



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:40 PM BST

PDB ID : 5XKG  
Title : Crystal structure of T2R-TTL-CH1 complex  
Authors : Wang, Y.; Yang, J.; Wang, T.; Chen, L.  
Deposited on : 2017-05-07  
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](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 : 2.13.1  
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) : 2.13.1

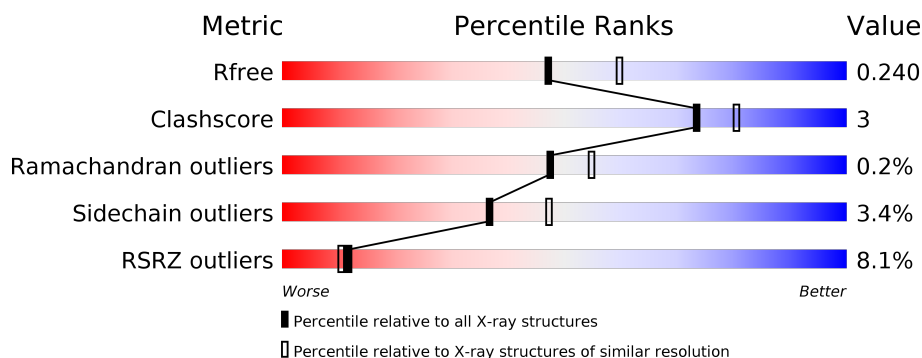
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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 on 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	451	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>
2	D	445	<div> <div>15%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
3	E	143	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
4	F	384	<div> <div>17%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>• 13%</div> </div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18087 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	437	Total	C	N	O	S	0	2	0
			3428	2169	583	652	24			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	1	0
			3375	2118	578	651	28			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

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		
5	D	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	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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

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

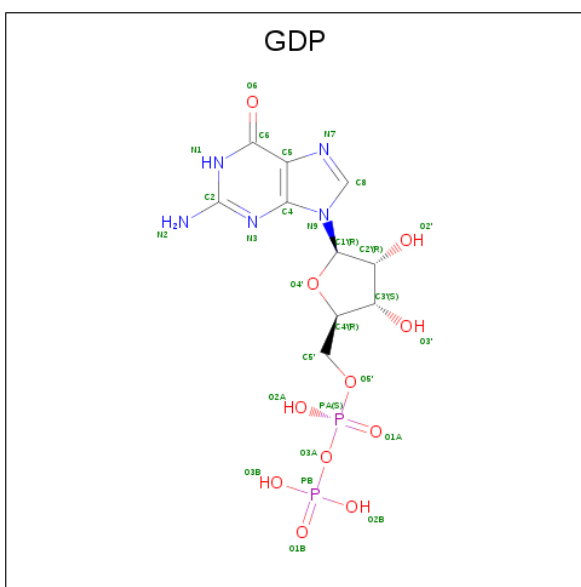
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



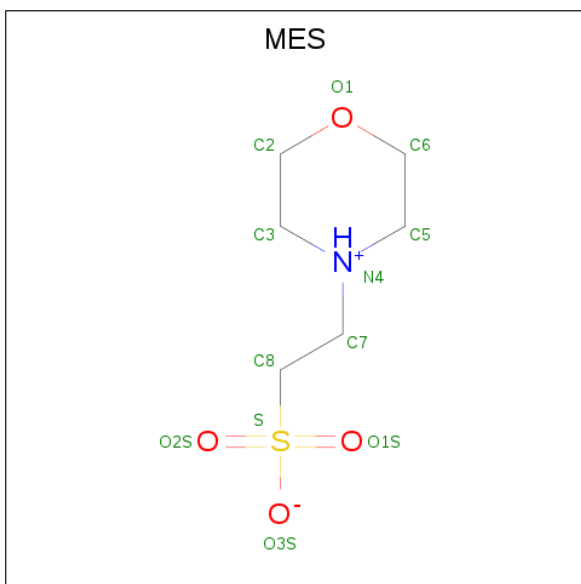
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



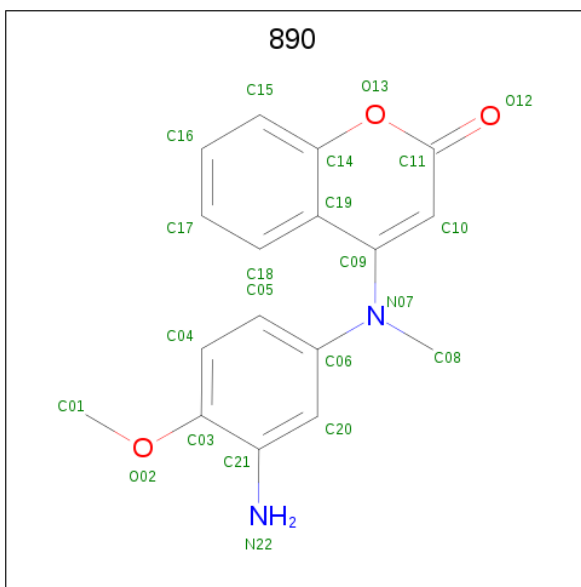
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 11 is 4-[(3-azanyl-4-methoxy-phenyl)-methyl-amino]chromen-2-one (three-letter code: 890) (formula:  $C_{17}H_{16}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			22	17	2	3		
11	D	1	Total	C	N	O	0	0
			22	17	2	3		

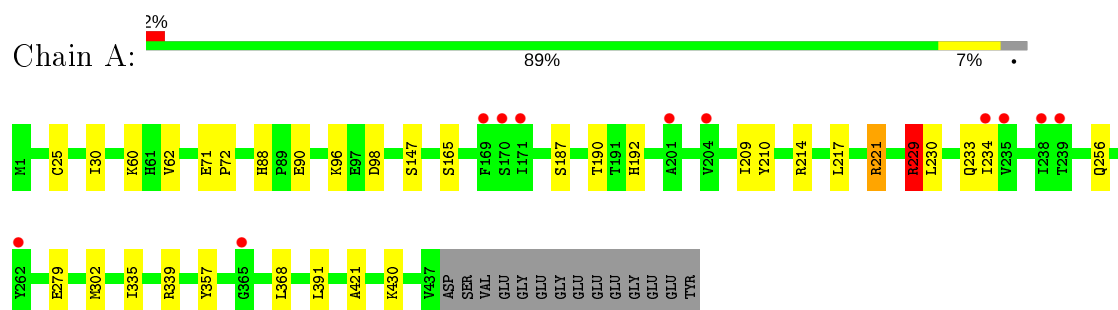
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	143	Total	O	0	0
			143	143		
12	B	121	Total	O	0	0
			121	121		
12	C	234	Total	O	0	0
			234	234		
12	D	30	Total	O	0	0
			30	30		
12	E	27	Total	O	0	0
			27	27		
12	F	38	Total	O	0	0
			38	38		

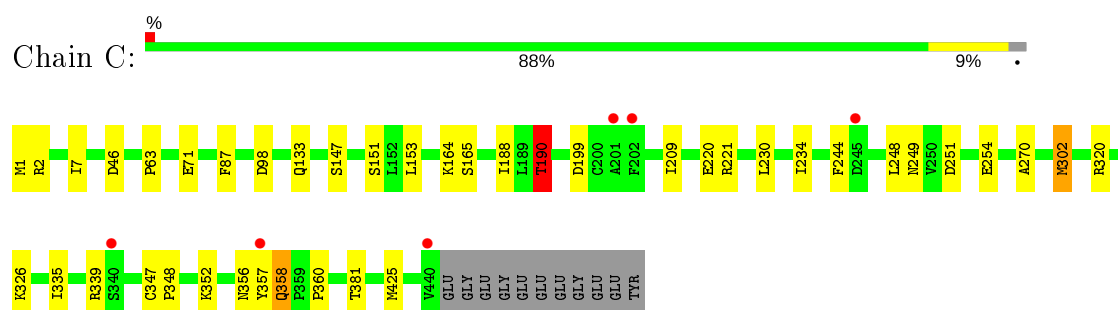
### 3 Residue-property plots [i](#)

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.

