Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:44 AM EDT

PDB ID	:	6TIS
Title	:	DROSOPHILA GDP-TUBULIN
Authors	:	Gigant, B.
Deposited on	:	2019-11-22
Resolution	:	2.30 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 (i) symbol.

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

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

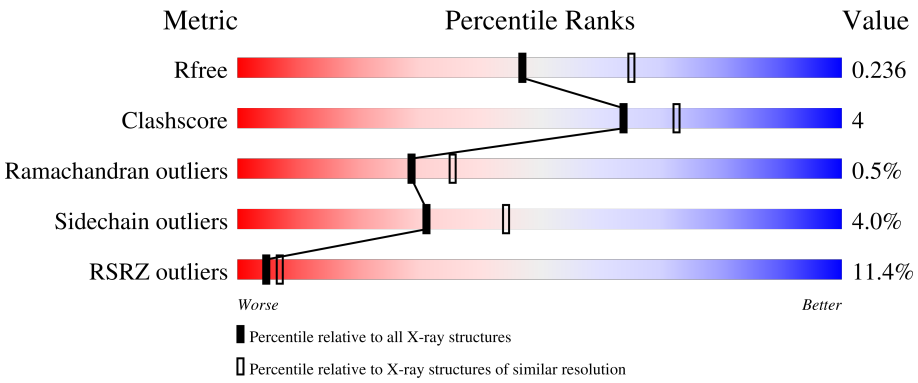
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	7% 81% 15% • •
1	C	450	10% 84% 11% • 5%
2	B	447	16% 84% 12% •
2	D	447	7% 87% 8% • •
3	E	143	21% 81% 9% • 9%

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
7	GOL	A	507	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 15255 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
			Total	C	N	O	S			
1	A	433	3388	2146	576	643	23	0	0	0
1	C	428	3351	2123	568	637	23	0	1	0

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
			Total	C	N	O	S			
2	B	430	3361	2112	573	650	26	0	0	0
2	D	429	3356	2108	574	648	26	0	1	0

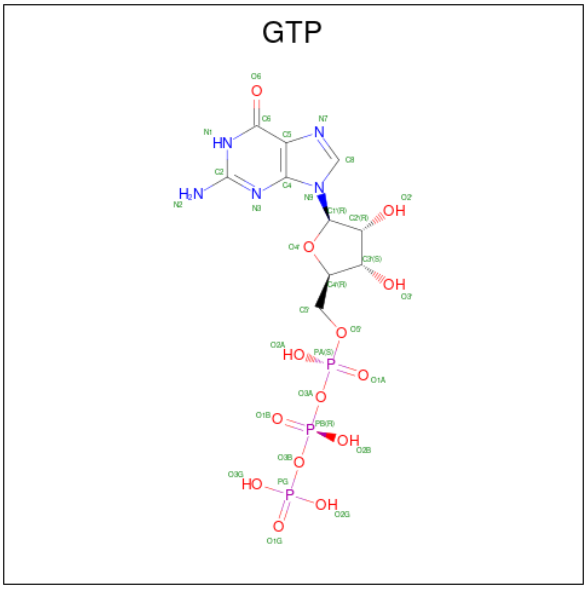
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	130	1062	655	194	209	4	0	0	0

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: $C_{10}H_{16}N_5O_{14}P_3$).

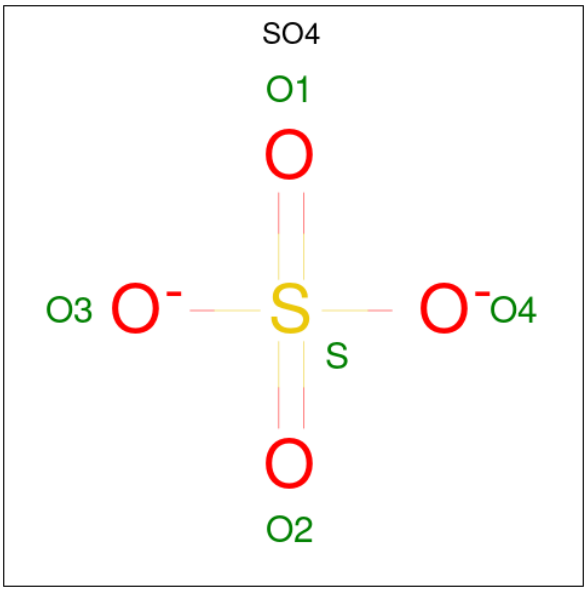


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
4	C	1	32	10	5	14	3	0	0

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

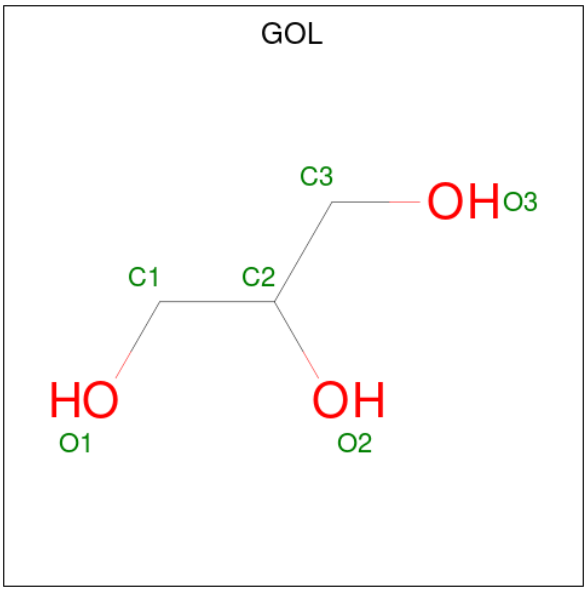
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
			Total	Mg		
5	C	1	1	1	0	0

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



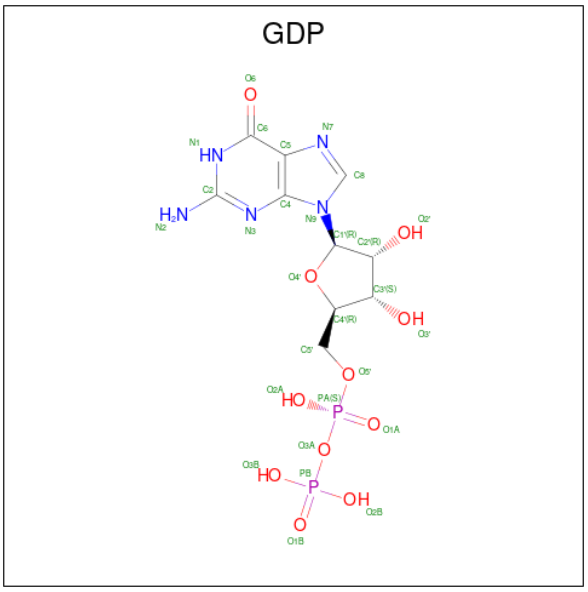
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	C	1	5	4	1	0	0
			Total	O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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	B	1	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
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0

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

- Molecule 9 is water.

