



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 12, 2021 – 04:36 PM JST

PDB ID : 6LSN  
Title : Crystal structure of tubulin-inhibitor complex  
Authors : Gang, L.; Wang, Y.X.; Cheng, J.J.  
Deposited on : 2020-01-17  
Resolution : 2.44 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](mailto: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.

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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

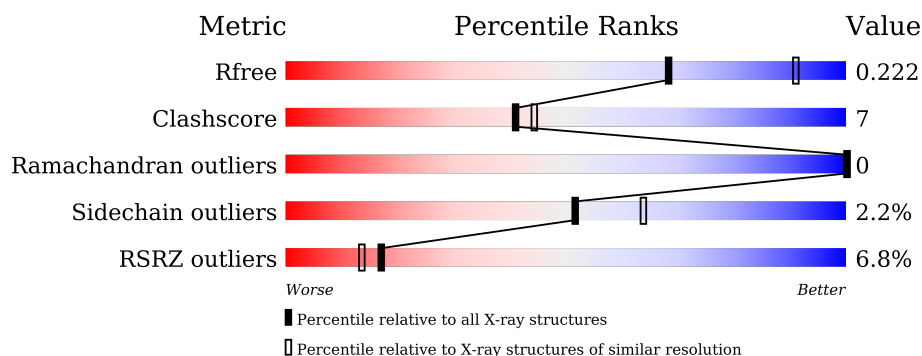
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	<div> <div>3%</div> <div>83% 14% .</div> </div>
1	C	450	<div> <div>%</div> <div>85% 12% .</div> </div>
2	B	445	<div> <div>6%</div> <div>81% 14% 5%</div> </div>
2	D	445	<div> <div>7%</div> <div>76% 18% 5%</div> </div>
3	E	143	<div> <div>8%</div> <div>73% 12% . 13%</div> </div>
4	F	384	<div> <div>16%</div> <div>66% 24% . 9%</div> </div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18041 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	1	0
			3435	2175	581	657	22			
1	C	440	Total	C	N	O	S	0	4	0
			3451	2184	585	660	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3344	2104	569	645	26			
2	D	421	Total	C	N	O	S	0	3	0
			3306	2079	562	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	1	0
			1025	631	185	204	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	0	2	0
			2887	1849	498	525	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

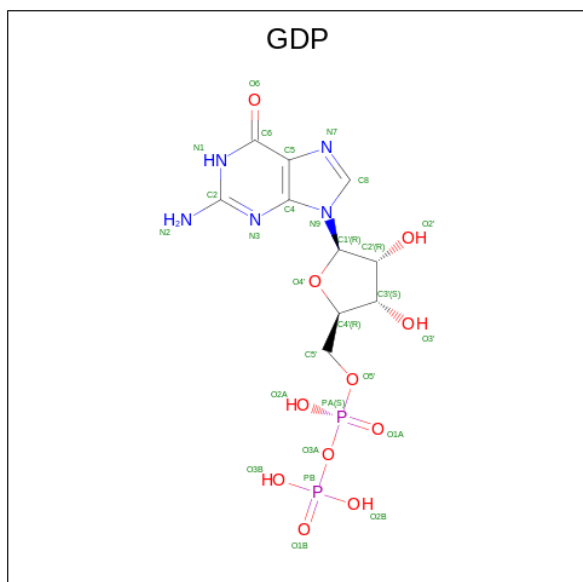
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	2	Total Ca 2 2	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



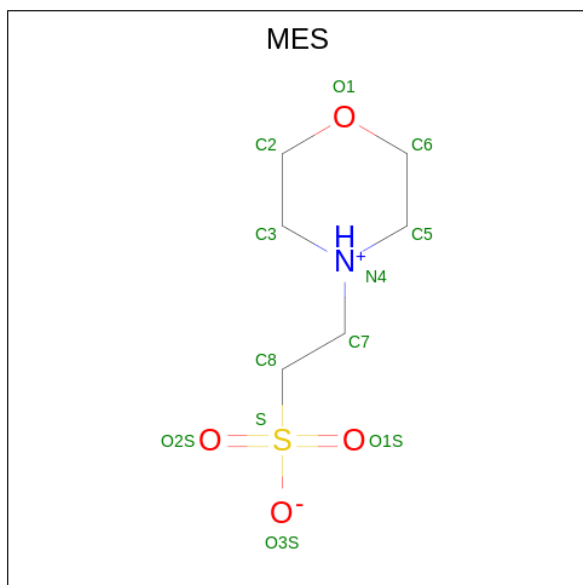
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0

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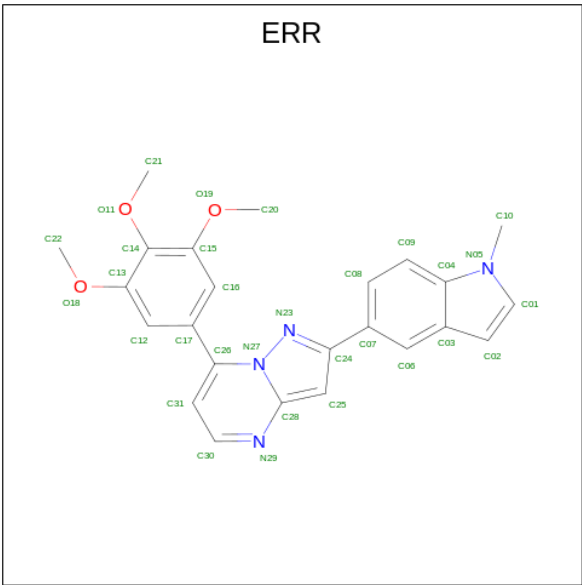
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



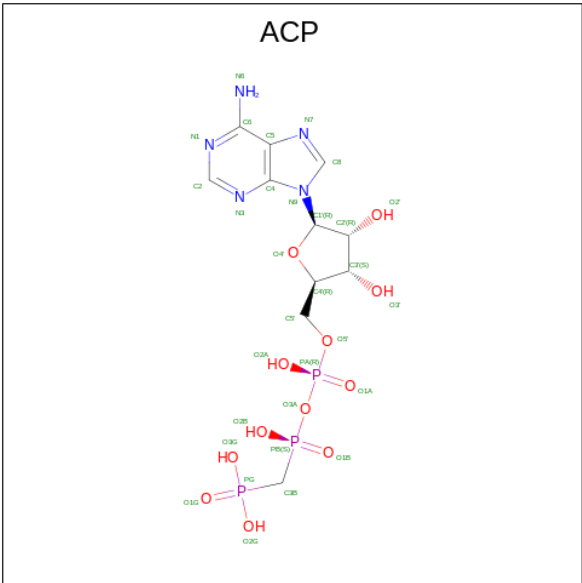
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-(1-methylindol-5-yl)-7-(3,4,5-trimethoxyphenyl)pyrazolo[1,5-a]pyrimidine (three-letter code: ERR) (formula: C<sub>24</sub>H<sub>22</sub>N<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			31	24	4	3		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 13 is water.

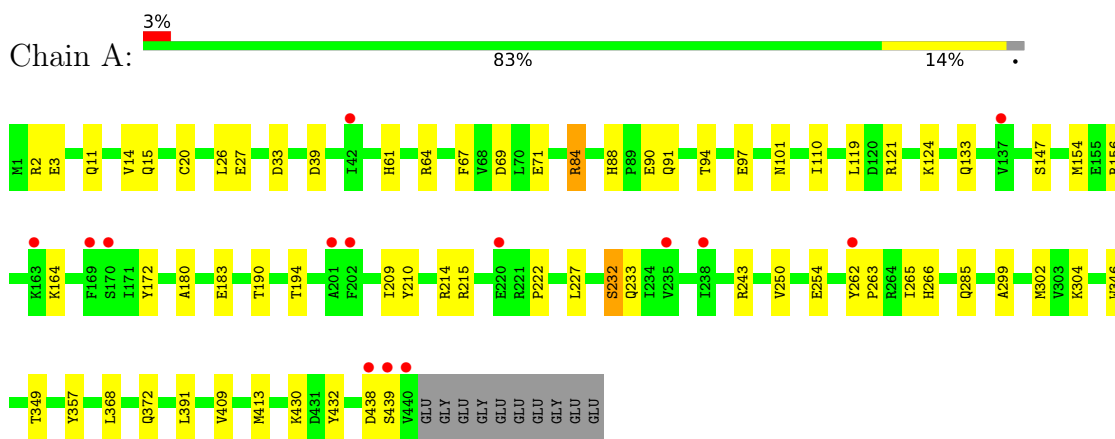
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	80	Total 80	O 80	0	0
13	B	68	Total 68	O 68	0	0
13	C	153	Total 153	O 153	0	0
13	D	28	Total 28	O 28	0	0
13	E	14	Total 14	O 14	0	0
13	F	33	Total 33	O 33	0	0



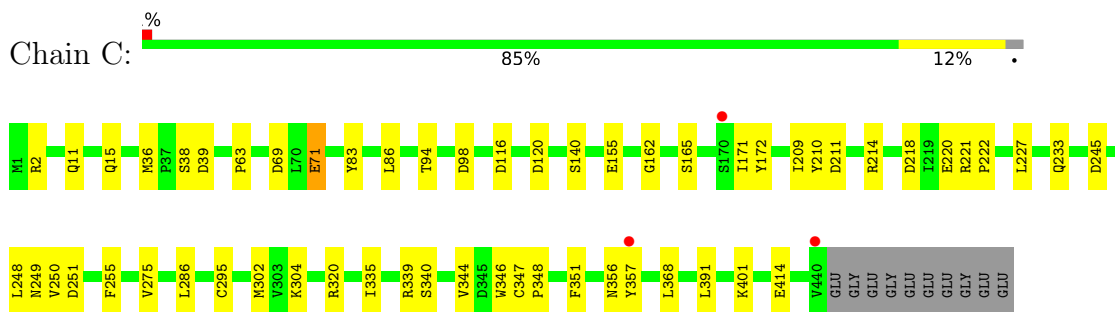
### 3 Residue-property plots [i](#)

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.