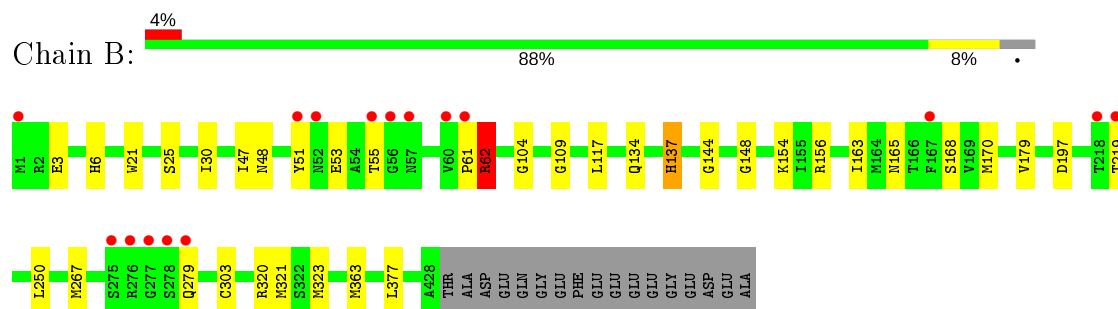
- Molecule 1: Tubulin alpha-1B chain



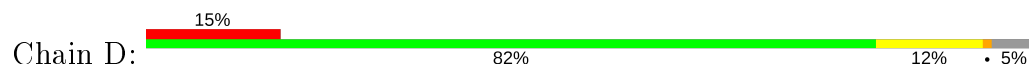
- Molecule 1: Tubulin alpha-1B chain



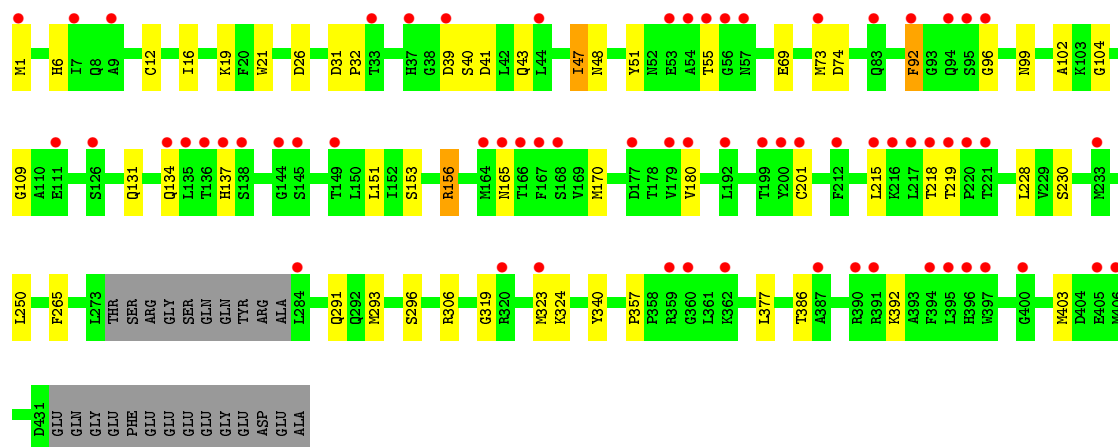
- Molecule 2: Tubulin beta chain



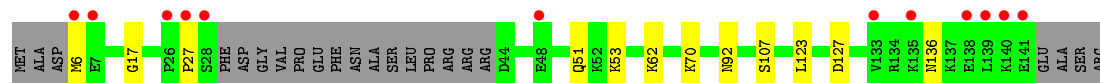
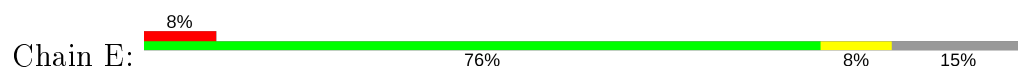
- Molecule 2: Tubulin beta chain







- Molecule 3: Stathmin-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.12Å 157.66Å 181.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.68 – 2.20 39.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.68-2.20) 99.9 (39.68-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.196 , 0.240 0.197 , 0.240	Depositor DCC
$R_{free}$ test set	7554 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: 890, GOL, MG, CA, GDP, GTP, 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	0.58	0/3506	0.72	2/4759 (0.0%)
1	C	0.67	0/3524	0.76	1/4785 (0.0%)
2	B	0.60	0/3450	0.69	0/4672
2	D	0.52	0/3382	0.68	0/4581
3	E	0.52	0/1008	0.70	0/1337
4	F	0.51	0/2806	0.69	1/3791 (0.0%)
All	All	0.58	0/17676	0.71	4/23925 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	190	THR	CB-CA-C	-6.03	95.33	111.60
4	F	132	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	229	ARG	CG-CD-NE	5.02	122.34	111.80

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	3428	0	3340	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3446	0	3354	22	0
2	B	3375	0	3254	34	0
2	D	3309	0	3189	27	0
3	E	1000	0	1018	3	0
4	F	2744	0	2709	16	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	4	0
11	B	22	0	0	1	0
11	D	22	0	0	0	0
12	A	143	0	0	0	0
12	B	121	0	0	0	0
12	C	234	0	0	2	0
12	D	30	0	0	0	0
12	E	27	0	0	0	0
12	F	38	0	0	0	0
All	All	18087	0	16933	115	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 3.

