Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 12:37 PM GMT

PDB ID	:	6TIY
Title	:	DROSOPHILA GMPCPP-TUBULIN
Authors	:	Gigant, B.
Deposited on	:	2019-11-22
Resolution	:	2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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:

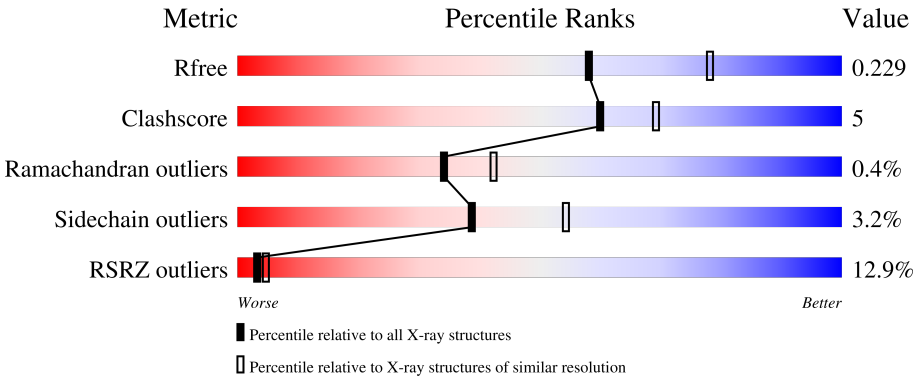
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	450	8% 83% 13% ·
1	C	450	14% 82% 13% · ·
2	B	447	16% 83% 12% · ·
2	D	447	8% 86% 9% ·
3	E	143	21% 83% 8% · 7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15210 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 Tubulin alpha-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3392	2148	577	644	23			
1	C	434	Total	C	N	O	S	0	2	0
			3386	2144	575	642	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ARG	LYS	engineered mutation	UNP P06603
C	40	ARG	LYS	engineered mutation	UNP P06603

- Molecule 2 is a protein called Tubulin beta-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3362	2112	573	651	26			
2	D	427	Total	C	N	O	S	0	3	0
			3362	2117	570	648	27			

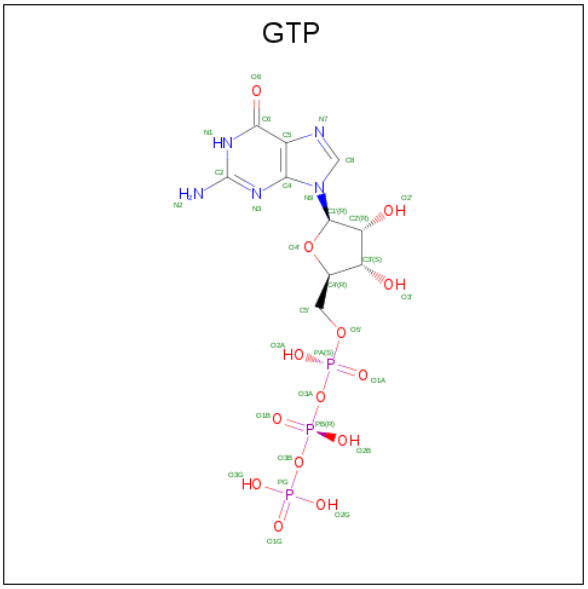
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	133	Total	C	N	O	S	0	0	0
			1085	670	197	214	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	SER	engineered mutation	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

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

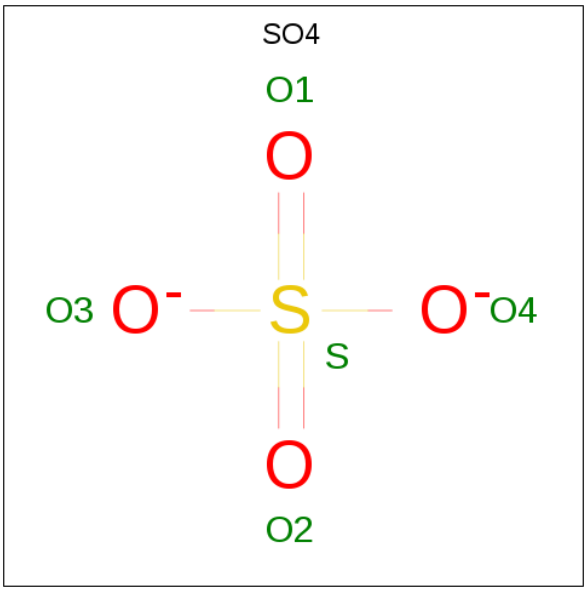


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

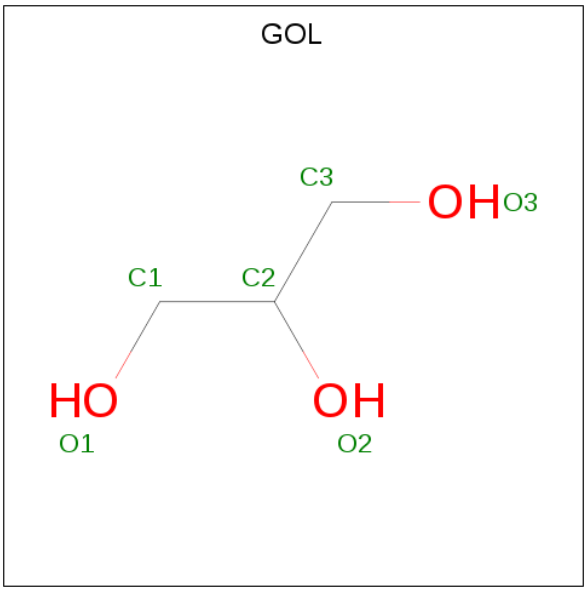
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



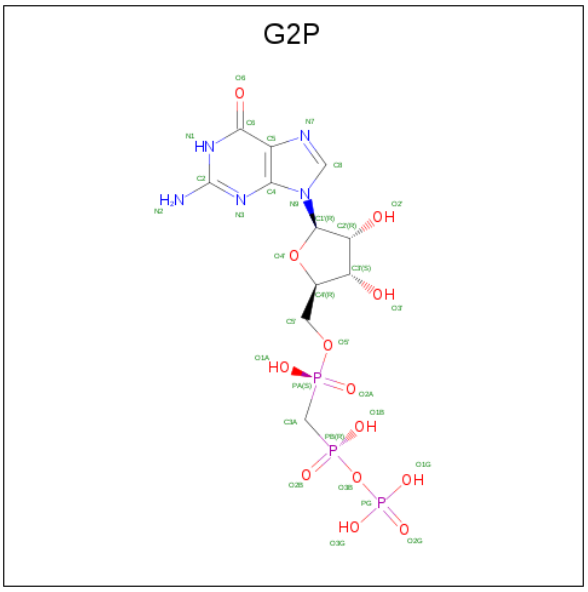
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
8	D	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 9 is water.

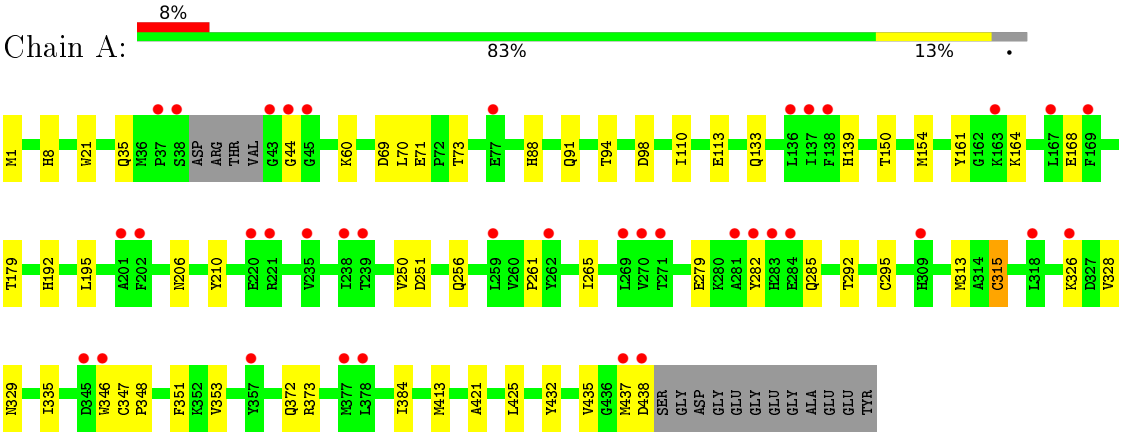
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	143	Total O 143 143	0	0
9	B	92	Total O 92 92	0	0
9	C	85	Total O 85 85	0	0
9	D	96	Total O 96 96	0	0
9	E	14	Total O 14 14	0	0

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.