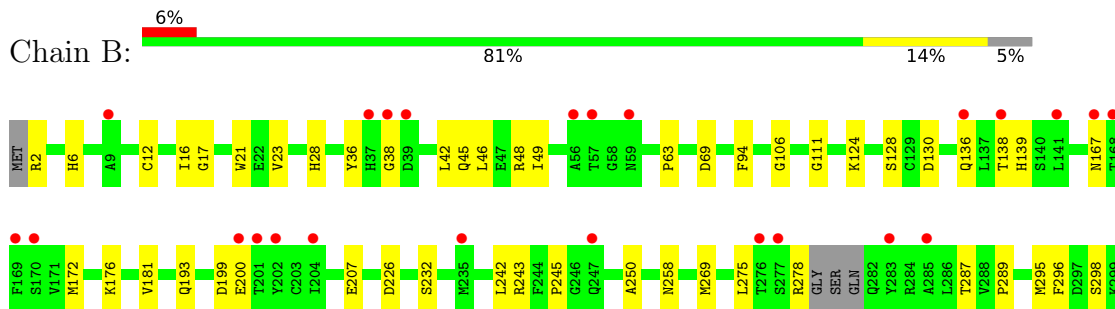
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

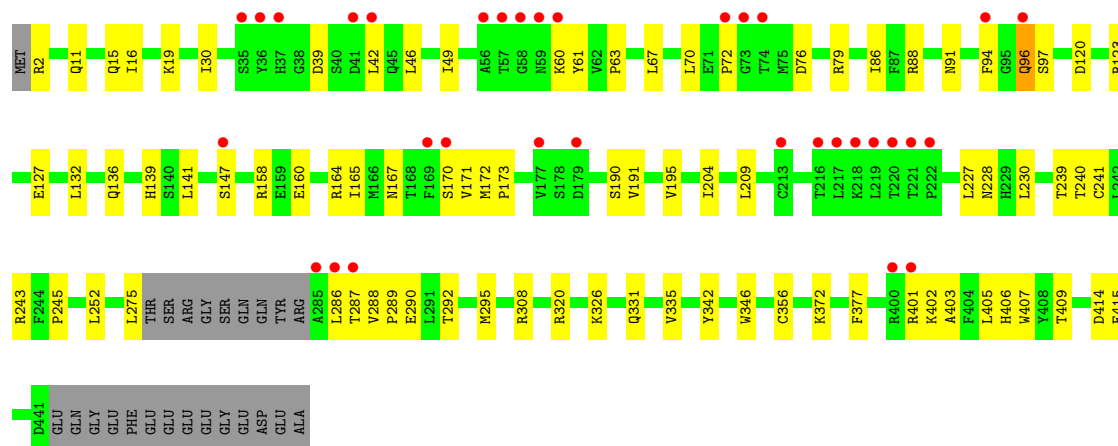
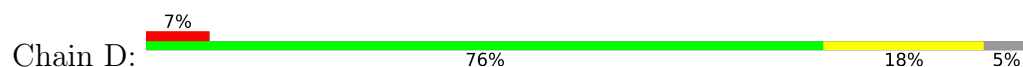


- Molecule 2: Tubulin beta chain

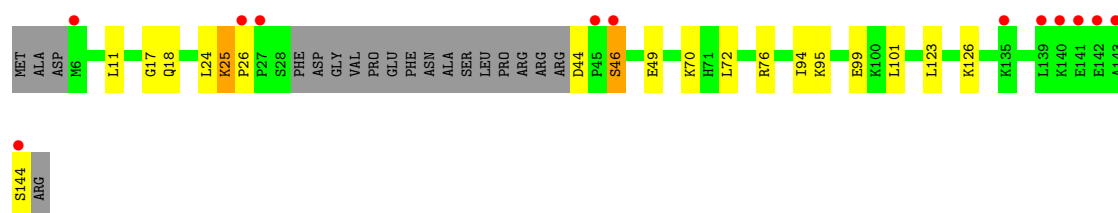
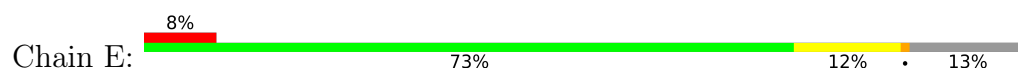




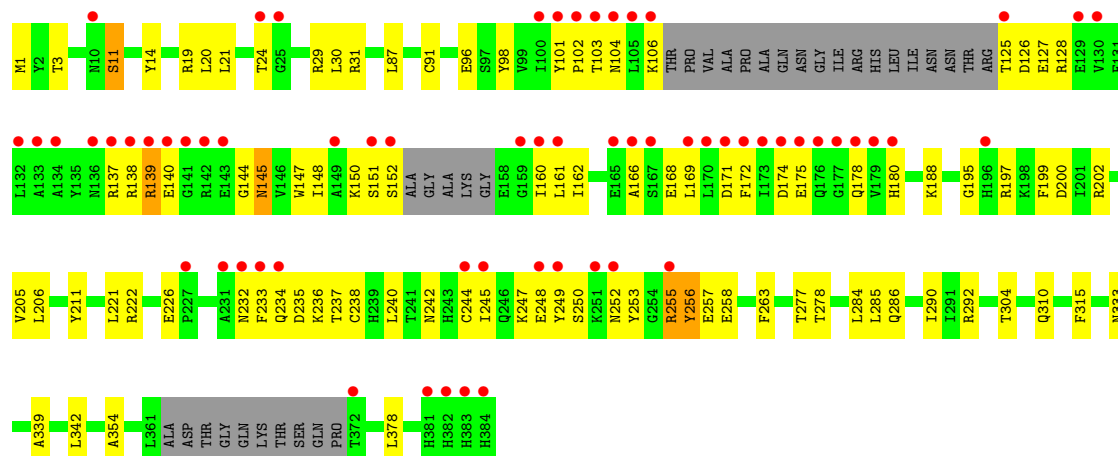
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.30Å 158.46Å 181.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.17 – 2.44 33.17 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.17-2.44) 99.5 (33.17-2.45)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.177 , 0.220 0.178 , 0.222	Depositor DCC
$R_{free}$ test set	2000 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18041	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, ERR, CL, CA, GTP, ACP, MES

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	0.50	0/3516	0.64	0/4775
1	C	0.62	2/3538 (0.1%)	0.71	0/4803
2	B	0.53	0/3424	0.66	0/4638
2	D	0.49	0/3385	0.62	1/4588 (0.0%)
3	E	0.50	0/1036	0.58	0/1375
4	F	0.41	0/2960	0.62	0/3999
All	All	0.52	2/17859 (0.0%)	0.65	1/24178 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	CYS	CB-SG	-6.82	1.70	1.82
1	C	295	CYS	CB-SG	-5.54	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	160	GLU	OE1-CD-OE2	-5.44	116.77	123.30

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	3435	0	3345	44	0
1	C	3451	0	3365	32	0
2	B	3344	0	3226	44	0
2	D	3306	0	3183	55	0
3	E	1025	0	1040	13	0
4	F	2887	0	2846	66	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	11	3	0
9	D	28	0	12	3	0
10	B	24	0	26	4	0
11	B	31	0	0	2	0
12	F	31	0	12	1	0
13	A	80	0	0	2	0
13	B	68	0	0	3	0
13	C	153	0	0	4	0
13	D	28	0	0	2	0
13	E	14	0	0	1	0
13	F	33	0	0	0	0
All	All	18041	0	17090	246	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 7.