All (115) 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:21:TRP:CZ3	2:B:61:PRO:HB3	1.87	1.10
1:C:234:ILE:HD13	1:C:302:MET:SD	2.17	0.83
2:B:25:SER:HA	2:B:51:TYR:OH	1.78	0.82
2:B:197:ASP:OD2	10:B:503:MES:H52	1.83	0.78
2:B:21:TRP:CZ3	2:B:61:PRO:CB	2.70	0.74
1:C:147:SER:O	1:C:190:THR:HG23	1.90	0.72
4:F:31:ARG:HG3	4:F:31:ARG:HH11	1.58	0.68
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:GLN:NE2	2:D:250:LEU:H	1.93	0.67
2:B:156:ARG:CZ	10:B:503:MES:H21	2.26	0.66
2:B:51:TYR:HA	2:B:61:PRO:HA	1.78	0.65
2:B:156:ARG:HG3	10:B:503:MES:H62	1.77	0.65
2:B:197:ASP:OD1	10:B:503:MES:H32	1.96	0.65
2:D:92:PHE:HD1	2:D:92:PHE:O	1.80	0.64
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.80	0.63
2:B:62:ARG:HB2	2:B:62:ARG:HH11	1.64	0.60
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.83	0.59
2:B:25:SER:CA	2:B:51:TYR:OH	2.51	0.58
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.03	0.58
1:A:209:ILE:HD11	1:A:302:MET:SD	2.43	0.58
2:B:30:ILE:HG13	2:B:51:TYR:CE2	2.38	0.58
2:B:62:ARG:HB2	2:B:62:ARG:NH1	2.19	0.56
2:B:21:TRP:CH2	2:B:61:PRO:HB3	2.40	0.55
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.73	0.53
1:A:221:ARG:HG3	2:B:323:MET:HB3	1.90	0.53
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.91	0.53
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.44	0.53
2:B:267:MET:SD	2:B:303[B]:CYS:SG	3.06	0.53
2:B:104:GLY:O	2:B:109:GLY:HA3	2.09	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
2:D:104:GLY:O	2:D:109:GLY:HA3	2.10	0.51
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.46	0.51
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.92	0.51
2:B:134:GLN:HA	2:B:165:ASN:O	2.11	0.51
2:B:51:TYR:CD2	2:B:61:PRO:HG3	2.46	0.51
2:D:99:ASN:HD22	2:D:99:ASN:N	2.08	0.51
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.94	0.50
1:A:229:ARG:CG	1:A:229:ARG:HH11	2.25	0.50
2:B:321:MET:HB3	2:B:363:MET:HE1	1.94	0.49
4:F:31:ARG:NH1	4:F:31:ARG:HG3	2.27	0.49
1:A:147:SER:HB2	1:A:190:THR:HB	1.94	0.49
4:F:226:GLU:HG3	4:F:237:THR:HB	1.94	0.49
2:B:219:THR:HG22	12:C:780:HOH:O	2.12	0.49
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.48
4:F:10:ASN:N	4:F:10:ASN:HD22	2.11	0.48
2:D:69:GLU:HG2	2:D:96:GLY:CA	2.43	0.48
2:D:134:GLN:HA	2:D:165:ASN:O	2.13	0.48
4:F:40:MET:HE1	4:F:47:LEU:HG	1.94	0.48
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HG3	1:C:360:PRO:HD3	1.96	0.48
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.94	0.47
4:F:225:SER:HB3	4:F:252:ASN:HB3	1.96	0.47
2:B:137:HIS:HE1	2:B:168:SER:OG	1.97	0.47
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.50	0.47
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.96	0.47
4:F:136:ASN:HA	4:F:139:ARG:HB3	1.97	0.47
2:D:215:LEU:HD11	2:D:228:LEU:HD21	1.96	0.47
2:D:40:SER:HB3	2:D:43:GLN:HG3	1.96	0.47
2:B:219:THR:HG21	1:C:326:LYS:HB2	1.97	0.46
4:F:166:ALA:HA	4:F:169:LEU:HD12	1.98	0.46
2:D:69:GLU:OE2	2:D:96:GLY:HA3	2.16	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.99	0.45
2:B:137:HIS:HD2	2:B:144:GLY:O	1.99	0.45
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.98	0.45
2:D:47:ILE:HD13	2:D:51:TYR:CD2	2.52	0.45
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.44
1:A:25:CYS:HB3	1:A:30:ILE:O	2.17	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.47	0.44
11:B:504:890:C18	11:B:504:890:C06	2.95	0.44
1:C:221:ARG:HD3	2:D:323:MET:HG3	2.00	0.44
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.00	0.44
1:C:1:MET:HA	1:C:46:ASP:OD1	2.17	0.44
2:D:73:MET:HG3	2:D:92:PHE:HB3	2.00	0.44
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.53	0.43
1:C:220:GLU:HG2	2:D:324:LYS:HD2	2.01	0.43
4:F:296:MET:HE3	4:F:380:HIS:CG	2.53	0.43
1:A:234:ILE:HD13	1:A:302:MET:SD	2.58	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.43
1:A:165:SER:OG	1:A:256:GLN:NE2	2.51	0.43
2:B:117:LEU:HD11	2:B:154:LYS:HD3	2.01	0.43
4:F:245:ILE:O	4:F:245:ILE:HG22	2.18	0.43
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.52	0.43
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.99	0.43
4:F:14:TYR:HA	4:F:17:VAL:HB	2.01	0.43
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.00	0.43
1:C:151:SER:HB3	1:C:190:THR:HG22	1.99	0.42
1:C:270:ALA:HB3	1:C:302:MET:HG2	2.01	0.42
2:D:102:ALA:HB2	2:D:403:MET:SD	2.60	0.42
2:D:99:ASN:ND2	2:D:99:ASN:N	2.67	0.42
2:B:144:GLY:O	2:B:148:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:CYS:O	2:D:16:ILE:HG12	2.20	0.42
2:D:92:PHE:C	2:D:92:PHE:CD1	2.93	0.42
2:D:134:GLN:HB3	2:D:165:ASN:HD22	1.84	0.42
2:B:21:TRP:HZ3	2:B:61:PRO:HB3	1.67	0.42
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.50	0.42
2:D:92:PHE:C	2:D:92:PHE:HD1	2.23	0.42
2:D:19:LYS:HB3	2:D:230:SER:HB3	2.03	0.41
4:F:10:ASN:N	4:F:10:ASN:ND2	2.68	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.41
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.02	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
2:B:47:ILE:HG12	2:B:51:TYR:HB2	2.02	0.41
2:B:179:VAL:HG11	12:C:774:HOH:O	2.21	0.41
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.55	0.41
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.41
1:C:165:SER:HA	1:C:199:ASP:OD2	2.21	0.41
4:F:26:GLN:HE22	4:F:362:ALA:H	1.69	0.41
4:F:244:CYS:SG	4:F:245:ILE:HG13	2.60	0.41
2:B:51:TYR:CD1	2:B:51:TYR:N	2.89	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.61	0.41
2:B:3:GLU:HG2	2:B:62:ARG:NH2	2.37	0.40
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.40
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.62	0.40
1:A:192:HIS:CG	1:A:421:ALA:HA	2.57	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	437/451 (97%)	428 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	427/445 (96%)	410 (96%)	16 (4%)	1 (0%)	47	55
2	D	417/445 (94%)	408 (98%)	8 (2%)	1 (0%)	47	55
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	17	16
4	F	324/384 (84%)	302 (93%)	20 (6%)	2 (1%)	25	26
All	All	2161/2319 (93%)	2093 (97%)	63 (3%)	5 (0%)	47	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	392	LYS
2	B	62	ARG
4	F	245	ILE
4	F	32	LYS
3	E	27	PRO

### 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	370/379 (98%)	363 (98%)	7 (2%)	57	71
1	C	372/379 (98%)	363 (98%)	9 (2%)	49	62
2	B	371/383 (97%)	364 (98%)	7 (2%)	57	71
2	D	364/383 (95%)	344 (94%)	20 (6%)	21	26
3	E	109/127 (86%)	100 (92%)	9 (8%)	11	11
4	F	301/342 (88%)	289 (96%)	12 (4%)	31	40
All	All	1887/1993 (95%)	1823 (97%)	64 (3%)	37	47

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LYS

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Mol	Chain	Res	Type
1	A	62	VAL
1	A	96	LYS
1	A	221	ARG
1	A	229	ARG
1	A	279	GLU
1	A	430	LYS
2	B	48	ASN
2	B	53	GLU
2	B	55	THR
2	B	62	ARG
2	B	137	HIS
2	B	279	GLN
2	B	320	ARG
1	C	2	ARG
1	C	133	GLN
1	C	164	LYS
1	C	190	THR
1	C	251	ASP
1	C	302	MET
1	C	347	CYS
1	C	358	GLN
1	C	381	THR
2	D	1	MET
2	D	26	ASP
2	D	39	ASP
2	D	41	ASP
2	D	47	ILE
2	D	48	ASN
2	D	55	THR
2	D	74	ASP
2	D	92	PHE
2	D	137	HIS
2	D	151	LEU
2	D	153	SER
2	D	156	ARG
2	D	180	VAL
2	D	218	THR
2	D	219	THR
2	D	291	GLN
2	D	293	MET
2	D	296	SER
2	D	386	THR

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Mol	Chain	Res	Type
3	E	6	MET
3	E	51	GLN
3	E	53	LYS
3	E	62	LYS
3	E	70	LYS
3	E	92	ASN
3	E	107	SER
3	E	127	ASP
3	E	136	ASN
4	F	31	ARG
4	F	70	LYS
4	F	130	VAL
4	F	132	LEU
4	F	162	ILE
4	F	175	GLU
4	F	176	GLN
4	F	211	TYR
4	F	235	ASP
4	F	237	THR
4	F	238	CYS
4	F	372	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
2	B	137	HIS
2	D	99	ASN
2	D	131	GLN
2	D	292	GLN
4	F	10	ASN
4	F	176	GLN
4	F	209	HIS

### 5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 6 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
5	GTP	C	501	6	26,34,34	1.15	3 (11%)	33,54,54	1.89	8 (24%)
11	890	D	503	-	21,24,24	2.11	11 (52%)	27,34,34	2.15	6 (22%)
5	GTP	A	501	6	26,34,34	1.22	3 (11%)	33,54,54	2.11	11 (33%)
10	MES	B	503	-	12,12,12	1.69	2 (16%)	14,16,16	6.29	9 (64%)
8	GOL	A	504	-	5,5,5	0.41	0	5,5,5	0.47	0
5	GTP	D	501	6	26,34,34	1.26	2 (7%)	33,54,54	1.90	8 (24%)
11	890	B	504	-	21,24,24	1.97	8 (38%)	27,34,34	1.52	6 (22%)
9	GDP	B	501	6	24,30,30	1.24	4 (16%)	31,47,47	2.16	6 (19%)

