



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 04:16 am BST

PDB ID : 3RYC  
Title : Tubulin: RB3 stathmin-like domain complex  
Authors : Nawrotek, A.; Knossow, M.; Gigant, B.  
Deposited on : 2011-05-11  
Resolution : 2.10 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 : 2.11  
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) : 2.11

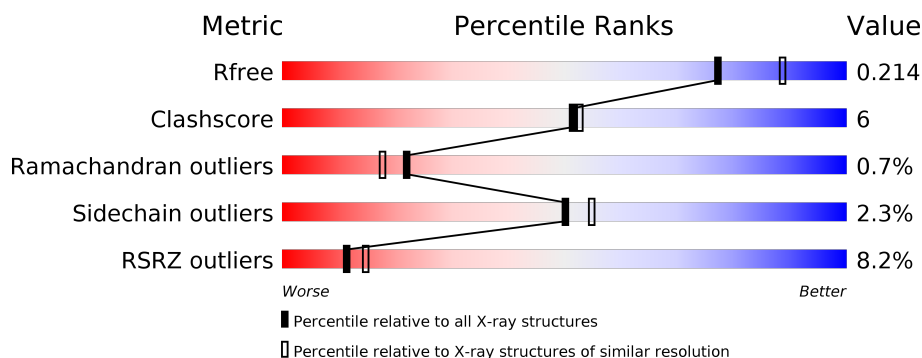
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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>5%</div> <div> <div>82%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	451	<div> <div>11%</div> <div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	445	<div> <div>10%</div> <div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
2	D	445	<div> <div>4%</div> <div> <div>86%</div> <div>11%</div> <div>.</div> </div> </div>
3	E	143	<div> <div>13%</div> <div> <div>84%</div> <div>9%</div> <div>.. 5%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15686 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	2	0
			3394	2150	576	645	23			
1	C	431	Total	C	N	O	S	0	4	0
			3366	2133	570	638	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	7	0
			3443	2163	585	668	27			
2	D	431	Total	C	N	O	S	0	10	0
			3445	2161	588	670	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

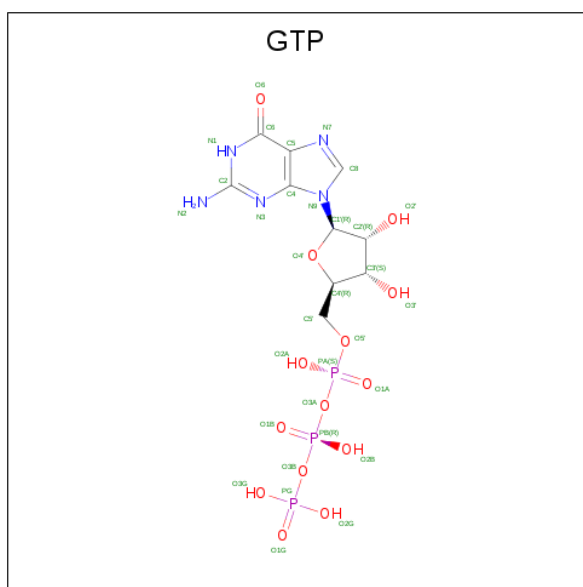
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	136	Total	C	N	O	S	0	0	0
			1096	677	200	215	4			

There are 4 discrepancies between the modelled and reference sequences:

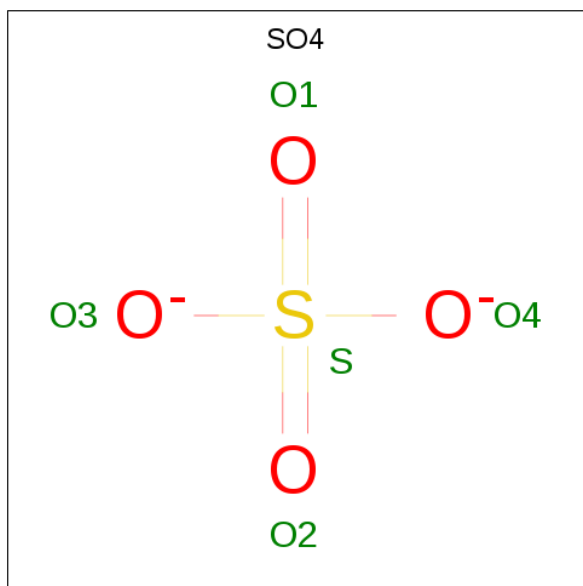
Chain	Residue	Modelled	Actual	Comment	Reference
E	3	ACE	-	SEE REMARK 999	UNP P63043
E	4	ALA	-	SEE REMARK 999	UNP P63043
E	14	ALA	CYS	ENGINEERED MUTATION	UNP P63043
E	20	TRP	PHE	ENGINEERED MUTATION	UNP P63043

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



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



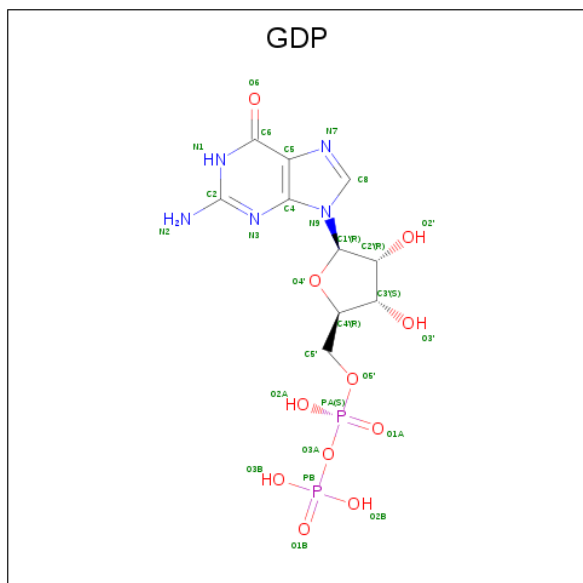
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

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

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

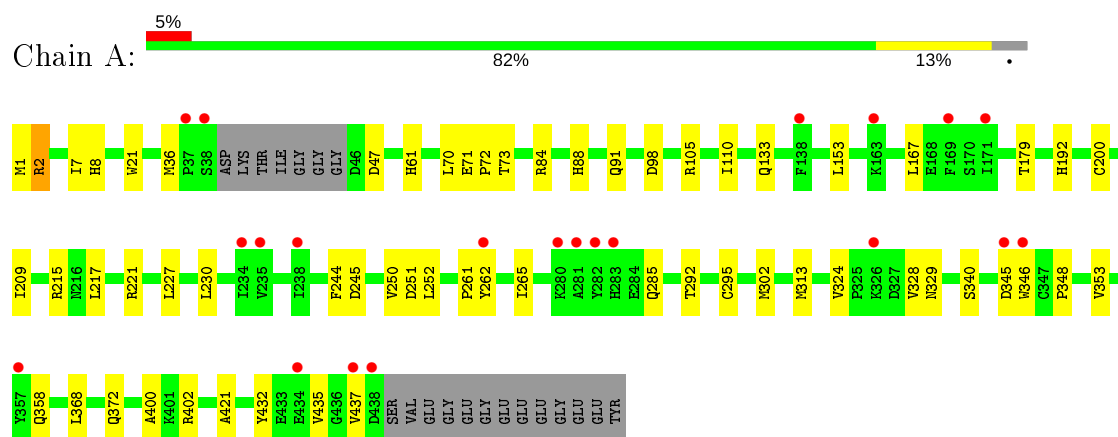
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	221	Total	O	0	0
			221	221		
8	B	146	Total	O	0	1
			147	147		
8	C	146	Total	O	0	0
			146	146		
8	D	182	Total	O	0	4
			186	186		
8	E	32	Total	O	0	0
			32	32		

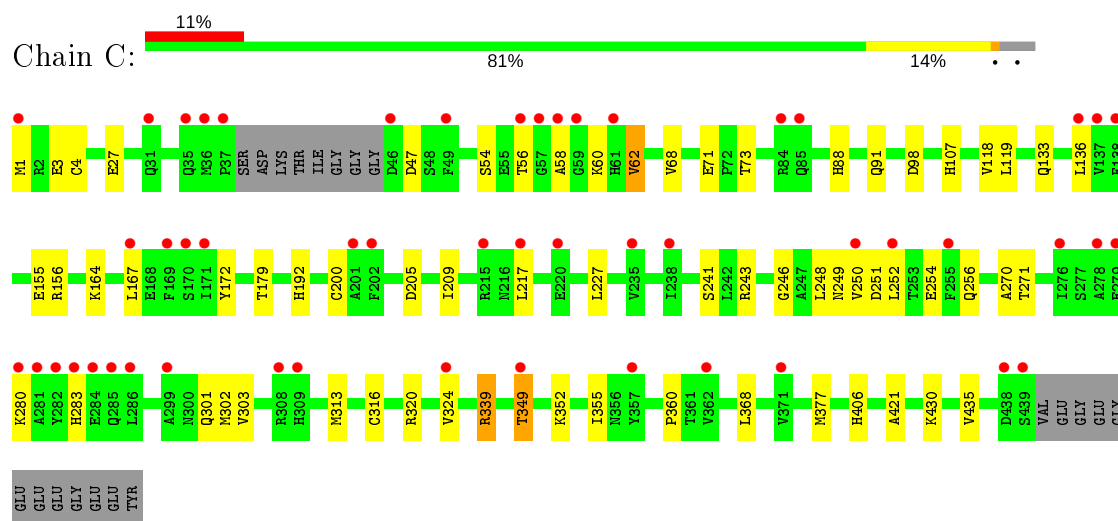
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