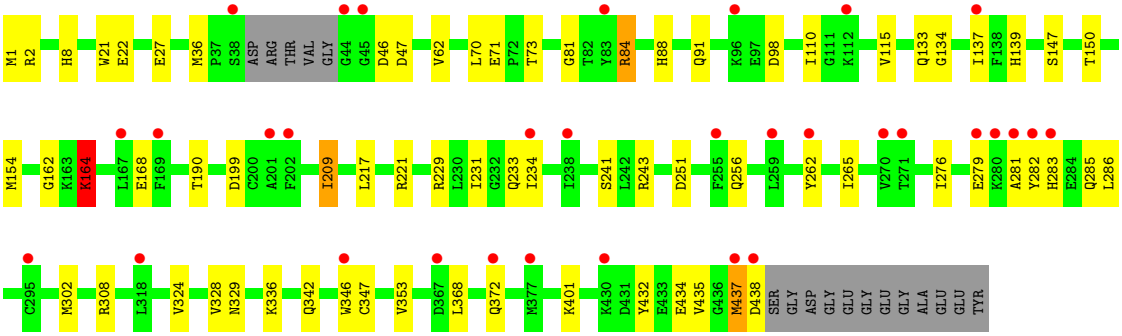
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	148	148	148	0	0
			Total	O		
9	B	113	113	113	0	0
			Total	O		
9	C	141	141	141	0	0
			Total	O		
9	D	120	120	120	0	0
			Total	O		
9	E	26	26	26	0	0

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.

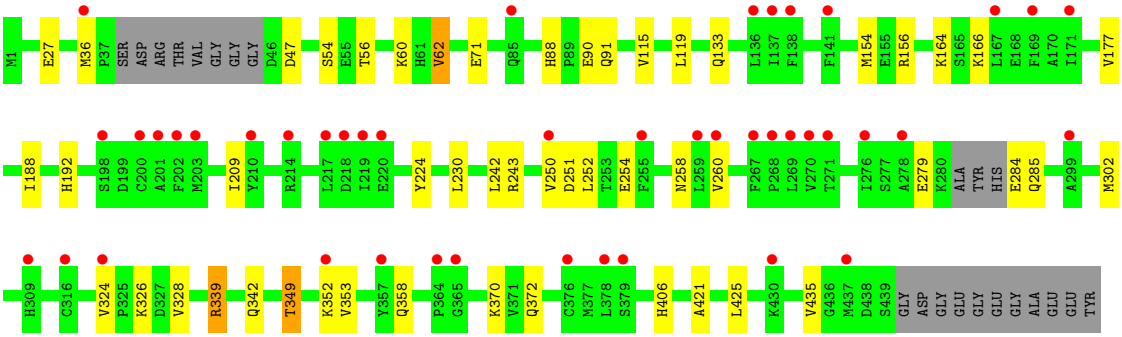
- Molecule 1: Tubulin alpha-1 chain

Chain A:



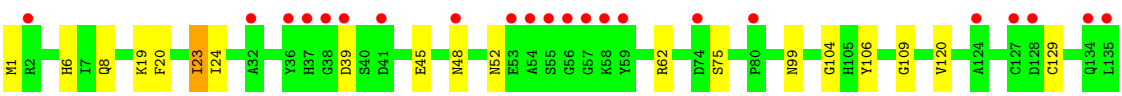
- Molecule 1: Tubulin alpha-1 chain

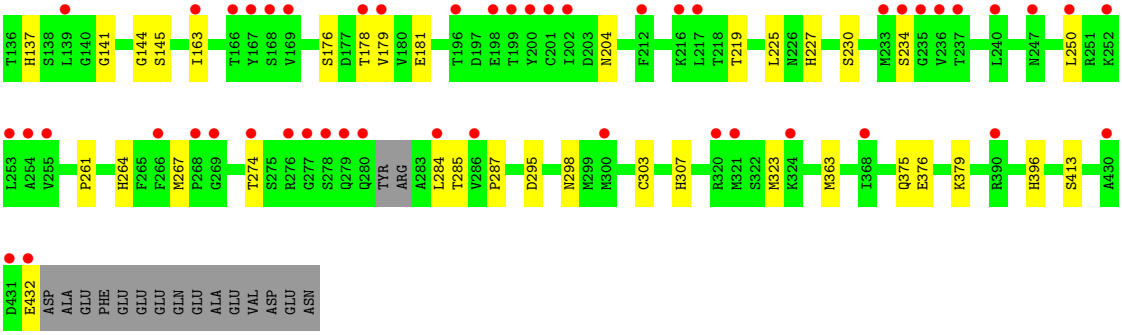
Chain C:



- Molecule 2: Tubulin beta-1 chain

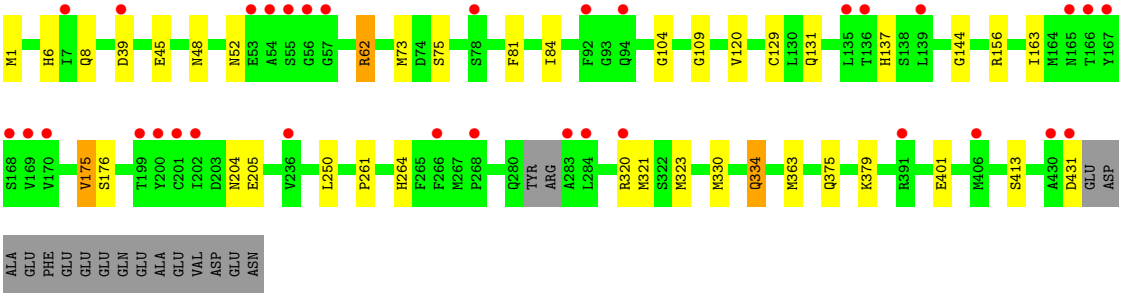
Chain B:





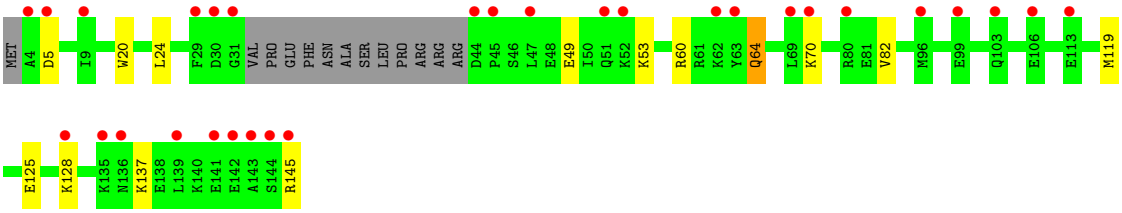
- Molecule 2: Tubulin beta-1 chain

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	66.59Å 126.52Å 250.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.30 33.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.1 (33.00-2.30) 92.1 (33.29-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.183 , 0.218 0.197 , 0.236	Depositor DCC
R_{free} test set	4349 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	1.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15255	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, SO4, MG, GOL, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.41	0/3465	0.59	0/4703
1	C	0.41	0/3428	0.58	0/4653
2	B	0.42	0/3433	0.56	0/4650
2	D	0.41	0/3436	0.56	0/4653
3	E	0.36	0/1072	0.55	0/1425
All	All	0.41	0/14834	0.57	0/20084