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
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
11	890	D	503	-	-	2/10/10/10	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	MES	B	503	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	504	-	-	1/4/4/4	-
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3
11	890	B	504	-	-	2/10/10/10	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-4.86	1.70	1.77
5	D	501	GTP	C6-C5	4.77	1.49	1.41
5	A	501	GTP	C6-C5	4.32	1.48	1.41
5	C	501	GTP	C6-C5	3.67	1.47	1.41
11	D	503	890	C17-C18	3.48	1.44	1.36
11	D	503	890	O02-C03	3.31	1.42	1.37
11	B	504	890	C05-C06	3.27	1.45	1.39
11	D	503	890	C21-C03	3.24	1.44	1.40
11	B	504	890	O02-C03	3.23	1.42	1.37
11	B	504	890	C10-C09	3.20	1.43	1.40
9	B	501	GDP	C6-C5	3.05	1.46	1.41
11	B	504	890	C17-C18	3.04	1.43	1.36
9	B	501	GDP	C2'-C1'	-2.95	1.49	1.53
11	D	503	890	C05-C06	2.86	1.44	1.39
5	D	501	GTP	C5-C4	2.58	1.47	1.40
11	D	503	890	C21-N22	2.50	1.46	1.37
10	B	503	MES	O2S-S	2.41	1.52	1.45
11	D	503	890	C16-C15	2.39	1.42	1.36
9	B	501	GDP	O4'-C1'	2.37	1.44	1.41
11	D	503	890	C20-C21	2.37	1.43	1.40
11	D	503	890	C20-C06	2.37	1.43	1.39
5	C	501	GTP	O4'-C1'	2.26	1.44	1.41
5	A	501	GTP	C5-C4	2.24	1.46	1.40
11	B	504	890	C16-C15	2.22	1.41	1.36
11	D	503	890	O13-C14	2.20	1.40	1.36
9	B	501	GDP	C5-C4	2.19	1.46	1.40
5	A	501	GTP	O4'-C1'	2.17	1.44	1.41
11	B	504	890	C21-N22	2.17	1.45	1.37
11	D	503	890	C09-C19	2.05	1.47	1.42
11	D	503	890	C05-C04	2.03	1.42	1.38
5	C	501	GTP	PG-O3G	-2.03	1.47	1.54
11	B	504	890	C05-C04	2.01	1.42	1.38
11	B	504	890	C04-C03	2.01	1.43	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O3S-S-O1S	-12.52	80.68	111.27
10	B	503	MES	O3S-S-O2S	-10.03	86.77	111.27
10	B	503	MES	O3S-S-C8	-9.75	90.01	105.77
10	B	503	MES	O1S-S-C8	9.39	118.22	106.92
10	B	503	MES	O2S-S-C8	8.58	117.25	106.92
11	D	503	890	C19-C09-N07	7.14	125.67	118.97
9	B	501	GDP	C6-C5-C4	-6.07	115.00	120.80
5	C	501	GTP	C5-C6-N1	-4.93	116.69	123.43
5	A	501	GTP	C6-C5-C4	-4.86	116.16	120.80
5	C	501	GTP	C6-N1-C2	4.85	123.63	115.93
5	D	501	GTP	C2-N3-C4	4.79	120.82	115.36
9	B	501	GDP	C2-N3-C4	4.75	120.78	115.36
5	A	501	GTP	C2-N3-C4	4.71	120.74	115.36
9	B	501	GDP	C6-N1-C2	4.65	123.32	115.93
9	B	501	GDP	N3-C2-N1	-4.62	121.06	127.22
5	D	501	GTP	C5-C6-N1	-4.35	117.48	123.43
5	D	501	GTP	C6-N1-C2	4.10	122.45	115.93
5	A	501	GTP	C6-N1-C2	3.92	122.16	115.93
5	A	501	GTP	C5-C6-N1	-3.84	118.17	123.43
11	D	503	890	C20-C21-C03	3.76	121.22	118.18
5	C	501	GTP	C2-N3-C4	3.73	119.62	115.36
5	C	501	GTP	N3-C2-N1	-3.63	122.38	127.22
5	A	501	GTP	N3-C2-N1	-3.52	122.53	127.22
5	D	501	GTP	C6-C5-C4	-3.49	117.46	120.80
10	B	503	MES	C6-O1-C2	3.47	121.46	109.89
11	D	503	890	C03-C21-N22	-3.46	116.49	119.46
11	D	503	890	C09-C19-C14	3.45	120.16	116.99
5	C	501	GTP	C6-C5-C4	-3.44	117.51	120.80
11	B	504	890	O02-C03-C21	3.32	116.25	114.05
5	D	501	GTP	N3-C2-N1	-3.28	122.85	127.22
11	D	503	890	C01-O02-C03	3.15	122.28	117.53
9	B	501	GDP	C5-C6-N1	-3.12	119.17	123.43
11	B	504	890	C18-C19-C14	3.09	120.08	116.50
5	D	501	GTP	C4-C5-N7	-3.09	106.18	109.40
9	B	501	GDP	C1'-N9-C4	-2.98	121.40	126.64
11	B	504	890	C20-C21-C03	2.95	120.56	118.18
11	D	503	890	C21-C20-C06	-2.86	118.54	122.13
5	A	501	GTP	N2-C2-N1	2.85	121.69	117.25
5	A	501	GTP	C1'-N9-C4	-2.79	121.74	126.64
10	B	503	MES	O2S-S-O1S	2.58	122.88	113.95
11	B	504	890	C21-C20-C06	-2.51	118.98	122.13
5	D	501	GTP	PA-O3A-PB	-2.50	124.23	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	O3G-PG-O2G	2.45	116.99	107.64
5	C	501	GTP	O3G-PG-O1G	2.42	120.17	110.68
5	A	501	GTP	C4-C5-N7	-2.39	106.91	109.40
10	B	503	MES	C5-N4-C3	2.37	114.17	108.83
11	B	504	890	C01-O02-C03	-2.26	114.12	117.53
5	A	501	GTP	PB-O3B-PG	-2.24	125.16	132.83
11	B	504	890	C19-C09-N07	2.22	121.06	118.97
10	B	503	MES	C7-N4-C5	2.21	116.88	111.23
5	C	501	GTP	C4-C5-N7	-2.19	107.11	109.40
5	A	501	GTP	O3G-PG-O1G	2.18	119.23	110.68
5	D	501	GTP	PB-O3B-PG	-2.02	125.89	132.83
5	C	501	GTP	PB-O3B-PG	-2.01	125.93	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
11	D	503	890	C10-C09-N07-C08
10	B	503	MES	N4-C7-C8-S
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O1S
11	B	504	890	C10-C09-N07-C08
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
11	B	504	890	C19-C09-N07-C06
9	B	501	GDP	PB-O3A-PA-O1A
11	D	503	890	C19-C09-N07-C06
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
5	D	501	GTP	C4'-C5'-O5'-PA

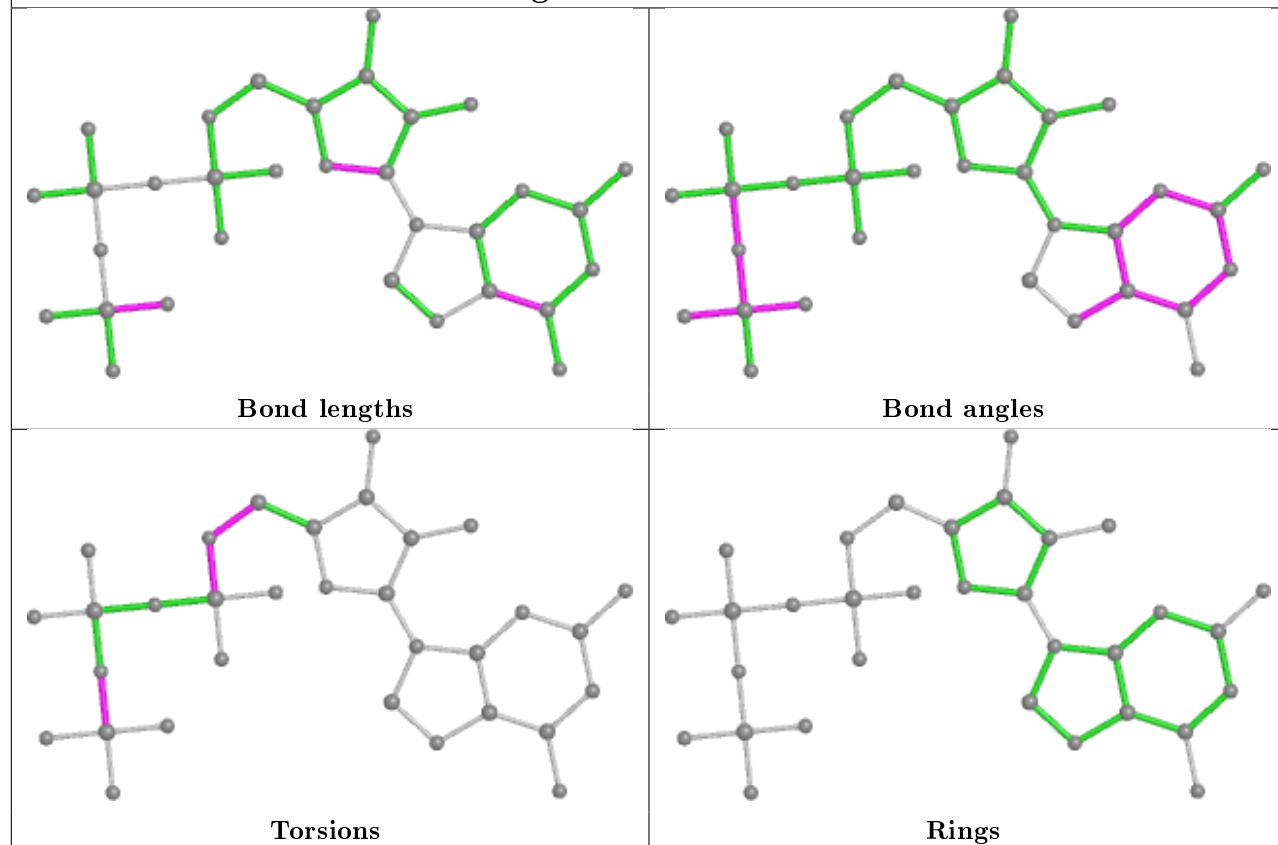
There are no ring outliers.