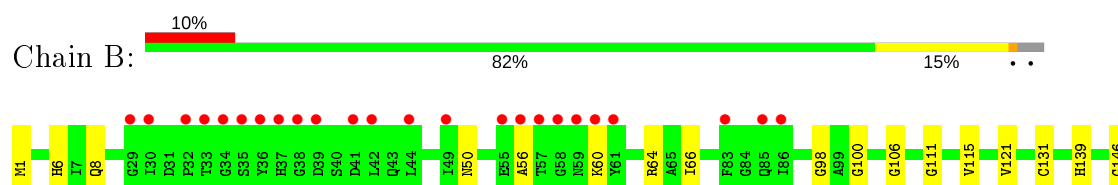
#### • Molecule 1: Tubulin alpha chain

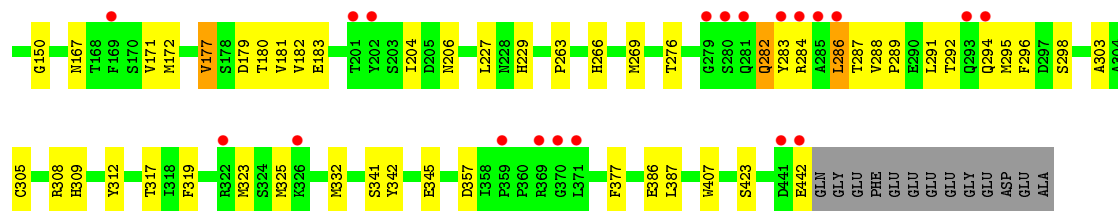


#### • Molecule 1: Tubulin alpha chain

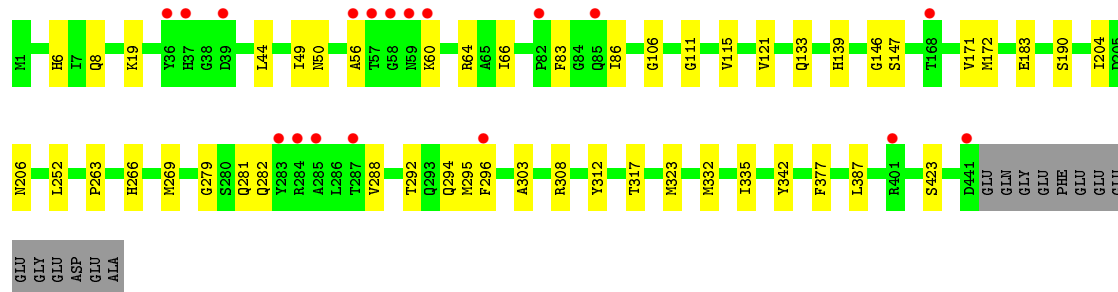
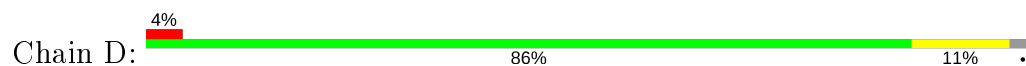


#### • Molecule 2: Tubulin beta chain

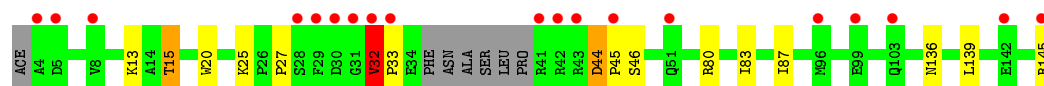
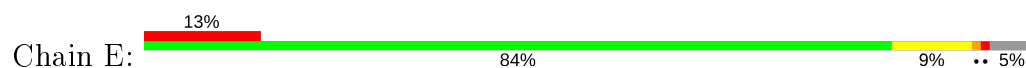




• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.45Å 127.24Å 250.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.14 – 2.10 43.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.14-2.10) 94.7 (43.14-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.171 , 0.201 0.183 , 0.214	Depositor DCC
$R_{free}$ test set	5924 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, GTP, MG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	1/3474 (0.0%)	0.66	0/4715
1	C	0.50	0/3453	0.68	0/4689
2	B	0.51	0/3531	0.69	0/4782
2	D	0.51	0/3543	0.70	1/4797 (0.0%)
3	E	0.48	0/1107	0.69	0/1475
All	All	0.51	1/15108 (0.0%)	0.68	1/20458 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	SER	CB-OG	8.83	1.53	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	281	GLN	C-N-CA	6.17	137.12	121.70

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	3394	0	3306	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3366	0	3279	38	0
2	B	3443	0	3293	47	0
2	D	3445	0	3305	41	0
3	E	1096	0	1091	9	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	D	60	0	24	5	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
6	E	5	0	0	0	0
7	B	28	0	12	2	0
8	A	221	0	0	2	0
8	B	147	0	0	1	0
8	C	146	0	0	0	0
8	D	186	0	0	1	0
8	E	32	0	0	0	0
All	All	15686	0	14334	163	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 6.