All (246) 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:D:228:ASN:ND2	9:D:600:GDP:HN1	1.61	0.96
2:D:228:ASN:HD21	9:D:600:GDP:HN1	1.08	0.96
2:B:172:MET:HG2	2:B:387:LEU:HD21	1.62	0.81
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.14	0.81
4:F:106:LYS:HA	4:F:106:LYS:HE2	1.65	0.79
4:F:202:ARG:NH2	4:F:333:ASN:HD22	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:277:THR:HG22	4:F:278:THR:H	1.48	0.78
4:F:248:GLU:HB3	4:F:249:TYR:HD1	1.55	0.72
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.19	0.72
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.71	0.72
2:B:352:LYS:HE2	11:B:507:ERR:C06	2.21	0.71
2:D:16:ILE:HG22	2:D:228:ASN:ND2	2.06	0.69
1:C:2:ARG:NH1	13:C:602:HOH:O	2.25	0.68
2:D:241[B]:CYS:SG	13:D:726:HOH:O	2.50	0.68
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.76	0.68
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.77	0.67
4:F:232:ASN:OD1	4:F:234:GLN:NE2	2.26	0.67
2:B:298:SER:N	10:B:505:MES:O1S	2.23	0.67
4:F:101:TYR:HD2	4:F:126:ASP:HB2	1.60	0.66
2:B:2:ARG:N	13:B:602:HOH:O	2.27	0.66
2:B:325:MET:HG2	2:B:355:VAL:HG21	1.79	0.65
4:F:145:ASN:HD21	4:F:147:TRP:HE1	1.45	0.64
4:F:145:ASN:ND2	4:F:147:TRP:HE1	1.95	0.63
4:F:29:ARG:HH21	4:F:31:ARG:HH22	1.47	0.63
2:B:396:THR:O	2:B:400:ARG:HG2	1.98	0.63
1:A:209:ILE:HD11	1:A:302:MET:SD	2.39	0.62
2:B:334:ASN:O	2:B:338:LYS:HB2	1.99	0.61
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.31	0.61
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.48	0.61
2:B:199:ASP:OD2	10:B:504:MES:H52	2.01	0.60
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.36	0.60
4:F:125:THR:HG23	4:F:126:ASP:H	1.67	0.60
2:B:136:GLN:HA	2:B:167:ASN:O	2.01	0.60
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.33	0.60
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.17	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.59
1:A:90:GLU:OE2	1:A:124:LYS:HE2	2.03	0.59
4:F:168:GLU:O	4:F:171:ASP:HB2	2.01	0.59
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.38	0.58
2:D:42:LEU:HD22	2:D:245:PRO:HG2	1.85	0.58
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.38	0.58
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.86	0.58
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.86	0.58
2:D:136:GLN:HA	2:D:167:ASN:O	2.04	0.58
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.39	0.57
4:F:292:ARG:HG3	4:F:378:LEU:HB3	1.86	0.57
4:F:126:ASP:OD1	4:F:127:GLU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.86	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.56
4:F:138:ARG:NH1	4:F:144:GLY:O	2.38	0.56
1:A:262:TYR:HE2	1:A:346:TRP:CZ2	2.24	0.56
2:D:228:ASN:OD1	9:D:600:GDP:O6	2.22	0.56
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.70	0.56
1:C:286:LEU:HD12	13:C:606:HOH:O	2.06	0.56
4:F:161:LEU:HD22	4:F:172:PHE:CG	2.41	0.56
4:F:151:SER:OG	4:F:180:HIS:ND1	2.39	0.56
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.42	0.55
2:B:28:HIS:NE2	2:B:243:ARG:HB3	2.22	0.55
4:F:151:SER:OG	4:F:180:HIS:CG	2.60	0.55
1:A:88:HIS:N	1:A:91:GLN:OE1	2.30	0.54
2:B:2:ARG:NH1	2:B:130:ASP:OD2	2.41	0.54
1:A:349:THR:HG22	3:E:24:LEU:HD12	1.90	0.54
2:D:123:ARG:O	2:D:127:GLU:HG2	2.07	0.54
2:D:331:GLN:O	2:D:335:VAL:HG23	2.08	0.54
1:A:263:PRO:O	1:A:266:HIS:HD2	1.90	0.54
2:B:16[A]:ILE:HD11	2:B:138:THR:HB	1.89	0.53
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.89	0.53
2:D:414:ASP:OD1	2:D:415:GLU:N	2.42	0.53
2:B:167:ASN:OD1	2:B:200:GLU:HG3	2.08	0.53
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.39	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.52
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.90	0.52
2:D:405:LEU:O	2:D:409:THR:HG22	2.10	0.52
2:B:176:LYS:HE2	2:B:207:GLU:HG3	1.91	0.52
2:D:76:ASP:HA	2:D:79:ARG:HH12	1.73	0.52
1:A:39:ASP:OD2	1:A:61:HIS:CE1	2.61	0.52
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.41	0.51
2:D:72:PRO:HG3	2:D:96:GLN:HG3	1.92	0.51
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.92	0.51
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.91	0.51
3:E:11:LEU:HD11	3:E:18:GLN:NE2	2.25	0.51
4:F:150:LYS:HD3	4:F:160:ILE:HG12	1.92	0.51
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.25	0.51
2:B:42:LEU:HD23	2:B:245:PRO:HG2	1.93	0.51
4:F:150:LYS:HD3	4:F:160:ILE:CG1	2.42	0.50
1:A:2:ARG:O	1:A:133:GLN:NE2	2.42	0.50
2:B:296:PHE:O	10:B:505:MES:H81	2.12	0.50
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:PRO:HG2	2:D:86:ILE:HG23	1.93	0.50
2:D:295:MET:CG	2:D:377:PHE:HB2	2.42	0.50
4:F:162:ILE:HB	4:F:233:PHE:HB3	1.94	0.50
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.93	0.50
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.92	0.50
2:D:67:LEU:N	2:D:67:LEU:HD12	2.27	0.50
2:B:46:LEU:HA	2:B:49:ILE:HB	1.93	0.50
2:D:76:ASP:HA	2:D:79:ARG:NH1	2.26	0.50
4:F:339:ALA:HB3	4:F:342:LEU:HD12	1.94	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.48	0.49
1:A:33:ASP:N	13:A:610:HOH:O	2.43	0.49
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.48	0.49
2:D:30:ILE:HD13	2:D:61:TYR:HB2	1.94	0.48
4:F:252:ASN:O	4:F:255:ARG:HB2	2.13	0.48
3:E:44:ASP:N	13:E:203:HOH:O	2.46	0.48
2:B:303:ALA:O	2:B:305:CYS:N	2.43	0.48
4:F:19:ARG:HG3	4:F:20:LEU:N	2.29	0.47
1:A:69:ASP:O	1:A:94:THR:HA	2.13	0.47
2:D:287:THR:N	2:D:290:GLU:OE2	2.44	0.47
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.47
1:A:409:VAL:HA	1:A:413:MET:O	2.15	0.47
1:A:285:GLN:NE2	1:A:372:GLN:H	2.12	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.50	0.47
2:B:242:LEU:HA	2:B:250:ALA:HB1	1.97	0.47
2:D:11:GLN:O	2:D:15:GLN:HG3	2.14	0.47
1:C:245:ASP:N	1:C:245:ASP:OD1	2.41	0.47
1:A:154:MET:HG3	1:A:194:THR:HG23	1.96	0.47
2:B:128:SER:O	2:B:128:SER:OG	2.33	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.47
4:F:286:GLN:O	4:F:290:ILE:HG13	2.15	0.47
4:F:150:LYS:NZ	4:F:151:SER:O	2.29	0.47
4:F:151:SER:OG	4:F:180:HIS:CE1	2.68	0.46
2:B:12:CYS:HB2	9:B:501:GDP:N7	2.31	0.46
1:C:63:PRO:HD3	1:C:86:LEU:HG	1.97	0.46
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.96	0.46
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.46
1:C:140:SER:HA	1:C:171:ILE:HB	1.97	0.46
2:B:226:ASP:OD1	2:B:278:ARG:NH2	2.46	0.46
2:D:286:LEU:HA	2:D:286:LEU:HD12	1.74	0.46
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.51	0.46
4:F:150:LYS:HZ3	4:F:151:SER:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:LEU:O	2:D:164:ARG:NH1	2.41	0.46
1:A:304:LYS:HB2	13:A:617:HOH:O	2.16	0.46
2:D:46:LEU:HA	2:D:49:ILE:HB	1.98	0.46
2:D:239:THR:O	2:D:243:ARG:HG3	2.16	0.46
2:B:12:CYS:HB2	9:B:501:GDP:C5	2.51	0.46
2:D:70:LEU:HA	2:D:70:LEU:HD23	1.80	0.46
4:F:145:ASN:ND2	4:F:147:TRP:NE1	2.61	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.45
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.51	0.45
4:F:247:LYS:HG3	4:F:253:TYR:CZ	2.51	0.45
1:A:124:LYS:HE3	1:A:124:LYS:HB3	1.62	0.45
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.97	0.45
2:D:372:LYS:HA	2:D:372:LYS:HD3	1.62	0.45
4:F:169:LEU:HA	4:F:169:LEU:HD23	1.65	0.45
2:D:209:LEU:HD12	2:D:230:LEU:HB2	1.99	0.45
1:C:351:PHE:CD1	1:C:351:PHE:N	2.85	0.45
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.35	0.45
4:F:125:THR:HG23	4:F:126:ASP:N	2.32	0.45
1:A:180:ALA:O	1:A:183:GLU:HG3	2.17	0.45
4:F:103:THR:HG23	4:F:174:ASP:OD2	2.17	0.45
4:F:284:LEU:HA	4:F:284:LEU:HD12	1.73	0.45
4:F:200:ASP:OD2	12:F:402:ACP:O3'	2.35	0.45
2:D:147[A]:SER:HB2	2:D:190:SER:OG	2.17	0.45
2:D:402:LYS:HE2	2:D:415:GLU:OE2	2.16	0.45
4:F:304:THR:O	4:F:310:GLN:NE2	2.50	0.45
1:C:250:VAL:HG22	1:C:255:PHE:CZ	2.52	0.44
1:C:155:GLU:HB3	3:E:101:LEU:HD22	1.98	0.44
2:B:411:GLU:OE1	13:B:601:HOH:O	2.21	0.44
1:C:250:VAL:CG2	1:C:255:PHE:CZ	3.00	0.44
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.99	0.44
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	3.06	0.44
2:B:124:LYS:HD3	2:B:124:LYS:HA	1.58	0.44
4:F:255:ARG:HD2	4:F:256:TYR:CZ	2.53	0.44
1:A:250:VAL:HG22	1:A:254:GLU:OE2	2.18	0.44
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.51	0.44
2:B:28:HIS:HE1	2:B:243:ARG:O	2.01	0.43
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.53	0.43
4:F:197:ARG:CZ	4:F:257:GLU:OE2	2.67	0.43
2:D:401:ARG:NE	2:D:403:ALA:HB2	2.34	0.43
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.01	0.43
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:THR:HG22	2:D:335:VAL:HG21	2.00	0.43
1:C:414:GLU:HB3	13:C:641:HOH:O	2.19	0.43
4:F:226:GLU:HB3	4:F:238:CYS:HB3	1.99	0.43
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.84	0.43
2:D:172:MET:HG3	2:D:173:PRO:HD2	2.01	0.43
4:F:202:ARG:NH2	4:F:333:ASN:ND2	2.58	0.43
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.19	0.43
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.01	0.43
4:F:263:PHE:HE2	4:F:342:LEU:HD11	1.83	0.43
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.49	0.43
1:C:116:ASP:CG	13:C:604:HOH:O	2.57	0.43
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.01	0.43
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.92	0.42
4:F:172:PHE:HA	4:F:175:GLU:OE2	2.19	0.42
1:A:20:CYS:HA	1:A:232:SER:OG	2.19	0.42
4:F:178:GLN:OE1	4:F:178:GLN:N	2.52	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.42
2:D:2:ARG:CZ	2:D:2:ARG:HB2	2.50	0.42
2:D:320:ARG:HA	2:D:356:CYS:O	2.19	0.42
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.19	0.42
4:F:150:LYS:NZ	4:F:151:SER:H	2.17	0.42
4:F:195:GLY:HA3	4:F:197:ARG:HD3	2.02	0.42
1:A:285:GLN:HG3	1:A:372:GLN:OE1	2.20	0.42
1:C:220:GLU:HG2	2:D:326:LYS:HE3	2.01	0.42
3:E:101:LEU:HA	3:E:101:LEU:HD12	1.79	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.20	0.42
2:D:94:PHE:O	2:D:94:PHE:CD1	2.72	0.42
3:E:46:SER:HB3	3:E:49:GLU:HG3	2.01	0.42
4:F:21:LEU:O	4:F:24:THR:OG1	2.24	0.42
4:F:237:THR:CG2	4:F:250:SER:HB2	2.50	0.42
2:D:141:LEU:HD12	2:D:172:MET:SD	2.60	0.42
2:D:275:LEU:O	13:D:701:HOH:O	2.22	0.42
4:F:244:CYS:SG	4:F:245:ILE:N	2.93	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.41
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.85	0.41
4:F:285:LEU:HA	4:F:285:LEU:HD23	1.80	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.20	0.41
2:D:94:PHE:C	2:D:94:PHE:CD1	2.94	0.41
1:A:97:GLU:O	1:A:110:ILE:HD13	2.20	0.41
3:E:72:LEU:O	3:E:76:ARG:HG2	2.19	0.41
4:F:205:VAL:HG22	4:F:315:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:248:GLU:HB3	4:F:249:TYR:CD1	2.44	0.41
4:F:11:SER:OG	4:F:14:TYR:HB2	2.20	0.41
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.84	0.41
4:F:139:ARG:HG3	4:F:140:GLU:N	2.34	0.41
4:F:3:THR:HB	4:F:30:LEU:HD13	2.01	0.41
4:F:87:LEU:O	4:F:91:CYS:HB2	2.20	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.01	0.41
2:B:295:MET:HE3	2:B:375:ALA:HB1	2.03	0.41
2:B:242:LEU:HD21	11:B:507:ERR:C20	2.51	0.41
3:E:95:LYS:HE2	3:E:99:GLU:OE1	2.20	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.56	0.41
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.03	0.41
1:C:69:ASP:O	1:C:94:THR:HA	2.21	0.41
4:F:166:ALA:O	4:F:169:LEU:N	2.52	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.20	0.41
2:B:16[A]:ILE:HG13	2:B:17:GLY:N	2.36	0.41
1:A:90:GLU:O	1:A:121:ARG:HD2	2.20	0.41
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.83	0.41
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.02	0.41
4:F:188:LYS:HD3	4:F:188:LYS:HA	1.79	0.41
4:F:277:THR:HG22	4:F:278:THR:N	2.25	0.41
4:F:96:GLU:HG2	4:F:98:TYR:CE2	2.56	0.41
2:B:193:GLN:HB3	13:B:625:HOH:O	2.21	0.40
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.51	0.40
1:A:84:ARG:HG2	1:A:84:ARG:H	1.69	0.40
2:B:199:ASP:OD1	10:B:504:MES:H32	2.20	0.40
1:C:36:MET:SD	1:C:39:ASP:HB2	2.61	0.40
3:E:123:LEU:O	3:E:126:LYS:HB2	2.21	0.40
1:C:11:GLN:O	1:C:15:GLN:HG3	2.21	0.40
2:D:402:LYS:O	2:D:405:LEU:HB2	2.20	0.40
2:D:60:LYS:HB3	2:D:60:LYS:HE3	1.96	0.40
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.04	0.40
2:B:287:THR:HB	2:B:289:PRO:HD2	2.04	0.40
4:F:148:ILE:HD11	4:F:160:ILE:HG21	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	439/450 (98%)	424 (97%)	15 (3%)	0	100	100
1	C	441/450 (98%)	429 (97%)	12 (3%)	0	100	100
2	B	422/445 (95%)	408 (97%)	14 (3%)	0	100	100
2	D	419/445 (94%)	407 (97%)	12 (3%)	0	100	100
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100
4	F	345/384 (90%)	330 (96%)	15 (4%)	0	100	100
All	All	2187/2317 (94%)	2118 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	371/378 (98%)	364 (98%)	7 (2%)	57	69
1	C	374/378 (99%)	365 (98%)	9 (2%)	49	61
2	B	368/383 (96%)	365 (99%)	3 (1%)	81	88
2	D	363/383 (95%)	357 (98%)	6 (2%)	60	73
3	E	112/127 (88%)	108 (96%)	4 (4%)	35	46
4	F	318/342 (93%)	305 (96%)	13 (4%)	30	40
All	All	1906/1991 (96%)	1864 (98%)	42 (2%)	52	64