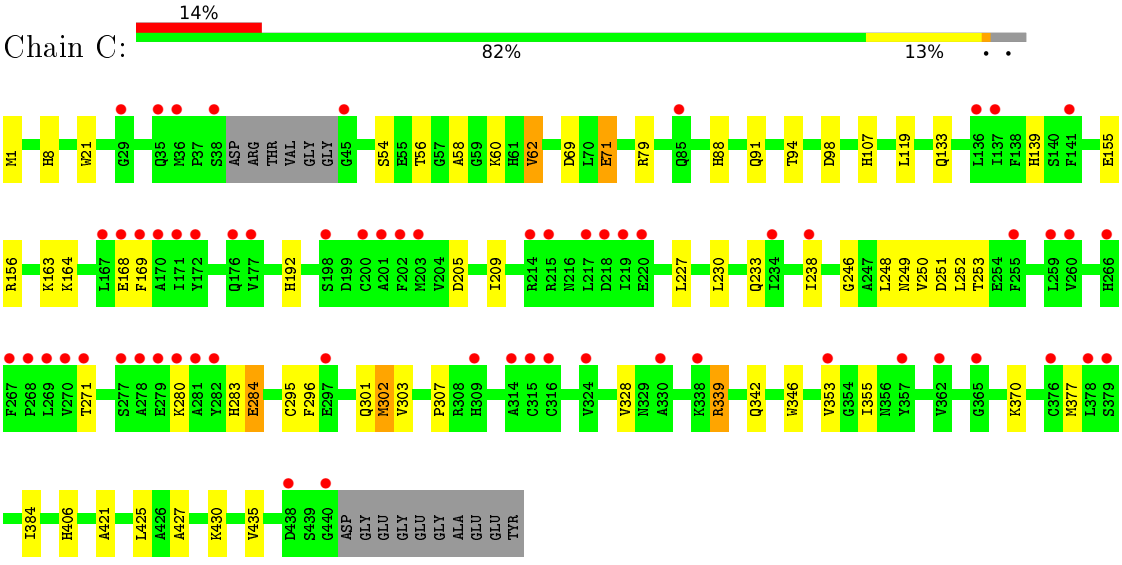
- Molecule 1: Tubulin alpha-1 chain

Chain A:



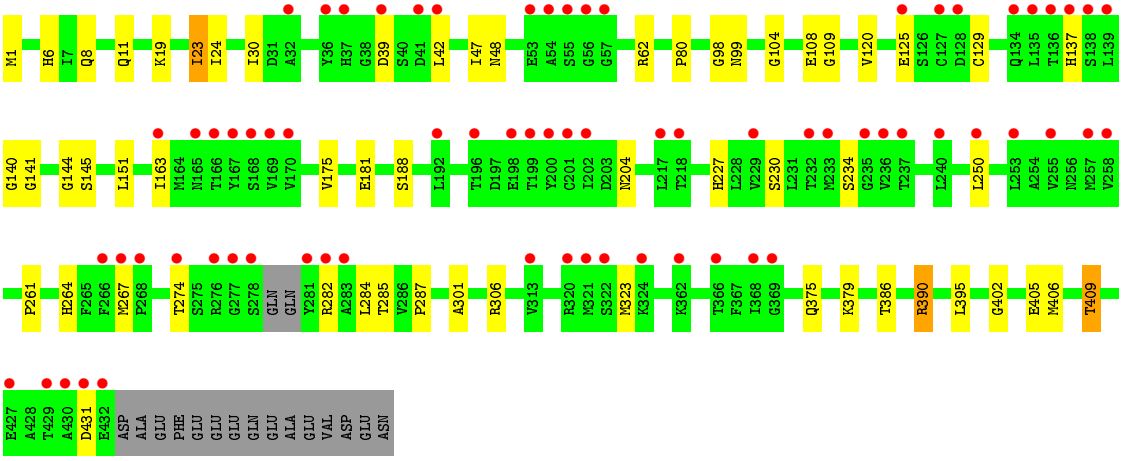
- Molecule 1: Tubulin alpha-1 chain

Chain C:



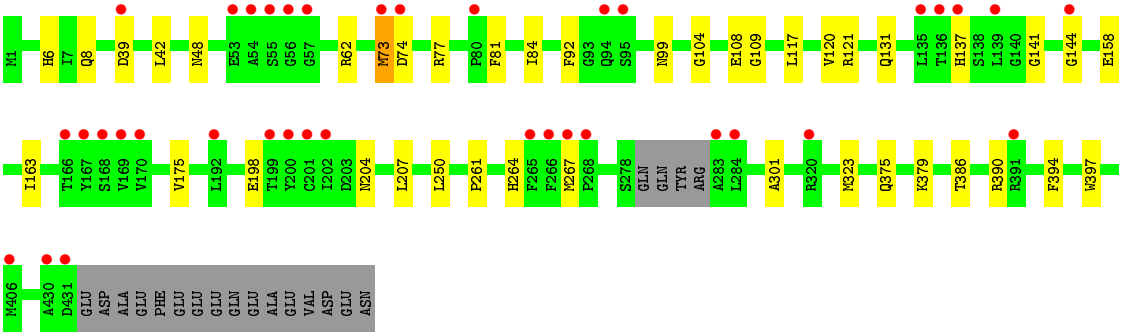
- Molecule 2: Tubulin beta-1 chain

Chain B:



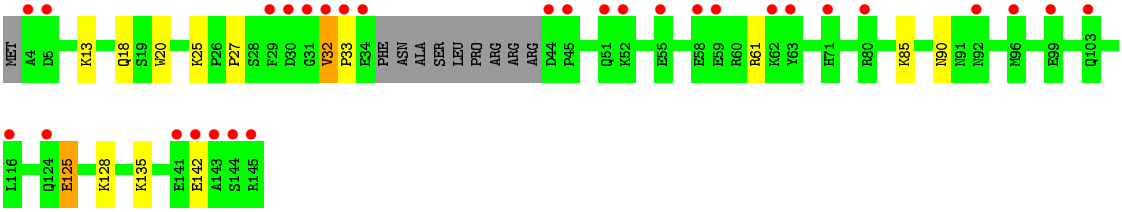
- Molecule 2: Tubulin beta-1 chain

Chain D:



- Molecule 3: Stathmin-4

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.67Å 126.56Å 251.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.29 33.04 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.3 (33.00-2.29) 95.3 (33.04-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.187 , 0.217 0.196 , 0.229	Depositor DCC
R_{free} test set	4565 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	1.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.9	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	0.96	EDS
Total number of atoms	15210	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, GOL, MG, SO4, G2P

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	0.42	0/3469	0.60	0/4708
1	C	0.43	0/3467	0.60	0/4705
2	B	0.43	0/3434	0.59	0/4651
2	D	0.41	0/3444	0.59	0/4663
3	E	0.41	0/1096	0.57	0/1459
All	All	0.42	0/14910	0.59	0/20186

