576	HIS
1	A	585	HIS
2	B	576	HIS
2	B	594	HIS
3	C	576	HIS
4	D	340	ASN
4	D	377	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 23 ligands modelled in this entry, 13 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
9	GOL	B	1001	-	5,5,5	0.04	0	5,5,5	0.14	0
9	GOL	C	1002	-	5,5,5	0.03	0	5,5,5	0.18	0
9	GOL	A	1003	-	5,5,5	0.05	0	5,5,5	0.11	0
8	FLC	C	1001	-	3,12,12	0.33	0	3,17,17	1.81	2 (66%)
7	G4P	C	1000	10	30,38,38	1.07	2 (6%)	43,61,61	1.69	9 (20%)
8	FLC	A	1002	-	3,12,12	0.43	0	3,17,17	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	G4P	A	1001	5	30,38,38	1.03	2 (6%)	43,61,61	1.74	9 (20%)
7	G4P	B	1000	-	30,38,38	1.03	2 (6%)	43,61,61	1.72	9 (20%)
9	GOL	C	1003	-	5,5,5	0.33	0	5,5,5	0.25	0
7	G4P	D	1001	10	30,38,38	1.08	2 (6%)	43,61,61	1.80	10 (23%)

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
9	GOL	B	1001	-	-	0/4/4/4	-
9	GOL	C	1002	-	-	0/4/4/4	-
9	GOL	A	1003	-	-	3/4/4/4	-
8	FLC	C	1001	-	-	5/6/16/16	-
7	G4P	C	1000	10	-	4/23/43/43	0/3/3/3
8	FLC	A	1002	-	-	3/6/16/16	-
7	G4P	A	1001	5	-	6/23/43/43	0/3/3/3
7	G4P	B	1000	-	-	7/23/43/43	0/3/3/3
9	GOL	C	1003	-	-	3/4/4/4	-
7	G4P	D	1001	10	-	7/23/43/43	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1001	G4P	C5-C6	4.10	1.48	1.41
7	C	1000	G4P	C5-C6	4.05	1.48	1.41
7	B	1000	G4P	C5-C6	3.85	1.48	1.41
7	A	1001	G4P	C5-C6	3.82	1.47	1.41
7	D	1001	G4P	C5-C4	2.45	1.47	1.40
7	B	1000	G4P	C5-C4	2.43	1.47	1.40
7	C	1000	G4P	C5-C4	2.40	1.47	1.40
7	A	1001	G4P	C5-C4	2.36	1.47	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1001	G4P	C2-N3-C4	5.68	121.84	115.36
7	A	1001	G4P	C2-N3-C4	5.29	121.40	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1000	G4P	C2-N3-C4	4.98	121.05	115.36
7	C	1000	G4P	C2-N3-C4	4.93	120.99	115.36
7	B	1000	G4P	C5-C6-N1	-4.11	117.82	123.43
7	C	1000	G4P	C5-C6-N1	-3.93	118.05	123.43
7	A	1001	G4P	C5-C6-N1	-3.93	118.06	123.43
7	B	1000	G4P	C2-N1-C6	3.83	122.02	115.93
7	D	1001	G4P	C5-C6-N1	-3.83	118.19	123.43
7	A	1001	G4P	C2-N1-C6	3.80	121.97	115.93
7	C	1000	G4P	C2-N1-C6	3.69	121.79	115.93
7	D	1001	G4P	C2-N1-C6	3.60	121.65	115.93
7	D	1001	G4P	PC-O3C-PD	-3.54	120.68	132.83
7	C	1000	G4P	C4-C5-C6	-3.38	117.57	120.80
7	A	1001	G4P	PC-O3C-PD	-3.18	121.90	132.83
7	A	1001	G4P	PA-O3A-PB	-3.15	122.00	132.83
7	A	1001	G4P	N3-C2-N1	-3.10	123.08	127.22
7	B	1000	G4P	PC-O3C-PD	-3.06	122.32	132.83
7	A	1001	G4P	C4-C5-C6	-3.02	117.91	120.80
7	C	1000	G4P	PA-O3A-PB	-3.01	122.50	132.83
7	D	1001	G4P	N3-C2-N1	-2.97	123.26	127.22
7	B	1000	G4P	C4-C5-C6	-2.96	117.97	120.80
7	B	1000	G4P	N3-C2-N1	-2.89	123.37	127.22
7	C	1000	G4P	N3-C2-N1	-2.85	123.42	127.22
7	D	1001	G4P	C4-C5-C6	-2.83	118.10	120.80
7	D	1001	G4P	PA-O3A-PB	-2.79	123.25	132.83
7	B	1000	G4P	PA-O3A-PB	-2.72	123.49	132.83
7	D	1001	G4P	C4-C5-N7	-2.62	106.67	109.40
7	C	1000	G4P	C4-C5-N7	-2.54	106.75	109.40
7	A	1001	G4P	C4-C5-N7	-2.53	106.77	109.40
7	C	1000	G4P	PC-O3C-PD	-2.41	124.55	132.83
8	C	1001	FLC	CB-CA-CAC	2.28	118.64	114.98
7	B	1000	G4P	C4-C5-N7	-2.23	107.07	109.40
7	D	1001	G4P	O4'-C1'-C2'	-2.23	103.67	106.93
7	D	1001	G4P	C1'-N9-C4	2.23	130.55	126.64
7	B	1000	G4P	O4'-C1'-C2'	-2.16	103.77	106.93
7	A	1001	G4P	C3'-C2'-C1'	2.15	104.65	99.89
8	C	1001	FLC	CB-CG-CGC	2.13	118.40	114.98
7	C	1000	G4P	C3'-C2'-C1'	2.04	104.42	99.89

