Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 12:38 PM GMT

PDB ID	:	6TIZ
Title	:	DROSOPHILA GDP-TUBULIN Y222F MUTANT
Authors	:	Gigant, B.
Deposited on	:	2019-11-22
Resolution	:	2.20 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:

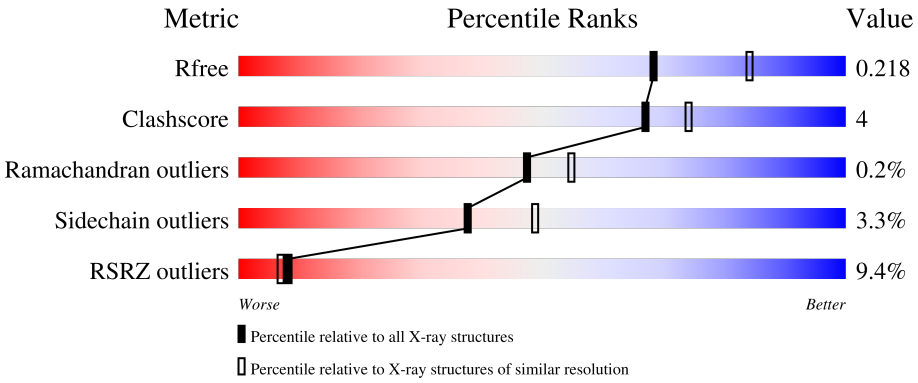
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.20 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 <=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	7% 83% 12% ·
1	C	450	11% 85% 10% ·
2	B	447	11% 85% 10% · ·
2	D	447	6% 87% 9% ·
3	E	143	13% 76% 13% · 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	504	-	-	X	-
6	SO4	B	503	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15487 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	430	Total	C	N	O	S	0	1	0
			3359	2127	570	639	23			
1	C	430	Total	C	N	O	S	0	3	0
			3372	2137	571	639	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	428	Total	C	N	O	S	0	1	0
			3359	2111	574	648	26			
2	D	427	Total	C	N	O	S	0	6	0
			3384	2126	577	655	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	PHE	TYR	engineered mutation	UNP Q24560
D	222	PHE	TYR	engineered mutation	UNP Q24560

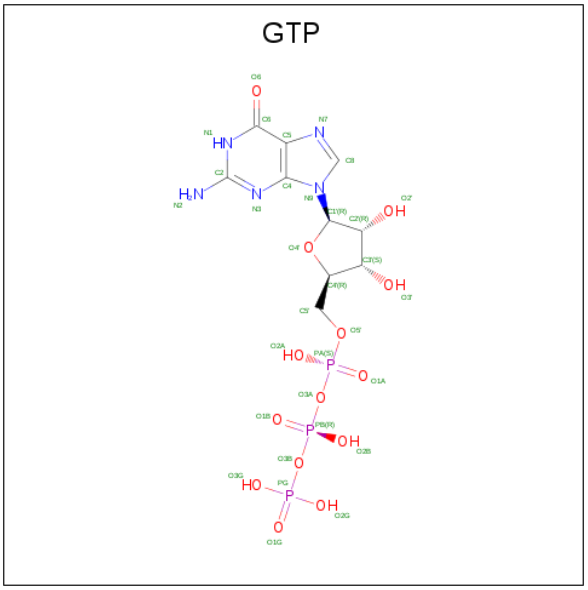
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	129	Total	C	N	O	S	0	1	0
			1055	653	192	206	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: $C_{10}H_{16}N_5O_{14}P_3$).

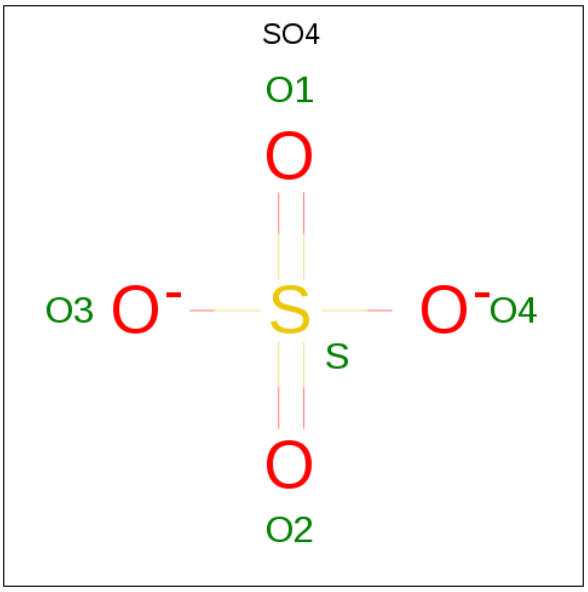


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

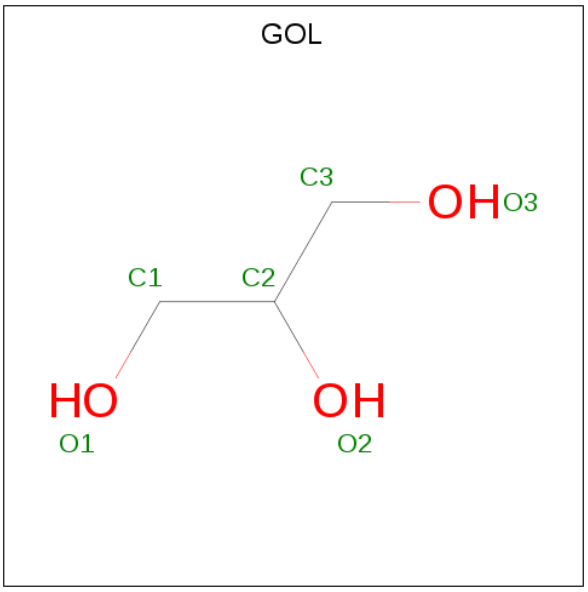
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

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



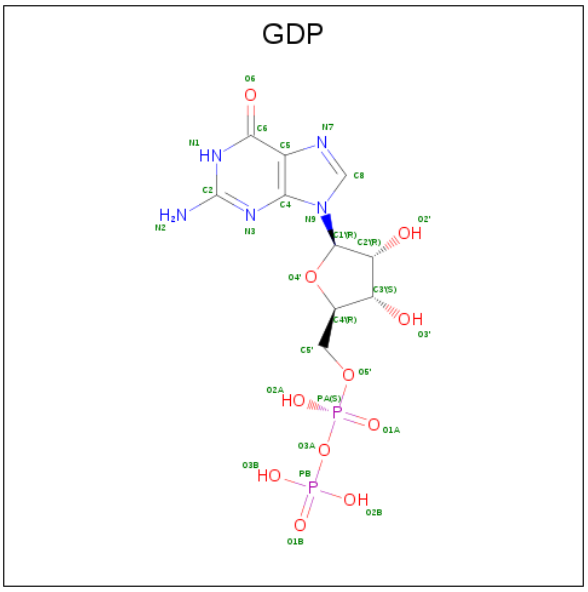
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	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 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

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

- Molecule 9 is water.