2 monomers are involved in 5 short contacts:

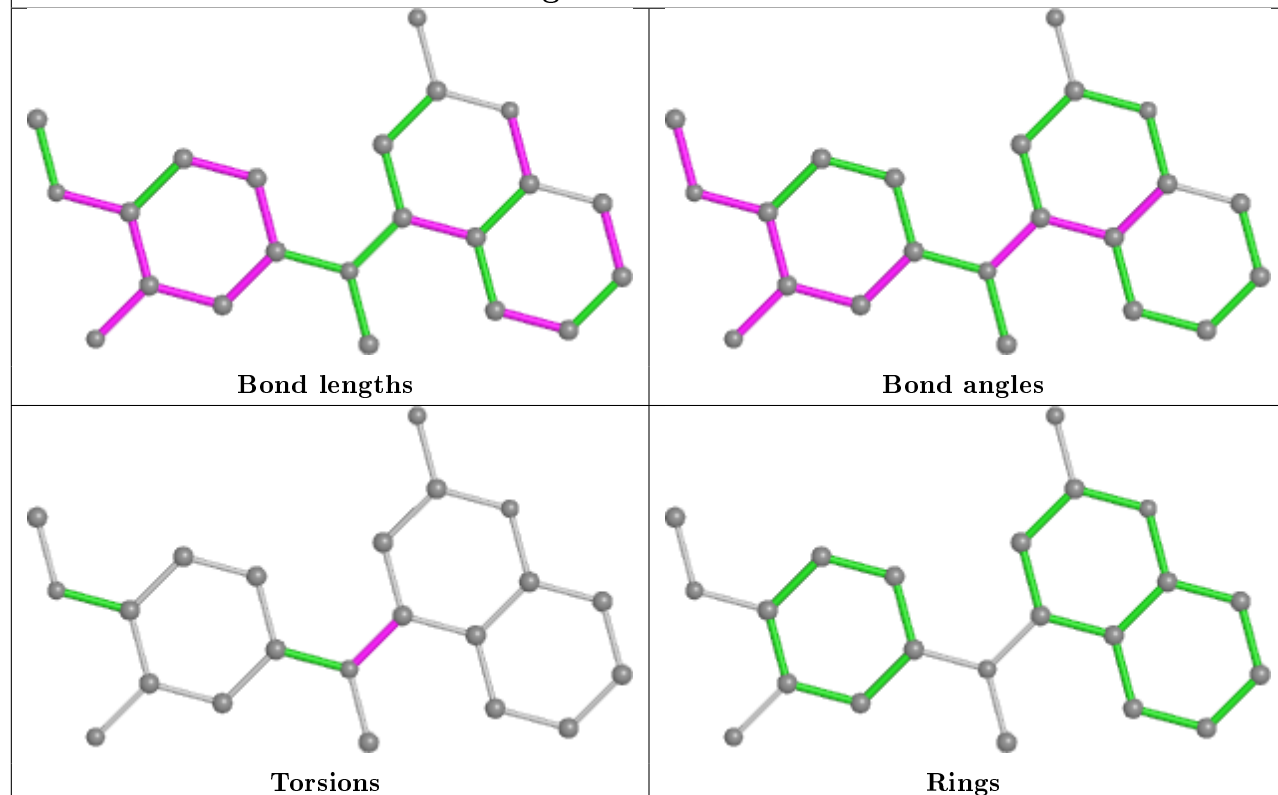
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	4	0
11	B	504	890	1	0

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 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.

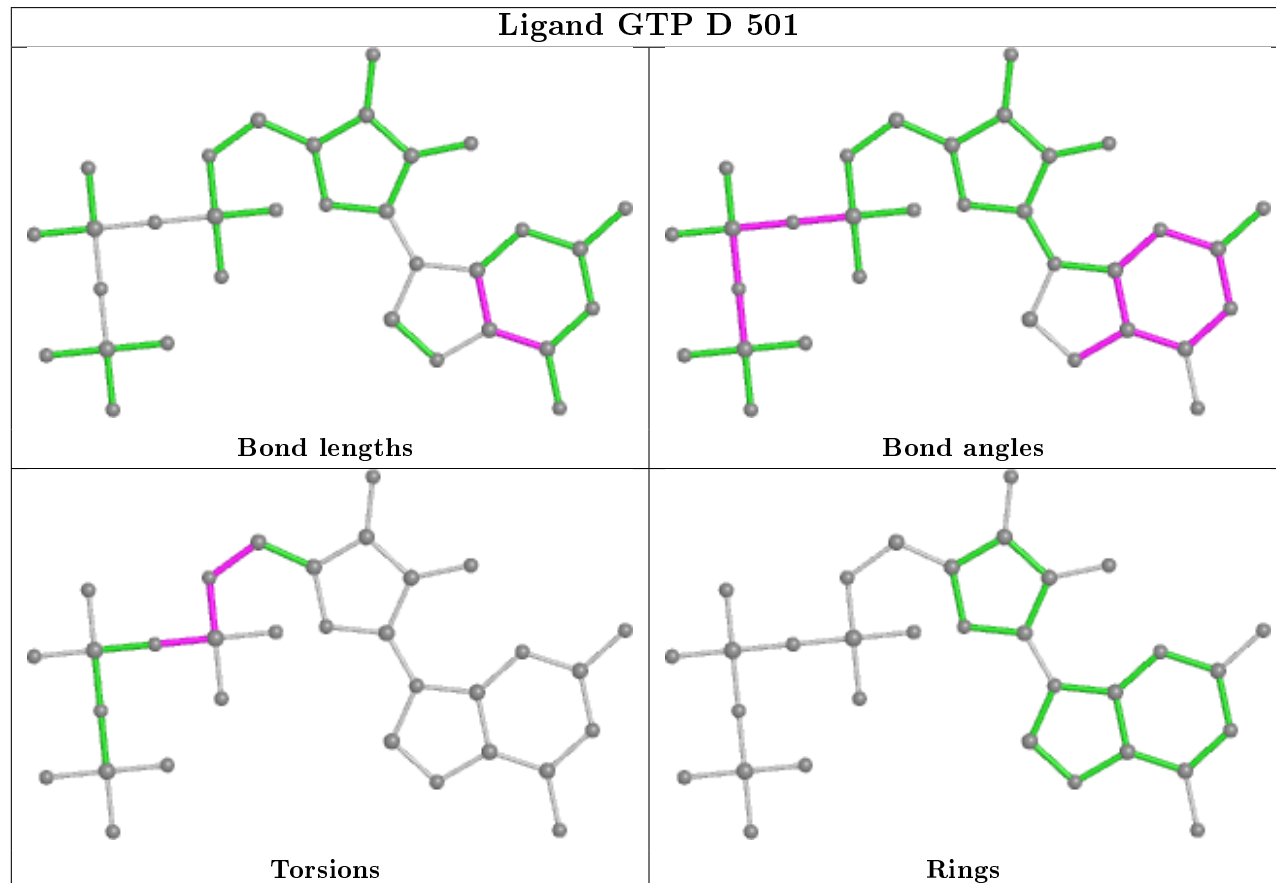
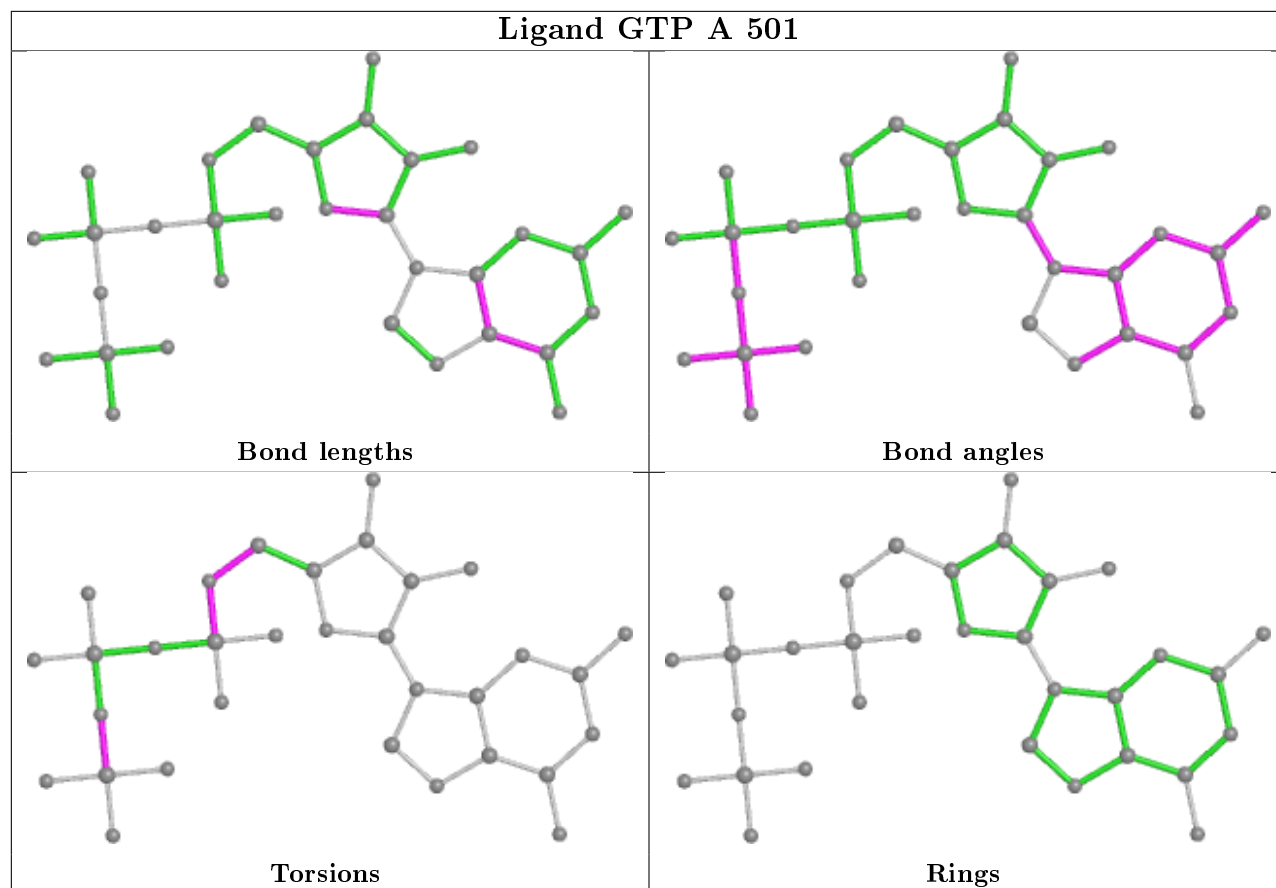
## Ligand GTP C 501