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3388	0	3298	45	0
1	C	3351	0	3261	27	0
2	B	3361	0	3237	38	0
2	D	3356	0	3231	18	0
3	E	1062	0	1067	8	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	20	0	0	1	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
6	D	15	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	B	28	0	12	1	0
8	D	28	0	12	1	0
9	A	148	0	0	1	0
9	B	113	0	0	0	0
9	C	141	0	0	0	0
9	D	120	0	0	0	0
9	E	26	0	0	0	0
All	All	15255	0	14158	122	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 (122) 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	1.06	0.99
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.15	0.93
1:A:81:GLY:O	1:A:84:ARG:HG3	1.72	0.90
2:B:6:HIS:CE1	2:B:8:GLN:HE21	1.92	0.86
2:D:204:ASN:HD21	8:D:501:GDP:HN22	1.20	0.86
2:B:204:ASN:HD21	8:B:501:GDP:HN22	1.21	0.85
1:C:339:ARG:H	1:C:339:ARG:HD3	1.44	0.83
2:D:6:HIS:CE1	2:D:8:GLN:HE21	1.99	0.81
2:B:99:ASN:HD22	1:C:258:ASN:HD21	1.30	0.77
1:A:71:GLU:OE2	1:A:73:THR:HB	1.84	0.76
3:E:60:ARG:O	3:E:64:GLN:HG2	1.86	0.74
1:A:133:GLN:HE22	1:A:251:ASP:HB2	1.53	0.74
2:D:261:PRO:O	2:D:264:HIS:HD2	1.72	0.72
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.72	0.71
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.40	0.69
1:A:401:LYS:HZ2	2:B:432:GLU:HB3	1.58	0.69
2:B:261:PRO:O	2:B:264:HIS:HD2	1.76	0.69
2:B:48:ASN:O	2:B:62:ARG:NH2	2.26	0.67
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:NZ	2:B:432:GLU:HB3	2.12	0.65
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.79	0.64
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.30	0.64
1:C:56:THR:CG2	1:C:60:LYS:HB3	2.28	0.63
2:D:48:ASN:O	2:D:62:ARG:NH2	2.31	0.63
2:B:267:MET:CE	2:B:303:CYS:HB2	2.30	0.62
1:C:154:MET:HE3	1:C:166:LYS:HE2	1.83	0.61
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.83	0.61
2:B:1:MET:N	2:B:129:CYS:SG	2.72	0.60
2:B:267:MET:HE3	2:B:303:CYS:HB2	1.83	0.60
2:D:137:HIS:HD2	2:D:144:GLY:O	1.84	0.60
1:A:221:ARG:NH2	6:A:506:SO4:O3	2.34	0.59
2:B:227:HIS:HE1	2:B:274:THR:HG23	1.66	0.59
2:D:131:GLN:NE2	2:D:250:LEU:H	2.01	0.58
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.85	0.58
2:B:307:HIS:HD2	2:B:376:GLU:OE1	1.87	0.57
1:A:88:HIS:H	1:A:91:GLN:HE21	1.52	0.57
2:B:227:HIS:CE1	2:B:274:THR:HG23	2.39	0.57
1:A:134:GLY:HA2	1:A:164:LYS:HG2	1.86	0.57
1:C:56:THR:HG22	1:C:60:LYS:HB3	1.87	0.57
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.88	0.56
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.23	0.56
1:A:71:GLU:OE2	1:A:73:THR:CB	2.52	0.56
2:D:1:MET:N	2:D:129:CYS:SG	2.75	0.54
1:A:88:HIS:H	1:A:91:GLN:NE2	2.06	0.54
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.54
2:B:23:ILE:HG12	2:B:230:SER:HB2	1.91	0.53
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.91	0.53
2:B:179:VAL:HG23	1:C:349:THR:O	2.09	0.52
2:B:99:ASN:ND2	1:C:258:ASN:HD21	2.05	0.52
1:A:285:GLN:NE2	1:A:372:GLN:H	2.08	0.52
1:C:285:GLN:NE2	1:C:372:GLN:H	2.08	0.52
1:A:46:ASP:O	1:A:47:ASP:HB3	2.08	0.52
1:A:62:VAL:HG11	1:A:88:HIS:HD2	1.76	0.51
2:B:137:HIS:HD2	2:B:144:GLY:O	1.94	0.51
2:B:19:LYS:O	2:B:23:ILE:HG13	2.11	0.51
2:B:141:GLY:O	2:B:145:SER:OG	2.26	0.50
1:A:209:ILE:HD13	1:A:231:ILE:HD11	1.92	0.50
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.04	0.50
3:E:125:GLU:HA	3:E:128:LYS:HD2	1.94	0.50
2:B:23:ILE:HD12	2:B:24:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:GLY:O	2:B:109:GLY:HA3	2.13	0.49
2:D:104:GLY:O	2:D:109:GLY:HA3	2.12	0.49
1:A:62:VAL:HG21	1:A:88:HIS:NE2	2.27	0.49
2:B:99:ASN:HB3	2:B:178:THR:HG21	1.95	0.49
2:D:330:MET:O	2:D:334:GLN:HG2	2.13	0.49
1:C:177:VAL:CG2	1:C:224:TYR:CE1	2.96	0.48
1:A:2:ARG:HB3	1:A:133:GLN:CD	2.34	0.48
1:C:56:THR:HG21	1:C:60:LYS:HB3	1.96	0.48
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.48
2:B:52:ASN:OD1	2:B:62:ARG:NH1	2.47	0.48
2:D:52:ASN:OD1	2:D:62:ARG:NH1	2.47	0.47
1:A:262:TYR:CE2	1:A:346:TRP:CH2	3.01	0.47
1:C:188:ILE:HG13	1:C:425:LEU:HD22	1.96	0.47
1:A:276:ILE:HD11	1:A:286:LEU:HD13	1.96	0.47
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.44	0.46
1:C:88:HIS:H	1:C:91:GLN:NE2	2.14	0.46
1:C:88:HIS:H	1:C:91:GLN:HE21	1.62	0.46
1:C:133:GLN:HE22	1:C:252:LEU:H	1.63	0.46
2:B:23:ILE:HD13	2:B:234:SER:HB2	1.96	0.46
1:A:276:ILE:HD13	1:A:283:HIS:NE2	2.31	0.46
1:A:46:ASP:HB3	9:A:629:HOH:O	2.15	0.45
2:B:20:PHE:HA	2:B:23:ILE:HD11	1.98	0.45
2:D:375:GLN:HE21	2:D:379:LYS:HE3	1.80	0.45
3:E:49:GLU:O	3:E:53:LYS:HD2	2.16	0.45
1:A:137:ILE:HD13	1:A:154:MET:SD	2.56	0.45
1:A:150:THR:O	1:A:154:MET:HG2	2.17	0.45
2:B:178:THR:HG23	2:B:181:GLU:HG3	2.00	0.44
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.52	0.44
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.36	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.44
1:C:339:ARG:HD3	1:C:339:ARG:N	2.23	0.43
2:D:401:GLU:HA	3:E:137:LYS:HD3	2.00	0.43
2:B:295:ASP:HB3	2:B:298:ASN:HD22	1.82	0.43
1:A:139:HIS:HE1	1:A:168:GLU:OE1	2.01	0.43
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.01	0.43
2:B:285:THR:CG2	2:B:287:PRO:HD2	2.48	0.43
2:D:163:ILE:HG21	2:D:250:LEU:HB3	2.00	0.43
2:B:267:MET:HE1	2:B:303:CYS:HB2	2.01	0.43
2:B:106:TYR:CD1	3:E:82:VAL:HG21	2.54	0.43
1:A:199:ASP:HB3	1:A:256:GLN:HG2	2.00	0.43
1:C:133:GLN:NE2	1:C:252:LEU:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLN:HE22	1:C:251:ASP:HB2	1.84	0.43
1:A:22:GLU:OE1	1:A:229:ARG:NH1	2.52	0.42
2:D:175:VAL:O	2:D:175:VAL:HG13	2.19	0.42
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.54	0.42
1:A:434:GLU:HA	1:A:437:MET:HG2	2.01	0.42
2:B:219:THR:HG21	1:C:326:LYS:O	2.20	0.42
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.66	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:B:375:GLN:HE21	2:B:379:LYS:HE3	1.84	0.41
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
1:C:54:SER:OG	1:C:62:VAL:HG13	2.19	0.41
2:B:396:HIS:HE1	1:C:260:VAL:O	2.03	0.41
2:D:137:HIS:CD2	2:D:144:GLY:O	2.68	0.41
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.51	0.41
2:B:99:ASN:ND2	1:C:254:GLU:HG2	2.36	0.40
2:B:106:TYR:CG	3:E:82:VAL:HG21	2.56	0.40
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.52	0.40
1:A:234:ILE:HD13	1:A:302:MET:SD	2.62	0.40
1:A:262:TYR:HB2	1:A:265:ILE:HD12	2.03	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/450 (95%)	414 (96%)	10 (2%)	5 (1%)	13 14
1	C	423/450 (94%)	412 (97%)	9 (2%)	2 (0%)	29 35
2	B	426/447 (95%)	417 (98%)	8 (2%)	1 (0%)	47 58
2	D	426/447 (95%)	419 (98%)	6 (1%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	126/143 (88%)	122 (97%)	4 (3%)	0	100	100
All	All	1830/1937 (94%)	1784 (98%)	37 (2%)	9 (0%)	29	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	437	MET
1	A	164	LYS
1	C	47	ASP
1	C	279	GLU
1	A	162	GLY
1	A	281	ALA
2	B	284	LEU
2	D	175	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	364/375 (97%)	351 (96%)	13 (4%)	35	49
1	C	361/375 (96%)	343 (95%)	18 (5%)	24	34
2	B	364/382 (95%)	354 (97%)	10 (3%)	44	61
2	D	365/382 (96%)	349 (96%)	16 (4%)	28	39
3	E	112/126 (89%)	107 (96%)	5 (4%)	27	39
All	All	1566/1640 (96%)	1504 (96%)	62 (4%)	31	44