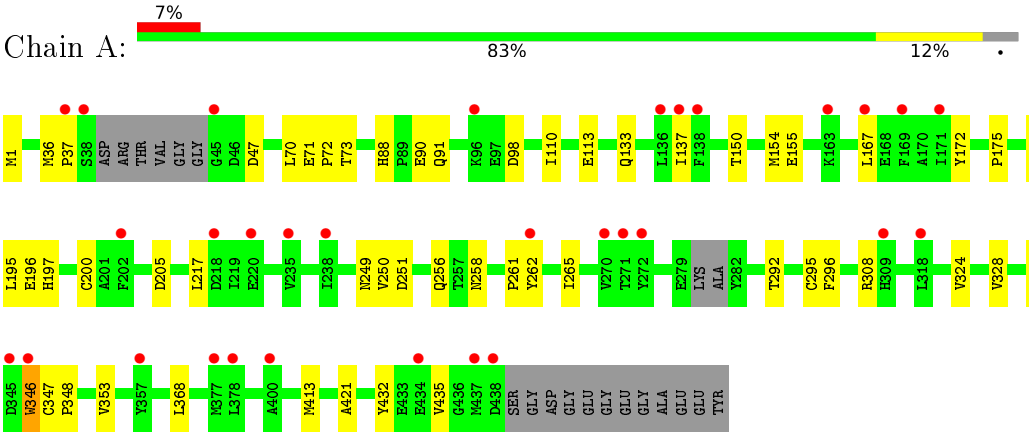
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	218	Total	O	0	0
			218	218		
9	B	164	Total	O	0	0
			164	164		
9	C	147	Total	O	0	0
			147	147		
9	D	185	Total	O	0	2
			185	185		
9	E	45	Total	O	0	0
			45	45		

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.

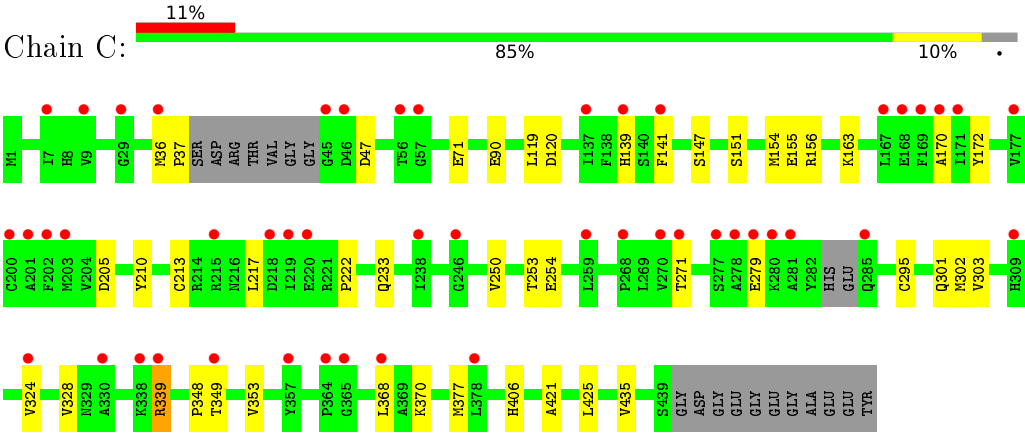
- Molecule 1: Tubulin alpha-1 chain

Chain A:



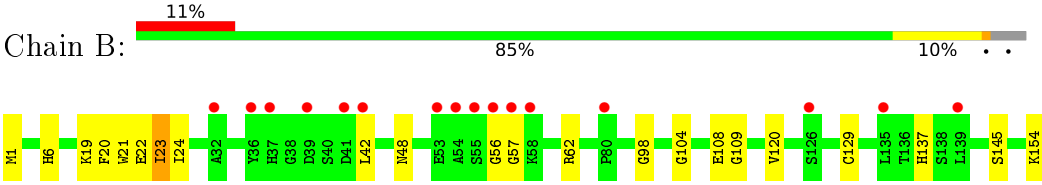
- Molecule 1: Tubulin alpha-1 chain

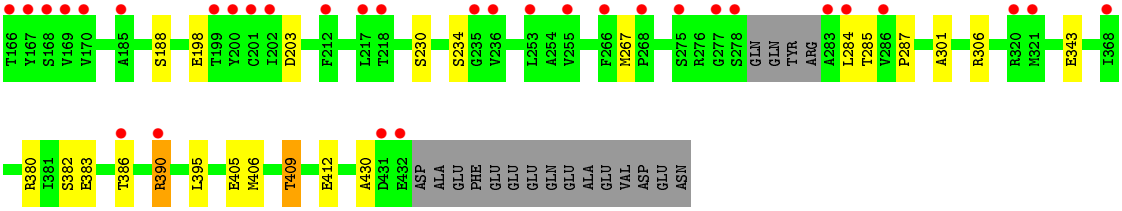
Chain C:



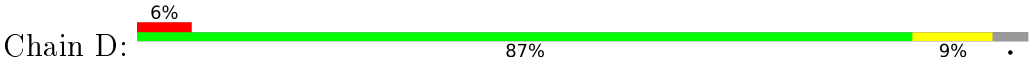
- Molecule 2: Tubulin beta-1 chain

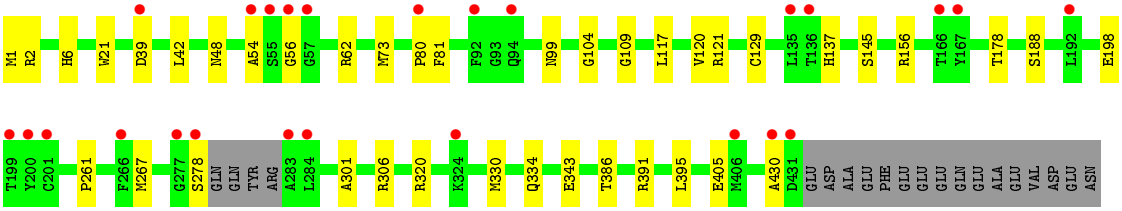
Chain B:



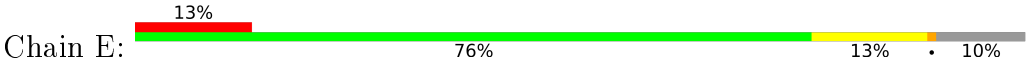


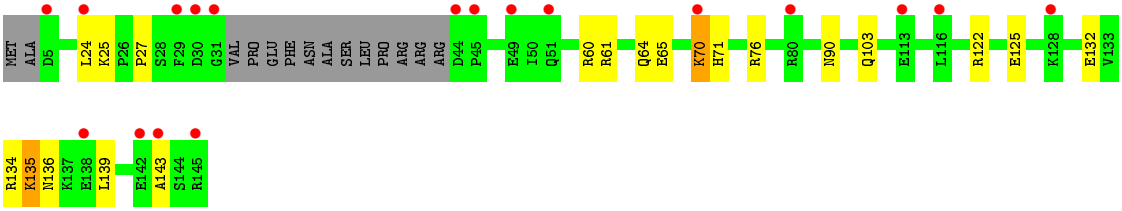
• Molecule 2: Tubulin beta-1 chain





• Molecule 3: Stathmin-4





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.18Å 126.73Å 250.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.20 32.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (32.00-2.20) 97.1 (32.01-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.175 , 0.208 0.183 , 0.218	Depositor DCC
R_{free} test set	5278 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.998	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.6	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	15487	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: GDP, GOL, MG, GTP, SO4