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	84	ARG
1	A	164	LYS
1	A	232	SER
1	A	430	LYS
1	A	438	ASP
1	A	439	SER
2	B	48	ARG
2	B	139	HIS
2	B	372	LYS
1	C	38	SER
1	C	71	GLU
1	C	120	ASP
1	C	165	SER
1	C	218	ASP
1	C	221	ARG
1	C	251	ASP
1	C	302	MET
1	C	340	SER
2	D	19	LYS
2	D	39	ASP
2	D	96	GLN
2	D	97	SER
2	D	139	HIS
2	D	158	ARG
3	E	25	LYS
3	E	46	SER
3	E	70	LYS
3	E	144	SER
4	F	1	MET
4	F	11	SER
4	F	128	ARG
4	F	137	ARG
4	F	139	ARG
4	F	145	ASN
4	F	152	SER
4	F	211	TYR
4	F	222	ARG
4	F	235	ASP
4	F	255	ARG
4	F	256	TYR
4	F	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	101	ASN
1	A	266	HIS
1	A	285	GLN
2	B	334	ASN
1	C	128	GLN
2	D	228	ASN
3	E	18	GLN
4	F	145	ASN
4	F	310	GLN
4	F	333	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, 11 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	GDP	B	501	6	24,30,30	4.12	13 (54%)	31,47,47	2.08	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	C	501	6	26,34,34	5.03	10 (38%)	33,54,54	1.62	6 (18%)
10	MES	B	505	-	12,12,12	1.55	2 (16%)	14,16,16	2.42	6 (42%)
5	GTP	A	501	6	26,34,34	5.26	11 (42%)	33,54,54	1.68	9 (27%)
11	ERR	B	507	-	31,35,35	2.08	10 (32%)	38,51,51	1.50	6 (15%)
9	GDP	D	600	6	24,30,30	1.78	8 (33%)	31,47,47	1.78	7 (22%)
12	ACP	F	402	6	27,33,33	4.76	12 (44%)	32,52,52	2.18	8 (25%)
10	MES	B	504	-	12,12,12	1.28	2 (16%)	14,16,16	2.27	6 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
10	MES	B	505	-	-	2/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
11	ERR	B	507	-	-	3/14/14/14	0/5/5/5
9	GDP	D	600	6	-	5/12/32/32	0/3/3/3
12	ACP	F	402	6	-	6/15/38/38	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	C2'-C1'	-15.28	1.30	1.53
5	A	501	GTP	C2'-C1'	-15.26	1.30	1.53
12	F	402	ACP	O4'-C1'	15.09	1.62	1.41
5	C	501	GTP	C2'-C1'	-14.94	1.31	1.53
5	C	501	GTP	O4'-C1'	13.40	1.59	1.41
5	A	501	GTP	O4'-C1'	13.40	1.59	1.41
9	B	501	GDP	C3'-C4'	-8.64	1.30	1.53
9	B	501	GDP	C2-N2	8.15	1.50	1.33
5	A	501	GTP	C6-C5	8.05	1.55	1.41
5	C	501	GTP	C6-C5	7.86	1.54	1.41
5	A	501	GTP	C4-N3	7.78	1.47	1.35
5	A	501	GTP	C6-N1	7.69	1.46	1.33
9	B	501	GDP	C6-N1	7.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C4-N3	6.87	1.46	1.35
9	B	501	GDP	C4-N3	6.82	1.46	1.35
9	B	501	GDP	O4'-C4'	6.74	1.60	1.45
5	C	501	GTP	C6-N1	6.61	1.44	1.33
12	F	402	ACP	O4'-C4'	-6.56	1.30	1.45
9	B	501	GDP	C6-C5	5.79	1.51	1.41
5	C	501	GTP	O4'-C4'	-5.50	1.32	1.45
5	A	501	GTP	C2-N2	5.45	1.44	1.33
5	A	501	GTP	O4'-C4'	-5.44	1.32	1.45
12	F	402	ACP	PB-O3A	5.14	1.64	1.58
5	A	501	GTP	C2-N1	4.97	1.44	1.35
11	B	507	ERR	C01-N05	-4.76	1.29	1.37
5	C	501	GTP	C2-N2	4.64	1.43	1.33
9	B	501	GDP	O4'-C1'	-4.62	1.34	1.41
5	C	501	GTP	C2-N1	4.24	1.42	1.35
11	B	507	ERR	C26-N27	-4.18	1.33	1.41
11	B	507	ERR	C24-N23	-4.10	1.28	1.34
9	B	501	GDP	O2'-C2'	-3.84	1.33	1.43
10	B	505	MES	C8-S	3.58	1.82	1.77
9	D	600	GDP	C2'-C1'	-3.54	1.48	1.53
9	B	501	GDP	C2-N1	3.46	1.41	1.35
11	B	507	ERR	C03-C04	-3.44	1.33	1.41
11	B	507	ERR	C16-C17	-3.30	1.34	1.39
12	F	402	ACP	C6-N6	3.29	1.46	1.34
11	B	507	ERR	C13-C14	-3.17	1.34	1.41
9	B	501	GDP	C2'-C1'	-3.12	1.49	1.53
12	F	402	ACP	PB-O2B	-3.02	1.49	1.56
9	D	600	GDP	PB-O2B	-2.99	1.43	1.54
12	F	402	ACP	O2'-C2'	2.96	1.50	1.43
12	F	402	ACP	PG-O2G	-2.85	1.48	1.54
12	F	402	ACP	PG-O3G	-2.85	1.48	1.54
11	B	507	ERR	C15-C14	-2.83	1.35	1.41
5	C	501	GTP	C2-N3	2.82	1.47	1.34
12	F	402	ACP	O3'-C3'	-2.82	1.36	1.43
9	D	600	GDP	C6-C5	2.77	1.46	1.41
5	A	501	GTP	O2'-C2'	2.76	1.49	1.43
9	B	501	GDP	O6-C6	-2.69	1.17	1.24
9	D	600	GDP	C4-N3	-2.68	1.31	1.35
5	A	501	GTP	C2-N3	2.62	1.46	1.34
12	F	402	ACP	C2-N3	2.48	1.36	1.32
5	A	501	GTP	O3'-C3'	-2.44	1.37	1.43
12	F	402	ACP	C5-C4	-2.43	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	600	GDP	PB-O3B	-2.39	1.45	1.54
9	D	600	GDP	PA-O2A	-2.38	1.44	1.55
9	B	501	GDP	C5-C4	-2.33	1.34	1.40
9	D	600	GDP	O4'-C4'	-2.33	1.39	1.45
5	C	501	GTP	O3'-C3'	-2.25	1.37	1.43
9	B	501	GDP	C2-N3	2.13	1.44	1.34
11	B	507	ERR	C31-C26	-2.09	1.35	1.38
11	B	507	ERR	C12-C13	-2.08	1.35	1.38
10	B	504	MES	C8-S	2.06	1.80	1.77
10	B	504	MES	C5-N4	-2.06	1.41	1.46
11	B	507	ERR	C12-C17	-2.02	1.36	1.39
9	D	600	GDP	PB-O1B	-2.01	1.44	1.50
10	B	505	MES	C5-N4	-2.01	1.41	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	C5-C6-N6	7.27	131.40	120.35
9	B	501	GDP	N3-C2-N1	-5.48	119.92	127.22
12	F	402	ACP	N3-C2-N1	-5.30	120.40	128.68
10	B	504	MES	O2S-S-C8	5.20	113.18	106.92
10	B	505	MES	O2S-S-C8	4.86	112.77	106.92
9	B	501	GDP	C1'-N9-C4	4.44	134.45	126.64
5	A	501	GTP	N3-C2-N1	-4.40	121.35	127.22
12	F	402	ACP	N6-C6-N1	-4.38	109.48	118.57
9	D	600	GDP	C2-N3-C4	4.27	120.23	115.36
5	C	501	GTP	C5-C6-N1	-3.98	117.99	123.43
9	D	600	GDP	O4'-C1'-C2'	-3.91	101.21	106.93
9	D	600	GDP	C4-C5-N7	-3.83	105.41	109.40
5	C	501	GTP	N3-C2-N1	-3.71	122.27	127.22
9	D	600	GDP	C5-C6-N1	-3.67	118.41	123.43
9	B	501	GDP	C6-C5-C4	-3.58	117.38	120.80
10	B	505	MES	O3S-S-O2S	-3.55	102.60	111.27
9	B	501	GDP	N2-C2-N1	3.55	122.77	117.25
10	B	505	MES	O1-C6-C5	3.38	119.24	111.80
10	B	505	MES	C6-C5-N4	3.28	115.07	110.10
5	C	501	GTP	PB-O3B-PG	-3.26	121.64	132.83
11	B	507	ERR	C30-N29-C28	3.19	120.81	116.73
5	A	501	GTP	C2-N3-C4	3.19	119.00	115.36
11	B	507	ERR	C31-C30-N29	-3.13	119.73	124.58
5	A	501	GTP	N2-C2-N1	3.09	122.06	117.25
10	B	504	MES	C5-N4-C3	3.08	115.75	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	C3'-C2'-C1'	3.06	105.58	100.98
9	B	501	GDP	C2-N3-C4	2.96	118.73	115.36
5	A	501	GTP	C5-C6-N1	-2.88	119.49	123.43
10	B	504	MES	C6-O1-C2	2.85	119.39	109.89
5	A	501	GTP	PA-O3A-PB	-2.84	123.06	132.83
10	B	504	MES	C2-C3-N4	2.83	114.39	110.10
10	B	504	MES	O3S-S-O2S	-2.80	104.43	111.27
9	D	600	GDP	C6-C5-C4	-2.78	118.14	120.80
9	B	501	GDP	O2B-PB-O3A	2.73	113.79	104.64
5	C	501	GTP	C6-N1-C2	2.67	120.17	115.93
5	A	501	GTP	PB-O3B-PG	-2.65	123.75	132.83
9	B	501	GDP	C6-N1-C2	2.61	120.07	115.93
9	B	501	GDP	C5-C6-N1	-2.60	119.87	123.43
12	F	402	ACP	O3G-PG-C3B	2.57	112.64	106.40
10	B	505	MES	C6-O1-C2	2.57	118.46	109.89
10	B	504	MES	O1-C2-C3	2.53	117.37	111.80
12	F	402	ACP	PA-O3A-PB	-2.53	124.55	132.56
11	B	507	ERR	C07-C24-N23	2.50	124.89	120.92
11	B	507	ERR	O18-C13-C14	2.44	119.45	115.16
12	F	402	ACP	O1G-PG-C3B	-2.40	106.08	111.24
5	A	501	GTP	C6-C5-C4	-2.35	118.56	120.80
11	B	507	ERR	C15-C14-C13	2.34	121.96	119.57
11	B	507	ERR	C12-C17-C16	2.31	121.72	118.31
5	A	501	GTP	C4-C5-N7	-2.26	107.04	109.40
12	F	402	ACP	C5'-C4'-C3'	-2.23	106.83	115.18
9	B	501	GDP	PA-O3A-PB	-2.16	125.41	132.83
5	C	501	GTP	C4-C5-N7	-2.16	107.15	109.40
9	D	600	GDP	PA-O3A-PB	-2.12	125.56	132.83
5	A	501	GTP	C6-N1-C2	2.10	119.27	115.93
9	D	600	GDP	C6-N1-C2	2.07	119.22	115.93
10	B	505	MES	O3S-S-C8	2.02	109.04	105.77
5	C	501	GTP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	GDP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	D	600	GDP	C5'-O5'-PA-O1A
9	D	600	GDP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O3A
12	F	402	ACP	O4'-C4'-C5'-O5'
12	F	402	ACP	C3'-C4'-C5'-O5'
11	B	507	ERR	C14-C13-O18-C22
11	B	507	ERR	C12-C13-O18-C22
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
10	B	505	MES	C7-C8-S-O2S
12	F	402	ACP	PB-O3A-PA-O2A
9	D	600	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
11	B	507	ERR	C16-C17-C26-N27
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
9	D	600	GDP	C5'-O5'-PA-O3A
9	D	600	GDP	PB-O3A-PA-O1A
10	B	505	MES	C7-C8-S-O1S