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	36	MET
1	A	84	ARG

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Mol	Chain	Res	Type
1	A	115	VAL
1	A	164	LYS
1	A	209	ILE
1	A	241	SER
1	A	279	GLU
1	A	308	ARG
1	A	324	VAL
1	A	342	GLN
1	A	435	VAL
1	A	438	ASP
2	B	23	ILE
2	B	39	ASP
2	B	45	GLU
2	B	75	SER
2	B	120	VAL
2	B	176	SER
2	B	225	LEU
2	B	323	MET
2	B	363	MET
2	B	413	SER
1	C	36	MET
1	C	62	VAL
1	C	71	GLU
1	C	90	GLU
1	C	115	VAL
1	C	164	LYS
1	C	242	LEU
1	C	250	VAL
1	C	284	GLU
1	C	302	MET
1	C	324	VAL
1	C	339	ARG
1	C	342	GLN
1	C	349	THR
1	C	352	LYS
1	C	358	GLN
1	C	370	LYS
1	C	435	VAL
2	D	39	ASP
2	D	45	GLU
2	D	62	ARG
2	D	73	MET

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Mol	Chain	Res	Type
2	D	75	SER
2	D	120	VAL
2	D	156	ARG
2	D	176	SER
2	D	205	GLU
2	D	320	ARG
2	D	321	MET
2	D	323	MET
2	D	334	GLN
2	D	363	MET
2	D	413	SER
2	D	431	ASP
3	E	5	ASP
3	E	64	GLN
3	E	70	LYS
3	E	119	MET
3	E	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	GLN
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
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	37	HIS
2	B	99	ASN
2	B	134	GLN
2	B	137	HIS
2	B	204	ASN
2	B	227	HIS
2	B	245	GLN
2	B	264	HIS
2	B	292	GLN
2	B	298	ASN

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Mol	Chain	Res	Type
2	B	307	HIS
2	B	332	ASN
2	B	375	GLN
2	B	396	HIS
2	B	423	GLN
2	B	424	GLN
1	C	8	HIS
1	C	11	GLN
1	C	88	HIS
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	256	GLN
1	C	285	GLN
1	C	301	GLN
1	C	329	ASN
1	C	358	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	37	HIS
2	D	131	GLN
2	D	134	GLN
2	D	137	HIS
2	D	204	ASN
2	D	245	GLN
2	D	264	HIS
2	D	292	GLN
2	D	298	ASN
2	D	332	ASN
2	D	375	GLN
2	D	423	GLN
2	D	424	GLN
2	D	426	GLN
3	E	18	GLN
3	E	111	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	B	503	-	4,4,4	0.22	0	6,6,6	0.08	0
8	GDP	B	501	-	25,30,30	0.95	2 (8%)	30,47,47	0.82	1 (3%)
4	GTP	C	501	5	29,34,34	0.85	1 (3%)	35,54,54	0.66	0
6	SO4	D	504	-	4,4,4	0.32	0	6,6,6	0.15	0
7	GOL	A	507	-	5,5,5	0.12	0	5,5,5	0.16	0
8	GDP	D	501	-	25,30,30	1.00	1 (4%)	30,47,47	0.67	0
4	GTP	A	501	5	29,34,34	0.93	2 (6%)	35,54,54	0.65	0
6	SO4	B	502	-	4,4,4	0.31	0	6,6,6	0.13	0
6	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.22	0
6	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.22	0
6	SO4	A	503	-	4,4,4	0.36	0	6,6,6	0.21	0
6	SO4	C	503	-	4,4,4	0.26	0	6,6,6	0.19	0
6	SO4	D	502	-	4,4,4	0.21	0	6,6,6	0.26	0
6	SO4	D	503	-	4,4,4	0.18	0	6,6,6	0.19	0
6	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.17	0
6	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.17	0
7	GOL	B	505	-	5,5,5	0.08	0	5,5,5	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
4	GTP	C	501	5	-	8/18/38/38	0/3/3/3
7	GOL	A	507	-	-	0/4/4/4	-
8	GDP	D	501	-	-	3/12/32/32	0/3/3/3
4	GTP	A	501	5	-	8/18/38/38	0/3/3/3
7	GOL	B	505	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	C5-C6	-2.62	1.42	1.47
8	B	501	GDP	C8-N7	-2.37	1.31	1.34
4	A	501	GTP	C8-N7	-2.34	1.31	1.34
8	B	501	GDP	C5-C4	-2.29	1.37	1.43
4	C	501	GTP	C8-N7	-2.25	1.31	1.34
8	D	501	GDP	PB-O3B	-2.07	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	GDP	O3B-PB-O2B	2.64	117.69	107.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	PB-O3B-PG-O1G
4	C	501	GTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	PB-O3B-PG-O2G
4	C	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	PB-O3A-PA-O1A
4	C	501	GTP	PB-O3A-PA-O1A
4	C	501	GTP	PB-O3A-PA-O2A