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	0/3436	0.59	0/4664
1	C	0.42	0/3455	0.59	0/4687
2	B	0.43	0/3434	0.59	0/4649
2	D	0.42	0/3462	0.59	0/4688
3	E	0.37	0/1069	0.52	0/1422
All	All	0.42	0/14856	0.58	0/20110

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	3359	0	3264	38	0
1	C	3372	0	3296	30	0
2	B	3359	0	3249	26	0
2	D	3384	0	3273	14	0
3	E	1055	0	1056	16	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	C	1	0	0	0	0
6	A	15	0	0	2	0
6	B	10	0	0	0	0
6	C	15	0	0	0	0
6	D	20	0	0	0	0
6	E	5	0	0	0	0
7	A	12	0	16	1	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	A	218	0	0	2	0
9	B	164	0	0	2	0
9	C	147	0	0	1	0
9	D	185	0	0	0	0
9	E	45	0	0	0	0
All	All	15487	0	14202	114	0

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

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ARG:H	1:C:339:ARG:HD3	1.37	0.86
1:A:71:GLU:OE2	1:A:73:THR:HB	1.84	0.78
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.72	0.70
1:C:163:LYS:HG2	3:E:90:ASN:OD1	1.91	0.70
1:A:336:LYS:HE3	3:E:25:LYS:HZ1	1.57	0.70
1:A:336:LYS:HE3	3:E:25:LYS:NZ	2.09	0.68
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.75	0.67
1:A:308:ARG:NH1	6:A:504:SO4:O3	2.29	0.65
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.15	0.64
3:E:132:GLU:HA	3:E:135:LYS:HD3	1.80	0.64
1:A:110:ILE:O	1:A:113:GLU:HG2	1.99	0.62
2:B:48:ASN:O	2:B:62:ARG:NH2	2.31	0.62
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.00	0.62
1:A:292:THR:O	1:A:295:CYS:HB2	2.01	0.60
1:C:295:CYS:HB3	1:C:377:MET:CE	2.33	0.59
1:C:295:CYS:HB3	1:C:377:MET:HE1	1.85	0.58
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.86	0.58
2:D:395:LEU:HD21	2:D:405:GLU:HG3	1.85	0.58
2:B:104:GLY:O	2:B:109:GLY:HA3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:640:HOH:O	1:C:348:PRO:HD2	2.05	0.56
2:B:1:MET:N	2:B:129:CYS:SG	2.77	0.55
2:B:162:ARG:HE	2:B:162:ARG:HA	1.72	0.55
2:B:23:ILE:HG12	2:B:230:SER:HB2	1.89	0.55
2:B:395:LEU:HD21	2:B:405:GLU:HG3	1.89	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.41	0.55
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.88	0.54
3:E:60:ARG:O	3:E:64:GLN:HG2	2.07	0.54
2:D:104:GLY:O	2:D:109:GLY:HA3	2.07	0.54
1:A:71:GLU:OE2	1:A:73:THR:CB	2.55	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
2:D:48:ASN:O	2:D:62:ARG:NH2	2.39	0.53
1:C:295:CYS:CB	1:C:377:MET:HE1	2.39	0.52
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.91	0.52
2:B:382:SER:O	2:B:386:THR:HG23	2.08	0.52
3:E:70:LYS:NZ	3:E:71[A]:HIS:CE1	2.78	0.52
2:B:406:MET:HA	2:B:409:THR:HG23	1.93	0.51
1:A:339:ARG:NH2	6:A:504:SO4:O4	2.43	0.50
2:D:1:MET:N	2:D:129:CYS:SG	2.79	0.50
2:B:19:LYS:O	2:B:23:ILE:HG13	2.12	0.50
2:B:154:LYS:HD3	3:E:76:ARG:CZ	2.41	0.50
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.93	0.50
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.78	0.49
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.94	0.49
2:B:23:ILE:HD12	2:B:24:ILE:HG23	1.95	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.94	0.49
2:B:23:ILE:HD13	2:B:234:SER:HB2	1.95	0.49
1:C:271:THR:OG1	1:C:377:MET:HB3	2.13	0.49
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.94	0.49
1:C:271:THR:HG22	1:C:301:GLN:HA	1.94	0.48
1:A:249:ASN:ND2	1:A:258:ASN:HD22	2.11	0.48
1:C:192:HIS:CG	1:C:421:ALA:HA	2.49	0.48
2:D:117:LEU:O	2:D:121:ARG:HG3	2.14	0.48
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.95	0.48
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.96	0.47
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.96	0.47
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.08	0.47
2:D:80:PRO:O	2:D:81:PHE:HB2	2.15	0.46
2:D:145:SER:HB2	2:D:188:SER:OG	2.15	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.51	0.46
2:B:343:GLU:HG3	2:B:430:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:135:LYS:NZ	3:E:136:ASN:ND2	2.63	0.46
1:A:336:LYS:CE	3:E:25:LYS:NZ	2.78	0.45
2:B:386:THR:O	2:B:390:ARG:HB2	2.16	0.45
7:A:506:GOL:H2	3:E:61:ARG:HG3	1.98	0.45
1:A:296:PHE:O	1:A:339:ARG:NH1	2.49	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.45
1:A:346:TRP:CE3	1:A:347:CYS:SG	3.10	0.45
2:B:165:ASN:ND2	9:B:605:HOH:O	2.49	0.45
1:C:213:CYS:HA	1:C:217:LEU:HD12	1.99	0.45
1:A:150:THR:O	1:A:154:MET:HG2	2.17	0.44
1:C:233:GLN:NE2	9:C:601:HOH:O	2.49	0.44
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.46	0.44
2:D:330:MET:O	2:D:334:GLN:HG2	2.17	0.44
1:C:313:MET:SD	1:C:435:VAL:CG1	3.05	0.44
1:C:217:LEU:HD21	1:C:368:LEU:HD23	1.99	0.44
2:B:380:ARG:O	2:B:383:GLU:HG2	2.17	0.43
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.53	0.43
2:D:99:ASN:HB3	2:D:178[A]:THR:HG21	2.00	0.43
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.43
1:A:88:HIS:O	1:A:91:GLN:HG2	2.18	0.43
1:A:137:ILE:HD13	1:A:154:MET:SD	2.59	0.43
1:C:151:SER:O	1:C:155:GLU:HG3	2.19	0.43
3:E:139:LEU:O	3:E:143:ALA:HB3	2.19	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.42
1:A:262:TYR:HB2	1:A:265:ILE:HD12	2.00	0.42
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.20	0.42
1:C:154:MET:HE3	1:C:154:MET:HB3	1.86	0.42
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.01	0.42
3:E:135:LYS:HZ3	3:E:136:ASN:CG	2.23	0.42
1:C:339:ARG:N	1:C:339:ARG:HD3	2.19	0.42
1:A:179:THR:HG21	9:A:693:HOH:O	2.20	0.42
1:C:250:VAL:HG23	1:C:254:GLU:HB2	2.01	0.42
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.42
1:A:36:MET:HA	1:A:37:PRO:HD3	1.93	0.42
1:C:36:MET:HA	1:C:37:PRO:HD3	1.94	0.42
1:A:175:PRO:HA	1:A:178:SER:HB2	2.02	0.41
2:B:23:ILE:HG13	2:B:23:ILE:H	1.69	0.41
1:C:141:PHE:O	1:C:147:SER:HB3	2.20	0.41
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.02	0.41
2:B:203:ASP:HB2	2:B:301:ALA:HA	2.02	0.41
2:B:145:SER:HB2	2:B:188:SER:OG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:HIS:O	1:C:170:ALA:HA	2.21	0.41
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.50	0.41
1:C:377:MET:HE3	1:C:377:MET:HB2	1.84	0.41
2:B:406:MET:HA	2:B:409:THR:CG2	2.50	0.41
1:C:163:LYS:HE3	3:E:90:ASN:HA	2.02	0.40
3:E:132:GLU:HG3	3:E:135:LYS:NZ	2.35	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.40
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.56	0.40
2:B:20:PHE:HA	2:B:23:ILE:HD11	2.03	0.40
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.51	0.40
2:D:54:ALA:O	2:D:56:GLY:O	2.39	0.40
1:A:261:PRO:HD2	9:A:615:HOH:O	2.21	0.40
2:B:98:GLY:HA3	1:C:253:THR:HG22	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	425/450 (94%)	411 (97%)	14 (3%)	0	100 100
1	C	426/450 (95%)	408 (96%)	18 (4%)	0	100 100
2	B	425/447 (95%)	413 (97%)	9 (2%)	3 (1%)	22 22
2	D	429/447 (96%)	419 (98%)	10 (2%)	0	100 100
3	E	126/143 (88%)	122 (97%)	4 (3%)	0	100 100
All	All	1831/1937 (94%)	1773 (97%)	55 (3%)	3 (0%)	47 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	GLY