All (163) 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:206:ASN:HD21	4:D:600[B]:GTP:HN22	1.06	0.99
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.47	0.95
2:D:292:THR:HG22	2:D:335:ILE:HD12	1.49	0.91
2:B:206:ASN:HD21	7:B:600:GDP:HN22	1.18	0.88
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.21	0.80
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.63	0.80
1:A:71:GLU:OE2	1:A:73:THR:HB	1.84	0.75
2:D:263:PRO:O	2:D:266:HIS:HD2	1.72	0.72
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.37	0.72
2:B:1:MET:N	2:B:131:CYS:SG	2.62	0.72
1:C:71:GLU:OE2	1:C:73:THR:HB	1.91	0.71
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:HD21	4:D:600[B]:GTP:N2	1.87	0.69
2:B:263:PRO:O	2:B:266:HIS:HD2	1.76	0.68
1:A:245:ASP:HB3	3:E:15:THR:HG22	1.76	0.68
3:E:44:ASP:H	3:E:45:PRO:HA	1.57	0.68
3:E:32:VAL:HB	3:E:33:PRO:CD	2.24	0.67
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.29	0.67
2:D:50:ASN:O	2:D:64:ARG:NH2	2.29	0.66
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.80	0.65
2:D:206:ASN:ND2	4:D:600[B]:GTP:HN22	1.89	0.64
1:A:133[B]:GLN:HG3	1:A:252:LEU:HB2	1.79	0.63
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.63	0.63
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.47	0.62
1:A:221:ARG:HG2	2:B:325:MET:HB3	1.82	0.62
2:B:312:TYR:CE2	2:B:377[A]:PHE:HZ	2.18	0.61
2:D:312:TYR:CE2	2:D:377[A]:PHE:HZ	2.19	0.61
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.84	0.61
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.83	0.61
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.47	0.61
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.37	0.60
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.65	0.60
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.84	0.60
1:C:339:ARG:H	1:C:339:ARG:HD3	1.67	0.59
2:D:133:GLN:NE2	2:D:252:LEU:H	2.00	0.59
2:D:295[A]:MET:CG	2:D:377[A]:PHE:HB2	2.33	0.59
2:B:295[A]:MET:CG	2:B:377[A]:PHE:HB2	2.34	0.58
2:D:139:HIS:HD2	2:D:146:GLY:O	1.87	0.58
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.85	0.57
2:B:282:GLN:CB	2:B:283:TYR:HA	2.35	0.56
1:C:313:MET:SD	1:C:435:VAL:CG1	2.93	0.56
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.39	0.56
1:C:54:SER:OG	1:C:62:VAL:HG13	2.06	0.56
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.24	0.56
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.41	0.55
1:A:71:GLU:OE2	1:A:73:THR:CB	2.53	0.55
1:C:246:GLY:H	1:C:249:ASN:HD21	1.52	0.55
1:A:262:TYR:CE1	1:A:346:TRP:CH2	2.94	0.55
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.89	0.55
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.89	0.55
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.54
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.25	0.54
2:B:286:LEU:HD12	2:B:291:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:THR:HG21	2:D:332:MET:HE1	1.89	0.54
2:D:206:ASN:HD21	4:D:600[A]:GTP:HN22	1.53	0.54
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.54
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.90	0.54
2:B:50:ASN:O	2:B:64:ARG:NH2	2.32	0.53
1:A:285:GLN:NE2	1:A:372:GLN:H	2.05	0.53
2:B:106:GLY:O	2:B:111:GLY:HA3	2.10	0.52
2:D:292:THR:HG22	2:D:335:ILE:CD1	2.31	0.52
2:B:100:GLY:HA2	1:C:254:GLU:HG3	1.91	0.52
2:B:269:MET:CE	2:B:305:CYS:HB2	2.40	0.52
1:A:261:PRO:HD2	8:A:692:HOH:O	2.10	0.52
2:B:206:ASN:HD21	7:B:600:GDP:N2	1.99	0.52
2:D:317:THR:HG21	2:D:332:MET:CE	2.40	0.52
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.92	0.51
2:B:66:ILE:HG12	2:B:121:VAL:HG12	1.90	0.51
2:B:269:MET:HE3	2:B:305:CYS:HB2	1.92	0.51
1:C:313:MET:SD	1:C:435:VAL:HG11	2.51	0.51
2:B:139:HIS:HD2	2:B:146:GLY:O	1.94	0.51
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.94	0.50
2:D:147[A]:SER:HB2	2:D:190:SER:HG	1.76	0.50
3:E:80:ARG:O	3:E:83:ILE:HG22	2.10	0.50
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.47	0.50
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.94	0.50
2:B:317:THR:HG21	2:B:332:MET:HE1	1.93	0.49
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.49
1:A:133[A]:GLN:OE1	1:A:251:ASP:HB2	2.12	0.49
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.93	0.49
2:D:288:VAL:HG22	2:D:323:MET:HE3	1.93	0.49
2:B:317:THR:HG21	2:B:332:MET:CE	2.42	0.49
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.47	0.49
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.94	0.48
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.93	0.48
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.36	0.48
2:B:295[A]:MET:HG3	2:B:377[A]:PHE:HB2	1.96	0.48
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.94	0.48
2:D:106:GLY:O	2:D:111:GLY:HA3	2.13	0.48
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.48
2:B:292:THR:HG22	2:B:319:PHE:CZ	2.49	0.47
2:D:296[B]:PHE:HB3	2:D:308:ARG:HE	1.79	0.47
2:B:296[B]:PHE:CE1	2:B:342:TYR:HB2	2.50	0.47
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HG2	1:A:110:ILE:HD13	1.96	0.47
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.32	0.47
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:HB2	1.96	0.47
2:B:229:HIS:HE1	2:B:276:THR:HG23	1.79	0.47
2:B:296[B]:PHE:HB3	2:B:308:ARG:HE	1.78	0.47
1:C:56:THR:HG23	1:C:58:ALA:H	1.79	0.47
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.61	0.47
1:C:217:LEU:HD21	1:C:368:LEU:HD23	1.96	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.55	0.47
2:D:56:ALA:HB3	2:D:60:LYS:HG3	1.97	0.46
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.98	0.46
1:C:192:HIS:CG	1:C:421:ALA:HA	2.51	0.46
1:C:71:GLU:OE2	1:C:73:THR:CB	2.61	0.46
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.46
1:A:88:HIS:H	1:A:91:GLN:NE2	2.14	0.46
2:D:133:GLN:HE22	2:D:252:LEU:H	1.64	0.45
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.98	0.45
3:E:83:ILE:O	3:E:87:ILE:HG12	2.16	0.45
1:C:133:GLN:HE22	1:C:251:ASP:HB2	1.81	0.45
2:D:312:TYR:CE2	2:D:377[A]:PHE:CZ	3.02	0.45
2:B:177:VAL:HG11	2:B:227:LEU:HD21	1.98	0.45
2:B:312:TYR:CE2	2:B:377[A]:PHE:CZ	3.02	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.17	0.45
2:D:183:GLU:OE2	4:D:600[B]:GTP:H3'	2.16	0.45
1:A:402:ARG:NH2	8:A:723:HOH:O	2.51	0.44
1:A:88:HIS:H	1:A:91:GLN:HE21	1.65	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.44
2:D:139:HIS:CD2	2:D:146:GLY:O	2.69	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.44
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.82	0.44
2:B:180:THR:HG23	2:B:183:GLU:HG3	1.99	0.44
2:B:181:VAL:HG13	2:B:182:VAL:HG13	1.99	0.43
1:C:107:HIS:CE1	1:C:155:GLU:OE2	2.67	0.43
1:A:2:ARG:HB2	1:A:133[A]:GLN:CD	2.39	0.43
2:D:19:LYS:HE3	8:D:723:HOH:O	2.18	0.43
1:A:244:PHE:CG	1:A:358:GLN:HG3	2.52	0.43
1:C:133:GLN:NE2	1:C:252:LEU:H	2.16	0.43
1:C:68:VAL:HG11	1:C:118:VAL:HG21	2.01	0.43
2:D:296[B]:PHE:CE1	2:D:342:TYR:HB2	2.54	0.43
1:C:271:THR:HG22	1:C:301:GLN:HA	2.00	0.43
1:C:56:THR:HG22	1:C:60:LYS:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:CYS:HA	1:C:352:LYS:O	2.19	0.43
2:D:292:THR:CG2	2:D:335:ILE:HD12	2.34	0.43
1:A:400:ALA:HB2	2:B:442:GLU:HG2	2.01	0.43
2:B:309:HIS:CD2	2:B:386:GLU:OE1	2.67	0.43
3:E:136:ASN:HA	3:E:139:LEU:HD12	2.01	0.43
1:C:271:THR:OG1	1:C:377:MET:HB3	2.19	0.42
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.82	0.42
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.37	0.42
1:A:261:PRO:HG3	1:A:313:MET:HG3	2.00	0.42
2:D:83:PHE:O	2:D:86:ILE:HG22	2.20	0.42
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.00	0.42
2:B:167:ASN:ND2	8:B:689:HOH:O	2.52	0.42
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.02	0.42
2:D:44:LEU:HA	2:D:49:ILE:HB	2.02	0.42
1:A:262:TYR:HE1	1:A:346:TRP:CZ2	2.37	0.42
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.02	0.41
1:A:292:THR:O	1:A:295:CYS:HB2	2.20	0.41
2:B:345:GLU:HG2	2:B:345:GLU:H	1.62	0.41
1:A:36:MET:HG2	1:A:61:HIS:CD2	2.56	0.41
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.41
1:C:320:ARG:HG3	1:C:360:PRO:HD3	2.02	0.41
2:B:146:GLY:O	2:B:150:GLY:HA3	2.21	0.41
2:D:49:ILE:HD12	2:D:49:ILE:HA	1.92	0.41
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.86	0.40
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:CB	2.51	0.40
2:B:181:VAL:HG23	1:C:349:THR:O	2.21	0.40
2:D:296[B]:PHE:CE1	2:D:342:TYR:CB	3.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/451 (95%)	417 (97%)	11 (3%)	1 (0%)	47	49
1	C	430/451 (95%)	414 (96%)	13 (3%)	3 (1%)	22	18
2	B	437/445 (98%)	418 (96%)	14 (3%)	5 (1%)	14	9
2	D	439/445 (99%)	425 (97%)	12 (3%)	2 (0%)	29	26
3	E	132/143 (92%)	125 (95%)	5 (4%)	2 (2%)	10	5
All	All	1867/1935 (96%)	1799 (96%)	55 (3%)	13 (1%)	22	18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	VAL
1	C	47	ASP
2	D	282	GLN
3	E	32	VAL
2	B	282	GLN
2	B	284	ARG
2	B	286	LEU
1	C	280	LYS
1	C	283	HIS
2	D	279	GLY
3	E	44	ASP
2	B	177	VAL
2	B	98	GLY

### 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	367/379 (97%)	357 (97%)	10 (3%)	44	48
1	C	363/379 (96%)	352 (97%)	11 (3%)	41	44
2	B	378/385 (98%)	370 (98%)	8 (2%)	53	59
2	D	381/385 (99%)	377 (99%)	4 (1%)	76	82
3	E	114/125 (91%)	108 (95%)	6 (5%)	22	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1603/1653 (97%)	1564 (98%)	39 (2%)	50 53

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	47	ASP
1	A	84	ARG
1	A	179	THR
1	A	215	ARG
1	A	250	VAL
1	A	324	VAL
1	A	345	ASP
1	A	435	VAL
2	B	115	VAL
2	B	179	ASP
2	B	294[A]	GLN
2	B	294[B]	GLN
2	B	298	SER
2	B	341	SER
2	B	357	ASP
2	B	423	SER
1	C	1[A]	MET
1	C	1[B]	MET
1	C	62	VAL
1	C	164	LYS
1	C	179	THR
1	C	241	SER
1	C	250	VAL
1	C	324	VAL
1	C	339	ARG
1	C	349	THR
1	C	430	LYS
2	D	115	VAL
2	D	294[A]	GLN
2	D	294[B]	GLN
2	D	423	SER
3	E	13	LYS
3	E	15	THR
3	E	25	LYS
3	E	32	VAL