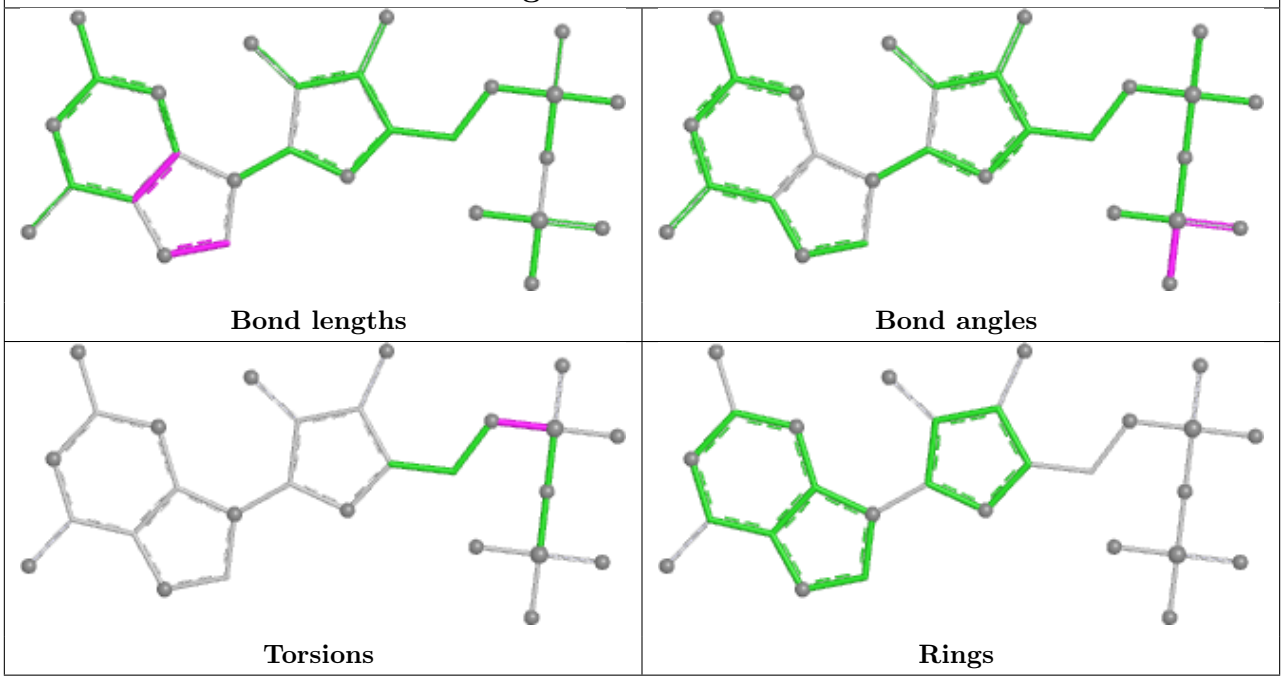
There are no ring outliers.

3 monomers are involved in 3 short contacts:

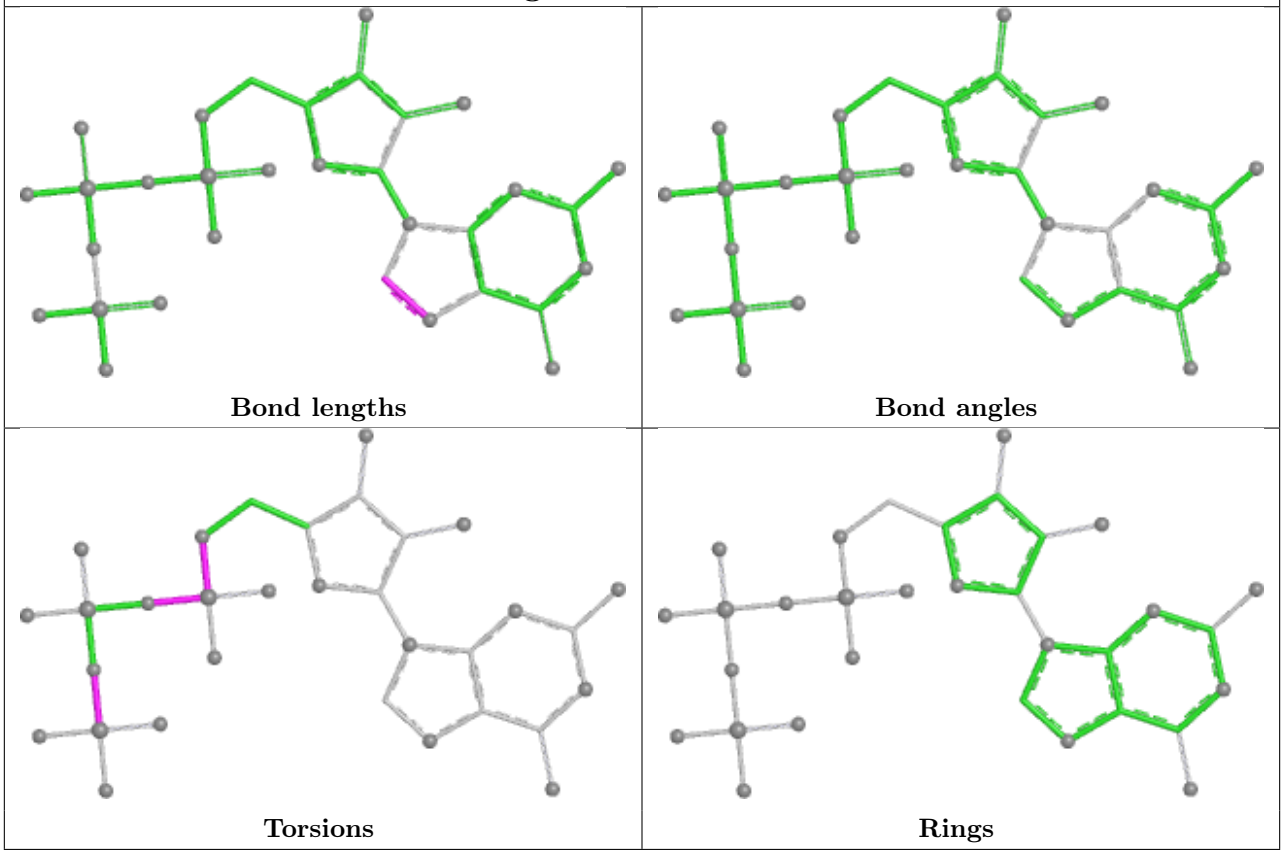
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	1	0
8	D	501	GDP	1	0
6	A	506	SO4	1	0