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	3392	0	3301	32	0
1	C	3386	0	3303	42	0
2	B	3362	0	3240	30	0
2	D	3362	0	3254	27	0
3	E	1085	0	1089	9	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	15	0	0	0	0
6	E	5	0	0	0	0
7	A	6	0	8	1	0
8	B	32	0	14	4	0
8	D	32	0	14	3	0
9	A	143	0	0	2	0
9	B	92	0	0	0	0
9	C	85	0	0	1	0
9	D	96	0	0	1	0
9	E	14	0	0	0	0
All	All	15210	0	14247	134	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 (134) 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:6:HIS:HE1	2:B:8:GLN:HE21	1.10	0.97
2:D:204:ASN:HD21	8:D:501:G2P:H2N2	1.07	0.96
2:B:204:ASN:HD21	8:B:501:G2P:H2N2	1.12	0.90
2:D:141:GLY:HA3	8:D:501:G2P:H3A1	1.52	0.89
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.15	0.89
1:A:71:GLU:OE2	1:A:73:THR:HB	1.76	0.86
2:B:6:HIS:CE1	2:B:8:GLN:HE21	1.98	0.80
1:C:339:ARG:H	1:C:339:ARG:HD3	1.44	0.80
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.00	0.80
2:D:261:PRO:O	2:D:264:HIS:HD2	1.71	0.73
2:B:261:PRO:O	2:B:264:HIS:HD2	1.74	0.70
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.74	0.68
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.75	0.68
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.44	0.66
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.79	0.64
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.00	0.61
2:B:227:HIS:HE1	2:B:274:THR:HG23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:506:GOL:H2	3:E:61:ARG:HG3	1.83	0.60
1:A:110:ILE:O	1:A:113:GLU:HG2	2.03	0.58
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.84	0.58
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.85	0.58
2:B:23:ILE:HD13	2:B:234:SER:HB2	1.86	0.57
1:C:427:ALA:O	1:C:430:LYS:HG3	2.03	0.57
1:A:71:GLU:OE2	1:A:73:THR:CB	2.52	0.56
2:B:406:MET:HA	2:B:409:THR:HG23	1.87	0.56
2:D:48:ASN:O	2:D:62:ARG:NH2	2.37	0.56
1:C:163:LYS:HG2	3:E:90:ASN:OD1	2.06	0.56
2:B:11:GLN:HB3	8:B:501:G2P:O2A	2.06	0.56
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.52	0.56
1:A:292:THR:O	1:A:295:CYS:HB2	2.05	0.55
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.72	0.55
1:A:346:TRP:CZ3	1:A:347:CYS:SG	2.99	0.55
2:D:73[A]:MET:HG3	2:D:74:ASP:N	2.23	0.54
2:B:145:SER:HG	2:B:188:SER:HG	1.54	0.54
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.89	0.54
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.26	0.54
1:A:437:MET:HG3	1:A:438:ASP:N	2.23	0.53
2:B:104:GLY:O	2:B:109:GLY:HA3	2.08	0.53
1:C:283:HIS:O	1:C:284:GLU:O	2.26	0.53
2:D:73[A]:MET:SD	2:D:77:ARG:NH1	2.80	0.53
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.90	0.53
1:C:427:ALA:HA	1:C:430:LYS:HG2	1.90	0.53
1:C:209:ILE:HD11	1:C:302:MET:HG3	1.91	0.53
2:B:141:GLY:HA3	8:B:501:G2P:H3A1	1.89	0.53
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.91	0.52
2:D:204:ASN:ND2	8:D:501:G2P:H2N2	1.91	0.52
2:B:48:ASN:O	2:B:62:ARG:NH2	2.41	0.52
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.75	0.51
1:C:296:PHE:CE1	1:C:377:MET:HE1	2.46	0.51
2:B:145:SER:OG	2:B:188:SER:OG	2.24	0.50
1:A:285:GLN:NE2	1:A:372:GLN:H	2.10	0.50
1:A:437:MET:HG3	1:A:438:ASP:H	1.76	0.50
2:D:73[A]:MET:HB3	2:D:92[A]:PHE:CZ	2.46	0.50
2:B:227:HIS:CE1	2:B:274:THR:HG23	2.47	0.50
1:A:139:HIS:HE1	1:A:168:GLU:OE1	1.95	0.50
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.94	0.49
1:C:133:GLN:HE22	1:C:252:LEU:H	1.60	0.49
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLN:NE2	1:C:252:LEU:H	2.11	0.48
2:B:386:THR:O	2:B:390:ARG:HB2	2.13	0.48
1:A:88:HIS:H	1:A:91:GLN:NE2	2.12	0.48
2:D:99:ASN:ND2	9:D:604:HOH:O	2.41	0.48
2:D:104:GLY:O	2:D:109:GLY:HA3	2.14	0.47
1:C:271:THR:HG21	1:C:295:CYS:O	2.14	0.47
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.96	0.47
1:C:54:SER:OG	1:C:62:VAL:HG13	2.14	0.47
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.96	0.47
2:B:395:LEU:HD21	2:B:405:GLU:HG3	1.95	0.47
2:D:386:THR:O	2:D:390:ARG:HB2	2.14	0.47
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.95	0.47
1:A:88:HIS:H	1:A:91:GLN:HE21	1.63	0.47
2:D:137:HIS:HD2	2:D:144:GLY:O	1.98	0.47
1:A:150:THR:O	1:A:154:MET:HG2	2.14	0.47
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.97	0.47
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.44	0.47
2:B:23:ILE:HD12	2:B:24:ILE:HG23	1.97	0.47
1:C:139:HIS:HE1	1:C:168:GLU:OE1	1.98	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.46
2:D:375:GLN:HE21	2:D:379:LYS:HE3	1.81	0.46
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.80	0.46
2:D:131:GLN:NE2	2:D:250:LEU:H	2.14	0.46
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.80	0.46
1:A:261:PRO:HD2	9:A:609:HOH:O	2.16	0.45
3:E:32:VAL:N	3:E:33:PRO:HD3	2.32	0.45
2:B:137:HIS:HD2	2:B:144:GLY:O	2.00	0.45
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.99	0.45
2:D:204:ASN:HD22	2:D:207:LEU:HD12	1.82	0.45
2:D:73[A]:MET:HB3	2:D:92[A]:PHE:CE1	2.51	0.45
1:C:107:HIS:CE1	1:C:155:GLU:OE2	2.68	0.45
2:D:73[A]:MET:HG3	2:D:74:ASP:H	1.80	0.45
2:D:73[A]:MET:SD	2:D:77:ARG:NH2	2.88	0.45
1:C:246:GLY:H	1:C:249:ASN:HD21	1.63	0.45
1:C:296:PHE:CE1	1:C:377:MET:CE	2.99	0.45
1:C:301:GLN:HE22	1:C:307:PRO:CG	2.30	0.44
2:B:402:GLY:O	3:E:85:LYS:HE2	2.17	0.44
1:C:280:LYS:NZ	1:C:283:HIS:HA	2.33	0.44
2:B:23:ILE:HG12	2:B:230:SER:HB2	2.00	0.43
2:B:375:GLN:HE21	2:B:379:LYS:HE3	1.84	0.43
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.43
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.43
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.43
2:B:1:MET:N	2:B:129:CYS:SG	2.84	0.43
2:B:98:GLY:HA3	1:C:253:THR:HG22	2.01	0.43
3:E:32:VAL:N	3:E:33:PRO:CD	2.82	0.43
1:C:280:LYS:HZ2	1:C:283:HIS:HA	1.84	0.42
1:C:79:ARG:HD3	9:C:632:HOH:O	2.18	0.42
1:C:69:ASP:O	1:C:94:THR:HA	2.19	0.42
2:B:19:LYS:O	2:B:23:ILE:HG13	2.20	0.42
1:A:69:ASP:O	1:A:94:THR:HA	2.20	0.42
2:B:30:ILE:HD11	2:B:47:ILE:HD11	2.02	0.42
1:A:206:ASN:O	1:A:210:TYR:HB2	2.20	0.41
1:C:56:THR:HG22	1:C:60:LYS:H	1.86	0.41
2:B:140:GLY:HA3	2:B:181:GLU:HG2	2.03	0.41
1:C:56:THR:HG23	1:C:58:ALA:H	1.85	0.41
3:E:125:GLU:HA	3:E:128:LYS:HD2	2.03	0.41
1:A:315:CYS:HG	1:A:351:PHE:HE1	1.68	0.41
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.55	0.41
1:C:88:HIS:O	1:C:91:GLN:HG2	2.20	0.41
1:C:205:ASP:CB	1:C:303:VAL:HA	2.50	0.41
2:D:73[A]:MET:HB3	2:D:92[A]:PHE:CE2	2.56	0.41
2:B:99:ASN:HA	8:B:501:G2P:O3G	2.21	0.41
1:C:169:PHE:HE2	1:C:238:ILE:HD12	1.85	0.41
1:C:133:GLN:HE22	1:C:251:ASP:HB2	1.86	0.41
2:D:394:PHE:O	2:D:397:TRP:HB2	2.21	0.41
1:A:179:THR:HG21	9:A:657:HOH:O	2.20	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.21	0.40
1:A:35:GLN:OE1	1:A:60:LYS:HG2	2.21	0.40
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.04	0.40
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.39	0.40
2:D:117:LEU:O	2:D:121:ARG:HG3	2.21	0.40
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.69	0.40
1:C:427:ALA:HA	1:C:430:LYS:CG	2.51	0.40
3:E:13:LYS:HD3	3:E:18:GLN:HG3	2.03	0.40