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Mol	Chain	Res	Type
2	B	284	LEU
2	B	57	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/375 (96%)	351 (97%)	10 (3%)	43	56
1	C	364/375 (97%)	353 (97%)	11 (3%)	41	53
2	B	366/382 (96%)	355 (97%)	11 (3%)	41	53
2	D	370/382 (97%)	357 (96%)	13 (4%)	36	46
3	E	111/126 (88%)	104 (94%)	7 (6%)	18	20
All	All	1572/1640 (96%)	1520 (97%)	52 (3%)	38	49

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	47	ASP
1	A	90	GLU
1	A	195	LEU
1	A	196	GLU
1	A	250	VAL
1	A	256	GLN
1	A	324	VAL
1	A	346	TRP
1	A	413	MET
2	B	22	GLU
2	B	23	ILE
2	B	42	LEU
2	B	108	GLU
2	B	120	VAL
2	B	137	HIS
2	B	162	ARG

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Mol	Chain	Res	Type
2	B	198	GLU
2	B	306	ARG
2	B	390	ARG
2	B	409	THR
1	C	47	ASP
1	C	71	GLU
1	C	90	GLU
1	C	120	ASP
1	C	279	GLU
1	C	302	MET
1	C	324	VAL
1	C	339	ARG
1	C	349	THR
1	C	370	LYS
1	C	425	LEU
2	D	2	ARG
2	D	39	ASP
2	D	42	LEU
2	D	73	MET
2	D	120	VAL
2	D	137	HIS
2	D	156	ARG
2	D	198	GLU
2	D	278	SER
2	D	306	ARG
2	D	320	ARG
2	D	386	THR
2	D	391	ARG
3	E	65	GLU
3	E	70	LYS
3	E	103	GLN
3	E	122	ARG
3	E	125	GLU
3	E	134	ARG
3	E	135	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	197	HIS
1	A	249	ASN
1	C	249	ASN

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Mol	Chain	Res	Type
1	C	256	GLN
1	C	342	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GOL	A	506	-	5,5,5	0.14	0	5,5,5	0.27	0
6	SO4	B	502	-	4,4,4	0.16	0	6,6,6	0.14	0
6	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.25	0
6	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.18	0
4	GTP	A	501	5	26,34,34	0.93	2 (7%)	33,54,54	2.00	6 (18%)
6	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.10	0
4	GTP	C	501	5	26,34,34	0.91	1 (3%)	33,54,54	2.01	6 (18%)
6	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.06	0
6	SO4	E	201	-	4,4,4	0.11	0	6,6,6	0.10	0
7	GOL	A	507	-	5,5,5	0.05	0	5,5,5	0.32	0
6	SO4	A	505	-	4,4,4	0.19	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GDP	B	501	-	24,30,30	1.05	1 (4%)	31,47,47	2.06	6 (19%)
6	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.06	0
6	SO4	C	504	-	4,4,4	0.16	0	6,6,6	0.11	0
6	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.11	0
6	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.13	0
8	GDP	D	501	-	24,30,30	0.96	1 (4%)	31,47,47	2.09	6 (19%)
6	SO4	D	503	-	4,4,4	0.16	0	6,6,6	0.14	0
6	SO4	D	502	-	4,4,4	0.21	0	6,6,6	0.20	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
7	GOL	A	506	-	-	1/4/4/4	-
4	GTP	A	501	5	-	6/18/38/38	0/3/3/3
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
4	GTP	C	501	5	-	6/18/38/38	0/3/3/3
7	GOL	A	507	-	-	1/4/4/4	-
8	GDP	D	501	-	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C6-N1	3.40	1.39	1.33
8	D	501	GDP	C6-N1	3.12	1.38	1.33
4	C	501	GTP	C6-N1	3.08	1.38	1.33
4	A	501	GTP	C6-N1	2.95	1.38	1.33
4	A	501	GTP	C8-N7	-2.01	1.31	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	GTP	C5-C6-N1	-8.22	112.19	123.43
8	D	501	GDP	C5-C6-N1	-8.12	112.32	123.43
4	A	501	GTP	C5-C6-N1	-8.09	112.36	123.43
8	B	501	GDP	C5-C6-N1	-7.90	112.62	123.43
8	D	501	GDP	C6-N1-C2	5.84	125.21	115.93
4	C	501	GTP	C6-N1-C2	5.83	125.19	115.93
4	A	501	GTP	C6-N1-C2	5.83	125.19	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	GDP	C6-N1-C2	5.75	125.07	115.93
8	B	501	GDP	N3-C2-N1	-2.98	123.25	127.22
4	A	501	GTP	N3-C2-N1	-2.91	123.34	127.22
8	B	501	GDP	C6-C5-C4	-2.84	118.08	120.80
8	D	501	GDP	N3-C2-N1	-2.84	123.44	127.22
4	C	501	GTP	N3-C2-N1	-2.84	123.44	127.22
8	D	501	GDP	C6-C5-C4	-2.67	118.25	120.80
4	A	501	GTP	C2-N3-C4	-2.51	112.50	115.36
4	C	501	GTP	C2-N3-C4	-2.49	112.52	115.36
4	A	501	GTP	C6-C5-C4	-2.42	118.48	120.80
4	C	501	GTP	C6-C5-C4	-2.36	118.55	120.80
8	D	501	GDP	C2-N3-C4	-2.30	112.73	115.36
8	B	501	GDP	C2-N3-C4	-2.25	112.78	115.36
4	C	501	GTP	O5'-PA-O1A	2.17	117.55	109.07
8	D	501	GDP	O2A-PA-O5'	2.07	117.37	107.75
8	B	501	GDP	O3B-PB-O2B	2.05	115.48	107.64
4	A	501	GTP	O5'-PA-O1A	2.02	116.94	109.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	C4'-C5'-O5'-PA
7	A	506	GOL	C1-C2-C3-O3
4	C	501	GTP	C4'-C5'-O5'-PA
4	A	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
4	C	501	GTP	PB-O3A-PA-O2A
7	A	507	GOL	O1-C1-C2-O2