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

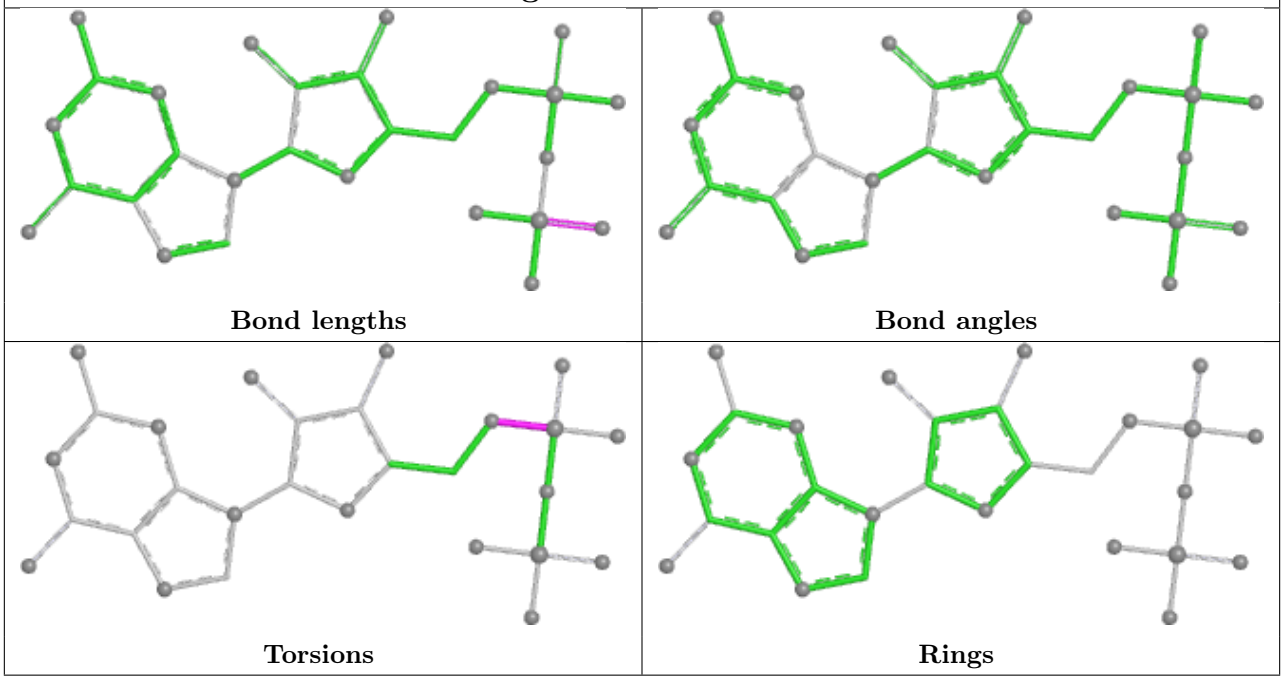
Ligand GDP B 501



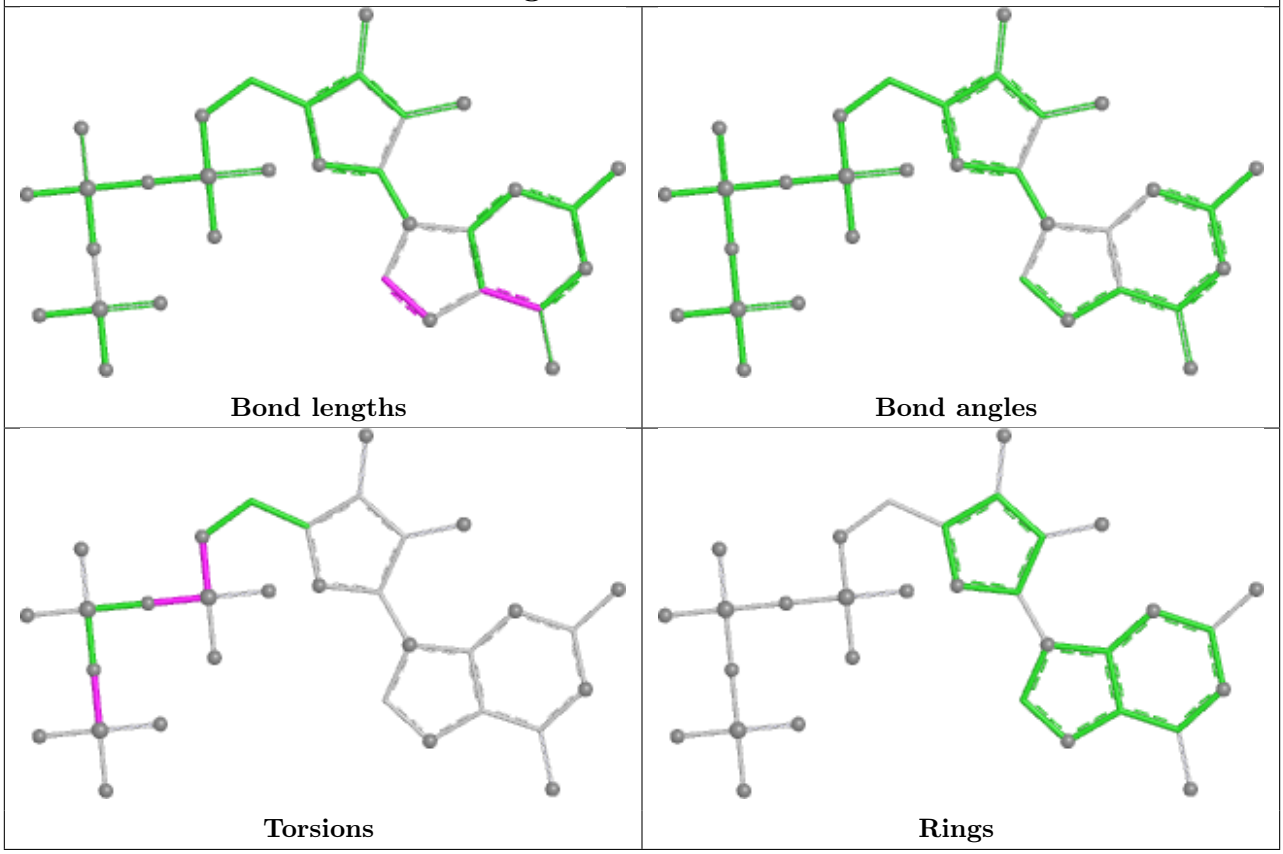
Ligand GTP C 501



Ligand GDP D 501



Ligand GTP A 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	433/450 (96%)	0.47	32 (7%)	14	19	48, 65, 87, 116	0
1	C	428/450 (95%)	0.55	44 (10%)	6	9	51, 69, 96, 104	0
2	B	430/447 (96%)	0.72	71 (16%)	1	2	49, 63, 93, 114	0
2	D	429/447 (95%)	0.37	33 (7%)	13	17	47, 61, 86, 97	0
3	E	130/143 (90%)	1.39	30 (23%)	0	1	63, 78, 113, 135	0
All	All	1850/1937 (95%)	0.59	210 (11%)	5	7	47, 65, 94, 135	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	9.1
3	E	4	ALA	8.4
1	A	44	GLY	8.1
3	E	142	GLU	7.5
3	E	31	GLY	7.3
1	A	281	ALA	7.3
3	E	5	ASP	7.1
3	E	144	SER	7.1
1	C	357	TYR	6.6
3	E	30	ASP	6.0
1	C	278	ALA	5.8
1	A	346	TRP	5.4
2	B	54	ALA	5.3
3	E	29	PHE	5.1
2	B	432	GLU	5.1
2	B	39	ASP	4.9
1	A	262	TYR	4.8
1	A	45	GLY	4.8
2	B	167	TYR	4.7
1	A	283	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	437	MET	4.4
2	D	54	ALA	4.4
3	E	145	ARG	4.4
1	C	324	VAL	4.4
2	B	320	ARG	4.3
2	B	236	VAL	4.3
1	C	202	PHE	4.1
2	B	278	SER	4.1
2	B	200	TYR	4.1
2	D	56	GLY	4.1
2	B	199	THR	3.9
2	B	431	ASP	3.9
1	C	200	CYS	3.8
1	C	270	VAL	3.8
2	B	36	TYR	3.8
3	E	45	PRO	3.8
3	E	69	LEU	3.7
2	B	57	GLY	3.7
2	B	235	GLY	3.7
2	D	166	THR	3.7
2	D	200	TYR	3.7
1	C	309	HIS	3.7
2	B	217	LEU	3.6
2	B	266	PHE	3.6
2	D	92	PHE	3.6
3	E	96	MET	3.6
2	B	253	LEU	3.5
1	C	203	MET	3.5
1	C	268	PRO	3.5
2	D	39	ASP	3.5
2	D	55	SER	3.5
1	A	38	SER	3.5
1	C	316	CYS	3.5
1	A	238	ILE	3.4
2	B	268	PRO	3.4
1	C	276	ILE	3.4
2	D	283	ALA	3.4
2	B	237	THR	3.4
3	E	99	GLU	3.4
2	D	320	ARG	3.4
2	D	167	TYR	3.4
1	C	269	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	279	GLN	3.4
2	B	168	SER	3.3
2	B	55	SER	3.3
2	D	431	ASP	3.2
2	B	321	MET	3.2
3	E	103	GLN	3.2
3	E	106	GLU	3.2
1	C	259	LEU	3.2
2	B	56	GLY	3.2
1	C	267	PHE	3.1
3	E	136	ASN	3.1
2	D	135	LEU	3.1
3	E	47	LEU	3.1
1	C	378	LEU	3.1
1	C	169	PHE	3.1
3	E	143	ALA	3.1
2	B	169	VAL	3.1
1	C	167	LEU	3.1
3	E	62	LYS	3.1
2	B	38	GLY	3.1
2	B	166	THR	3.0
1	C	201	ALA	3.0
2	B	32	ALA	3.0
2	B	280	GLN	3.0
2	D	7	ILE	3.0
3	E	139	LEU	3.0
2	B	196	THR	3.0