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Mol	Chain	Res	Type
3	E	46	SER
3	E	145	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	ASN
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	101	ASN
2	B	136	GLN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	300	ASN
2	B	309	HIS
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	15	GLN
1	C	91	GLN
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	301	GLN
1	C	329	ASN
1	C	342	GLN
1	C	358	GLN
2	D	6	HIS
2	D	8	GLN

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Mol	Chain	Res	Type
2	D	14	ASN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	197	ASN
2	D	206	ASN
2	D	266	HIS
2	D	300	ASN
2	D	385	GLN
2	D	433	GLN
2	D	436	GLN
3	E	111	ASN
3	E	124	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	SO4	A	454	-	4,4,4	0.32	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	A	452	-	4,4,4	0.53	0	6,6,6	0.16	0
6	SO4	A	455	-	4,4,4	0.18	0	6,6,6	0.11	0
6	SO4	C	452	-	4,4,4	0.17	0	6,6,6	0.13	0
6	SO4	C	453	-	4,4,4	0.18	0	6,6,6	0.11	0
6	SO4	B	457	-	4,4,4	0.16	0	6,6,6	0.09	0
6	SO4	D	457	-	4,4,4	0.23	0	6,6,6	0.14	0
7	GDP	B	600	-	24,30,30	1.36	4 (16%)	31,47,47	2.18	10 (32%)
4	GTP	D	600[B]	5	26,30,34	1.18	3 (11%)	33,47,54	2.18	11 (33%)
6	SO4	A	453	-	4,4,4	0.22	0	6,6,6	0.08	0
4	GTP	D	600[A]	5	26,34,34	1.30	3 (11%)	33,54,54	2.39	11 (33%)
6	SO4	D	456	-	4,4,4	0.21	0	6,6,6	0.24	0
6	SO4	E	146	-	4,4,4	0.12	0	6,6,6	0.08	0
6	SO4	B	456	-	4,4,4	0.28	0	6,6,6	0.22	0
4	GTP	C	600	5	26,34,34	1.28	3 (11%)	33,54,54	2.19	11 (33%)
4	GTP	A	600	5	26,34,34	1.39	6 (23%)	33,54,54	1.98	9 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	D	600[A]	5	-	6/18/38/38	0/3/3/3
7	GDP	B	600	-	-	4/12/32/32	0/3/3/3
4	GTP	C	600	5	-	6/18/38/38	0/3/3/3
4	GTP	D	600[B]	5	-	3/18/32/38	0/3/3/3
4	GTP	A	600	5	-	6/18/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	C6-N1	3.31	1.38	1.33
7	B	600	GDP	C6-N1	3.23	1.38	1.33
4	D	600[A]	GTP	C2-N2	2.87	1.39	1.33
7	B	600	GDP	O4'-C1'	2.79	1.45	1.41
4	D	600[A]	GTP	O4'-C1'	2.77	1.44	1.41
7	B	600	GDP	C8-N7	-2.68	1.29	1.34
4	D	600[B]	GTP	O4'-C1'	2.57	1.44	1.41
4	C	600	GTP	O4'-C4'	2.56	1.50	1.45
4	A	600	GTP	C6-C5	2.50	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	600[A]	GTP	O6-C6	-2.34	1.18	1.24
4	A	600	GTP	C2'-C1'	2.32	1.57	1.53
4	C	600	GTP	C6-C5	2.31	1.45	1.41
4	A	600	GTP	C8-N7	-2.24	1.30	1.34
4	C	600	GTP	C6-N1	2.20	1.36	1.33
4	D	600[B]	GTP	C2-N2	2.18	1.38	1.33
4	A	600	GTP	O4'-C1'	2.18	1.44	1.41
4	A	600	GTP	O4'-C4'	2.18	1.49	1.45
4	D	600[B]	GTP	C6-N1	2.08	1.36	1.33
7	B	600	GDP	C6-C5	2.03	1.44	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600[A]	GTP	C6-C5-C4	-5.75	115.31	120.80
4	D	600[A]	GTP	N3-C2-N1	-5.25	120.21	127.22
4	C	600	GTP	C2-N3-C4	4.83	120.87	115.36
4	D	600[B]	GTP	PB-O3B-PG	-4.83	116.26	132.83
4	D	600[B]	GTP	PA-O3A-PB	-4.79	116.38	132.83
7	B	600	GDP	C5-C6-N1	-4.75	116.93	123.43
4	D	600[A]	GTP	C2-N3-C4	4.67	120.69	115.36
4	C	600	GTP	N3-C2-N1	-4.62	121.06	127.22
4	D	600[A]	GTP	PB-O3B-PG	-4.54	117.24	132.83
4	D	600[B]	GTP	N3-C2-N1	-4.39	121.37	127.22
7	B	600	GDP	C6-N1-C2	4.37	122.87	115.93
4	C	600	GTP	C5-C6-N1	-4.32	117.52	123.43
4	D	600[A]	GTP	C6-N1-C2	4.27	122.71	115.93
4	A	600	GTP	C2-N3-C4	4.25	120.22	115.36
4	A	600	GTP	N3-C2-N1	-4.16	121.67	127.22
7	B	600	GDP	N3-C2-N1	-4.15	121.69	127.22
4	A	600	GTP	C6-C5-C4	-4.14	116.85	120.80
4	A	600	GTP	C5-C6-N1	-4.03	117.93	123.43
4	D	600[B]	GTP	C6-N1-C2	3.98	122.25	115.93
4	C	600	GTP	C6-C5-C4	-3.96	117.02	120.80
7	B	600	GDP	C6-C5-C4	-3.86	117.11	120.80
4	D	600[B]	GTP	C5-C6-N1	-3.85	118.16	123.43
4	D	600[A]	GTP	N2-C2-N3	3.84	124.05	117.79
4	C	600	GTP	C6-N1-C2	3.81	121.99	115.93
7	B	600	GDP	C2-N3-C4	3.61	119.48	115.36
4	A	600	GTP	C6-N1-C2	3.47	121.44	115.93
4	D	600[B]	GTP	C2-N3-C4	3.41	119.26	115.36
7	B	600	GDP	PA-O3A-PB	-3.37	121.28	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600[A]	GTP	PA-O3A-PB	-3.36	121.31	132.83
4	D	600[B]	GTP	C6-C5-C4	-3.29	117.66	120.80
4	D	600[B]	GTP	O2G-PG-O3B	3.26	115.57	104.64
7	B	600	GDP	O2B-PB-O3A	3.08	114.98	104.64
4	D	600[A]	GTP	C1'-N9-C4	-3.08	121.22	126.64
4	C	600	GTP	PB-O3B-PG	-3.04	122.41	132.83
4	D	600[B]	GTP	O3G-PG-O3B	-2.82	95.18	104.64
4	C	600	GTP	C4-C5-N7	-2.82	106.46	109.40
4	D	600[A]	GTP	C5-C6-N1	-2.64	119.83	123.43
4	C	600	GTP	PA-O3A-PB	-2.60	123.91	132.83
4	A	600	GTP	C4-C5-N7	-2.49	106.80	109.40
7	B	600	GDP	C4-C5-N7	-2.49	106.81	109.40
4	A	600	GTP	PA-O3A-PB	-2.49	124.29	132.83
4	C	600	GTP	O5'-C5'-C4'	-2.40	100.72	108.99
4	D	600[B]	GTP	N2-C2-N3	2.38	121.66	117.79
4	A	600	GTP	C1'-N9-C4	-2.36	122.50	126.64
4	D	600[A]	GTP	O5'-C5'-C4'	-2.36	100.88	108.99
4	C	600	GTP	C1'-N9-C4	-2.35	122.51	126.64
4	C	600	GTP	C3'-C2'-C1'	2.29	104.42	100.98
4	A	600	GTP	PB-O3B-PG	-2.21	125.25	132.83
4	D	600[A]	GTP	C4-C5-N7	-2.07	107.24	109.40
4	D	600[B]	GTP	O4'-C1'-C2'	-2.07	103.91	106.93
7	B	600	GDP	O5'-C5'-C4'	-2.06	101.89	108.99
7	B	600	GDP	C3'-C2'-C1'	-2.01	97.95	100.98

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	600	GDP	C5'-O5'-PA-O1A
4	D	600[B]	GTP	PB-O3B-PG-O3G
4	D	600[A]	GTP	C5'-O5'-PA-O1A
4	D	600[A]	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	PB-O3B-PG-O3G
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	C5'-O5'-PA-O1A
4	A	600	GTP	C5'-O5'-PA-O2A
4	D	600[A]	GTP	PB-O3B-PG-O1G
4	D	600[A]	GTP	C5'-O5'-PA-O3A
7	B	600	GDP	C5'-O5'-PA-O2A