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1001	G4P	C5'-O5'-PA-O1A
7	A	1001	G4P	O4'-C4'-C5'-O5'
7	B	1000	G4P	C3'-C4'-C5'-O5'
7	B	1000	G4P	C3'-O3'-PC-O3C
7	C	1000	G4P	C4'-C5'-O5'-PA
7	D	1001	G4P	C5'-O5'-PA-O1A
7	D	1001	G4P	C5'-O5'-PA-O2A
8	A	1002	FLC	CAC-CA-CB-CBC
8	A	1002	FLC	CAC-CA-CB-CG
8	C	1001	FLC	CA-CB-CG-CGC
8	C	1001	FLC	OHB-CB-CG-CGC
9	A	1003	GOL	C1-C2-C3-O3
9	C	1003	GOL	O1-C1-C2-O2
9	C	1003	GOL	O1-C1-C2-C3
7	A	1001	G4P	C3'-C4'-C5'-O5'
7	B	1000	G4P	O4'-C4'-C5'-O5'
8	A	1002	FLC	CAC-CA-CB-OHB
8	C	1001	FLC	CAC-CA-CB-OHB
7	C	1000	G4P	C3'-C4'-C5'-O5'
7	B	1000	G4P	C3'-O3'-PC-O1C
8	C	1001	FLC	CAC-CA-CB-CG
7	B	1000	G4P	PB-O3A-PA-O5'
7	D	1001	G4P	PB-O3A-PA-O5'
7	A	1001	G4P	C5'-O5'-PA-O3A
7	B	1000	G4P	PD-O3C-PC-O2C
7	C	1000	G4P	PD-O3C-PC-O2C
7	D	1001	G4P	PD-O3C-PC-O1C
8	C	1001	FLC	CBC-CB-CG-CGC
9	A	1003	GOL	O2-C2-C3-O3
7	A	1001	G4P	PB-O3A-PA-O1A
9	A	1003	GOL	O1-C1-C2-C3
7	A	1001	G4P	PB-O3A-PA-O2A
9	C	1003	GOL	C1-C2-C3-O3
7	D	1001	G4P	C5'-O5'-PA-O3A
7	B	1000	G4P	PD-O3C-PC-O1C
7	D	1001	G4P	PD-O3C-PC-O2C
7	D	1001	G4P	C3'-O3'-PC-O3C
7	C	1000	G4P	C5'-O5'-PA-O1A

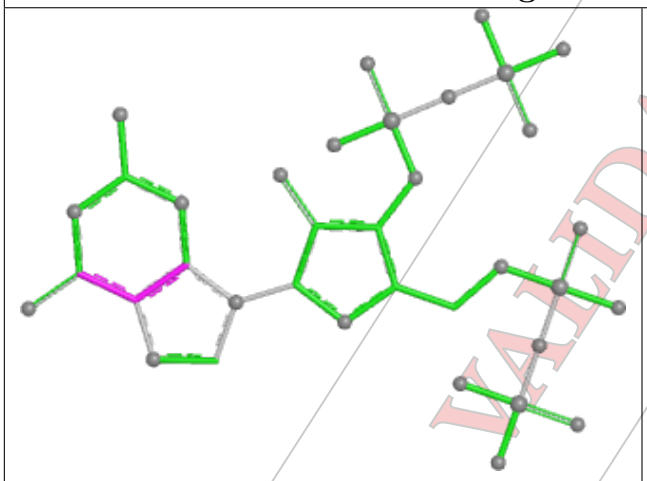
There are no ring outliers.

1 monomer is involved in 3 short contacts:

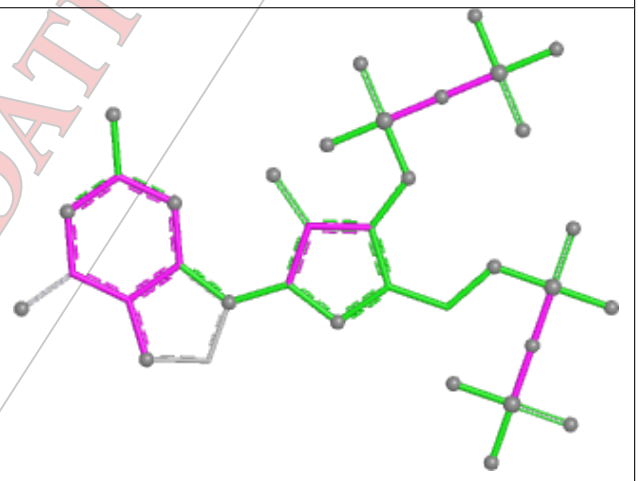
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1002	FLC	3	0

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.