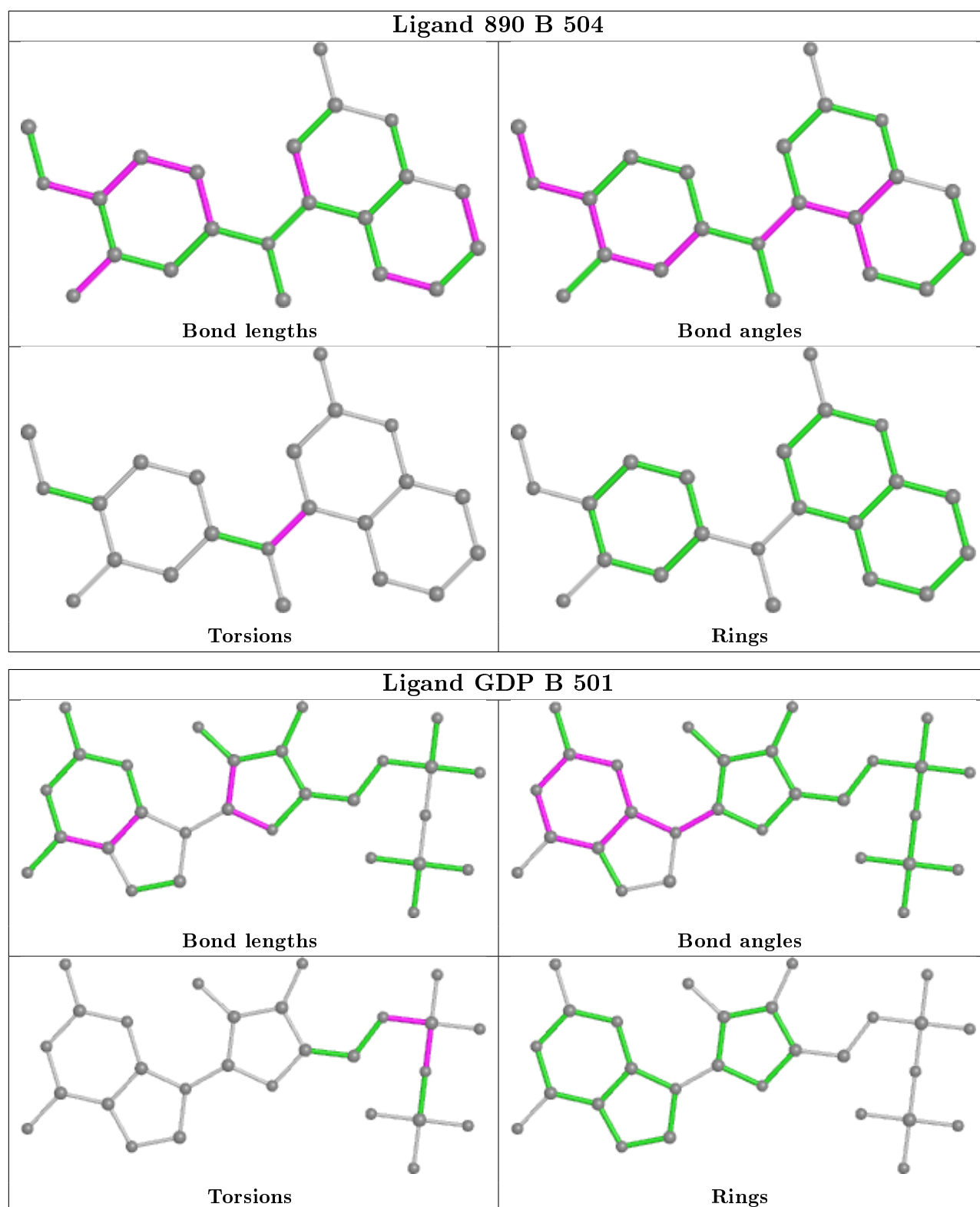


## Ligand 890 D 503









## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	437/451 (96%)	-0.04	11 (2%) 57 55	27, 41, 64, 85	0
1	C	440/451 (97%)	-0.31	6 (1%) 75 73	20, 33, 58, 78	0
2	B	428/445 (96%)	0.05	16 (3%) 41 39	23, 41, 76, 119	0
2	D	421/445 (94%)	0.67	65 (15%) 2 1	30, 64, 98, 126	0
3	E	121/143 (84%)	0.43	12 (9%) 7 6	31, 55, 92, 114	0
4	F	334/384 (86%)	0.75	66 (19%) 1 1	35, 64, 129, 147	0
All	All	2181/2319 (94%)	0.21	176 (8%) 12 10	20, 46, 97, 147	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.1
4	F	234	GLN	8.1
4	F	169	LEU	8.0
4	F	170	LEU	7.2
3	E	139	LEU	7.1
4	F	132	LEU	6.8
4	F	231	ALA	6.7
4	F	182	ILE	6.4
2	B	55	THR	6.0
2	D	55	THR	6.0
4	F	233	PHE	6.0
2	B	57	ASN	5.9
4	F	103	THR	5.8
4	F	167	SER	5.4
4	F	380	HIS	5.3
4	F	130	VAL	5.2
4	F	171	ASP	5.2
2	D	219	THR	5.1
4	F	372	THR	5.0