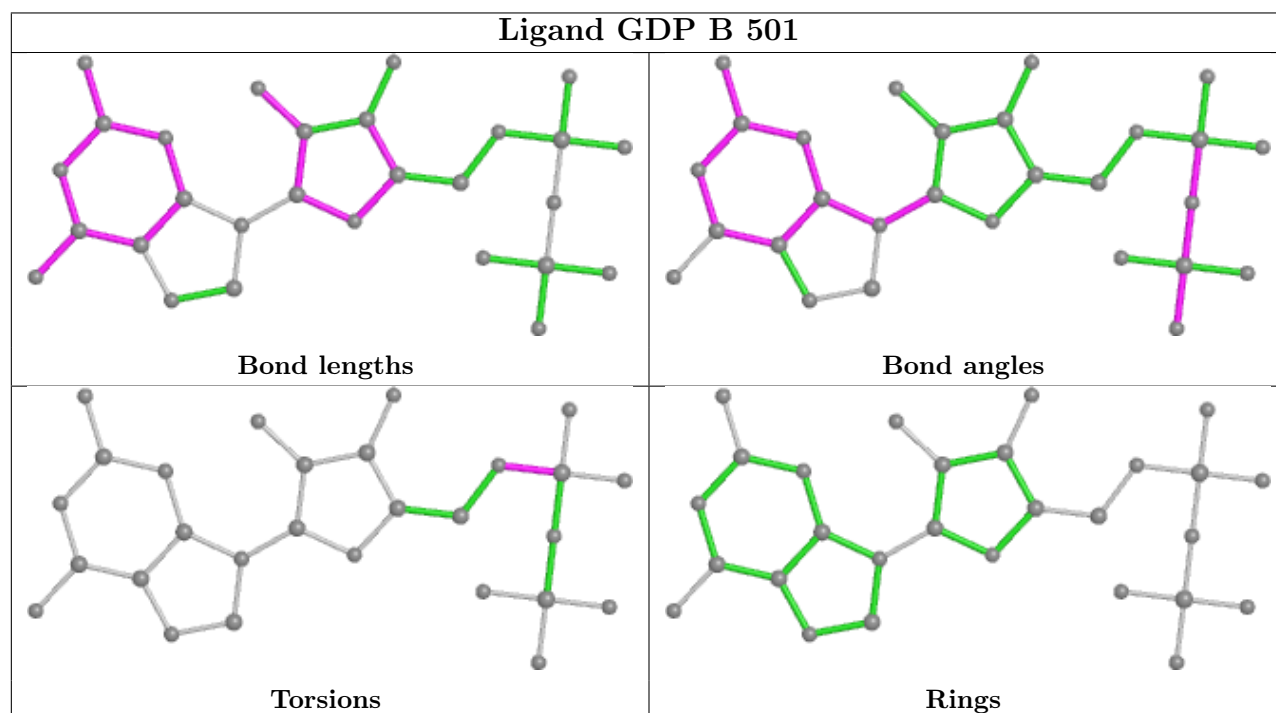
There are no ring outliers.

6 monomers are involved in 13 short contacts:

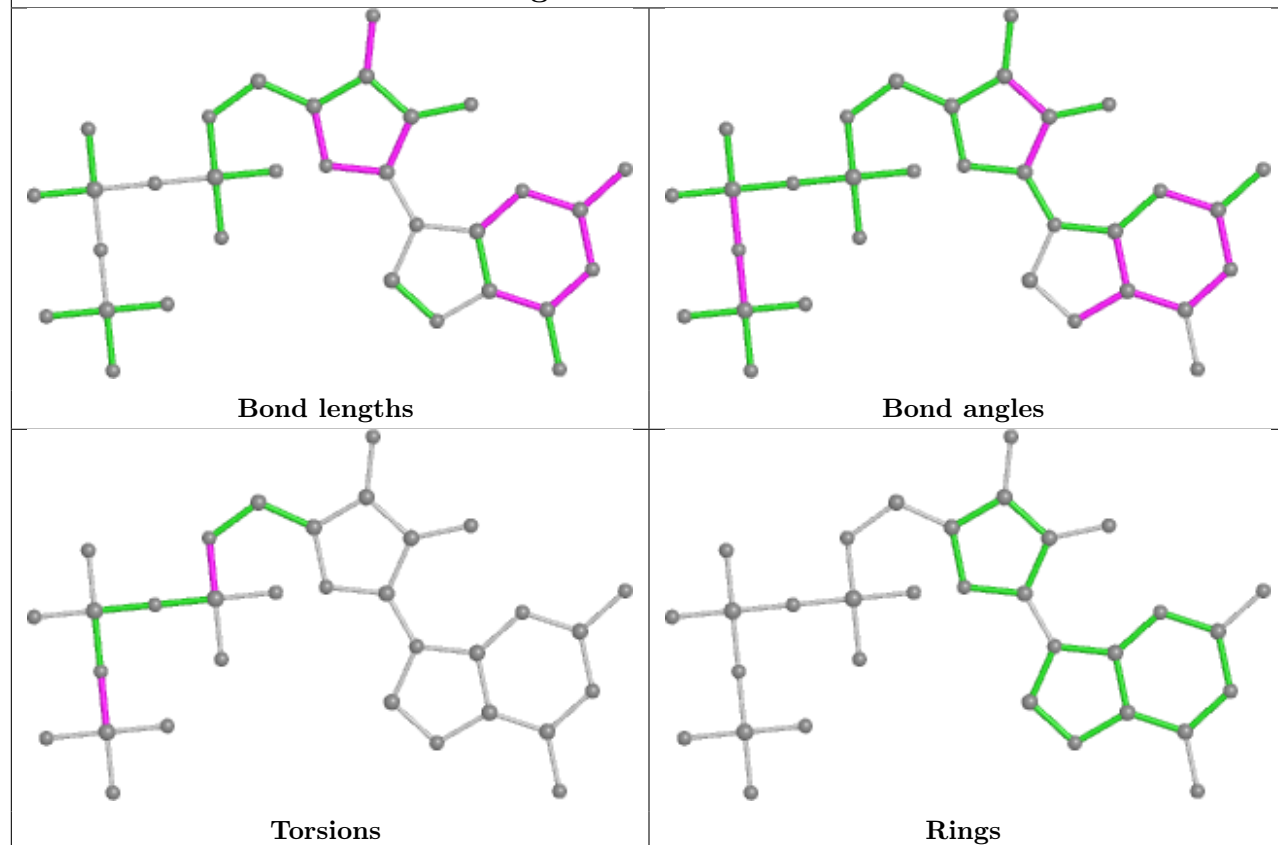
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	GDP	3	0
10	B	505	MES	2	0
11	B	507	ERR	2	0
9	D	600	GDP	3	0
12	F	402	ACP	1	0
10	B	504	MES	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