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	430/450 (96%)	417 (97%)	11 (3%)	2 (0%)	29	35
1	C	431/450 (96%)	415 (96%)	15 (4%)	1 (0%)	47	58
2	B	426/447 (95%)	419 (98%)	4 (1%)	3 (1%)	22	26
2	D	426/447 (95%)	420 (99%)	6 (1%)	0	100	100
3	E	129/143 (90%)	125 (97%)	3 (2%)	1 (1%)	19	23
All	All	1842/1937 (95%)	1796 (98%)	39 (2%)	7 (0%)	34	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	C	284	GLU
1	A	44	GLY
2	B	284	LEU
2	B	282	ARG
3	E	142	GLU
2	B	175	VAL

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	364/375 (97%)	352 (97%)	12 (3%)	38	53
1	C	364/375 (97%)	351 (96%)	13 (4%)	35	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	365/382 (96%)	352 (96%)	13 (4%)	35 49
2	D	367/382 (96%)	357 (97%)	10 (3%)	44 61
3	E	115/126 (91%)	111 (96%)	4 (4%)	36 50
All	All	1575/1640 (96%)	1523 (97%)	52 (3%)	39 53

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	195	LEU
1	A	250	VAL
1	A	256	GLN
1	A	279	GLU
1	A	313	MET
1	A	315	CYS
1	A	326	LYS
1	A	373	ARG
1	A	384	ILE
1	A	413	MET
1	A	425	LEU
2	B	23	ILE
2	B	39	ASP
2	B	42	LEU
2	B	80	PRO
2	B	108	GLU
2	B	120	VAL
2	B	125	GLU
2	B	151	LEU
2	B	306	ARG
2	B	323	MET
2	B	390	ARG
2	B	409	THR
2	B	431	ASP
1	C	1[A]	MET
1	C	1[B]	MET
1	C	62	VAL
1	C	71	GLU
1	C	164	LYS
1	C	233	GLN
1	C	250	VAL
1	C	302	MET

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Mol	Chain	Res	Type
1	C	339	ARG
1	C	342	GLN
1	C	370	LYS
1	C	384	ILE
1	C	425	LEU
2	D	39	ASP
2	D	42	LEU
2	D	73[A]	MET
2	D	73[B]	MET
2	D	108	GLU
2	D	120	VAL
2	D	158	GLU
2	D	175	VAL
2	D	198	GLU
2	D	323	MET
3	E	25	LYS
3	E	32	VAL
3	E	125	GLU
3	E	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	134	GLN
2	B	137	HIS
2	B	204	ASN
2	B	227	HIS
2	B	264	HIS
2	B	292	GLN
2	B	298	ASN

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Mol	Chain	Res	Type
2	B	375	GLN
2	B	423	GLN
1	C	8	HIS
1	C	15	GLN
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	301	GLN
1	C	329	ASN
1	C	342	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	15	GLN
2	D	131	GLN
2	D	134	GLN
2	D	137	HIS
2	D	195	ASN
2	D	204	ASN
2	D	264	HIS
2	D	292	GLN
2	D	298	ASN
2	D	375	GLN
2	D	423	GLN
2	D	426	GLN
3	E	111	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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
8	G2P	B	501	5	26,34,34	2.02	5 (19%)	30,54,54	1.93	5 (16%)
6	SO4	D	504	-	4,4,4	0.18	0	6,6,6	0.19	0
6	SO4	D	505	-	4,4,4	0.20	0	6,6,6	0.15	0
6	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.24	0
8	G2P	D	501	5	26,34,34	1.93	5 (19%)	30,54,54	1.85	5 (16%)
6	SO4	E	201	-	4,4,4	0.14	0	6,6,6	0.08	0
4	GTP	C	501	5	26,34,34	0.95	1 (3%)	33,54,54	2.02	6 (18%)
4	GTP	A	501	5	26,34,34	0.98	1 (3%)	33,54,54	2.03	5 (15%)
7	GOL	A	506	-	5,5,5	0.11	0	5,5,5	0.26	0
6	SO4	B	503	-	4,4,4	0.18	0	6,6,6	0.21	0
6	SO4	C	504	-	4,4,4	0.16	0	6,6,6	0.07	0
6	SO4	D	503	-	4,4,4	0.20	0	6,6,6	0.19	0
6	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.20	0
6	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.17	0
6	SO4	C	503	-	4,4,4	0.17	0	6,6,6	0.10	0
6	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.11	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	GTP	A	501	5	-	6/18/38/38	0/3/3/3
8	G2P	B	501	5	-	6/18/38/38	0/3/3/3
8	G2P	D	501	5	-	7/18/38/38	0/3/3/3
7	GOL	A	506	-	-	0/4/4/4	-
4	GTP	C	501	5	-	6/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	G2P	C4-N9	-7.55	1.37	1.47
8	D	501	G2P	C4-N9	-6.95	1.38	1.47
8	D	501	G2P	C5-C6	-4.44	1.45	1.52
8	B	501	G2P	C5-C6	-4.36	1.45	1.52
4	A	501	GTP	C6-N1	3.24	1.38	1.33
8	B	501	G2P	C6-N1	3.22	1.38	1.33
8	D	501	G2P	C6-N1	3.02	1.38	1.33
4	C	501	GTP	C6-N1	2.88	1.38	1.33
8	B	501	G2P	C8-N9	-2.37	1.37	1.45
8	D	501	G2P	C5-C4	-2.37	1.38	1.53
8	B	501	G2P	C5-C4	-2.31	1.38	1.53
8	D	501	G2P	C8-N9	-2.29	1.37	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	GTP	C5-C6-N1	-8.23	112.17	123.43
4	A	501	GTP	C5-C6-N1	-8.17	112.25	123.43
8	D	501	G2P	C4-C5-N7	6.02	110.44	102.46
8	B	501	G2P	C4-C5-N7	6.00	110.41	102.46
4	A	501	GTP	C6-N1-C2	5.97	125.41	115.93
4	C	501	GTP	C6-N1-C2	5.75	125.06	115.93
8	B	501	G2P	C5-C6-N1	-5.30	111.65	118.19
8	D	501	G2P	C5-C6-N1	-5.02	112.00	118.19
8	B	501	G2P	O6-C6-C5	3.94	127.91	119.86
8	D	501	G2P	O6-C6-C5	3.93	127.87	119.86
8	B	501	G2P	O2B-PB-C3A	3.44	118.18	109.07
8	B	501	G2P	O2A-PA-C3A	3.34	117.91	109.07
4	A	501	GTP	N3-C2-N1	-2.92	123.33	127.22
8	D	501	G2P	O2B-PB-C3A	2.82	116.52	109.07
8	D	501	G2P	O2A-PA-C3A	2.78	116.43	109.07
4	A	501	GTP	C6-C5-C4	-2.72	118.20	120.80
4	C	501	GTP	N3-C2-N1	-2.68	123.65	127.22
4	C	501	GTP	O5'-PA-O1A	2.43	118.56	109.07
4	C	501	GTP	C6-C5-C4	-2.41	118.50	120.80
4	A	501	GTP	C2-N3-C4	-2.39	112.62	115.36
4	C	501	GTP	C2-N3-C4	-2.36	112.66	115.36