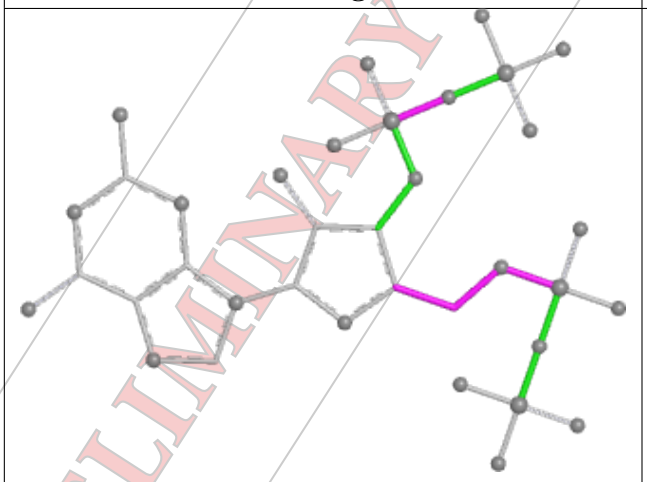
Ligand G4P C 1000



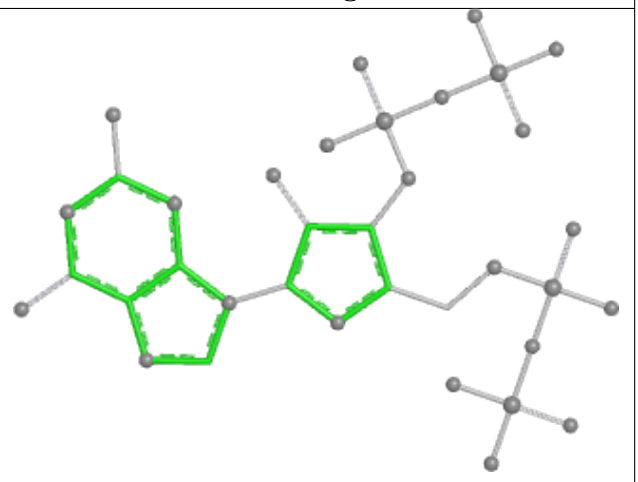
Bond lengths



Bond angles

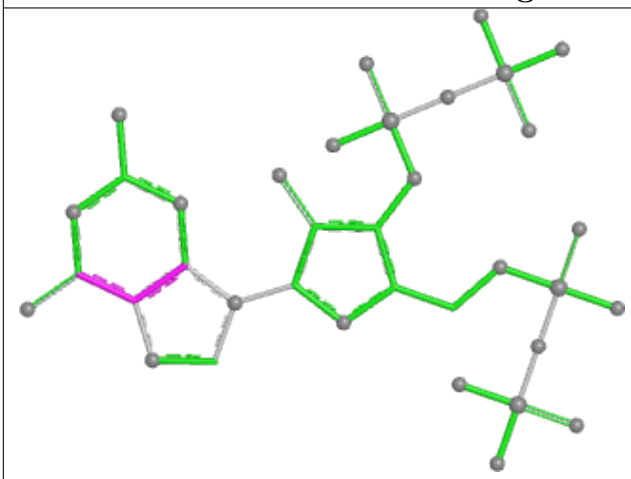


Torsions

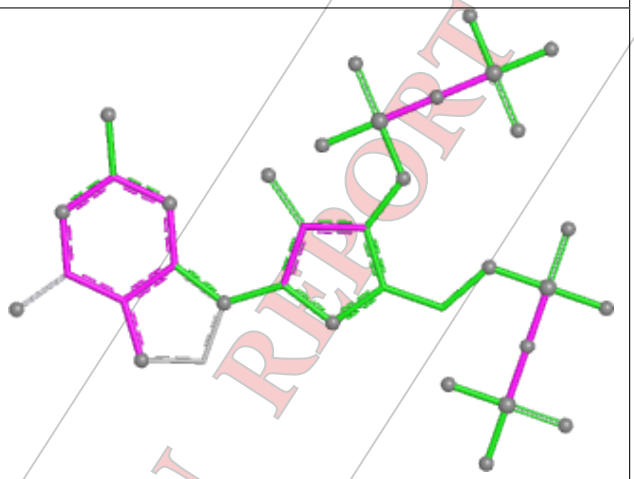


Rings

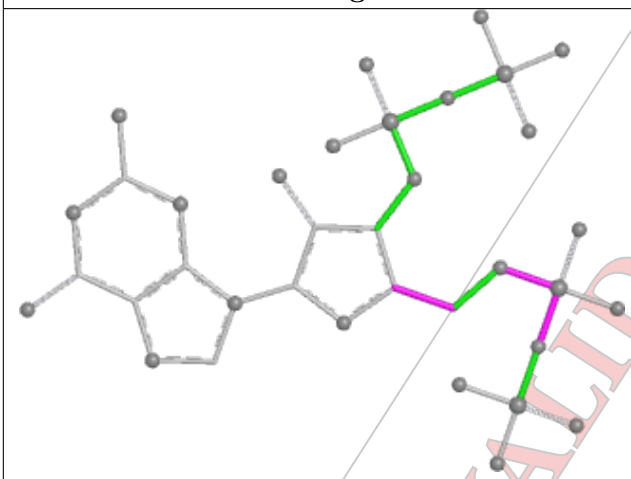
Ligand G4P A 1001



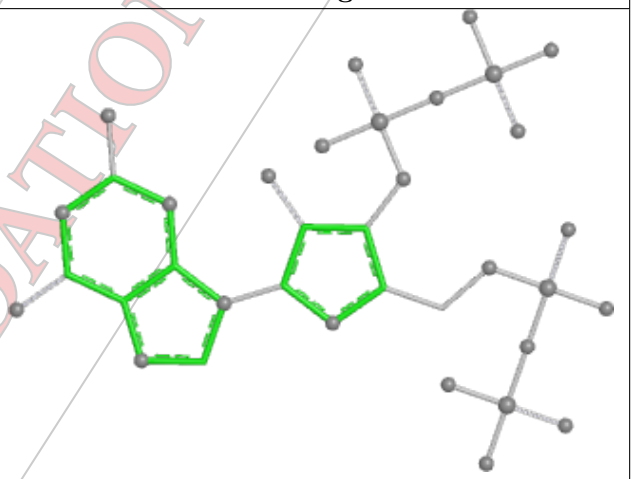
Bond lengths