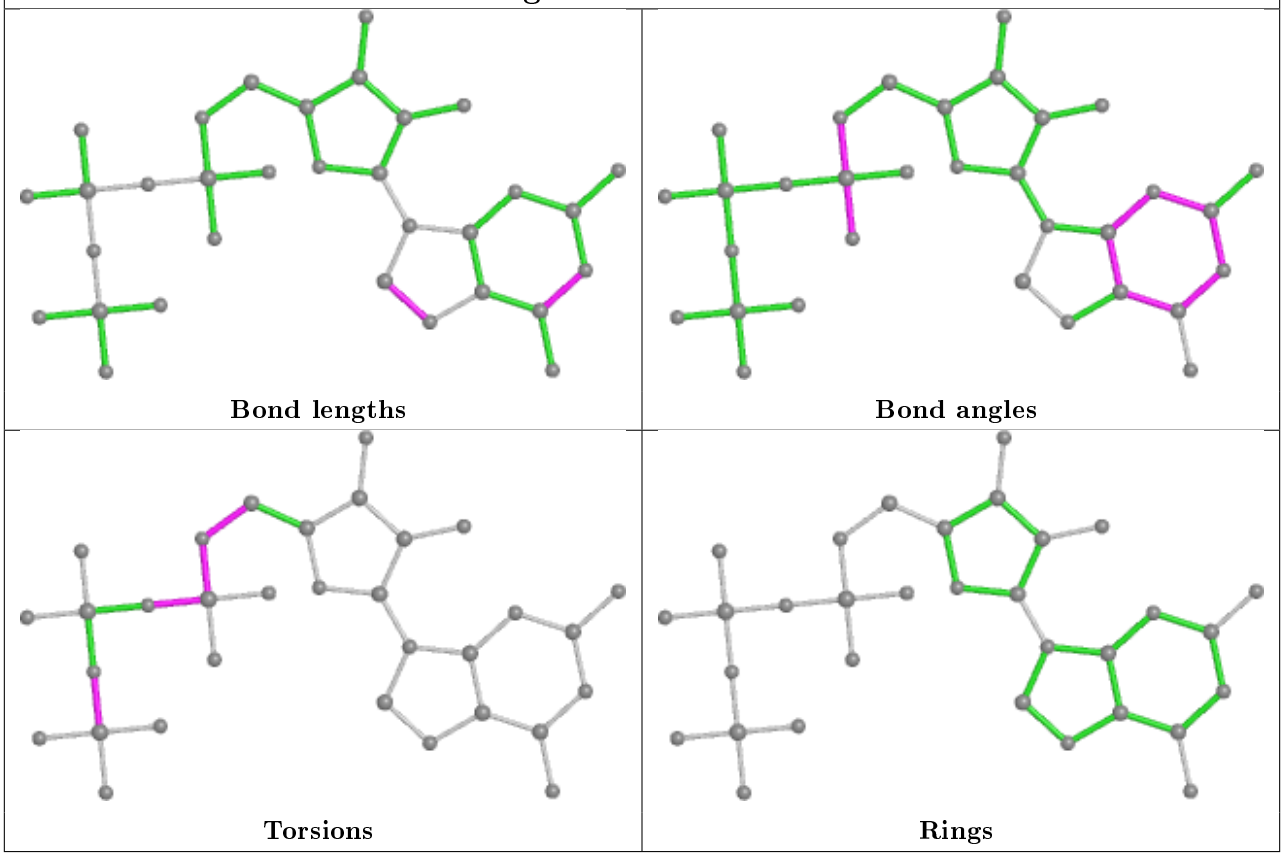
There are no ring outliers.

2 monomers are involved in 3 short contacts:

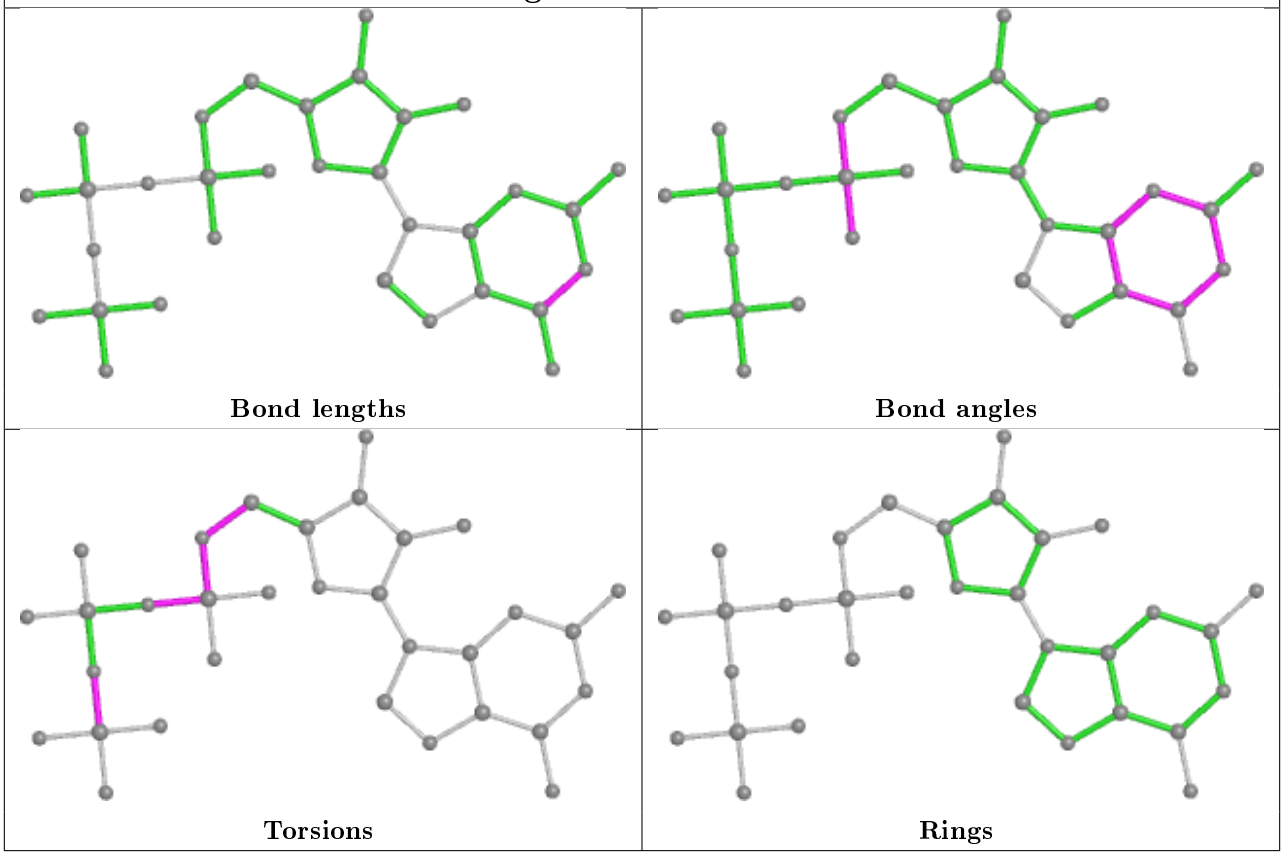
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	506	GOL	1	0
6	A	504	SO4	2	0