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	501	G2P	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
8	B	501	G2P	C2'-C1'-N9-C4
8	D	501	G2P	PB-O3B-PG-O1G
8	D	501	G2P	PB-O3B-PG-O3G
8	D	501	G2P	PB-C3A-PA-O2A
8	D	501	G2P	PB-C3A-PA-O5'
8	D	501	G2P	C2'-C1'-N9-C4
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O1A
8	B	501	G2P	O4'-C4'-C5'-O5'
8	B	501	G2P	C3'-C4'-C5'-O5'
8	B	501	G2P	C5'-O5'-PA-C3A
8	B	501	G2P	PB-O3B-PG-O2G
4	C	501	GTP	C5'-O5'-PA-O2A
4	A	501	GTP	C5'-O5'-PA-O2A
8	D	501	G2P	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	PB-O3A-PA-O2A
8	D	501	G2P	PB-O3B-PG-O2G
4	C	501	GTP	C4'-C5'-O5'-PA
4	A	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

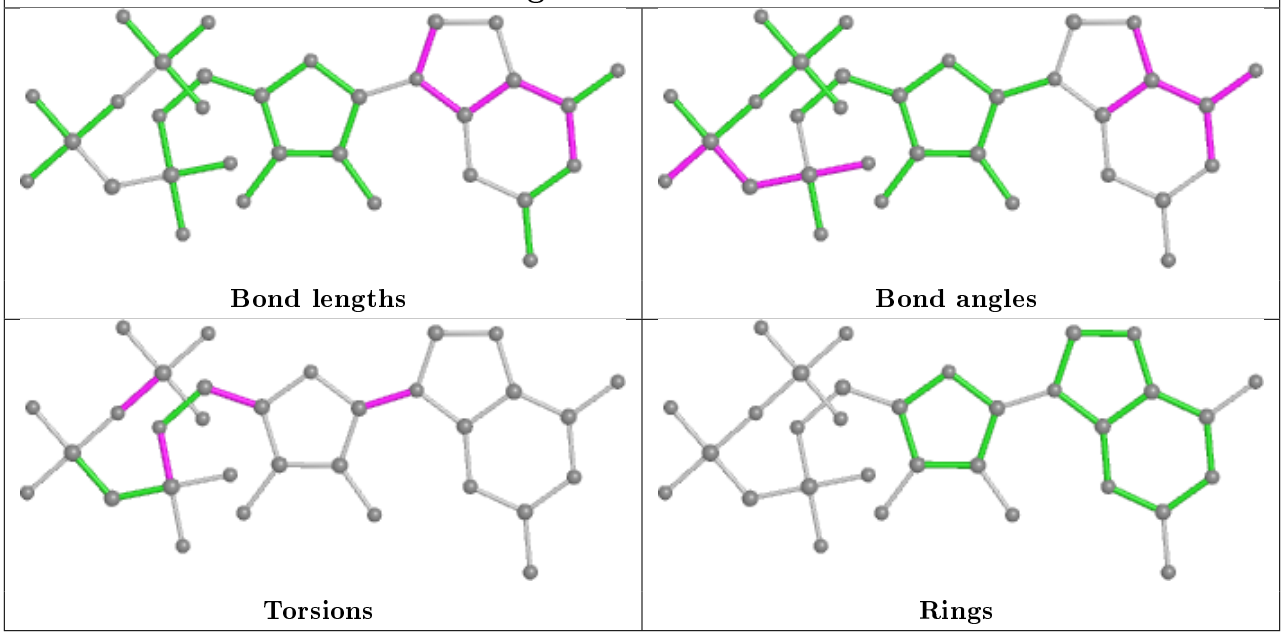
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	G2P	4	0
8	D	501	G2P	3	0
7	A	506	GOL	1	0

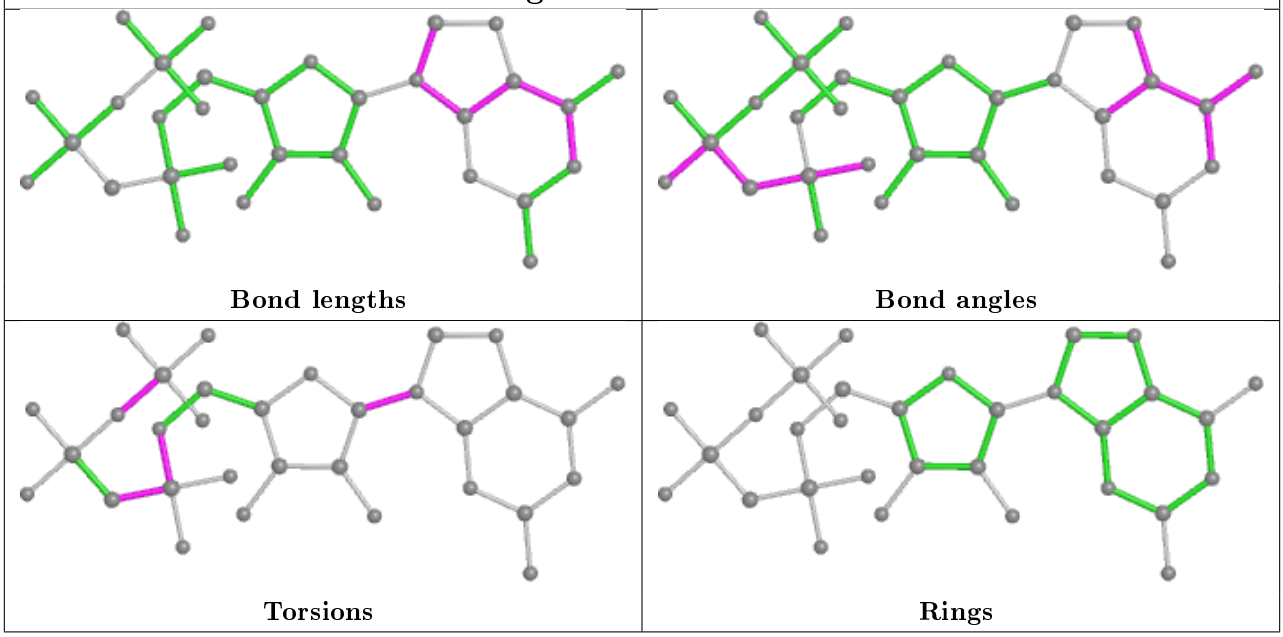
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