Bond angles

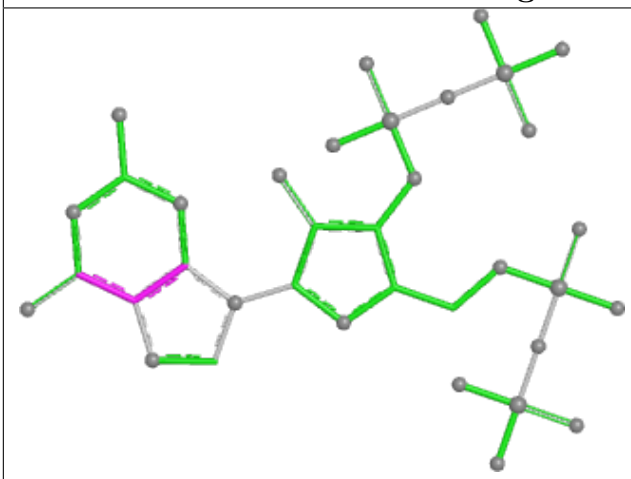


Torsions

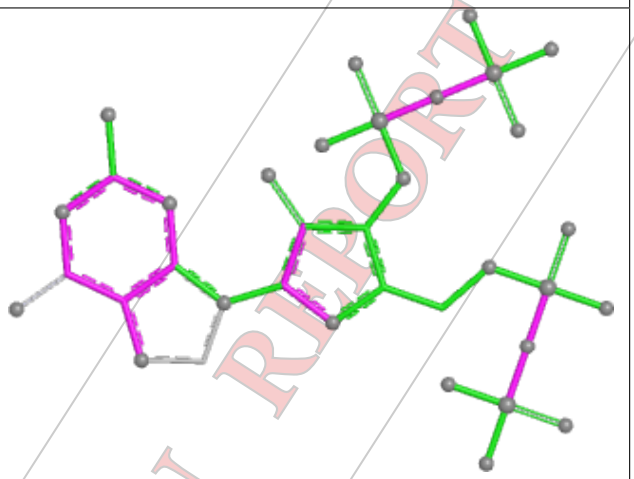


Rings

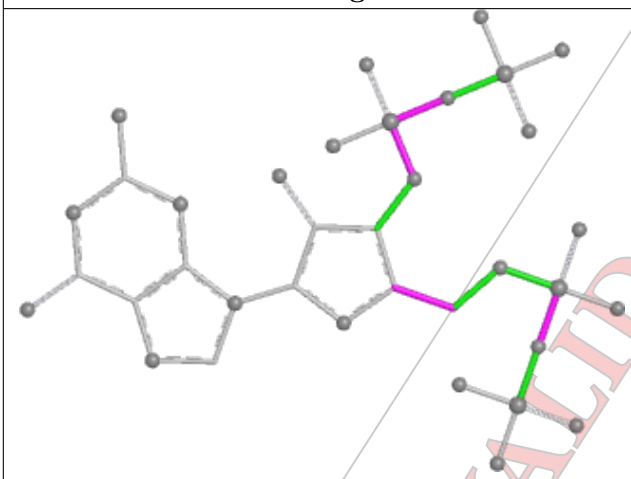
Ligand G4P B 1000



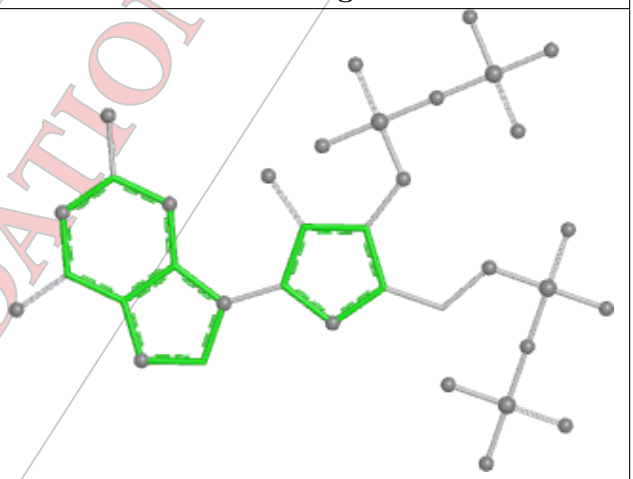
Bond lengths



Bond angles

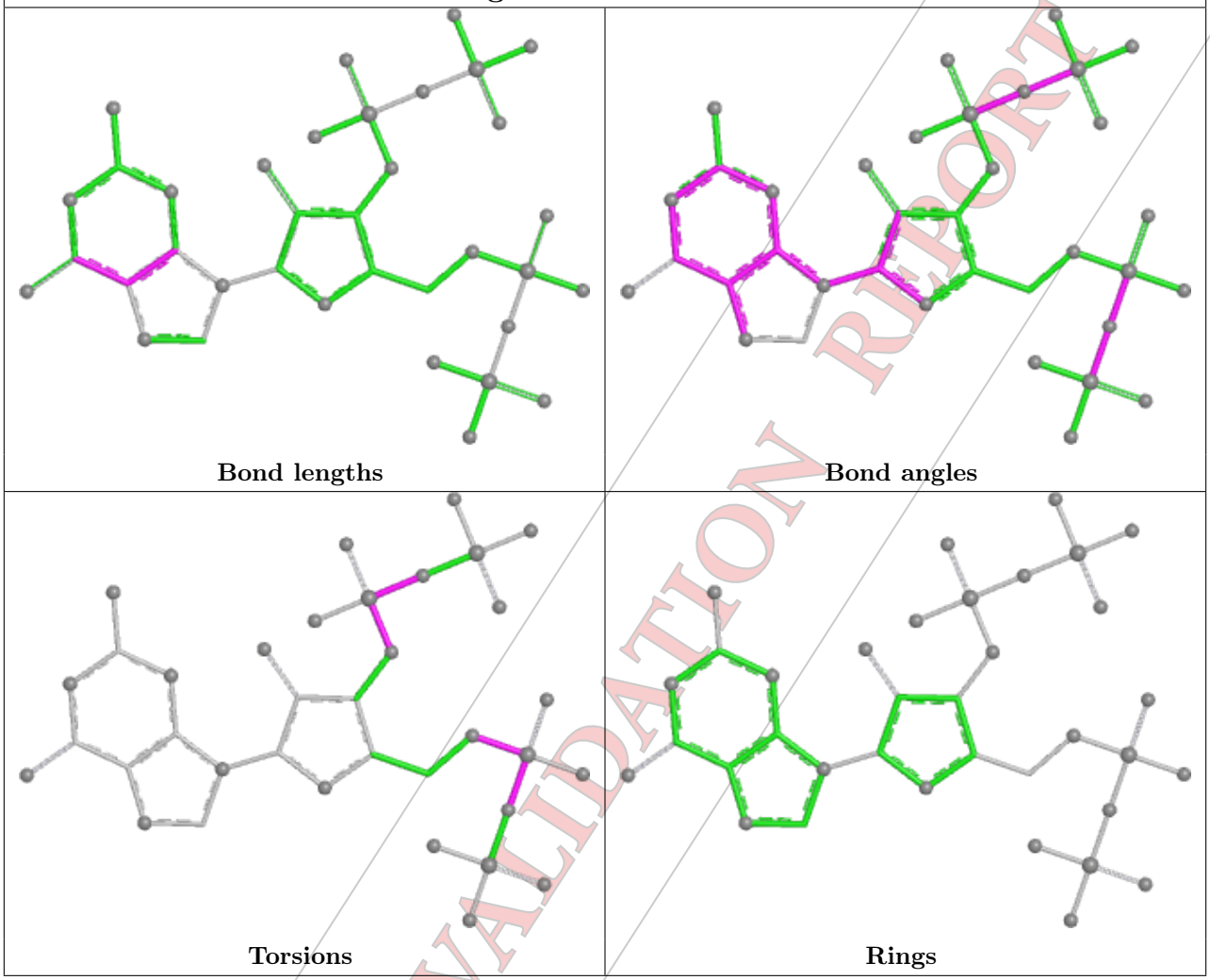


Torsions



Rings

Ligand G4P D 1001



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
2	B	3
3	C	2
1	A	2
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	537:ALA	C	547:SER	N	12.88
1	B	539:ASP	C	544:ALA	N	10.79
1	A	542:PRO	C	546:ASN	N	7.06
1	B	338:GLY	C	340:ASN	N	5.96
1	A	359:LEU	C	367:THR	N	5.74
1	D	361:ASP	C	368:THR	N	5.64
1	B	359:LEU	C	365:ALA	N	4.82
1	C	358:THR	C	368:THR	N	4.06