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Mol	Chain	Res	Type	RSRZ
4	F	163	SER	5.0
2	B	61	PRO	4.9
2	D	37	HIS	4.9
4	F	133	ALA	4.8
4	F	137	ARG	4.8
4	F	102	PRO	4.8
4	F	174	ASP	4.7
4	F	140	GLU	4.6
4	F	172	PHE	4.6
4	F	232	ASN	4.5
2	B	277	GLY	4.5
4	F	100	ILE	4.5
3	E	138	GLU	4.4
4	F	179	VAL	4.4
3	E	140	LYS	4.4
4	F	166	ALA	4.2
4	F	138	ARG	4.2
2	D	135	LEU	4.2
2	D	218	THR	4.2
2	B	279	GLN	4.1
4	F	176	GLN	4.0
2	D	216	LYS	4.0
4	F	101	TYR	3.9
2	D	390	ARG	3.9
4	F	177	GLY	3.8
2	D	284	LEU	3.8
2	D	391	ARG	3.7
2	D	56	GLY	3.7
4	F	141	GLY	3.7
4	F	178	GLN	3.7
4	F	129	GLU	3.6
2	D	387	ALA	3.6
2	D	217	LEU	3.6
2	D	1	MET	3.6
4	F	142	ARG	3.5
1	A	262	TYR	3.5
2	B	51	TYR	3.5
4	F	245	ILE	3.4
3	E	7	GLU	3.4
2	D	137	HIS	3.4
4	F	134	ALA	3.4
2	D	33	THR	3.4

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Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	3.4
2	D	395	LEU	3.4
4	F	145	ASN	3.4
2	D	396	HIS	3.3
2	D	136	THR	3.3
2	D	199	THR	3.3
2	D	168	SER	3.2
4	F	139	ARG	3.2
4	F	131	PHE	3.2
2	D	167	PHE	3.2
4	F	361	LEU	3.1
4	F	362	ALA	3.1
2	D	212	PHE	3.1
2	B	1	MET	3.1
2	D	96	GLY	3.1
2	D	54	ALA	3.1
4	F	135	TYR	3.1
2	D	215	LEU	3.0
2	D	323	MET	3.0
2	D	394	PHE	3.0
3	E	28	SER	3.0
4	F	181	VAL	3.0
1	A	238	ILE	2.9
4	F	236	LYS	2.9
2	D	177	ASP	2.9
2	B	275	SER	2.9
3	E	6	MET	2.9
3	E	135	LYS	2.9
3	E	141	GLU	2.9
4	F	165	GLU	2.9
2	B	276	ARG	2.9
1	A	235	VAL	2.8
2	B	60	VAL	2.8
2	D	73	MET	2.8
2	D	83	GLN	2.8
2	D	57	ASN	2.8
2	D	166	THR	2.8
4	F	147	TRP	2.8
4	F	256	TYR	2.8
2	D	165	ASN	2.8
2	D	397	TRP	2.8
3	E	48	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	144	GLY	2.7
2	D	92	PHE	2.7
2	D	400	GLY	2.7
4	F	99	VAL	2.7
2	B	56	GLY	2.7
4	F	194	PRO	2.7
2	D	9	ALA	2.7
2	D	220	PRO	2.7
2	D	359	ARG	2.6
4	F	244	CYS	2.6
2	D	94	GLN	2.6
2	D	149	THR	2.6
2	D	405	GLU	2.6
2	D	221	THR	2.6
4	F	230	SER	2.5
1	C	440	VAL	2.5
2	D	362	LYS	2.5
4	F	253	TYR	2.5
1	C	202	PHE	2.5
2	B	52	ASN	2.5
1	A	365	GLY	2.5
4	F	162	ILE	2.5
2	D	320	ARG	2.4
2	D	179	VAL	2.4
4	F	146	VAL	2.4
3	E	26	PRO	2.4
1	C	245	ASP	2.4
4	F	175	GLU	2.4
2	D	126	SER	2.4
2	D	7	ILE	2.4
4	F	98	TYR	2.4
2	D	360	GLY	2.4
2	D	134	GLN	2.4
4	F	164	SER	2.4
2	B	278	SER	2.3
2	D	192	LEU	2.3
2	D	233	MET	2.3
1	A	171	ILE	2.3
1	A	234	ILE	2.3
4	F	240	LEU	2.3
2	D	39	ASP	2.3
4	F	168	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	180	VAL	2.3
1	A	239	THR	2.3
4	F	161	LEU	2.3
2	D	111	GLU	2.3
1	A	169	PHE	2.3
1	A	201	ALA	2.3
1	A	170	SER	2.2
2	D	95	SER	2.2
4	F	9	GLU	2.2
4	F	136	ASN	2.2
1	C	340	SER	2.2
2	D	53	GLU	2.2
2	D	145	SER	2.2
2	B	167	PHE	2.2
2	D	164	MET	2.2
2	D	138	SER	2.2
4	F	10	ASN	2.1
2	D	200	TYR	2.1
3	E	133	VAL	2.1
2	B	219	THR	2.1
4	F	89	GLU	2.1
4	F	45	ASN	2.1
2	D	201	CYS	2.1
2	D	406	MET	2.1
2	B	218	THR	2.1
1	C	357	TYR	2.1
4	F	180	HIS	2.1
2	D	144	GLY	2.0
1	A	204	VAL	2.0
2	D	44	LEU	2.0
1	C	201	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 ⓘ

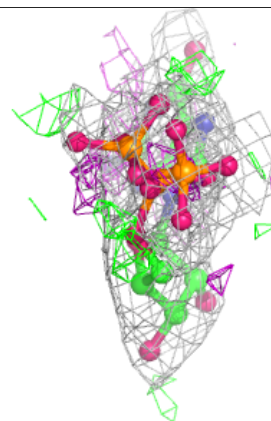
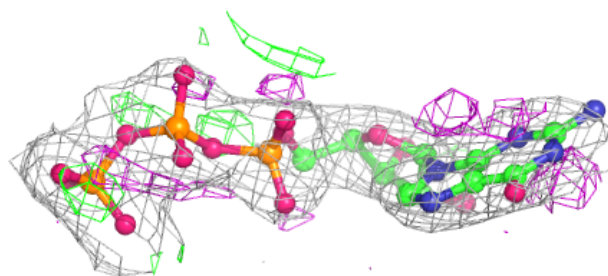
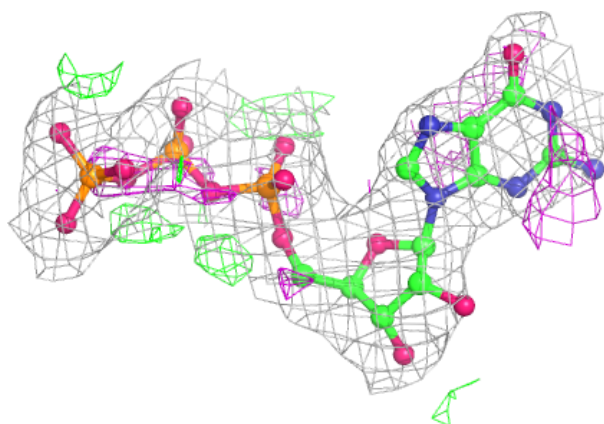
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	D	502	1/1	0.89	0.14	81,81,81,81	0
5	GTP	D	501	32/32	0.92	0.13	51,61,72,83	0
6	MG	A	502	1/1	0.94	0.11	33,33,33,33	0
8	GOL	A	504	6/6	0.94	0.11	39,49,54,57	0
10	MES	B	503	12/12	0.95	0.14	43,48,55,56	0
5	GTP	A	501	32/32	0.98	0.13	25,29,34,37	0
11	890	B	504	22/22	0.98	0.16	26,32,33,35	0
7	CA	A	503	1/1	0.98	0.03	53,53,53,53	0
7	CA	C	503	1/1	0.98	0.03	40,40,40,40	0
11	890	D	503	22/22	0.98	0.11	30,40,43,43	0
6	MG	B	502	1/1	0.98	0.13	27,27,27,27	0
6	MG	C	502	1/1	0.99	0.12	28,28,28,28	0
5	GTP	C	501	32/32	0.99	0.12	24,26,30,36	0
9	GDP	B	501	28/28	0.99	0.12	23,29,31,33	0