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

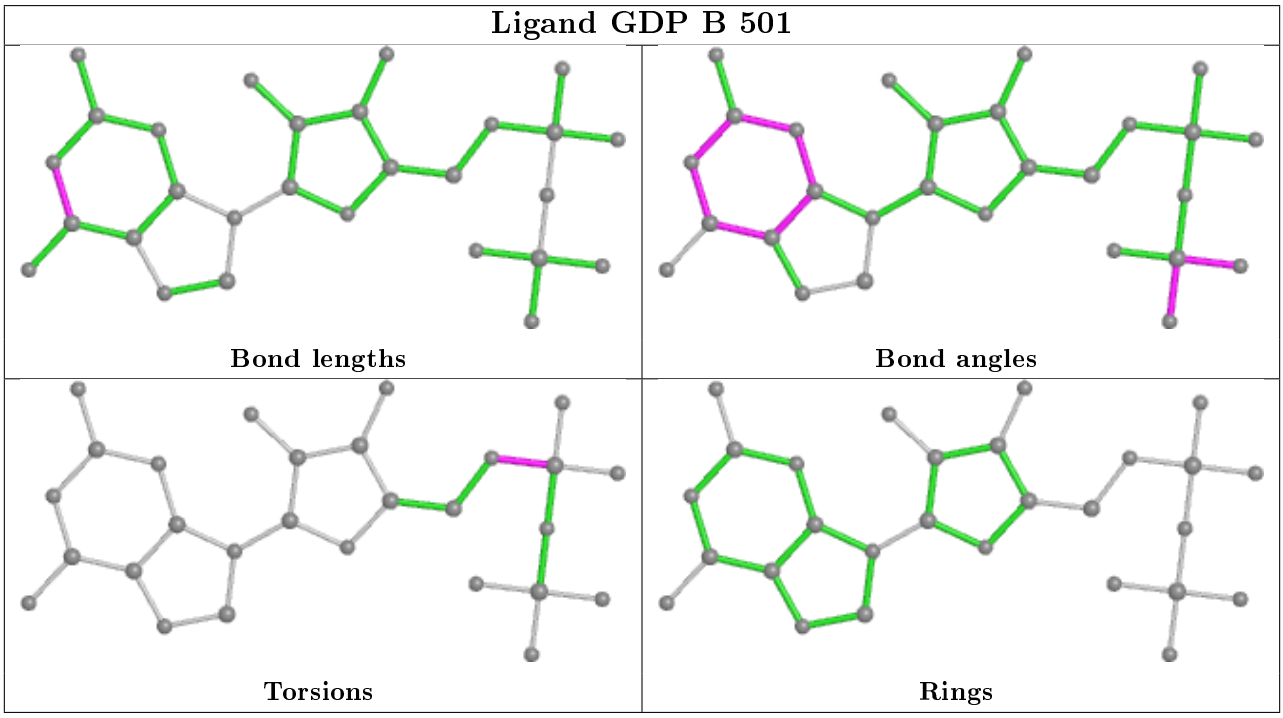
Ligand GTP A 501



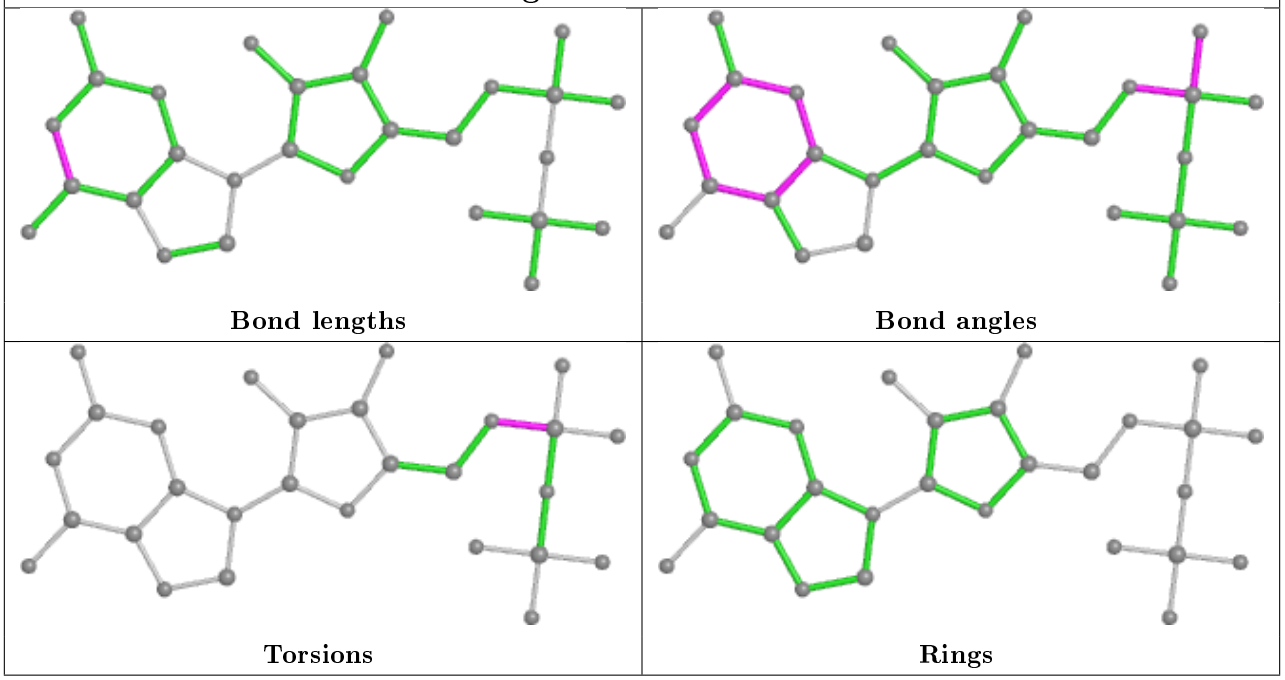
Ligand GTP C 501



Ligand GDP B 501



Ligand GDP D 501



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	430/450 (95%)	0.33	31 (7%)	15	14	33, 48, 69, 89	0
1	C	430/450 (95%)	0.58	51 (11%)	4	4	34, 55, 82, 103	0
2	B	428/447 (95%)	0.51	49 (11%)	5	4	33, 48, 75, 99	0
2	D	427/447 (95%)	0.26	25 (5%)	22	21	33, 45, 71, 87	0
3	E	129/143 (90%)	0.99	18 (13%)	2	2	47, 61, 86, 98	0
All	All	1844/1937 (95%)	0.46	174 (9%)	8	7	33, 50, 77, 103	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	281	ALA	7.0
3	E	142	GLU	6.8
1	A	346	TRP	6.7
1	C	278	ALA	6.7
2	D	431	ASP	5.3
1	A	45	GLY	5.2
2	B	278	SER	5.2
1	A	38	SER	5.0
1	C	357	TYR	5.0
2	D	56	GLY	4.9
2	B	320	ARG	4.9
2	D	54	ALA	4.8
2	D	55	SER	4.8
2	B	431	ASP	4.8
3	E	31	GLY	4.8
1	A	262	TYR	4.6
1	C	45	GLY	4.5
2	B	277	GLY	4.4
2	B	432	GLU	4.3
1	A	438	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	55	SER	4.2
1	C	202	PHE	4.1
1	C	309	HIS	4.1
2	D	57	GLY	4.0
2	B	283	ALA	4.0
2	B	39	ASP	3.9
1	C	201	ALA	3.9
3	E	145	ARG	3.9
1	A	238	ILE	3.8
1	C	218	ASP	3.7
1	C	378	LEU	3.6
3	E	29	PHE	3.6
3	E	5	ASP	3.6
3	E	30	ASP	3.5
1	A	437	MET	3.5
1	A	270	VAL	3.5
2	D	283	ALA	3.5
2	B	168	SER	3.4
2	B	218	THR	3.4
2	B	368	ILE	3.4
1	C	279	GLU	3.4
1	C	137	ILE	3.4
1	C	200	CYS	3.4
3	E	44	ASP	3.4
2	B	42	LEU	3.4
1	C	167	LEU	3.4
2	D	166	THR	3.3
1	C	280	LYS	3.3
2	B	199	THR	3.2
1	C	316	CYS	3.2
1	C	277	SER	3.2
3	E	143	ALA	3.1
2	B	200	TYR	3.1
2	B	236	VAL	3.1
1	A	137	ILE	3.0
2	B	54	ALA	3.0
2	B	80	PRO	3.0
1	C	324	VAL	3.0
1	C	368	LEU	3.0
1	C	170	ALA	3.0
1	C	270	VAL	3.0
1	C	220	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	36	TYR	2.9
2	D	167	TYR	2.9
2	D	430	ALA	2.9
2	B	37	HIS	2.9
2	D	284	LEU	2.9
1	A	378	LEU	2.9
2	B	217	LEU	2.9
1	A	235	VAL	2.8
1	C	169	PHE	2.8
