



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:37 AM BST

PDB ID : 5XKF  
Title : Crystal structure of T2R-TTL-MPC6827 complex  
Authors : Wang, Y.; Yang, J.; Wang, T.; Chen, L.  
Deposited on : 2017-05-07  
Resolution : 2.80 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

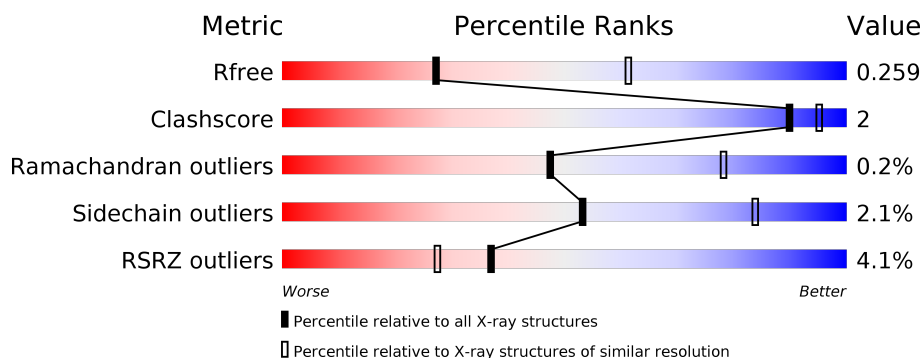
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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>92%</div> <div>5%</div> <div>.</div> </div>
1	C	451	<div> <div>92%</div> <div>6%</div> <div>.</div> </div>
2	B	445	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
2	D	445	<div> <div>5%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
3	E	143	<div> <div>6%</div> <div>82%</div> <div>.</div> <div>15%</div> </div>
4	F	384	<div> <div>11%</div> <div>82%</div> <div>5%</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17488 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	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
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

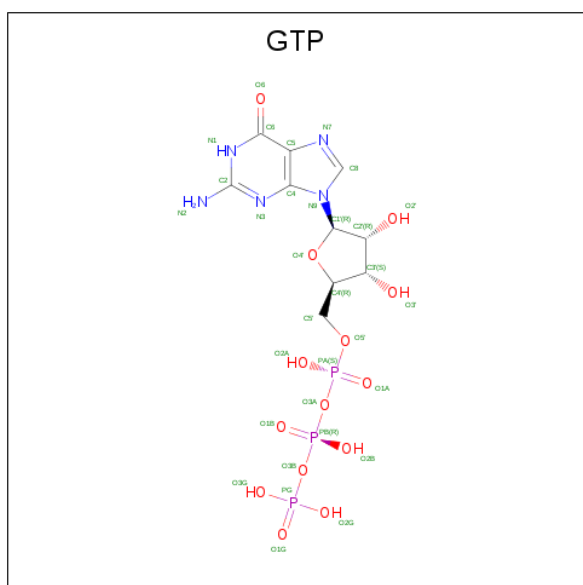
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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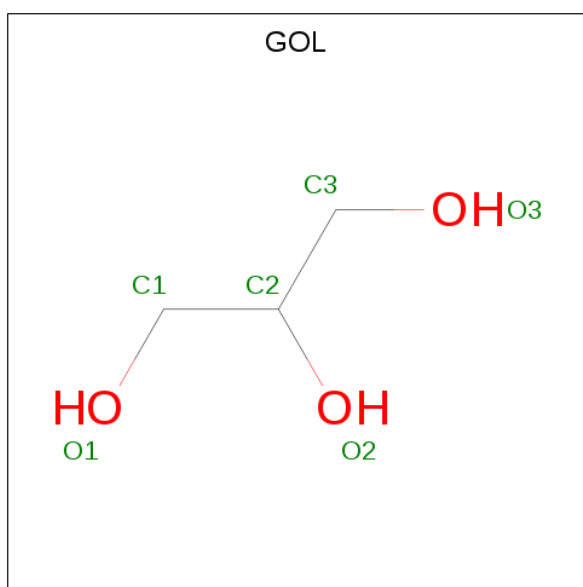
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