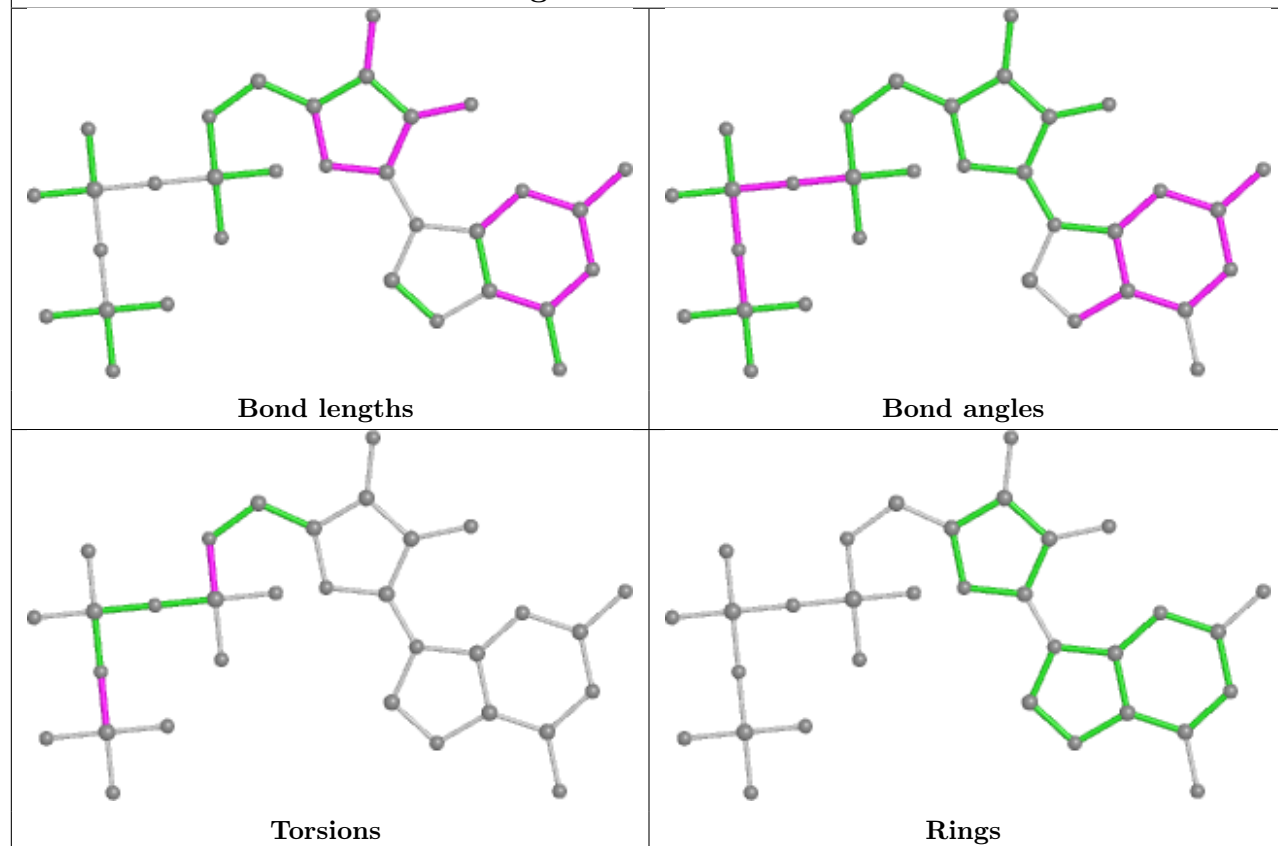
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

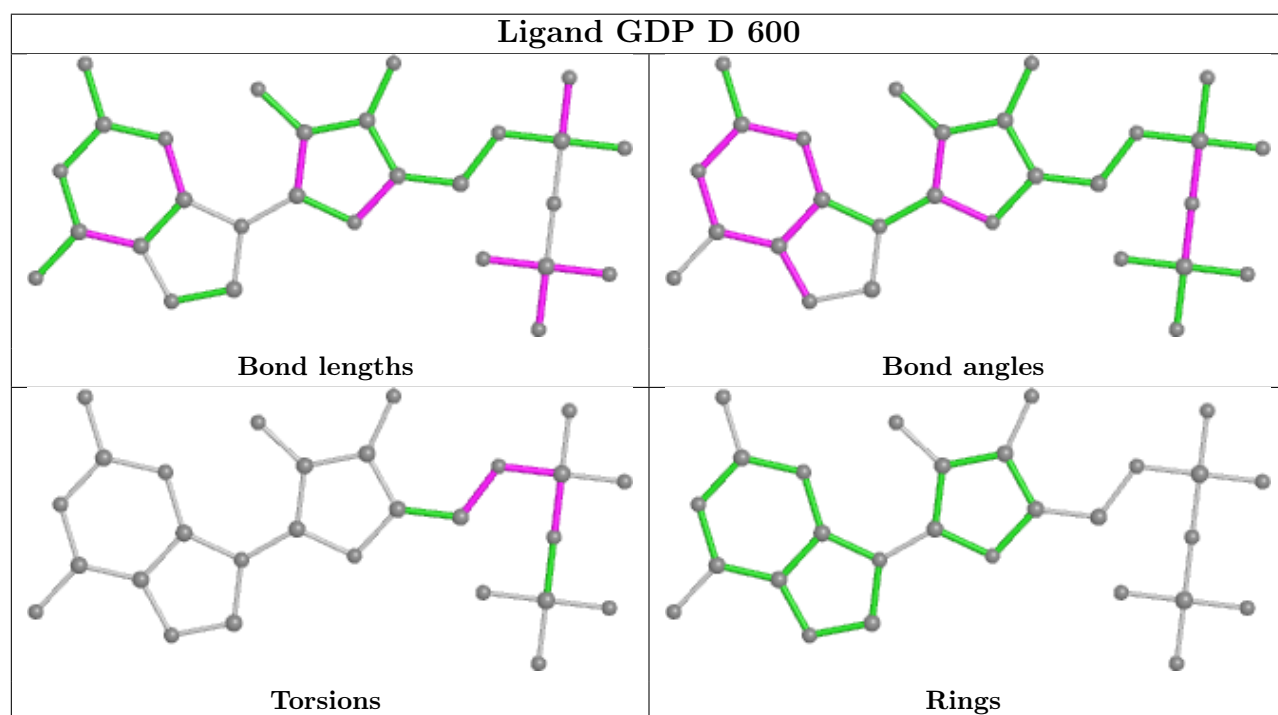
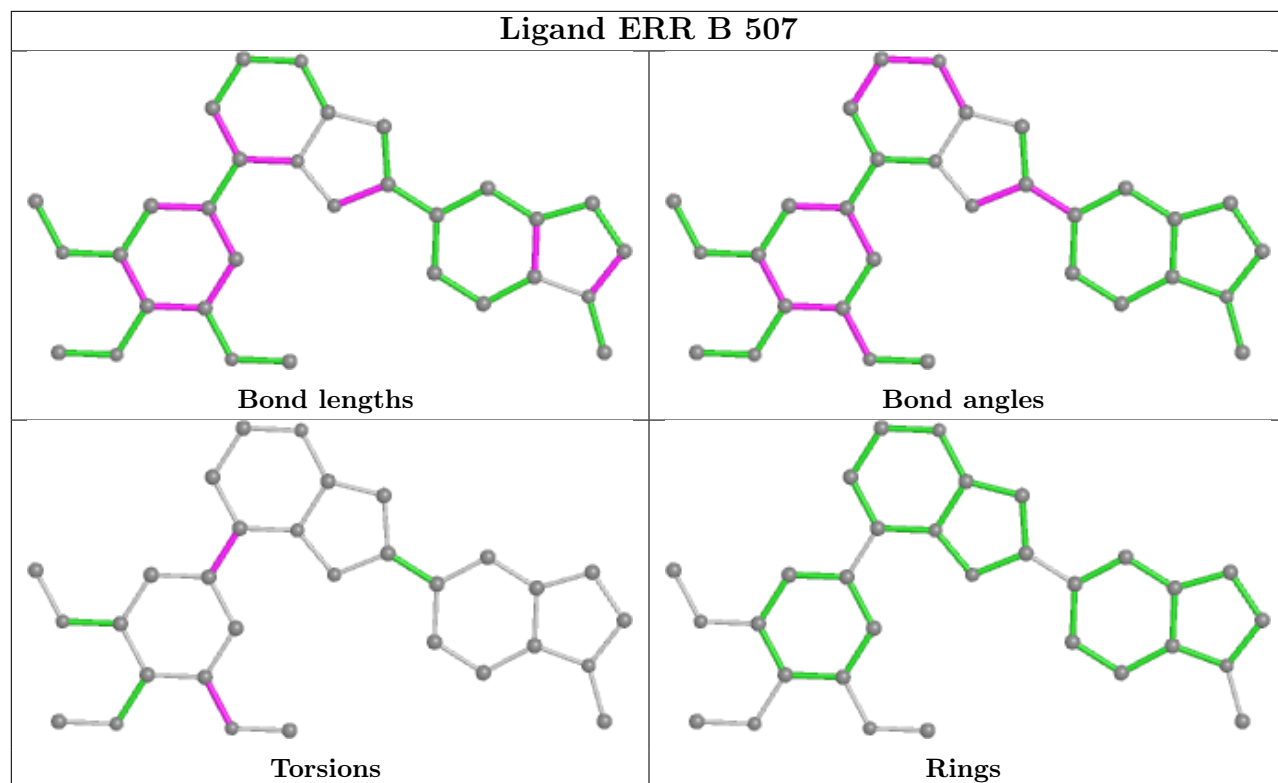