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	687/687 (100%)	0.07	21 (3%) 49 53	38, 59, 110, 148	0
2	B	687/687 (100%)	0.21	28 (4%) 37 41	39, 68, 103, 121	0
3	C	678/678 (100%)	0.14	28 (4%) 37 41	40, 63, 113, 143	0
4	D	689/689 (100%)	0.25	34 (4%) 29 32	42, 69, 113, 140	0
All	All	2741/2741 (100%)	0.17	111 (4%) 38 42	38, 65, 110, 148	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	368	THR	6.4
2	B	334	GLY	6.3
4	D	695	MET	5.0
1	A	695	MET	5.0
1	A	153	ALA	5.0
3	C	535	LEU	4.9
1	A	359	LEU	4.9
3	C	511	ILE	4.8
3	C	547	SER	4.7
2	B	335	VAL	4.6
4	D	546	ASN	4.6
2	B	370	ASN	4.5
4	D	542	PRO	4.5
2	B	85	GLN	4.4
3	C	503	LEU	4.0
3	C	531	VAL	4.0
2	B	153	ALA	3.9
4	D	538	ASN	3.9
2	B	697	ILE	3.9
3	C	505	LEU	3.9
3	C	487	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
4	D	543	ARG	3.8
1	A	539	ASP	3.8
1	A	49	GLU	3.7
2	B	84	THR	3.6
4	D	491	ASN	3.6
4	D	86	TYR	3.5
4	D	598	LEU	3.5
3	C	510	HIS	3.4
2	B	356	LEU	3.3
2	B	48	GLY	3.3
1	A	156	PRO	3.2
4	D	359	LEU	3.2
4	D	1	MET	3.2
3	C	358	THR	3.2
1	A	497	LEU	3.2
4	D	87	THR	3.2
2	B	367	THR	3.2
2	B	338	GLY	3.1
2	B	89	ASP	3.1
2	B	696	GLU	3.1
4	D	548	ASP	3.0
2	B	369	PHE	3.0
1	A	697	ILE	3.0
1	A	505	LEU	3.0
2	B	340	ASN	3.0
2	B	365	ALA	2.9
4	D	313	GLY	2.9
3	C	523	VAL	2.9
3	C	470	GLN	2.9
3	C	533	ASN	2.9
3	C	553	GLY	2.9
2	B	250	PHE	2.9
4	D	360	ILE	2.8
4	D	539	ASP	2.8
4	D	335	VAL	2.8
4	D	694	GLN	2.8
3	C	493	SER	2.8
3	C	507	GLN	2.7
1	A	367	THR	2.7
3	C	474	GLU	2.7
2	B	461	ARG	2.7
3	C	500	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	542	PRO	2.7
2	B	695	MET	2.7
1	A	152	GLY	2.6
1	A	502	TRP	2.6
4	D	91	ILE	2.6
3	C	536	PHE	2.6
1	A	546	ASN	2.6
4	D	369	PHE	2.5
1	A	500	ALA	2.5
1	A	490	PHE	2.4
3	C	495	ASN	2.4
3	C	489	LEU	2.4
4	D	48	GLY	2.4
3	C	469	ASP	2.4
4	D	358	THR	2.4
4	D	489	LEU	2.4
4	D	547	SER	2.3
1	A	535	LEU	2.3
4	D	370	ASN	2.3
2	B	530	LEU	2.3
1	A	498	SER	2.3
3	C	471	ASP	2.3
4	D	341	ALA	2.2
4	D	503	LEU	2.2
3	C	477	LEU	2.2
2	B	358	THR	2.2
2	B	359	LEU	2.2
3	C	512	ASP	2.2
3	C	1	MET	2.2
2	B	546	ASN	2.2
2	B	333	PHE	2.2
4	D	337	LEU	2.1
4	D	39	ALA	2.1
4	D	557	ILE	2.1
4	D	661	ILE	2.1
4	D	597	HIS	2.1
4	D	521	ILE	2.1
2	B	2	PRO	2.1
1	A	494	ILE	2.1
2	B	290	ILE	2.1
1	A	461	ARG	2.1
4	D	541	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	486	ALA	2.0
4	D	544	ALA	2.0
1	A	495	ASN	2.0
3	C	506	LEU	2.0
3	C	530	LEU	2.0
2	B	545	GLU	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
8	FLC	C	1001	13/?	0.62	0.37	105,106,107,107	0
9	GOL	C	1002	6/?	0.73	0.14	126,126,126,126	0
7	G4P	C	1000	36/?	0.74	0.20	189,190,192,192	0
7	G4P	D	1001	36/?	0.75	0.21	125,127,130,130	36
9	GOL	A	1003	6/?	0.77	0.39	104,104,104,104	0
7	G4P	B	1000	36/?	0.77	0.19	191,191,192,192	0
11	CL	F	1	1/?	0.79	0.40	129,129,129,129	0
7	G4P	A	1001	36/?	0.80	0.20	152,155,156,156	0
8	FLC	A	1002	13/?	0.80	0.25	114,114,115,115	0
11	CL	F	2	1/?	0.82	0.09	100,100,100,100	0
10	MG	E	5	1/?	0.85	0.09	109,109,109,109	0
9	GOL	C	1003	6/?	0.88	0.17	74,75,75,75	0
5	MN	B	799	1/?	0.88	0.10	133,133,133,133	0
9	GOL	B	1001	6/?	0.90	0.13	101,101,101,101	0
5	MN	D	800	1/?	0.90	0.12	134,134,134,134	0
5	MN	C	799	1/?	0.90	0.04	124,124,124,124	0
10	MG	E	6	1/?	0.93	0.10	74,74,74,74	0

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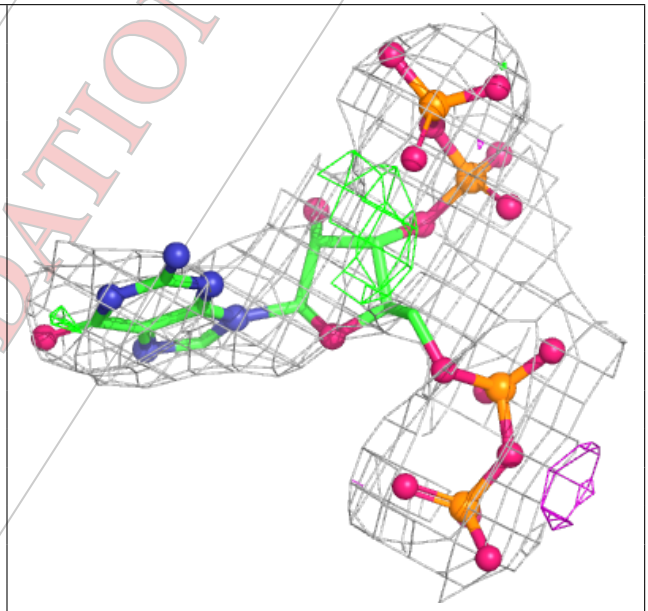
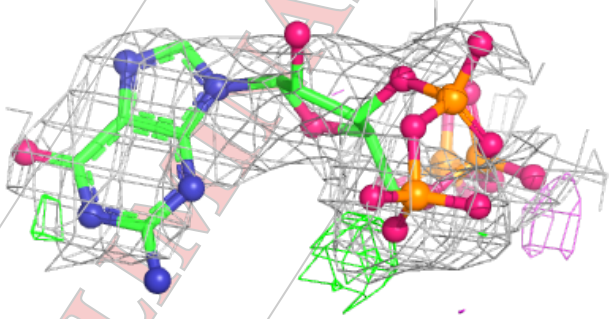
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MN	A	800	1/?	0.94	0.10	121,121,121,121	0
11	CL	F	3	1/?	0.98	0.48	83,83,83,83	0
6	ZN	A	900	1/?	0.99	0.18	54,54,54,54	0
6	ZN	B	900	1/?	0.99	0.14	68,68,68,68	0
6	ZN	D	900	1/?	0.99	0.15	70,70,70,70	0
6	ZN	C	900	1/?	1.00	0.13	51,51,51,51	0