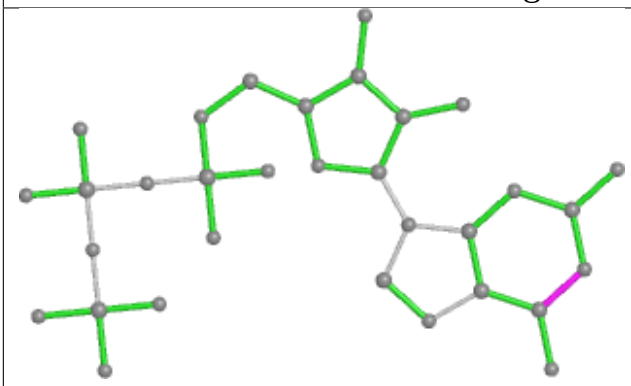
Ligand G2P B 501



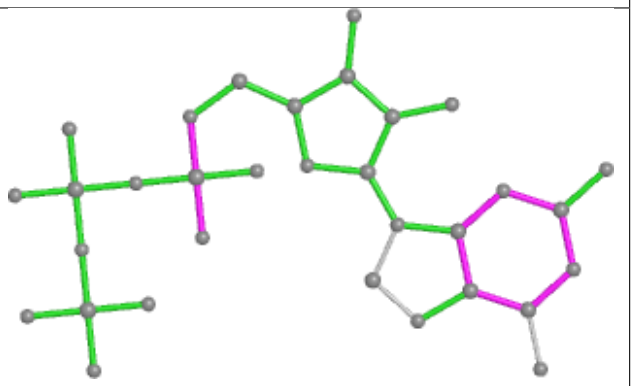
Ligand G2P D 501



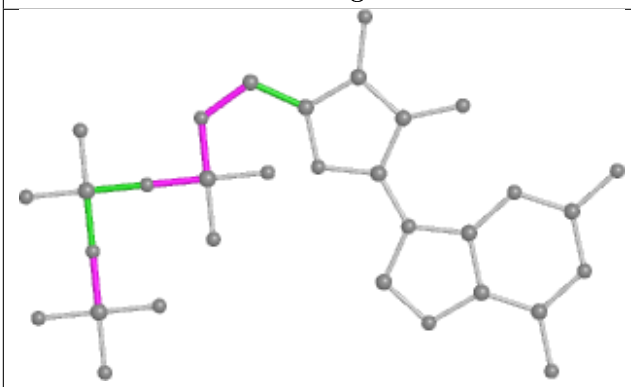
Ligand GTP C 501



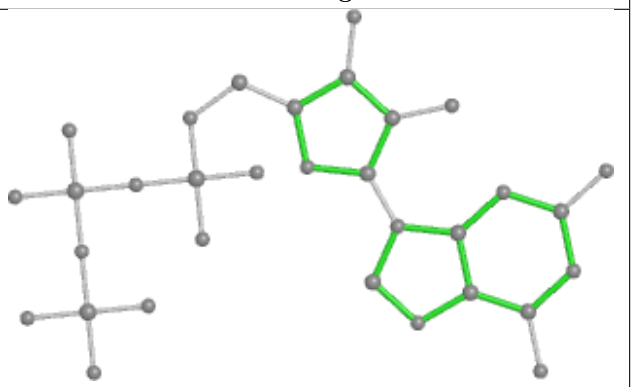
Bond lengths



Bond angles

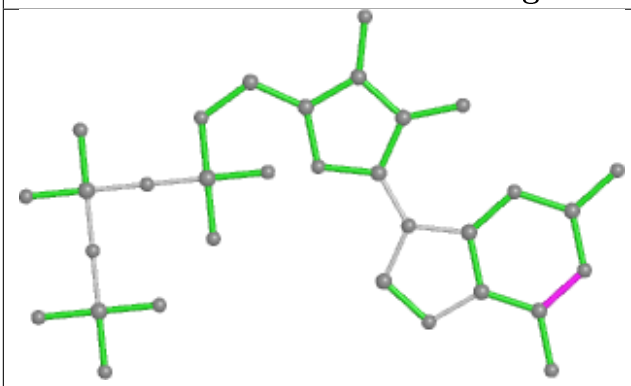


Torsions

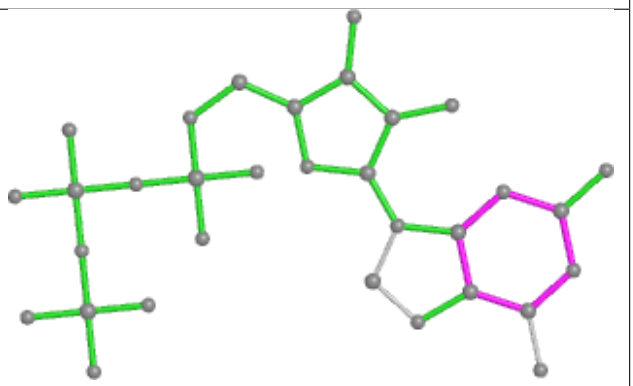


Rings

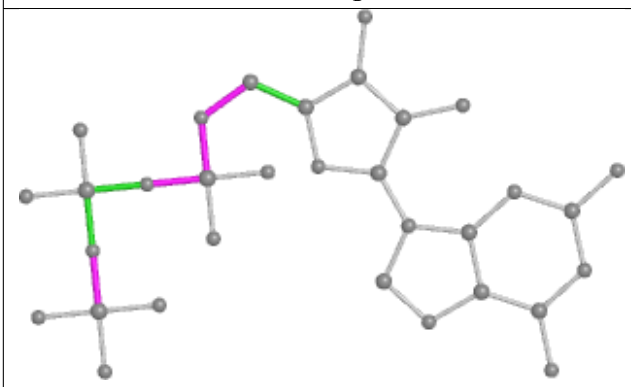
Ligand GTP A 501



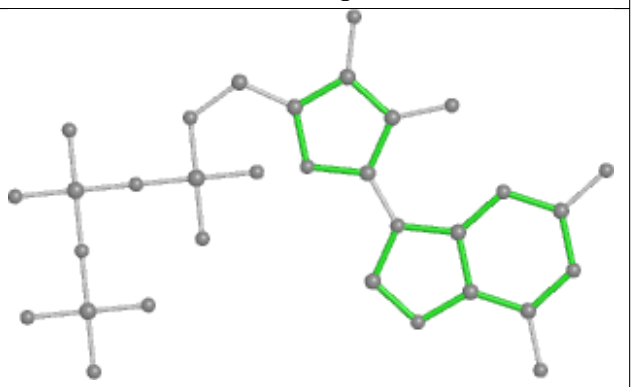
Bond lengths



Bond angles



Torsions



Rings

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	434/450 (96%)	0.46	38 (8%) 10 13	45, 59, 82, 105	0
1	C	434/450 (96%)	0.71	62 (14%) 2 3	45, 65, 94, 112	0
2	B	430/447 (96%)	0.78	72 (16%) 1 2	44, 60, 89, 112	0
2	D	427/447 (95%)	0.47	37 (8%) 10 14	44, 56, 81, 96	0
3	E	133/143 (93%)	1.27	30 (22%) 0 1	58, 75, 113, 125	0
All	All	1858/1937 (95%)	0.65	239 (12%) 3 5	44, 61, 90, 125	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	32	VAL	11.4
1	A	282	TYR	7.6
3	E	31	GLY	7.5
1	A	346	TRP	6.9
3	E	5	ASP	6.5
1	C	278	ALA	6.3
1	A	44	GLY	6.3
3	E	145	ARG	5.9
1	C	202	PHE	5.9
3	E	33	PRO	5.8
3	E	29	PHE	5.7
2	B	200	TYR	5.6
2	B	278	SER	5.6
1	A	438	ASP	5.5
3	E	4	ALA	5.4
3	E	142	GLU	5.3
2	B	432	GLU	5.3
1	C	200	CYS	5.1
2	B	167	TYR	5.1
2	B	368	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	440	GLY	5.0
2	B	281	TYR	4.9
2	B	236	VAL	4.8
1	C	357	TYR	4.8
2	B	199	THR	4.8
1	C	201	ALA	4.7
2	B	431	ASP	4.7
2	D	57	GLY	4.6
1	C	45	GLY	4.6
1	C	177	VAL	4.5
3	E	34	GLU	4.5
1	C	218	ASP	4.4
1	C	268	PRO	4.4
2	D	73[A]	MET	4.3
2	D	431	ASP	4.3
3	E	30	ASP	4.3
1	C	279	GLU	4.3
2	D	200	TYR	4.3
2	B	266	PHE	4.2
2	D	166	THR	4.2
2	D	167	TYR	4.2
2	B	166	THR	4.2
1	A	262	TYR	4.1
2	D	406	MET	4.1
1	A	238	ILE	4.1
1	A	202	PHE	4.1
2	D	320	ARG	4.1
1	C	167	LEU	4.1
1	A	45	GLY	4.0
1	C	169	PHE	4.0
2	B	168	SER	4.0
2	D	135	LEU	3.9
2	B	55	SER	3.9
2	B	268	PRO	3.8
2	B	135	LEU	3.8
1	A	283	HIS	3.8
1	A	43	GLY	3.8
2	B	320	ARG	3.8
2	D	54	ALA	3.7
1	A	38	SER	3.7
1	A	309	HIS	3.7
2	B	42	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	218	THR	3.6
1	C	378	LEU	3.6
1	A	270	VAL	3.6
1	C	38	SER	3.6
1	C	316	CYS	3.6
2	B	39	ASP	3.6
1	C	203	MET	3.6
1	A	235	VAL	3.6
2	B	276	ARG	3.6
1	C	170	ALA	3.5
2	D	53	GLU	3.5
2	D	80	PRO	3.4
1	C	270	VAL	3.4
2	D	39	ASP	3.4
2	B	430	ALA	3.4
2	B	53	GLU	3.4
1	A	437	MET	3.3
3	E	143	ALA	3.3
1	A	167	LEU	3.3
2	B	57	GLY	3.3
3	E	45	PRO	3.3
2	B	54	ALA	3.3
1	A	281	ALA	3.3
3	E	44	ASP	3.3
1	C	172	TYR	3.3
2	B	282	ARG	3.3
1	C	282	TYR	3.3
2	D	202	ILE	3.2
3	E	55	GLU	3.2
2	D	168	SER	3.2
2	D	201	CYS	3.2
2	D	199	THR	3.2
2	D	283	ALA	3.2
1	A	136	LEU	3.2
2	B	128	ASP	3.2
1	C	255	PHE	3.1
1	C	215	ARG	3.1
2	B	217	LEU	3.1
3	E	116	LEU	3.1
2	B	169	VAL	3.1
2	B	237	THR	3.1
2	B	429	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	3.1
1	C	281	ALA	3.1
1	C	137	ILE	3.1
1	C	259	LEU	3.0
1	C	269	LEU	3.0
2	B	139	LEU	3.0
1	C	171	ILE	3.0
2	D	55	SER	3.0
2	D	56	GLY	3.0
1	C	217	LEU	3.0
2	B	253	LEU	3.0
1	C	220	GLU	3.0
2	B	201	CYS	3.0
1	C	36	MET	3.0
1	C	238	ILE	3.0
2	B	322	SER	3.0
2	B	313	VAL	3.0
1	A	137	ILE	3.0
2	D	136	THR	2.9
1	A	201	ALA	2.9