2	D	284	LEU	3.0
1	C	365	GLY	3.0
2	B	240	LEU	2.9
2	D	168	SER	2.9
2	B	128	ASP	2.9
3	E	51	GLN	2.8
2	B	250	LEU	2.8
1	C	364	PRO	2.8
1	A	96	LYS	2.8
3	E	70	LYS	2.8
3	E	141	GLU	2.8
2	D	170	VAL	2.8
3	E	52	LYS	2.8
2	D	266	PHE	2.7
1	A	167	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	218	ASP	2.7
2	B	37	HIS	2.7
1	C	352	LYS	2.7
2	D	136	THR	2.7
1	C	171	ILE	2.7
2	B	135	LEU	2.7
2	B	277	GLY	2.7
2	D	268	PRO	2.7
1	C	220	GLU	2.6
2	D	199	THR	2.6
1	A	202	PHE	2.6
2	B	324	LYS	2.6
2	D	139	LEU	2.6
2	D	406	MET	2.6
1	C	214	ARG	2.6
2	B	390	ARG	2.6
1	A	234	ILE	2.6
1	A	169	PHE	2.6
1	C	260	VAL	2.6
2	B	201	CYS	2.6
2	D	169	VAL	2.6
1	C	379	SER	2.5
3	E	9	ILE	2.5
2	B	216	LYS	2.5
1	C	219	ILE	2.4
1	C	36	MET	2.4
1	A	270	VAL	2.4
1	C	299	ALA	2.4
2	D	202	ILE	2.4
1	C	437	MET	2.4
1	A	83	TYR	2.4
1	C	210	TYR	2.4
1	A	377	MET	2.4
2	B	212	PHE	2.4
2	B	127	CYS	2.4
1	C	430	LYS	2.3
3	E	128	LYS	2.3
1	A	367	ASP	2.3
1	C	136	LEU	2.3
2	B	430	ALA	2.3
1	C	271	THR	2.3
1	C	141	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	372	GLN	2.3
1	A	112	LYS	2.3
2	B	255	VAL	2.3
2	D	165	ASN	2.3
2	D	53	GLU	2.3
1	C	217	LEU	2.3
1	A	438	ASP	2.3
2	B	74	ASP	2.3
2	B	134	GLN	2.3
2	D	430	ALA	2.3
2	B	202	ILE	2.2
2	B	368	ILE	2.2
2	B	274	THR	2.2
2	B	58	LYS	2.2
1	C	198	SER	2.2
1	C	85	GLN	2.2
2	B	80	PRO	2.2
2	B	179	VAL	2.2
1	A	271	THR	2.2
2	B	284	LEU	2.2
1	A	279	GLU	2.2
2	D	201	CYS	2.2
1	A	259	LEU	2.2
2	B	286	VAL	2.1
1	C	376	CYS	2.1
1	A	430	LYS	2.1
2	B	2	ARG	2.1
1	A	280	LYS	2.1
2	B	139	LEU	2.1
2	B	233	MET	2.1
2	B	300	MET	2.1
2	B	124	ALA	2.1
2	B	178	THR	2.1
2	D	236	VAL	2.1
3	E	63	TYR	2.1
3	E	135	LYS	2.1
2	B	247	ASN	2.1
2	B	41	ASP	2.1
2	B	59	TYR	2.1
2	B	48	ASN	2.1
3	E	113	GLU	2.1
1	C	250	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	252	LYS	2.1
2	B	163	ILE	2.1
3	E	44	ASP	2.1
2	D	78	SER	2.1
1	A	255	PHE	2.1
2	B	53	GLU	2.0
1	C	137	ILE	2.0
2	D	391	ARG	2.0
3	E	80	ARG	2.0
2	B	198	GLU	2.0
1	A	295	CYS	2.0
1	C	255	PHE	2.0
2	B	276	ARG	2.0
1	A	137	ILE	2.0
2	D	57	GLY	2.0
2	B	234	SER	2.0
2	D	94	GLN	2.0
1	C	138	PHE	2.0
1	A	318	LEU	2.0
2	B	269	GLY	2.0
1	A	201	ALA	2.0
2	B	254	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	507	6/6	0.47	0.42	89,90,90,90	0