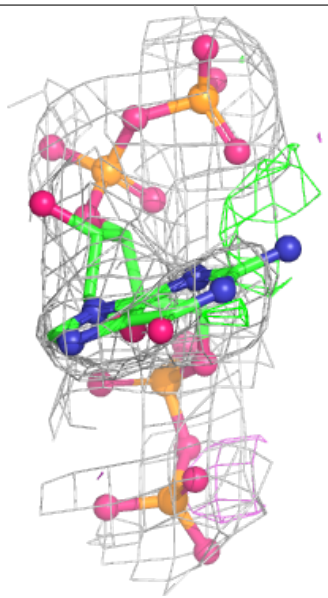
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G4P C 1000:

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

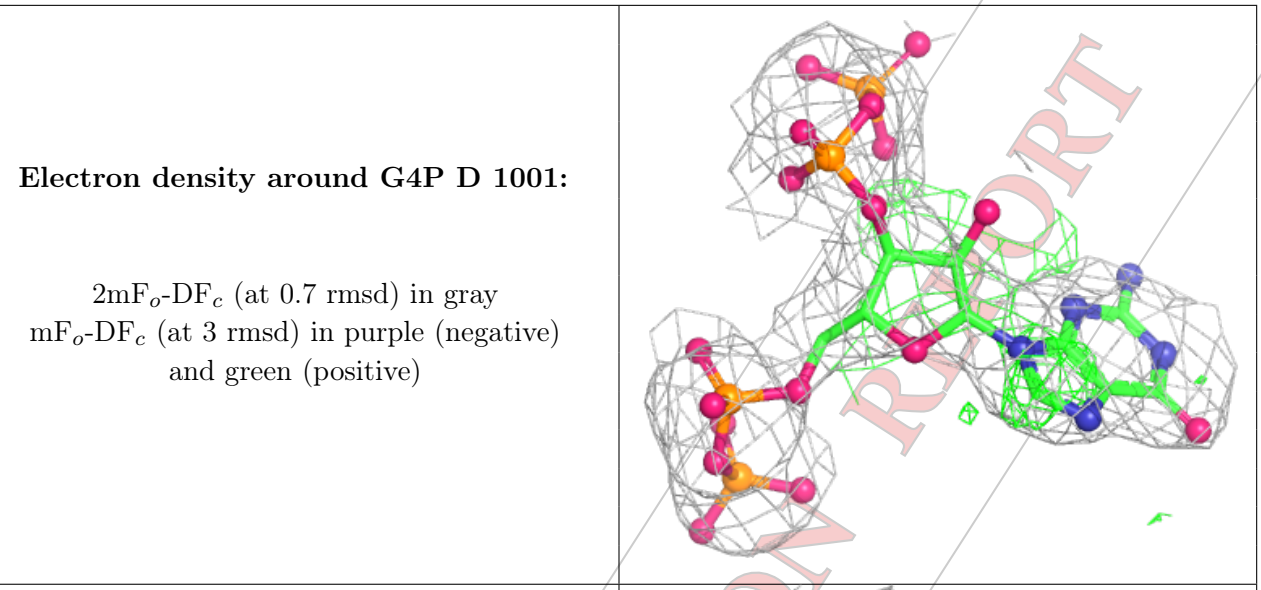






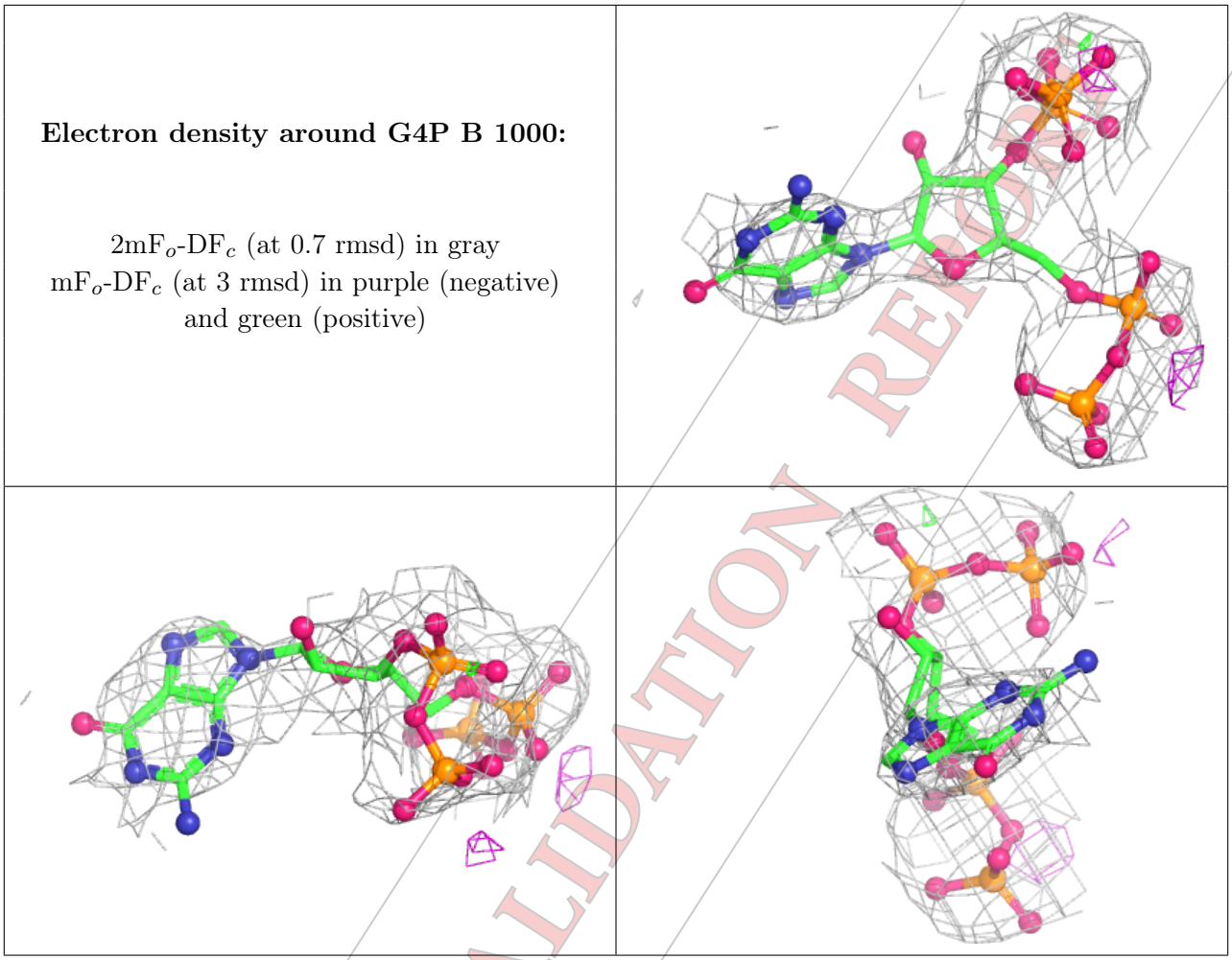
Electron density around G4P D 1001:

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



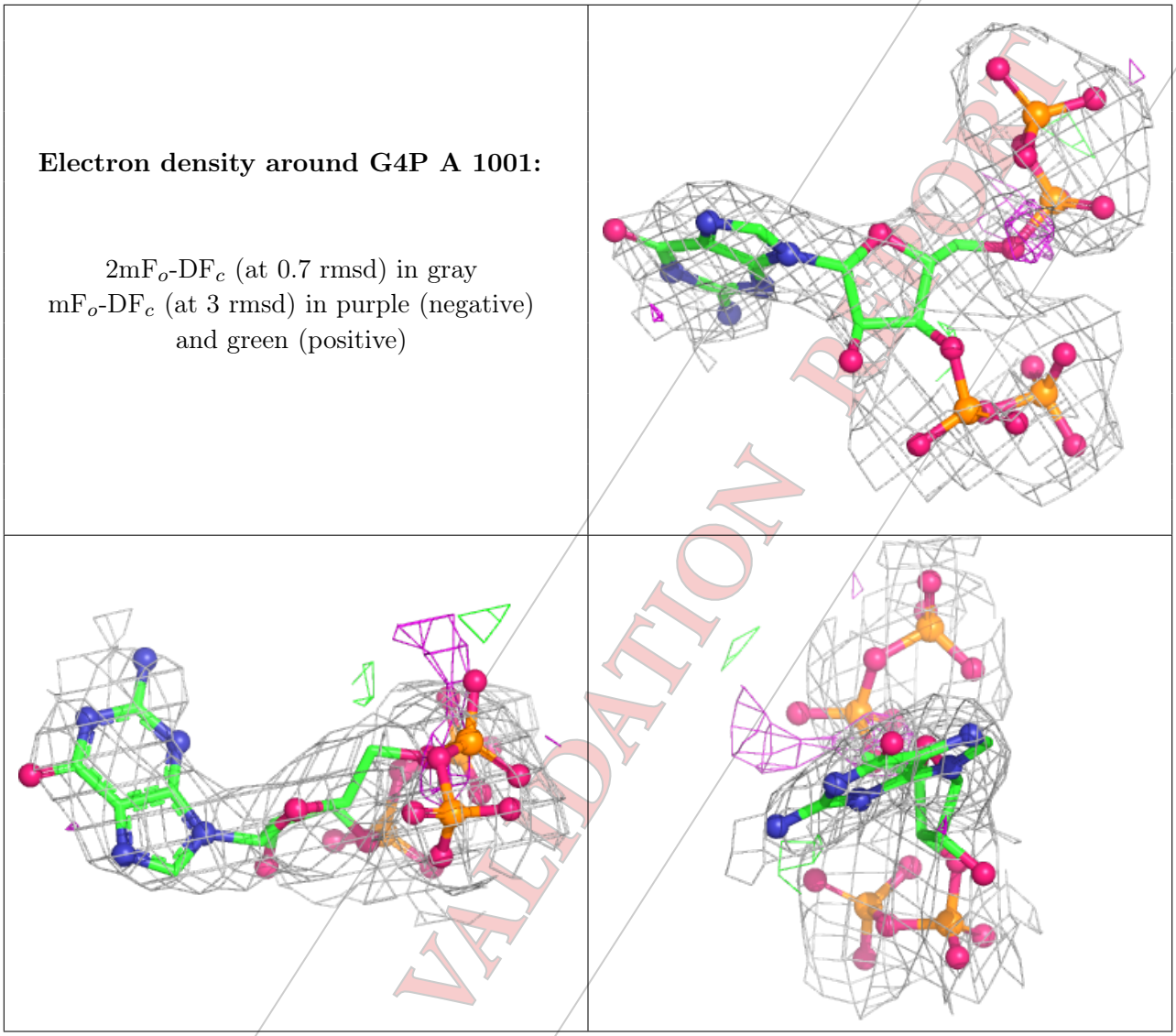
Electron density around G4P B 1000:

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



Electron density around G4P A 1001:

$2mF_o$-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.