3	E	59	GLU	2.9
1	C	309	HIS	2.9
2	B	170	VAL	2.9
2	B	137	HIS	2.9
1	A	138	PHE	2.9
2	D	170	VAL	2.8
3	E	62	LYS	2.8
3	E	141	GLU	2.8
1	C	267	PHE	2.8
2	B	235	GLY	2.8
2	B	196	THR	2.8
2	D	266	PHE	2.8
3	E	96	MET	2.8
1	A	37	PRO	2.8
2	D	284	LEU	2.8
2	B	36	TYR	2.8
2	D	137	HIS	2.8
1	A	345	ASP	2.7
1	C	379	SER	2.7
2	B	255	VAL	2.7
2	B	258	VAL	2.7
2	D	391	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	378	LEU	2.7
3	E	144	SER	2.7
3	E	103	GLN	2.7
1	A	271	THR	2.7
1	C	260	VAL	2.7
2	D	430	ALA	2.6
2	B	233	MET	2.6
3	E	63	TYR	2.6
2	B	165	ASN	2.6
2	B	283	ALA	2.6
2	B	41	ASP	2.6
1	C	234	ILE	2.6
2	B	163	ILE	2.6
2	B	136	THR	2.5
2	B	257	MET	2.5
1	C	136	LEU	2.5
1	C	376	CYS	2.5
1	A	220	GLU	2.5
2	B	125	GLU	2.5
2	D	169	VAL	2.5
1	C	280	LYS	2.5
1	A	357	TYR	2.5
1	C	198	SER	2.5
2	B	277	GLY	2.5
2	D	94	GLN	2.5
1	C	29	GLY	2.4
1	A	269	LEU	2.4
2	B	32	ALA	2.4
2	B	37	HIS	2.4
2	B	366	THR	2.4
2	D	95	SER	2.4
1	C	214	ARG	2.4
1	C	438	ASP	2.4
2	B	138	SER	2.4
1	A	318	LEU	2.4
1	C	271	THR	2.4
1	C	277	SER	2.4
3	E	58	GLU	2.4
2	B	127	CYS	2.4
1	C	219	ILE	2.3
2	B	192	LEU	2.3
2	D	192	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	365	GLY	2.3
1	A	284	GLU	2.3
1	C	85	GLN	2.3
3	E	51	GLN	2.3
2	B	240	LEU	2.3
3	E	52	LYS	2.3
1	A	221	ARG	2.3
1	A	259	LEU	2.3
1	C	324	VAL	2.3
2	B	198	GLU	2.3
1	A	239	THR	2.3
2	D	139	LEU	2.3
3	E	80	ARG	2.3
2	B	324	LYS	2.3
2	B	369	GLY	2.3
1	C	297	GLU	2.3
1	C	141	PHE	2.3
2	D	268	PRO	2.3
3	E	71	HIS	2.2
2	D	74	ASP	2.2
2	B	202	ILE	2.2
2	B	427	GLU	2.2
2	B	250	LEU	2.2
1	A	377	MET	2.2
1	A	163	LYS	2.2
2	B	229	VAL	2.2
2	B	267	MET	2.2
2	B	321	MET	2.2
2	D	265	PHE	2.2
1	C	266	HIS	2.2
1	C	314	ALA	2.1
1	C	330	ALA	2.1
1	C	168	GLU	2.1
3	E	99	GLU	2.1
1	C	315	CYS	2.1
1	C	176	GLN	2.1
1	C	338	LYS	2.1
1	C	362	VAL	2.1
2	B	274	THR	2.1
2	D	144	GLY	2.1
1	A	326	LYS	2.1
1	A	77	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	232	THR	2.1
2	B	56	GLY	2.1
2	B	362	LYS	2.1
1	C	353	VAL	2.1
3	E	124	GLN	2.0
2	D	267	MET	2.0
3	E	92	ASN	2.0
1	C	35	GLN	2.0
2	B	134	GLN	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
7	GOL	A	506	6/6	0.63	0.35	82,82,82,83	0
6	SO4	C	504	5/5	0.70	0.30	175,175,175,175	0
6	SO4	D	504	5/5	0.88	0.17	127,127,127,127	0
6	SO4	B	504	5/5	0.88	0.39	151,151,151,151	0
6	SO4	E	201	5/5	0.89	0.21	132,132,132,132	0
6	SO4	A	504	5/5	0.92	0.15	131,131,131,131	0
6	SO4	D	505	5/5	0.92	0.23	113,113,113,113	0
6	SO4	B	503	5/5	0.93	0.18	118,118,118,119	0
6	SO4	C	503	5/5	0.93	0.22	140,140,140,140	0
6	SO4	A	505	5/5	0.94	0.19	115,116,116,116	0
5	MG	A	502	1/1	0.94	0.11	52,52,52,52	0
5	MG	B	502	1/1	0.94	0.05	68,68,68,68	0
8	G2P	D	501	32/32	0.95	0.16	42,49,55,55	0
6	SO4	A	503	5/5	0.96	0.10	107,107,107,107	0

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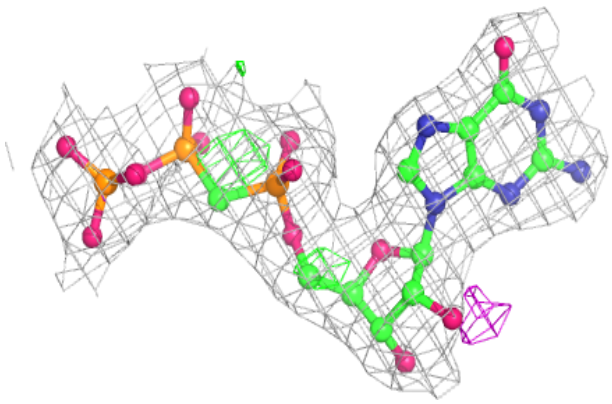
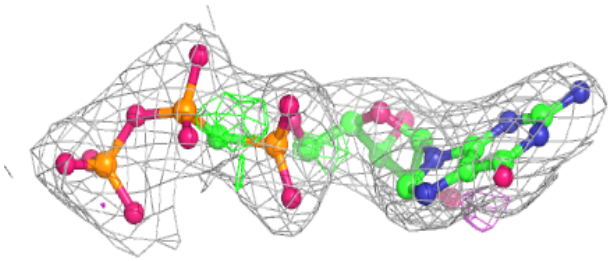
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GTP	C	501	32/32	0.97	0.13	52,59,62,64	0
8	G2P	B	501	32/32	0.97	0.15	54,56,61,62	0
4	GTP	A	501	32/32	0.98	0.14	45,49,49,50	0
5	MG	D	502	1/1	0.99	0.02	58,58,58,58	0
6	SO4	D	503	5/5	0.99	0.07	66,66,66,66	0
5	MG	C	502	1/1	0.99	0.07	47,47,47,47	0