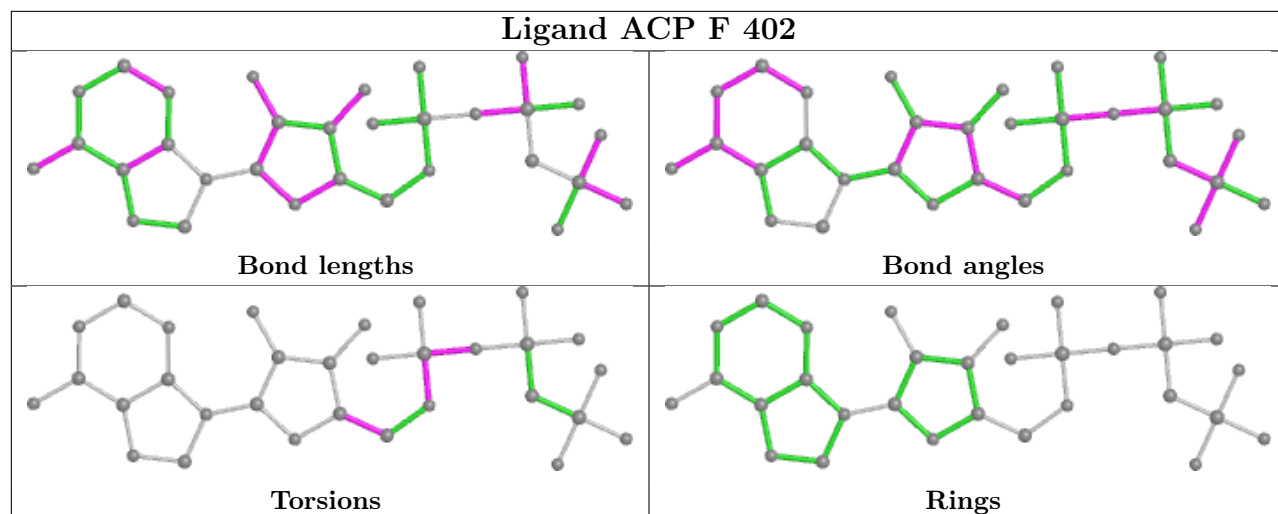
## Ligand GTP C 501



## 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	440/450 (97%)	-0.01	14 (3%) 47 44	33, 50, 82, 137	0
1	C	440/450 (97%)	-0.27	3 (0%) 87 87	25, 40, 68, 91	0
2	B	424/445 (95%)	0.05	25 (5%) 22 18	28, 49, 82, 155	1 (0%)
2	D	421/445 (94%)	0.25	33 (7%) 13 10	33, 66, 110, 142	7 (1%)
3	E	124/143 (86%)	0.42	12 (9%) 7 5	37, 66, 107, 143	0
4	F	351/384 (91%)	0.70	63 (17%) 1 1	39, 77, 154, 174	0
All	All	2200/2317 (94%)	0.14	150 (6%) 17 13	25, 56, 113, 174	8 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	9.9
2	D	285	ALA	7.7
4	F	177	GLY	7.6
4	F	161	LEU	7.5
4	F	233	PHE	6.9
1	A	440	VAL	6.8
3	E	144	SER	5.6
4	F	106	LYS	5.6
4	F	173	ILE	5.6
4	F	178	GLN	5.5
4	F	101	TYR	5.3
4	F	251	LYS	5.2
4	F	102	PRO	5.0
1	A	439	SER	5.0
3	E	143	ALA	4.9
4	F	166	ALA	4.9
4	F	136	ASN	4.9
4	F	103	THR	4.9
4	F	234	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	4.6
4	F	104	ASN	4.6
4	F	152	SER	4.5
4	F	232	ASN	4.5
2	B	59	ASN	4.4
2	D	286	LEU	4.2
4	F	170	LEU	4.2
2	B	57	THR	4.2
4	F	133	ALA	4.1
4	F	141	GLY	4.1
2	D	57	THR	4.1
4	F	372	THR	4.1
4	F	169	LEU	3.9
2	D	56	ALA	3.9
2	D	221	THR	3.9
4	F	176	GLN	3.9
4	F	137	ARG	3.8
4	F	134	ALA	3.8
2	D	213	CYS	3.7
2	B	169	PHE	3.7
4	F	142	ARG	3.7
4	F	381	HIS	3.7
3	E	46	SER	3.6
2	D	179	ASP	3.6
2	D	216	THR	3.6
4	F	179	VAL	3.6
1	A	235	VAL	3.5
4	F	244	CYS	3.5
4	F	167	SER	3.4
2	D	94	PHE	3.4
4	F	151	SER	3.4
4	F	25	GLY	3.3
4	F	140	GLU	3.3
4	F	174	ASP	3.3
4	F	132	LEU	3.3
4	F	143	GLU	3.3
4	F	231	ALA	3.3
4	F	130	VAL	3.3
2	D	219	LEU	3.3
2	D	400	ARG	3.2
1	A	220	GLU	3.2
4	F	100	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	167	ASN	3.2
2	B	276	THR	3.2
2	B	168	THR	3.1
4	F	139	ARG	3.1
2	D	73	GLY	3.0
4	F	383	HIS	3.0
2	D	220	THR	3.0
2	D	218	LYS	3.0
1	A	438	ASP	3.0
4	F	384	HIS	2.9
2	B	247	GLN	2.9
2	D	217	LEU	2.9
2	B	277	SER	2.9
2	D	169	PHE	2.8
2	D	72	PRO	2.8
2	D	58	GLY	2.8
4	F	165	GLU	2.8
1	A	262	TYR	2.8
2	B	202	TYR	2.8
4	F	248	GLU	2.8
4	F	382	HIS	2.8
2	D	287	THR	2.8
4	F	10	ASN	2.7
2	B	204	ILE	2.7
4	F	138	ARG	2.7
2	B	37	HIS	2.7
1	A	169	PHE	2.6
2	B	38	GLY	2.6
4	F	180	HIS	2.6
1	A	170	SER	2.6
2	D	36	TYR	2.6
2	D	59	ASN	2.6
3	E	26	PRO	2.6
4	F	125	THR	2.5
4	F	24	THR	2.5
2	B	200	GLU	2.5
3	E	6	MET	2.5
4	F	252	ASN	2.5
1	C	357	TYR	2.4
4	F	196	HIS	2.4
2	D	42	LEU	2.4
4	F	175	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	147[A]	SER	2.4
2	D	96	GLN	2.4
2	D	74	THR	2.4
1	A	202	PHE	2.4
2	D	401	ARG	2.4
2	B	136	GLN	2.4
4	F	129	GLU	2.4
2	D	41	ASP	2.3
3	E	142	GLU	2.3
2	D	37	HIS	2.3
3	E	135	LYS	2.3
3	E	140	LYS	2.3
2	B	56	ALA	2.3
4	F	255	ARG	2.3
2	B	235	MET	2.3
2	B	283	TYR	2.3
3	E	141	GLU	2.3
4	F	227	PRO	2.2
1	C	440	VAL	2.2
3	E	139	LEU	2.2
4	F	159	GLY	2.2
1	A	238	ILE	2.2
2	B	201	THR	2.2
2	D	177	VAL	2.2
1	A	163	LYS	2.2
2	B	138	THR	2.2
4	F	172	PHE	2.2
3	E	45	PRO	2.2
2	D	35	SER	2.2
2	D	170	SER	2.2
1	A	42	ILE	2.2
4	F	245	ILE	2.1
4	F	160	ILE	2.1
2	B	141	LEU	2.1
2	B	170	SER	2.1
2	B	437	ASP	2.1
1	A	201	ALA	2.1
2	B	285	ALA	2.1
4	F	149	ALA	2.1
1	A	137	VAL	2.1
4	F	171	ASP	2.1
1	C	170	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	9	ALA	2.0
2	D	60	LYS	2.0
2	D	222	PRO	2.0
2	B	39	ASP	2.0
3	E	27	PRO	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	MG	F	401	1/1	0.73	0.17	78,78,78,78	0
6	MG	D	601	1/1	0.78	0.15	68,68,68,68	0
7	CA	A	505	1/1	0.86	0.06	105,105,105,105	0
12	ACP	F	402	31/31	0.89	0.21	73,89,148,153	0
7	CA	B	503	1/1	0.90	0.12	97,97,97,97	0
6	MG	C	502	1/1	0.90	0.19	39,39,39,39	0
8	CL	A	504	1/1	0.93	0.11	76,76,76,76	0
11	ERR	B	507	31/31	0.93	0.14	41,57,72,80	0
9	GDP	D	600	28/28	0.94	0.11	49,63,77,83	0
10	MES	B	505	12/12	0.94	0.22	71,80,87,96	0
6	MG	A	502	1/1	0.95	0.21	36,36,36,36	0
10	MES	B	504	12/12	0.95	0.15	40,58,79,93	0
6	MG	B	506	1/1	0.95	0.05	72,72,72,72	0
7	CA	A	503	1/1	0.96	0.07	79,79,79,79	0
7	CA	C	503	1/1	0.97	0.04	51,51,51,51	0
5	GTP	C	501	32/32	0.98	0.19	26,36,41,48	0
6	MG	B	502	1/1	0.98	0.18	43,43,43,43	0
5	GTP	A	501	32/32	0.98	0.15	28,41,47,52	0

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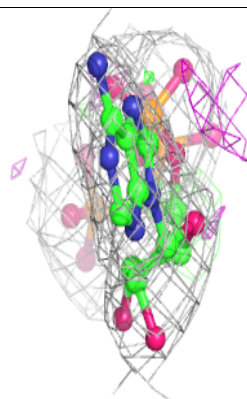
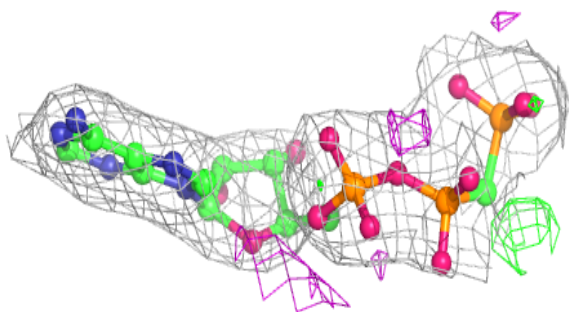
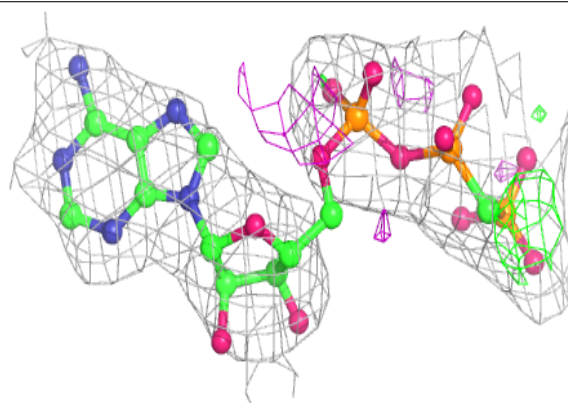
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	GDP	B	501	28/28	0.99	0.17	29,38,42,43	0

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.