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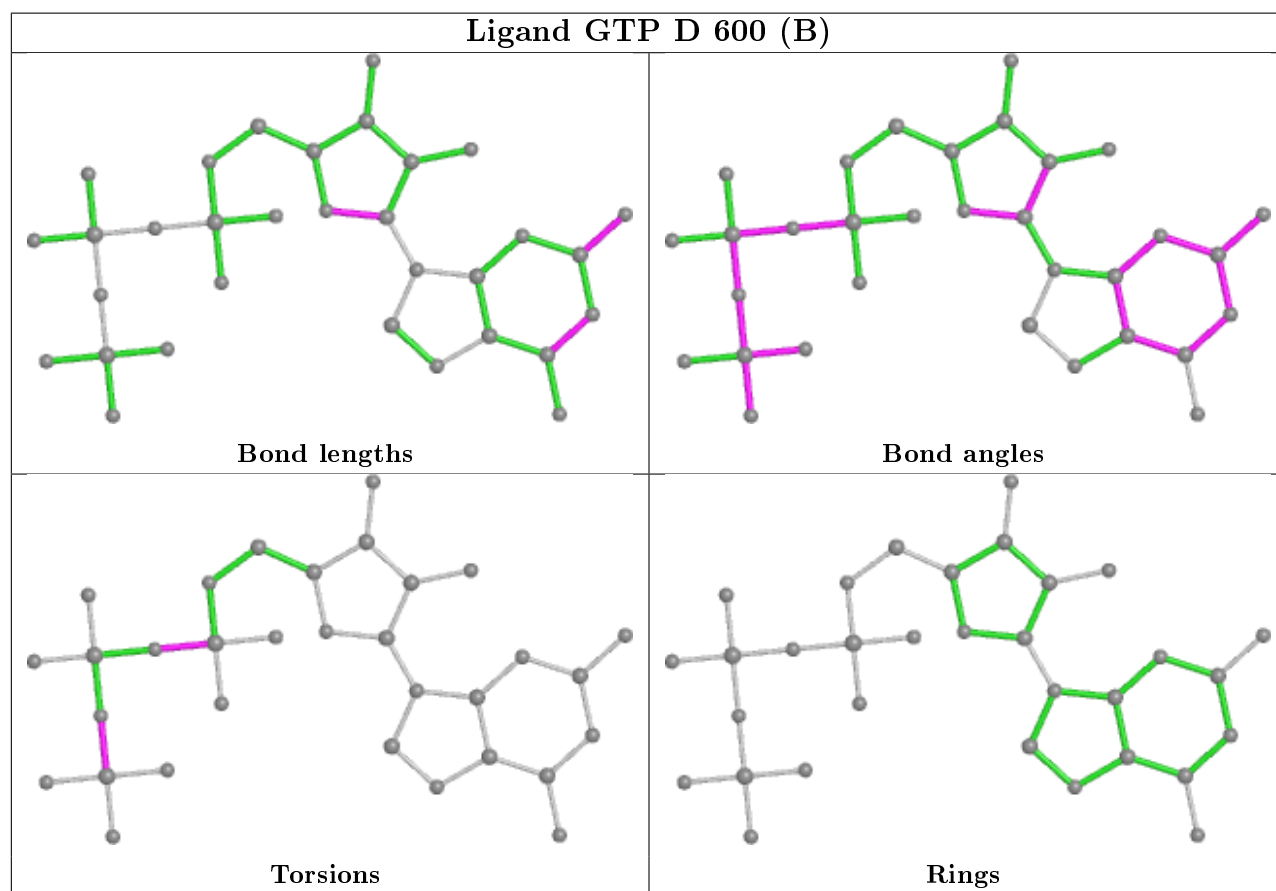
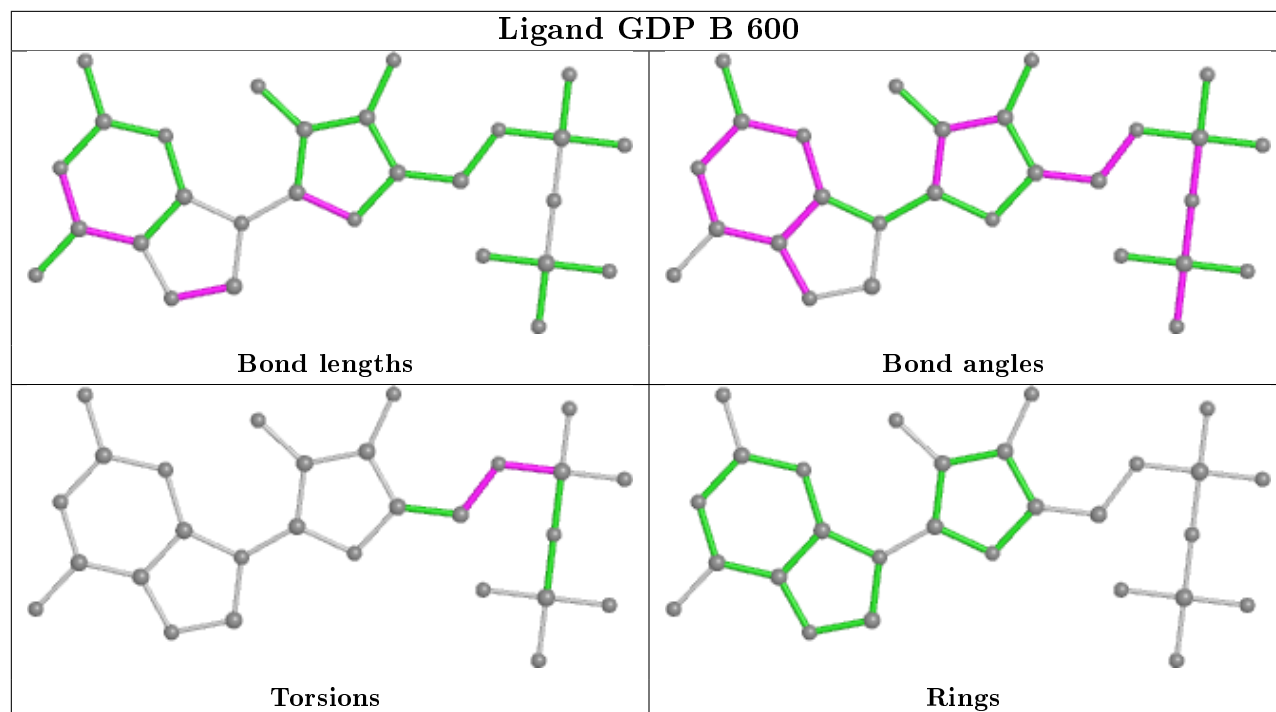
Mol	Chain	Res	Type	Atoms
4	D	600[B]	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
4	A	600	GTP	PB-O3A-PA-O2A
4	D	600[A]	GTP	PB-O3B-PG-O2G
4	D	600[A]	GTP	PB-O3B-PG-O3G
7	B	600	GDP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O3A
4	D	600[B]	GTP	PB-O3A-PA-O1A
4	C	600	GTP	PB-O3A-PA-O1A
4	A	600	GTP	PB-O3A-PA-O1A
7	B	600	GDP	C4'-C5'-O5'-PA

There are no ring outliers.

3 monomers are involved in 7 short contacts:

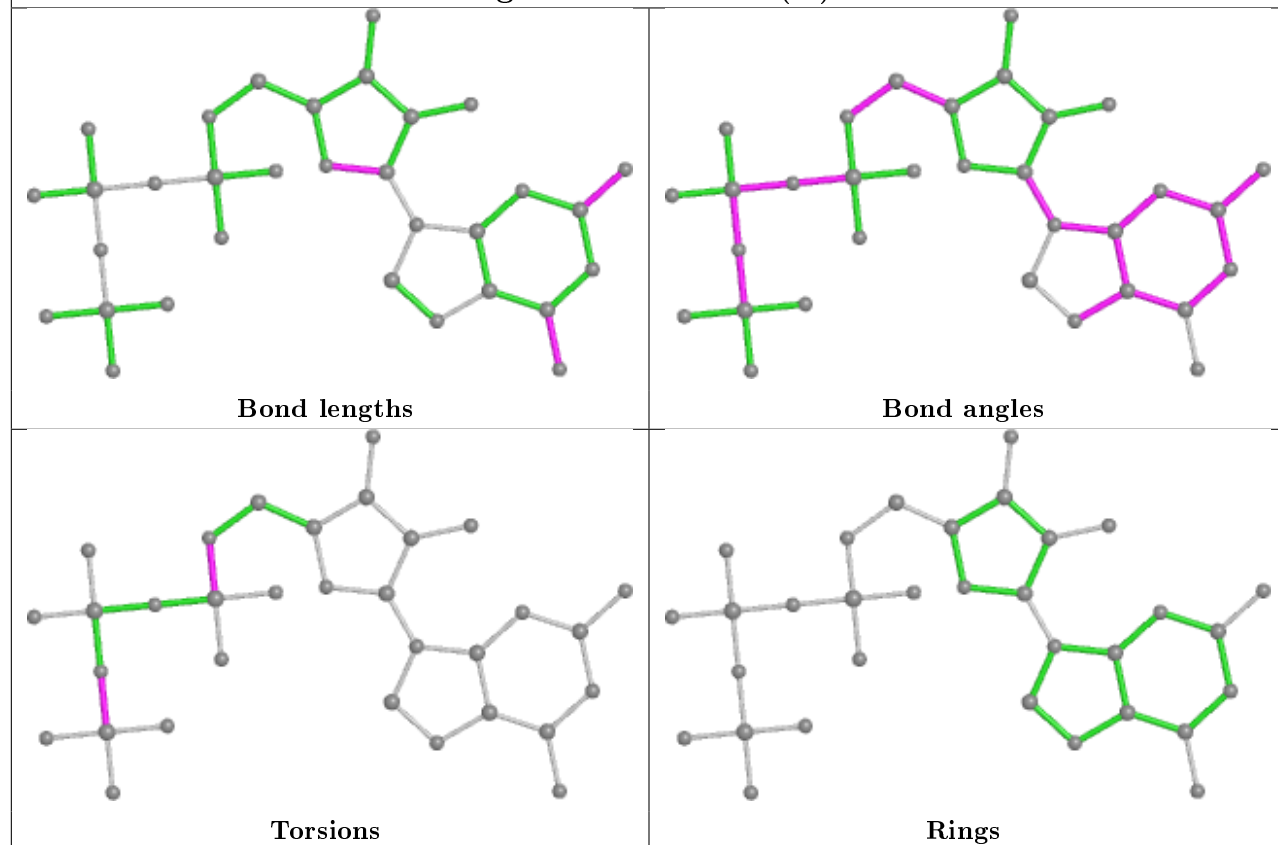
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	600	GDP	2	0
4	D	600[B]	GTP	4	0
4	D	600[A]	GTP	1	0