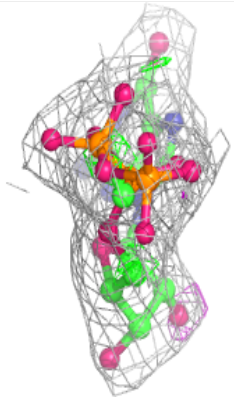
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G2P 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)

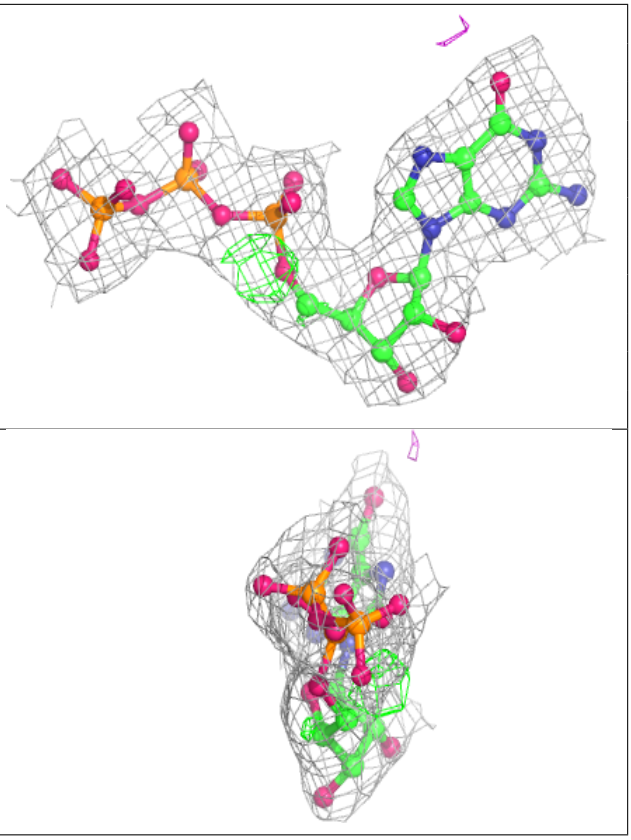






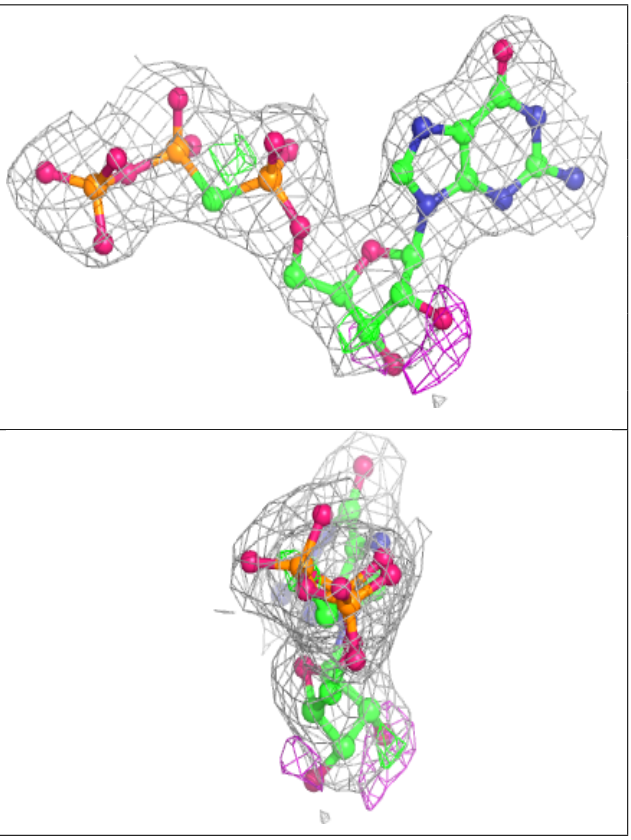
Electron density around GTP C 501:

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



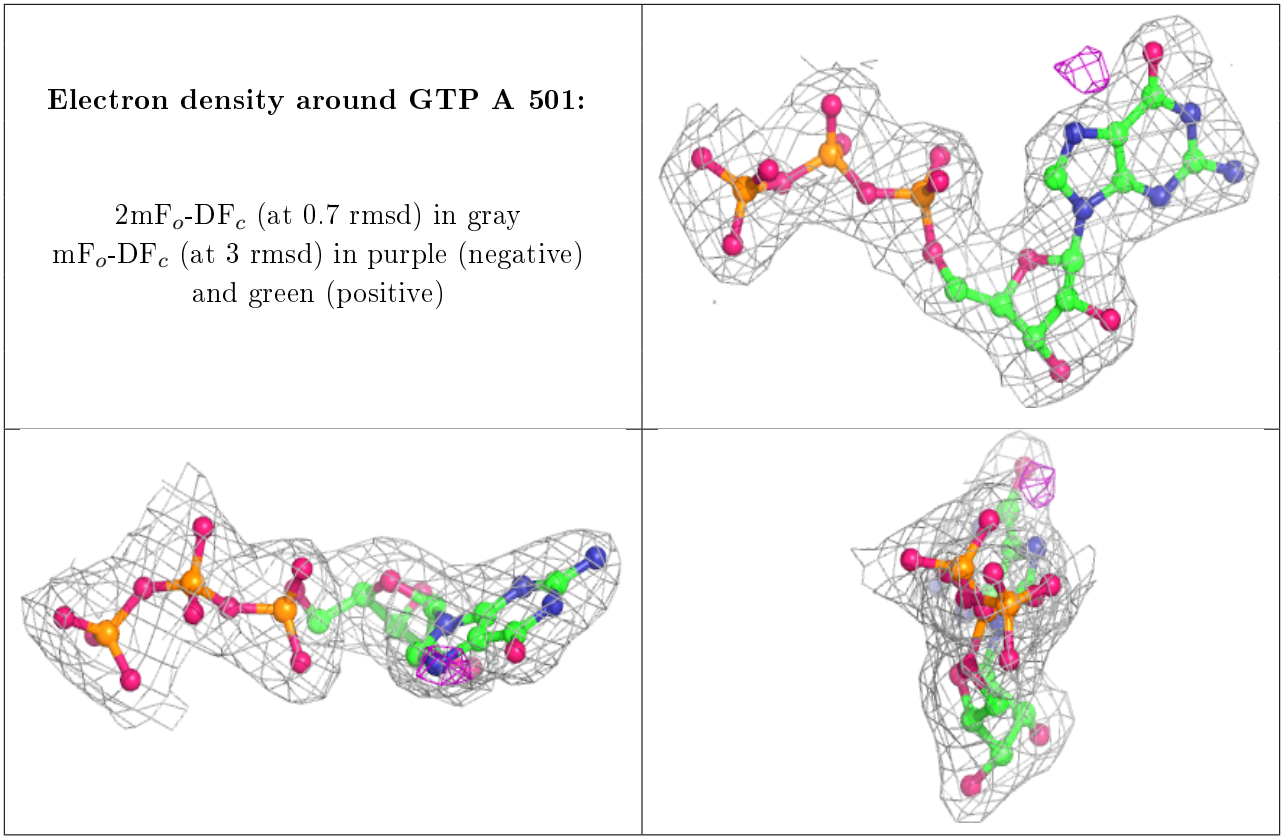
Electron density around G2P B 501:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.