1	A	37	PRO	2.8
2	B	57	GLY	2.8
2	B	41	ASP	2.8
2	B	286	VAL	2.7
2	B	167	TYR	2.7
2	B	321	MET	2.7
2	D	39	ASP	2.7
2	B	284	LEU	2.7
1	C	36	MET	2.7
2	B	255	VAL	2.7
2	B	126	SER	2.7
3	E	113	GLU	2.7
1	A	138	PHE	2.7
3	E	45	PRO	2.7
1	C	349	THR	2.7
2	B	169	VAL	2.6
2	B	58	LYS	2.6
1	C	365	GLY	2.6
1	C	177	VAL	2.6
2	D	278	SER	2.5
1	C	203	MET	2.5
1	C	238	ILE	2.5
1	C	219	ILE	2.5
2	D	92	PHE	2.5
2	B	201	CYS	2.5
2	B	166	THR	2.5
2	D	94	GLN	2.5
1	A	171	ILE	2.5
1	A	220	GLU	2.5
2	B	32	ALA	2.5
2	D	199	THR	2.4
1	C	246	GLY	2.4
2	B	53	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	116	LEU	2.4
1	C	339	ARG	2.4
1	C	171	ILE	2.4
1	A	167	LEU	2.4
1	C	259	LEU	2.4
2	D	80	PRO	2.4
1	C	168	GLU	2.3
3	E	128	LYS	2.3
2	B	275	SER	2.3
1	C	141	PHE	2.3
2	D	266	PHE	2.3
1	C	46	ASP	2.3
2	B	266	PHE	2.3
1	C	268	PRO	2.3
3	E	138	GLU	2.3
2	B	268	PRO	2.3
3	E	24	LEU	2.2
1	A	202	PHE	2.2
1	C	7	ILE	2.2
2	B	135	LEU	2.2
1	A	377	MET	2.2
1	C	315	CYS	2.2
1	C	139	HIS	2.2
1	A	169	PHE	2.2
1	A	357	TYR	2.2
2	D	406	MET	2.2
1	C	56	THR	2.2
1	C	330	ALA	2.2
1	A	345	ASP	2.2
1	C	198	SER	2.2
2	B	253	LEU	2.2
3	E	80	ARG	2.2
1	C	285	GLN	2.1
2	B	212	PHE	2.1
2	B	185	ALA	2.1
2	B	235	GLY	2.1
2	B	390	ARG	2.1
3	E	51	GLN	2.1
2	D	135	LEU	2.1
2	B	170	VAL	2.1
2	D	136	THR	2.1
1	A	96	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	309	HIS	2.1
1	A	318	LEU	2.1
3	E	49	GLU	2.1
1	C	57	GLY	2.1
2	D	324	LYS	2.1
1	C	364	PRO	2.1
2	D	201	CYS	2.1
1	C	29	GLY	2.1
2	B	56	GLY	2.1
1	A	136	LEU	2.1
2	B	139	LEU	2.1
1	A	434	GLU	2.1
2	D	200	TYR	2.0
1	A	218	ASP	2.0
2	B	165	ASN	2.0
3	E	70	LYS	2.0
2	B	202	ILE	2.0
2	D	192	LEU	2.0
1	A	271	THR	2.0
2	B	386	THR	2.0
1	C	9	VAL	2.0
1	C	215	ARG	2.0
2	D	277	GLY	2.0
1	A	163	LYS	2.0
1	A	272	TYR	2.0
1	A	400	ALA	2.0
1	C	271	THR	2.0
1	C	338	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

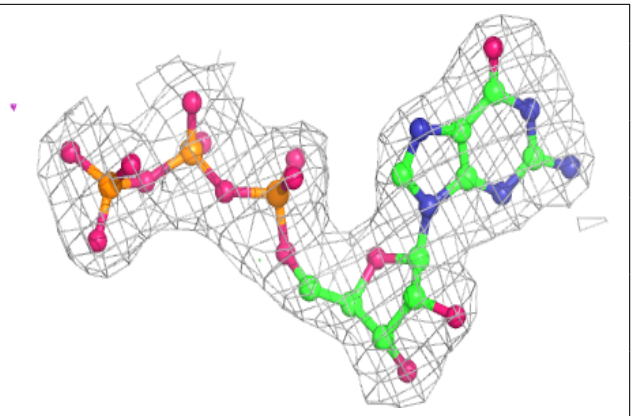
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