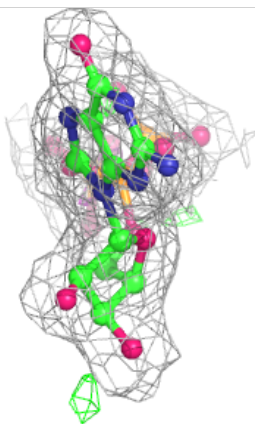
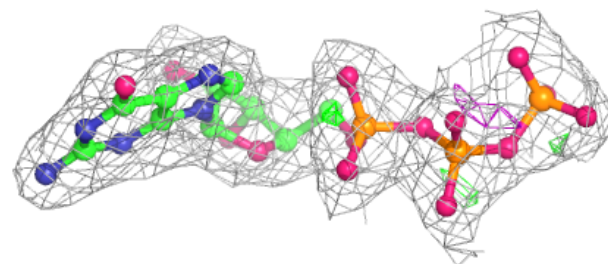
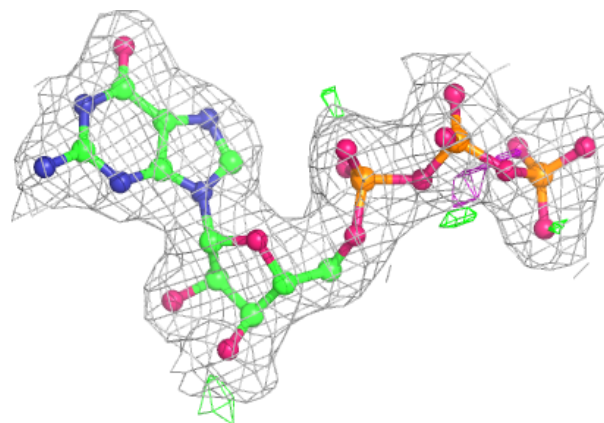
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GTP 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)

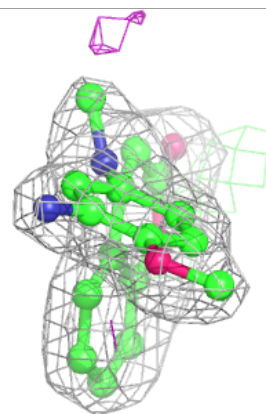
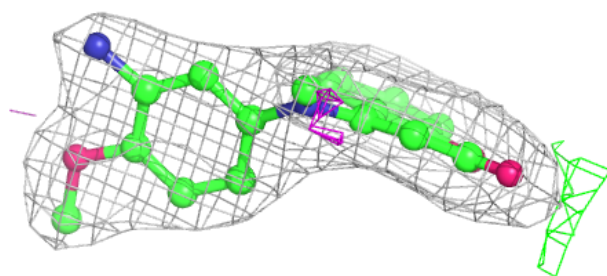
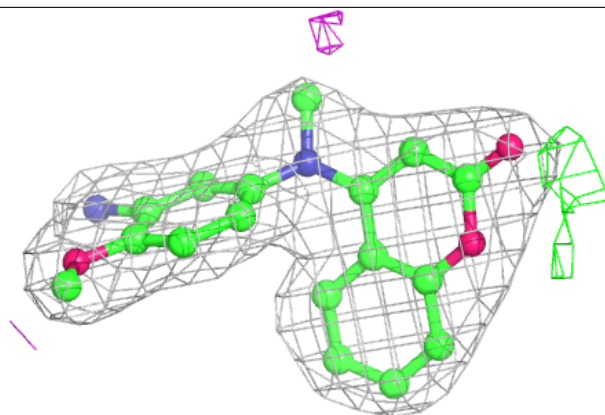
**Electron density around GTP A 501:**

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

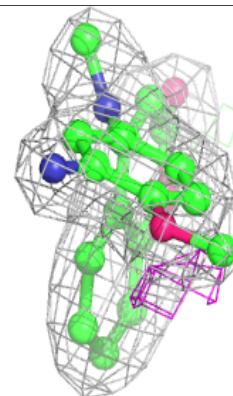
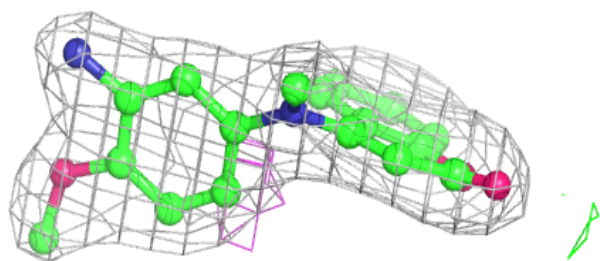
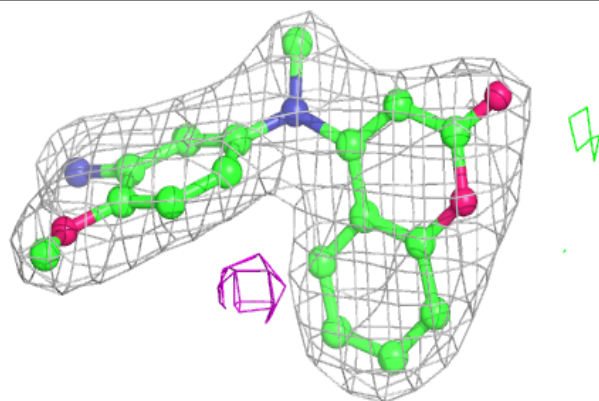


**Electron density around 890 B 504:**

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

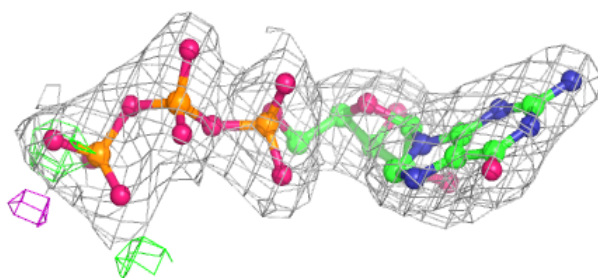
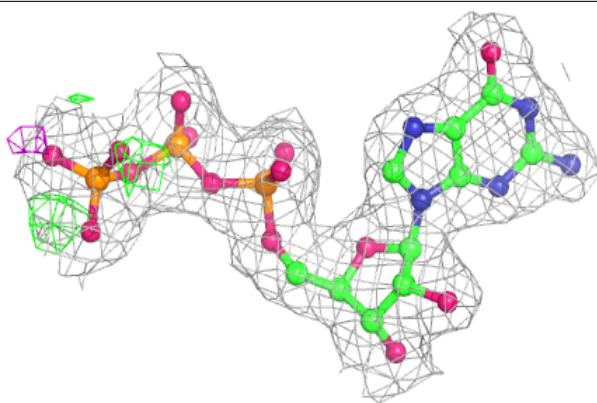
**Electron density around 890 D 503:**

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



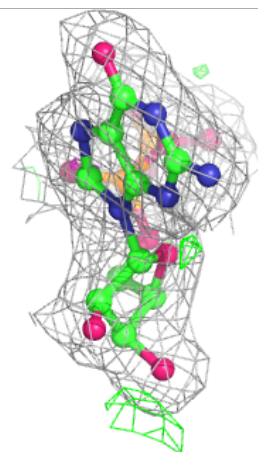
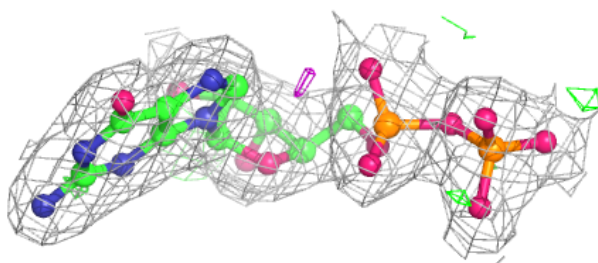
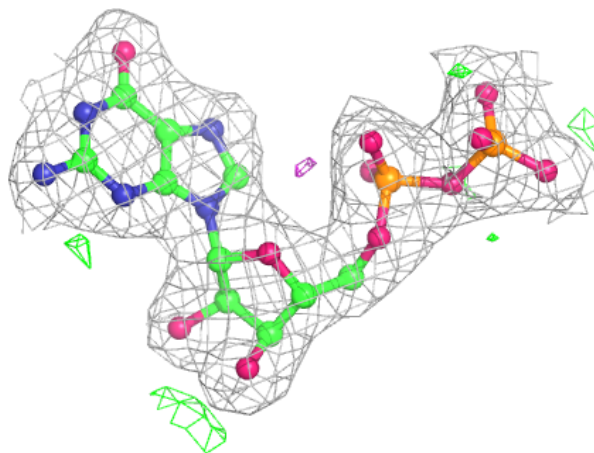
**Electron density around GTP C 501:**

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



**Electron density around 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.