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.

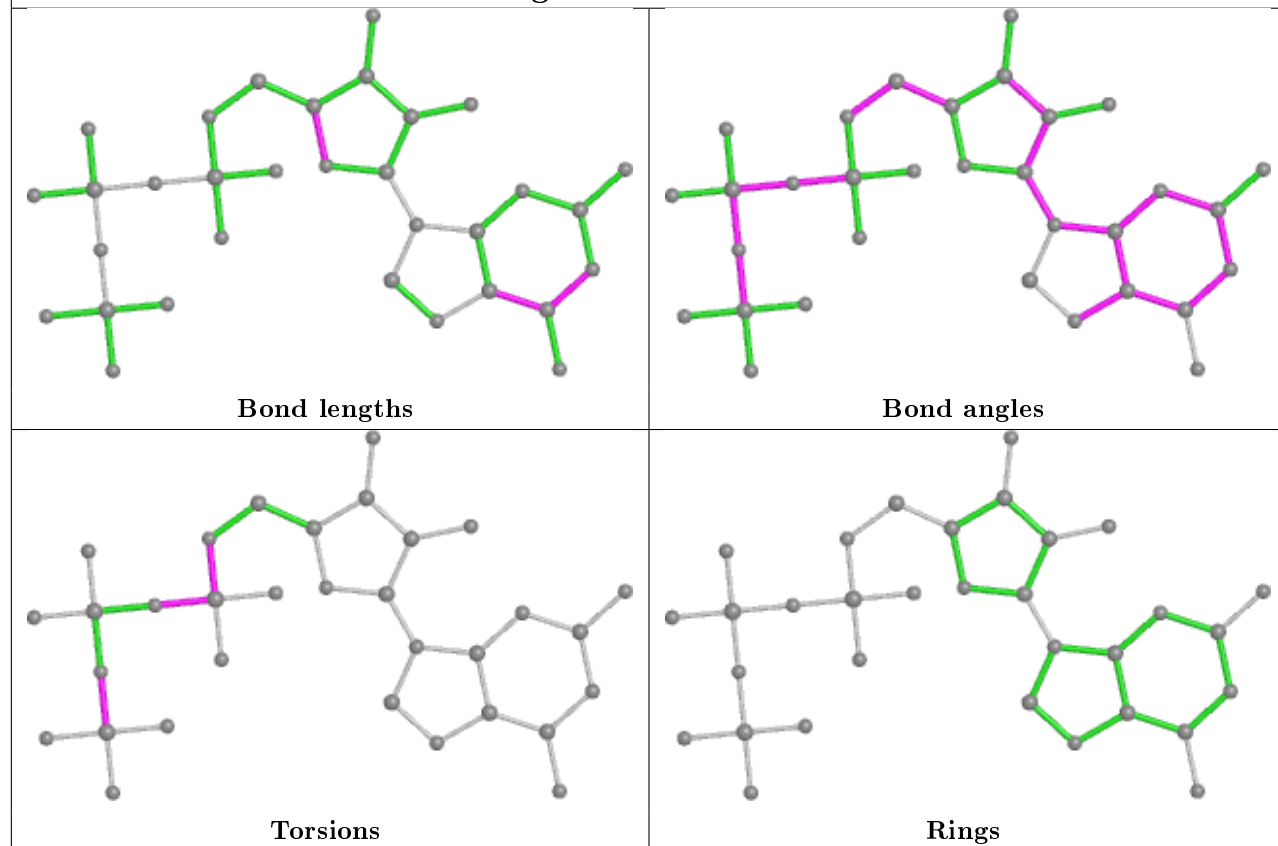


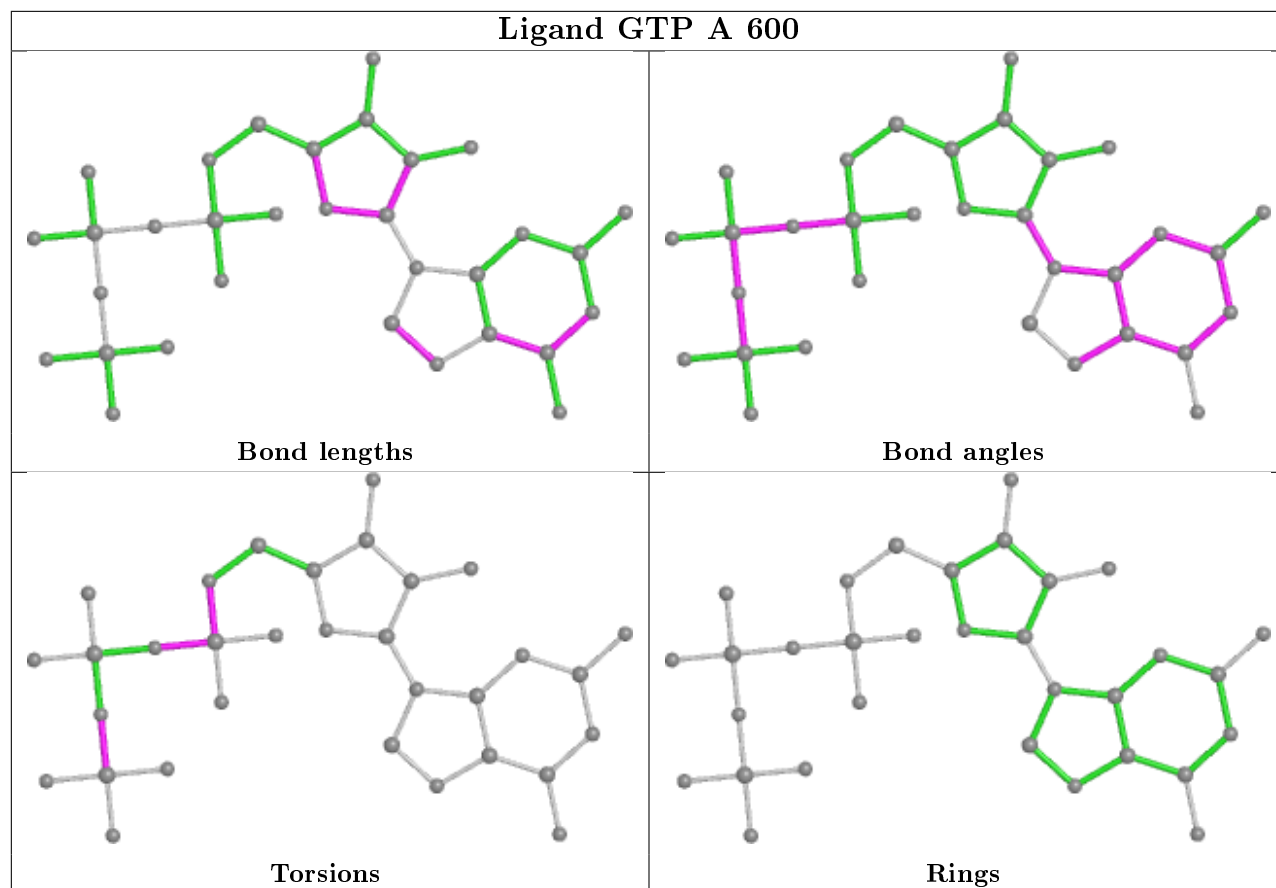


## Ligand GTP D 600 (A)



## Ligand GTP C 600





## 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	431/451 (95%)	0.13	21 (4%) 29 35	30, 45, 72, 130	0
1	C	431/451 (95%)	0.51	51 (11%) 4 5	31, 53, 88, 115	0
2	B	432/445 (97%)	0.41	44 (10%) 6 8	30, 48, 90, 117	4 (0%)
2	D	431/445 (96%)	0.09	18 (4%) 36 42	28, 41, 78, 111	4 (0%)
3	E	136/143 (95%)	1.04	19 (13%) 2 3	43, 62, 110, 138	0
All	All	1861/1935 (96%)	0.34	153 (8%) 11 15	28, 48, 86, 138	8 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	32	VAL	12.1
3	E	31	GLY	10.0
1	A	282	TYR	9.2
2	D	59	ASN	8.2
2	D	283	TYR	7.7
1	C	284	GLU	7.7
1	C	283	HIS	7.4
2	B	57	THR	7.3
2	B	59	ASN	7.2
2	B	283	TYR	7.0
3	E	33	PRO	6.6
1	A	281	ALA	6.2
2	B	285	ALA	6.0
2	D	57	THR	5.9
3	E	41	ARG	5.8
3	E	4	ALA	5.8
1	A	437	VAL	5.8
2	B	280	SER	5.7
2	B	37	HIS	5.5
1	A	438	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	39	ASP	5.2
2	B	56	ALA	5.2
3	E	42	ARG	5.1
1	C	439	SER	5.1
2	B	286	LEU	5.0
2	B	36	TYR	4.9
2	B	441	ASP	4.8
1	A	346	TRP	4.8
2	B	279	GLY	4.6
1	C	276	ILE	4.6
2	B	371	LEU	4.5
3	E	145	ARG	4.5
2	B	42	LEU	4.4
1	C	36	MET	4.2
1	C	282	TYR	4.2
2	D	39	ASP	4.2
1	A	283	HIS	4.2
1	C	357	TYR	4.1
3	E	29	PHE	4.1
2	B	60	LYS	4.0
2	D	284	ARG	4.0
2	B	58	GLY	4.0
2	D	58	GLY	4.0
2	B	284	ARG	4.0
1	C	281	ALA	3.9
1	A	37	PRO	3.9
1	C	169	PHE	3.9
3	E	45	PRO	3.7
2	B	29	GLY	3.7
2	B	35	SER	3.7
1	C	167	LEU	3.6
1	A	38	SER	3.6
2	B	41	ASP	3.6
3	E	43	ARG	3.6
1	C	137	VAL	3.6
1	C	46	ASP	3.6
2	B	369	ARG	3.5
2	B	38	GLY	3.5
2	B	293[A]	GLN	3.5
1	C	278	ALA	3.4
1	A	262	TYR	3.4
3	E	96	MET	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	44	LEU	3.3
1	C	201	ALA	3.3
2	B	49	ILE	3.2
1	C	309	HIS	3.2
3	E	5	ASP	3.2
1	C	202	PHE	3.2
1	C	324	VAL	3.1
1	C	215	ARG	3.1
2	B	85	GLN	3.1
2	D	285	ALA	3.0
1	C	56	THR	3.0
3	E	30	ASP	3.0
1	C	286	LEU	3.0
1	C	280	LYS	3.0
3	E	51	GLN	3.0
1	C	58	ALA	3.0
2	B	281	GLN	3.0
1	C	37	PRO	3.0
2	B	61	TYR	2.9
1	C	349	THR	2.9
3	E	28	SER	2.9
1	C	255	PHE	2.8
1	A	280	LYS	2.8
1	C	362	VAL	2.8
1	C	57	GLY	2.8
1	C	85	GLN	2.8