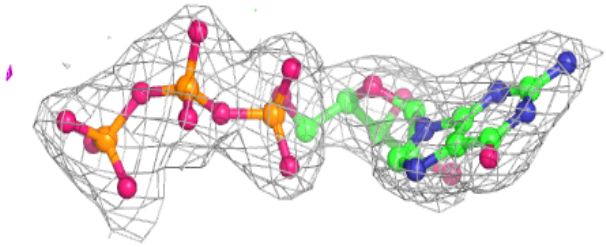
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	D	504	5/5	0.69	0.35	175,175,175,175	0
7	GOL	A	506	6/6	0.71	0.29	63,64,65,65	0
6	SO4	D	503	5/5	0.78	0.18	128,128,128,129	0
6	SO4	B	503	5/5	0.80	0.47	154,154,154,154	0
6	SO4	C	505	5/5	0.81	0.34	142,142,142,142	0
6	SO4	C	503	5/5	0.82	0.31	125,125,125,125	0
7	GOL	A	507	6/6	0.86	0.16	70,71,71,71	0
6	SO4	E	201	5/5	0.88	0.44	131,131,131,131	0
6	SO4	A	505	5/5	0.89	0.16	124,124,124,124	0
6	SO4	C	504	5/5	0.91	0.16	129,129,129,129	0
6	SO4	A	504	5/5	0.92	0.17	105,105,106,106	0
6	SO4	D	505	5/5	0.93	0.22	111,111,111,111	0
6	SO4	A	503	5/5	0.95	0.12	83,83,83,83	0
6	SO4	B	502	5/5	0.96	0.14	102,102,102,102	0
5	MG	A	502	1/1	0.97	0.08	39,39,39,39	0
4	GTP	C	501	32/32	0.98	0.09	41,47,49,50	0
8	GDP	B	501	28/28	0.99	0.10	38,41,42,42	0
8	GDP	D	501	28/28	0.99	0.09	33,35,36,37	0
4	GTP	A	501	32/32	0.99	0.14	35,38,41,41	0
5	MG	C	502	1/1	0.99	0.06	40,40,40,40	0
6	SO4	D	502	5/5	0.99	0.09	59,59,59,59	0

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

Electron density around GTP C 501:

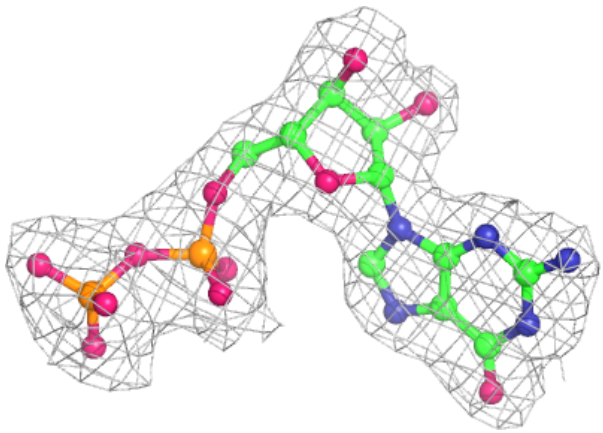
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

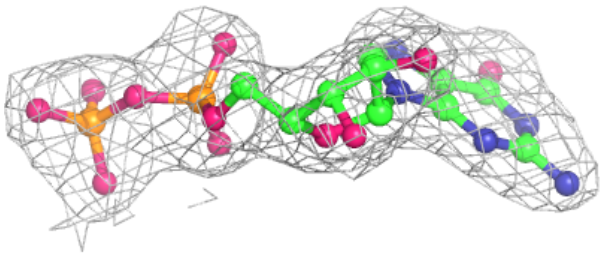


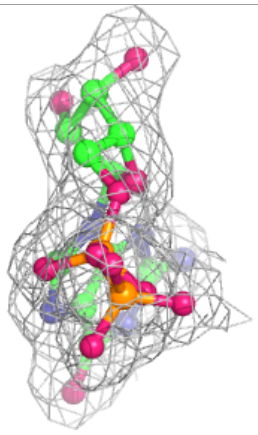


Electron density around GDP B 501:

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

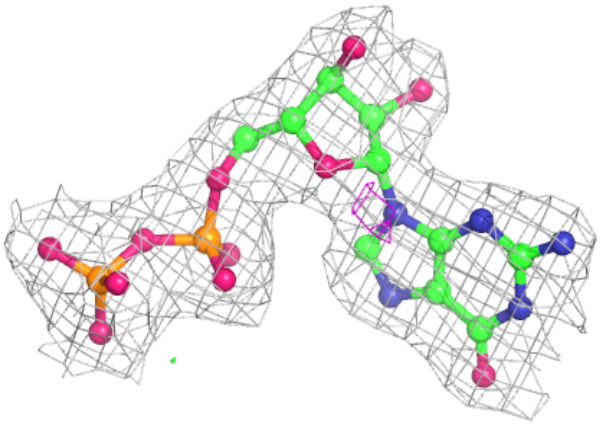


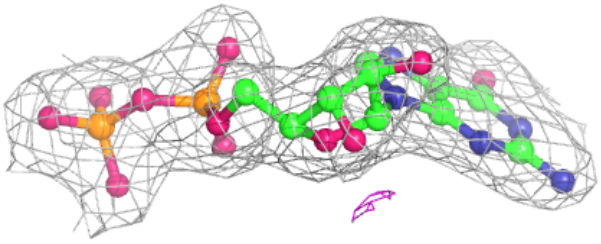


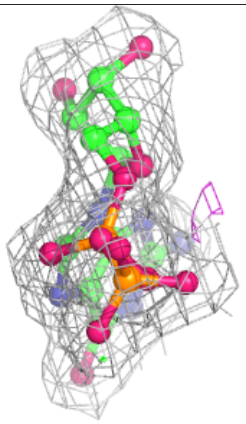


Electron density around GDP D 501:

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

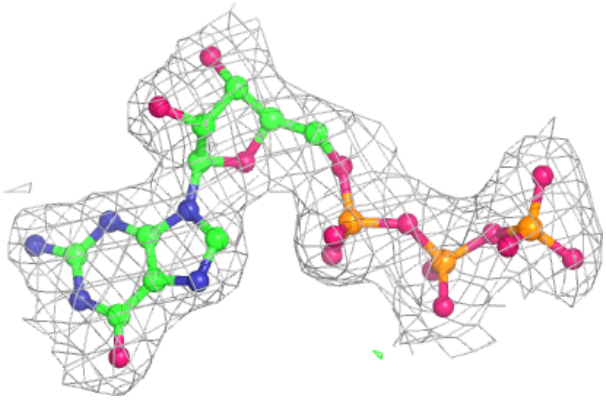


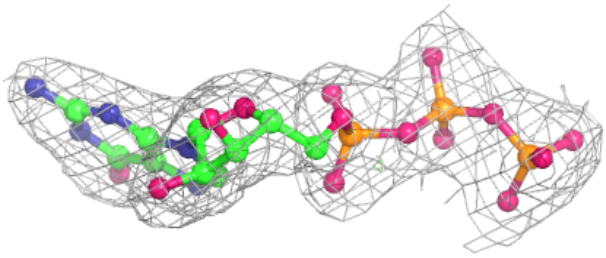


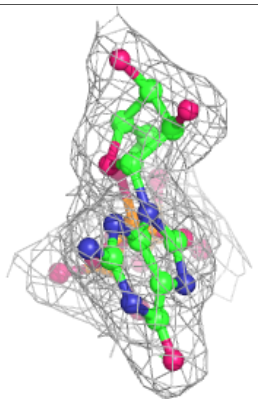


Electron density around GTP A 501:

$2mF_o$-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.