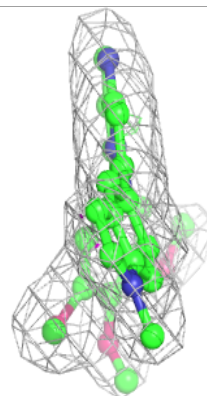
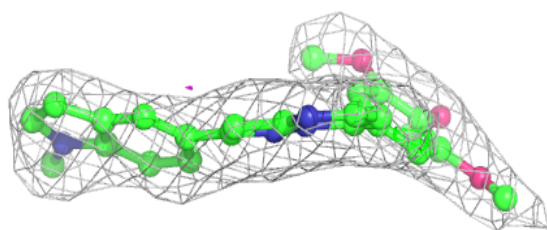
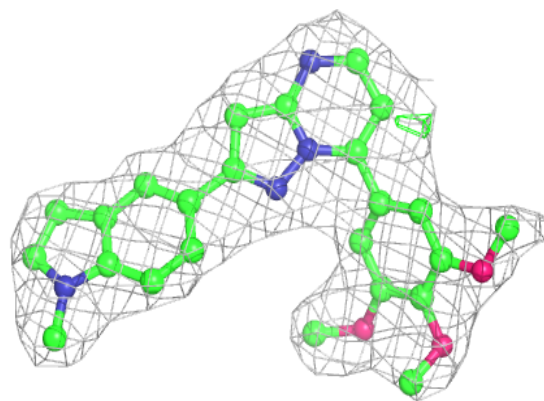
**Electron density around ACP F 402:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

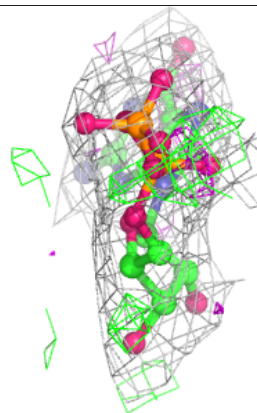
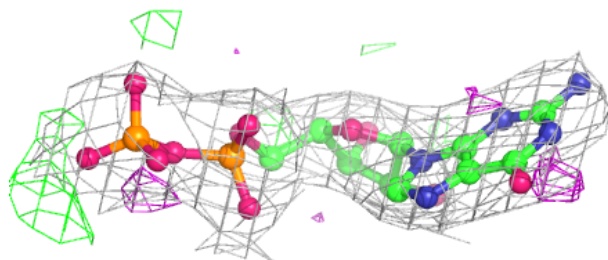
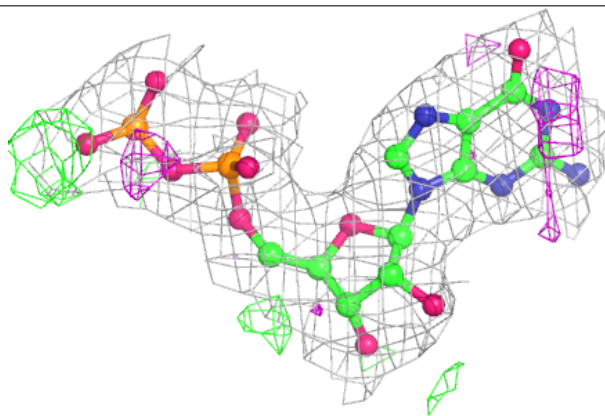


**Electron density around ERR B 507:**

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

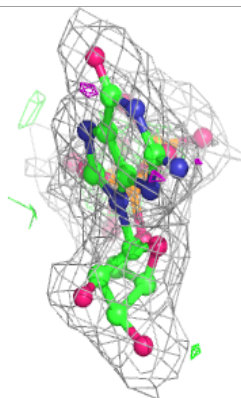
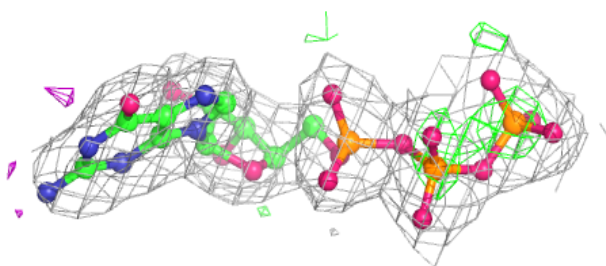
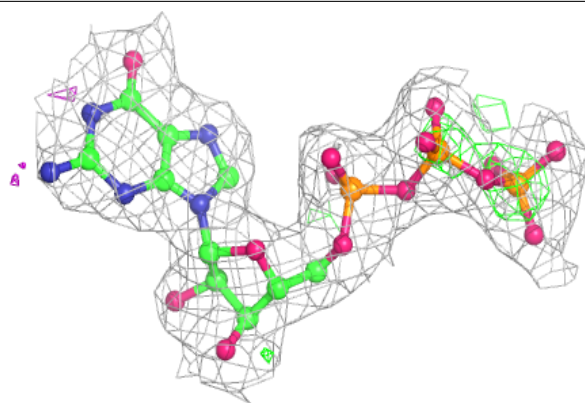
**Electron density around GDP D 600:**

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

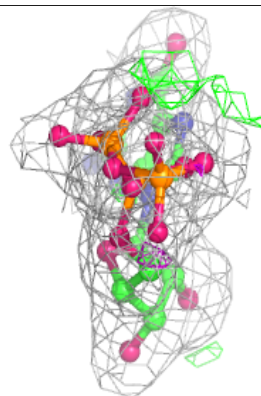
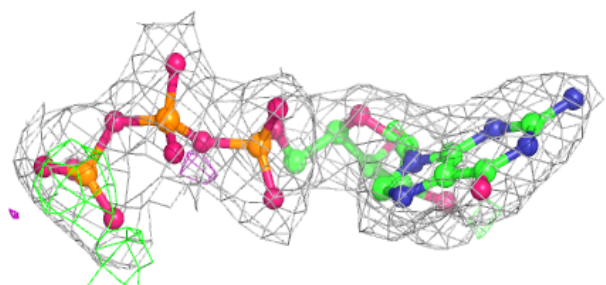
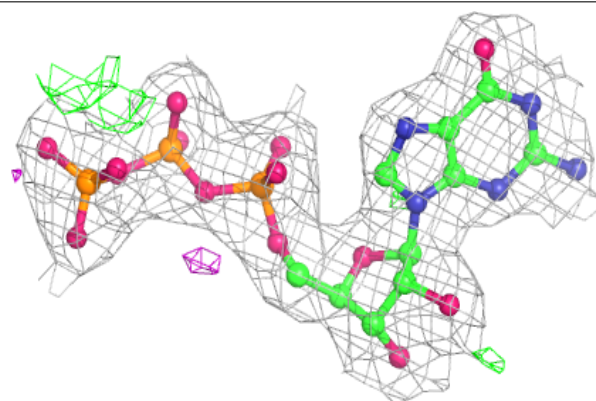


**Electron density around GTP C 501:**

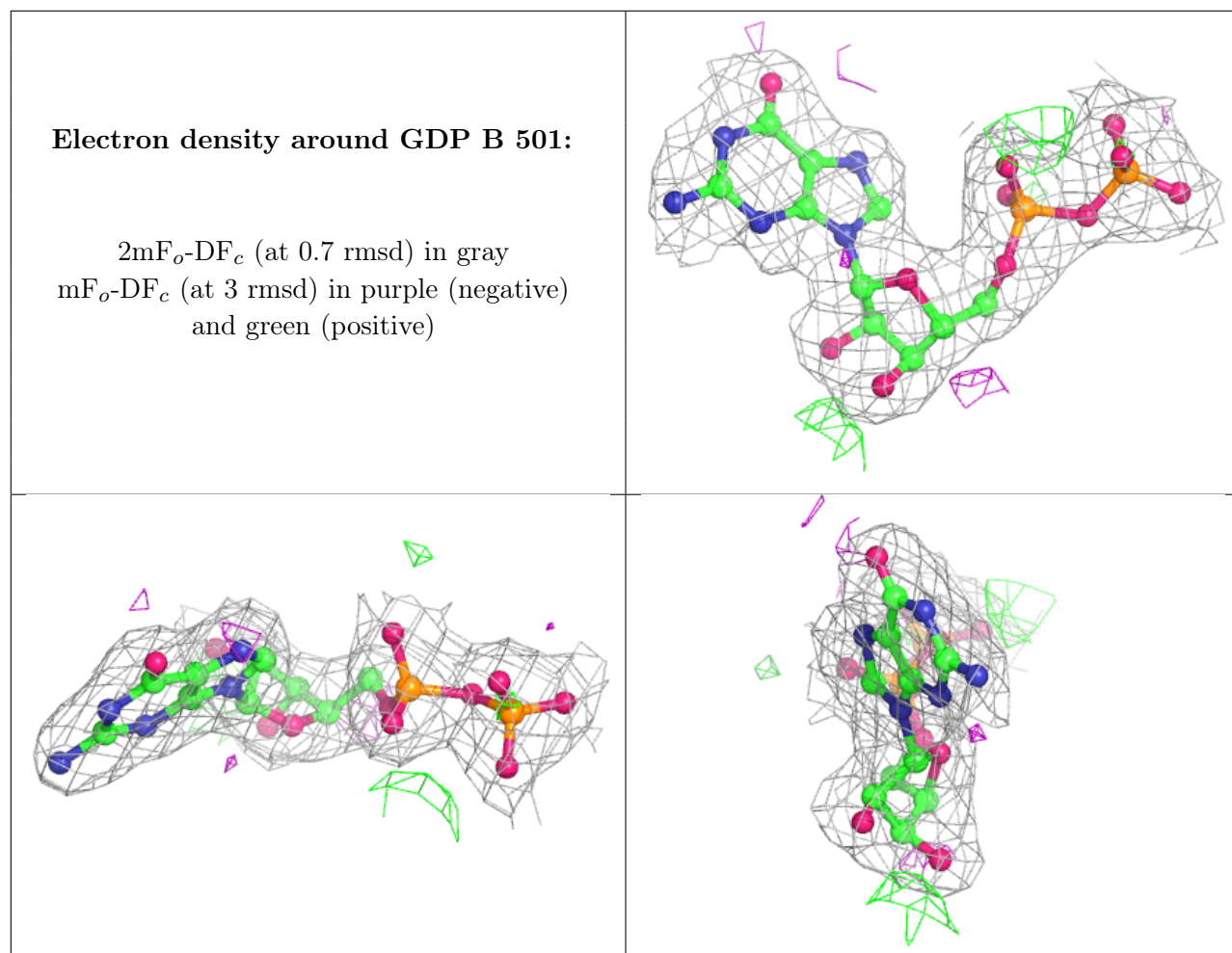
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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 ⓘ

There are no such residues in this entry.