1	A	169	PHE	2.7
1	C	136	LEU	2.7
1	C	252	LEU	2.7
1	A	235	VAL	2.7
1	A	138	PHE	2.7
1	C	59	GLY	2.7
2	D	37	HIS	2.7
1	C	138	PHE	2.7
2	B	34	GLY	2.7
2	B	32	PRO	2.6
1	C	299	ALA	2.6
2	B	55	GLU	2.6
1	C	438	ASP	2.6
2	B	442	GLU	2.6
1	C	217	LEU	2.6
1	A	171	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	250	VAL	2.5
1	A	345	ASP	2.5
1	C	35	GLN	2.5
1	A	238	ILE	2.5
2	B	30	ILE	2.5
3	E	142	GLU	2.5
2	B	326	LYS	2.5
1	A	234	ILE	2.4
2	B	33	THR	2.4
2	D	56	ALA	2.4
2	D	85	GLN	2.4
1	C	285	GLN	2.3
1	A	163	LYS	2.3
1	C	171	ILE	2.3
2	D	441	ASP	2.3
1	C	238	ILE	2.3
2	B	86	ILE	2.3
2	D	36	TYR	2.3
2	D	401	ARG	2.3
2	D	296[A]	PHE	2.3
1	C	235	VAL	2.2
2	B	359	PRO	2.2
1	C	31	GLN	2.2
2	B	201	THR	2.2
1	C	170	SER	2.2
3	E	103	GLN	2.2
1	C	84	ARG	2.2
2	B	322	ARG	2.2
2	B	83	PHE	2.2
3	E	8	VAL	2.2
1	C	220	GLU	2.1
1	A	357	TYR	2.1
1	C	49	PHE	2.1
2	D	60	LYS	2.1
1	C	1[A]	MET	2.1
2	D	82	PRO	2.1
2	B	370	GLY	2.1
2	B	294[A]	GLN	2.1
1	C	371	VAL	2.1
2	B	169	PHE	2.1
2	B	202	TYR	2.1
1	A	434	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	61	HIS	2.0
1	C	308	ARG	2.0
1	C	279	GLU	2.0
3	E	99	GLU	2.0
2	D	168	THR	2.0
2	D	287	THR	2.0
1	A	326	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

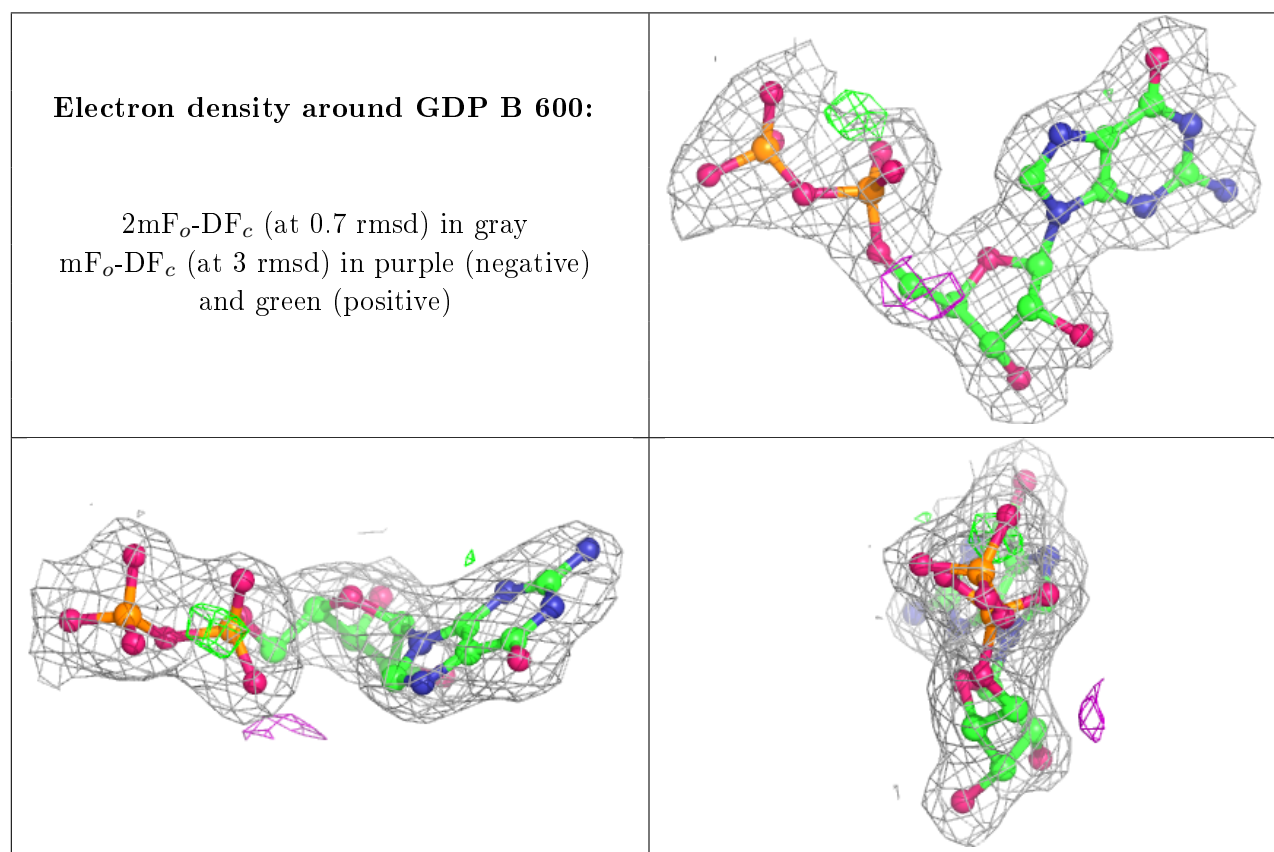
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	C	453	5/5	0.81	0.18	127,132,132,133	0
6	SO4	A	453	5/5	0.82	0.21	110,114,116,117	0
6	SO4	D	457	5/5	0.86	0.13	112,116,117,117	0
6	SO4	A	455	5/5	0.87	0.21	125,129,130,131	0
6	SO4	B	457	5/5	0.89	0.15	129,133,134,135	0
6	SO4	B	456	5/5	0.93	0.10	94,98,99,100	0
6	SO4	E	146	5/5	0.94	0.20	103,107,108,109	0
5	MG	D	601	1/1	0.94	0.14	38,38,38,38	1
6	SO4	A	452	5/5	0.95	0.10	72,75,76,79	0
6	SO4	A	454	5/5	0.96	0.07	84,88,89,89	0
6	SO4	C	452	5/5	0.96	0.09	80,84,85,86	0
7	GDP	B	600	28/28	0.98	0.12	37,39,41,42	0
5	MG	A	601	1/1	0.98	0.17	42,42,42,42	0
4	GTP	C	600	32/32	0.98	0.14	34,40,43,45	0
4	GTP	D	600[B]	28/32	0.99	0.11	30,32,35,35	28
4	GTP	D	600[A]	32/32	0.99	0.11	26,29,35,35	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	D	456	5/5	0.99	0.08	60,64,64,66	0
4	GTP	A	600	32/32	0.99	0.15	31,33,36,38	0
5	MG	C	601	1/1	1.00	0.13	36,36,36,36	0