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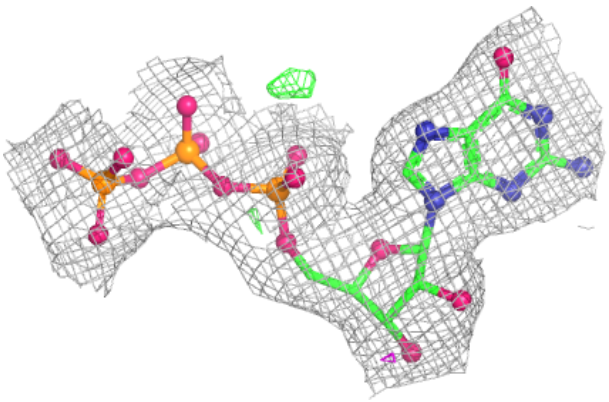
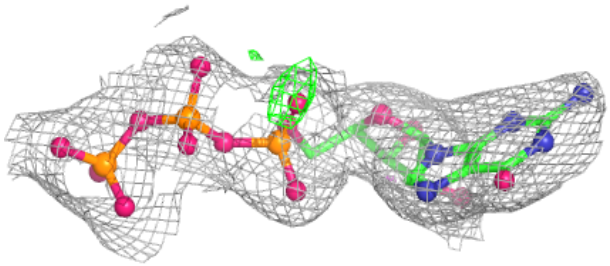
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	506	5/5	0.77	0.27	140,140,140,140	0
6	SO4	A	505	5/5	0.78	0.26	143,143,143,143	0
7	GOL	B	505	6/6	0.84	0.26	107,107,107,107	0
6	SO4	D	504	5/5	0.87	0.12	123,123,123,123	0
6	SO4	B	502	5/5	0.91	0.17	126,126,126,126	0
6	SO4	C	503	5/5	0.92	0.11	125,125,125,125	0
6	SO4	A	504	5/5	0.93	0.14	94,94,95,95	0
6	SO4	D	503	5/5	0.94	0.21	111,111,111,112	0
6	SO4	A	503	5/5	0.94	0.11	113,114,114,114	0
6	SO4	B	504	5/5	0.95	0.15	111,111,111,111	0
6	SO4	D	502	5/5	0.95	0.10	78,78,78,79	0
6	SO4	B	503	5/5	0.96	0.28	113,113,113,113	0
4	GTP	C	501	32/32	0.98	0.14	54,61,62,62	0
5	MG	A	502	1/1	0.98	0.13	56,56,56,56	0
4	GTP	A	501	32/32	0.98	0.16	50,53,56,56	0
8	GDP	B	501	28/28	0.98	0.14	51,52,55,57	0
8	GDP	D	501	28/28	0.98	0.14	48,50,52,53	0
5	MG	C	502	1/1	0.99	0.13	61,61,61,61	0

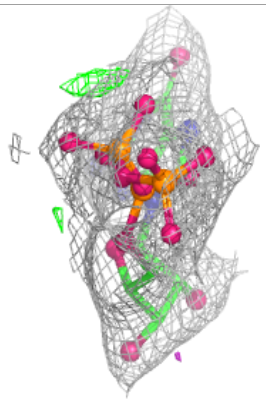
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

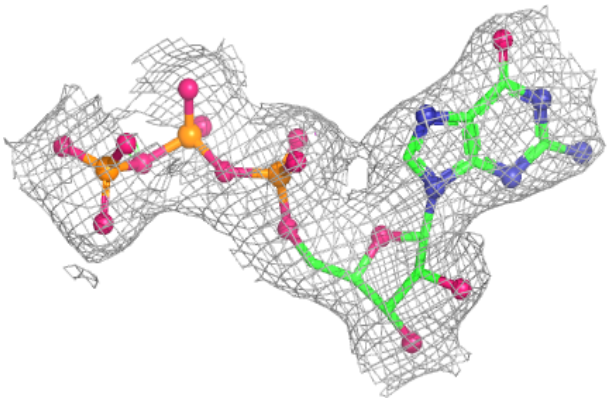


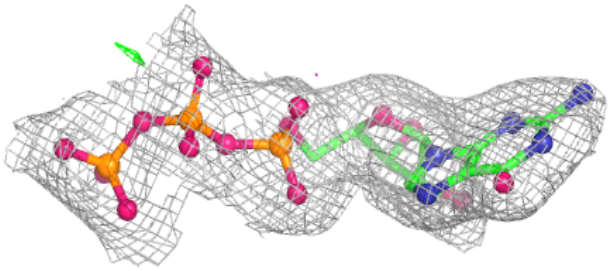


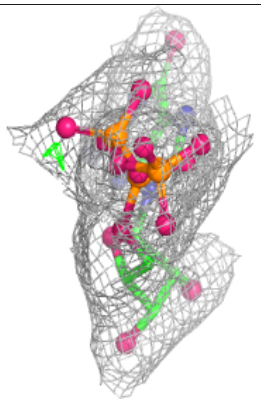


Electron density around GTP A 501:

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

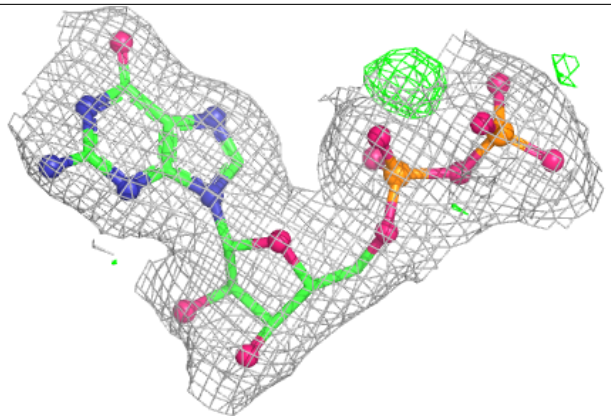


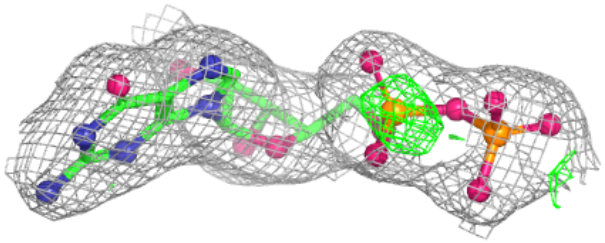


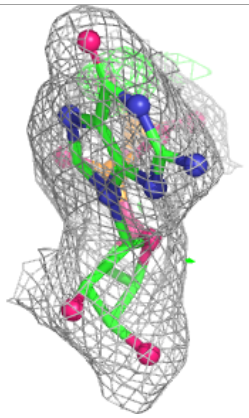


Electron density around GDP B 501:

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

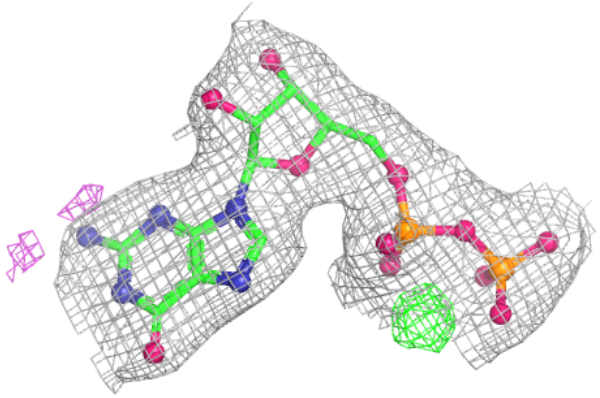


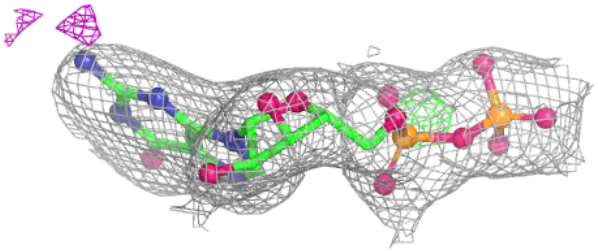


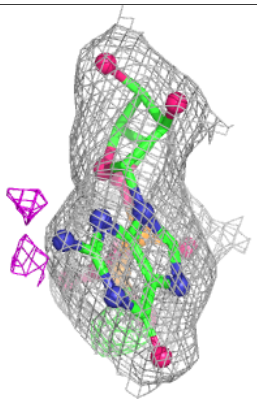


Electron density around GDP D 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.