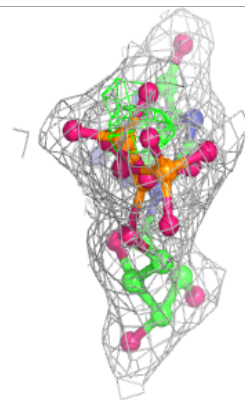
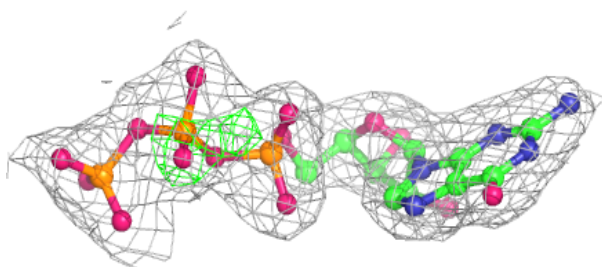
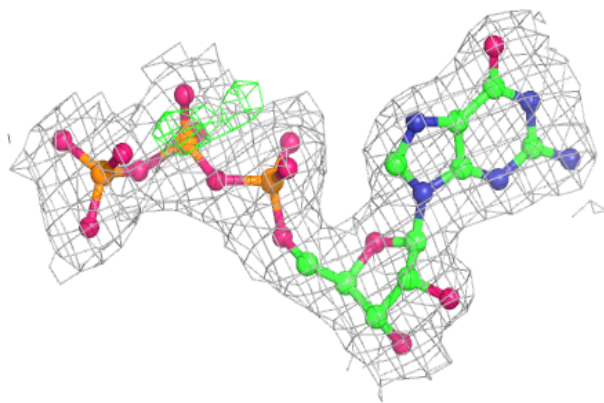
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



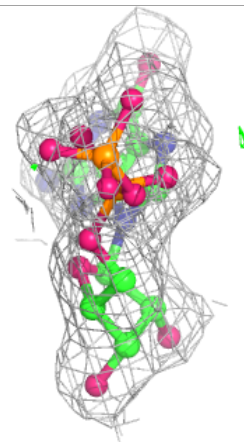
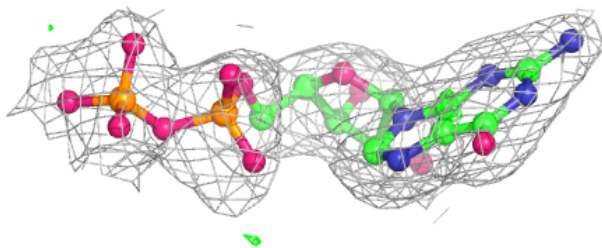
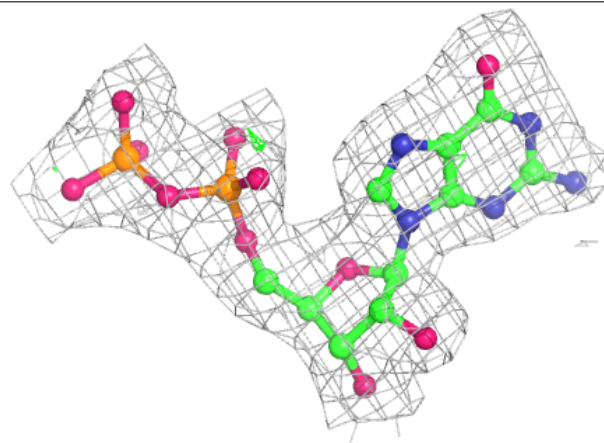


**Electron density around GTP C 600:**

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

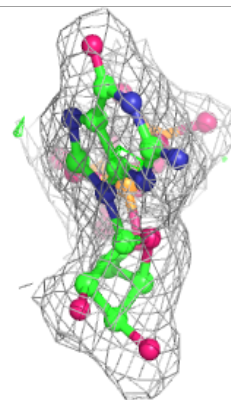
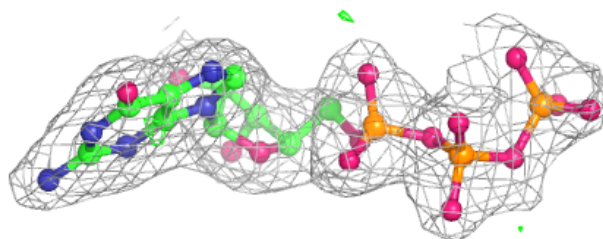
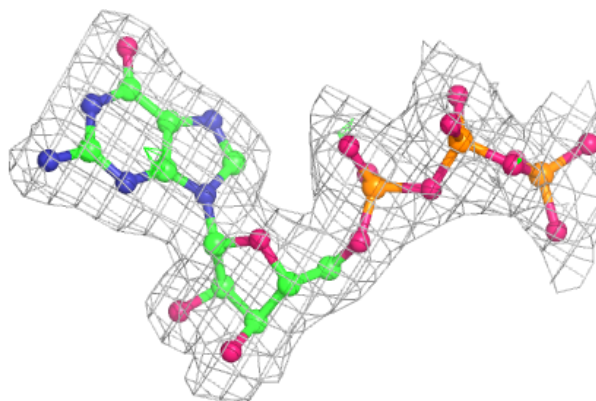
**Electron density around GTP D 600 (B):**

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

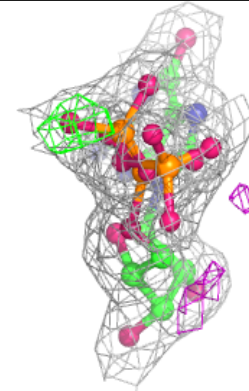
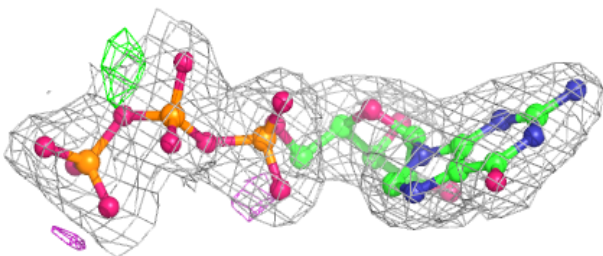
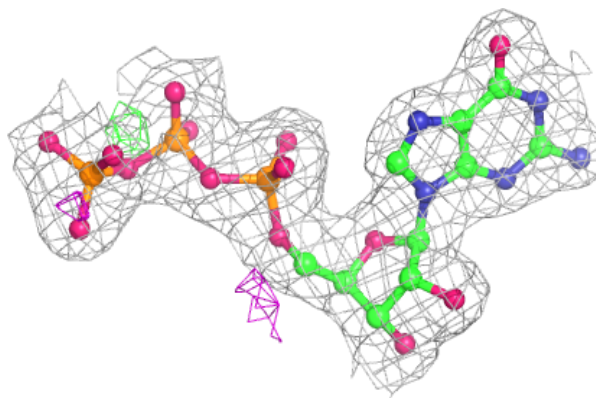


**Electron density around GTP D 600 (A):**

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

**Electron density around GTP A 600:**

$2mF_o-DF_c$  (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.