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

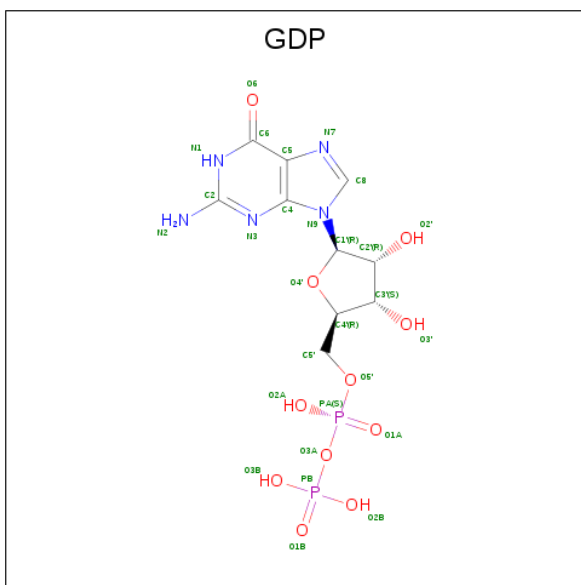
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



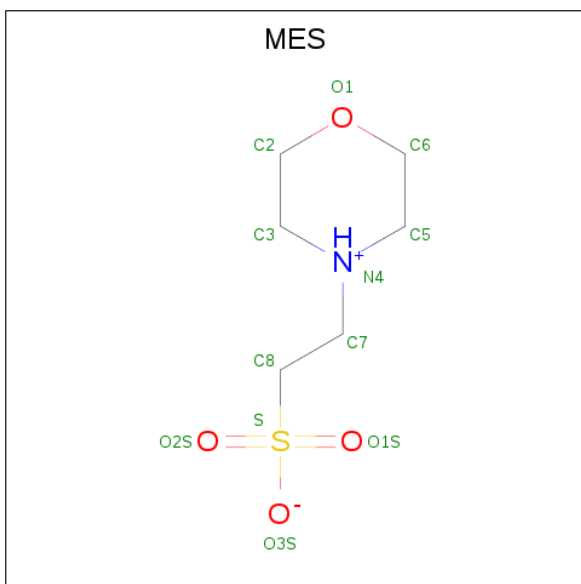
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- 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>).



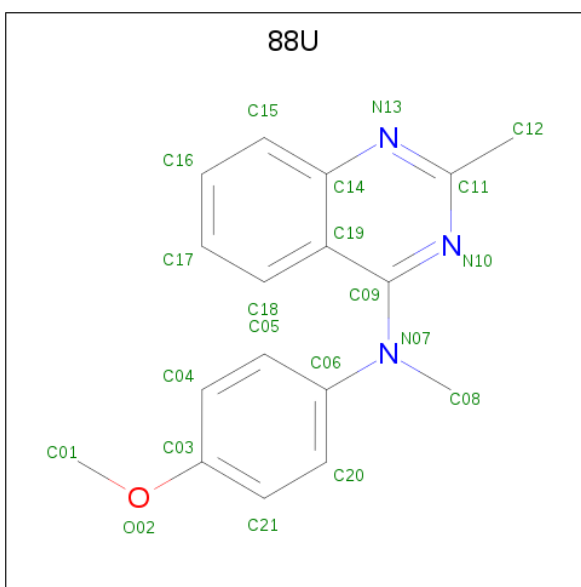
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



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

- Molecule 11 is N-(4-methoxyphenyl)-N,2-dimethyl-quinazolin-4-amine (three-letter code: 88U) (formula:  $C_{17}H_{17}N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			21	17	3	1		
11	D	1	Total	C	N	O	0	0
			21	17	3	1		

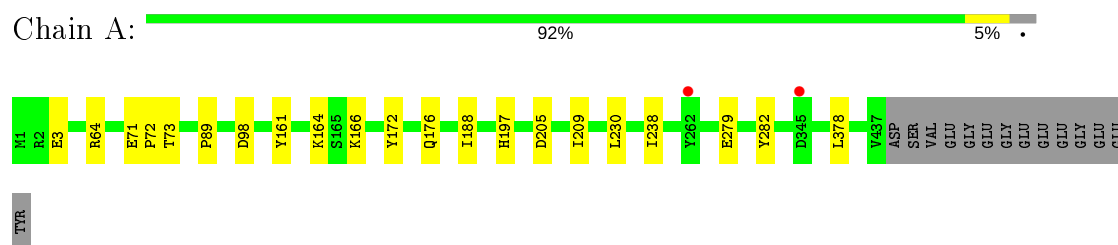
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	4	Total	O	0	0
			4	4		
12	B	11	Total	O	0	0
			11	11		
12	C	11	Total	O	0	0
			11	11		
12	D	4	Total	O	0	0
			4	4		
12	E	1	Total	O	0	0
			1	1		

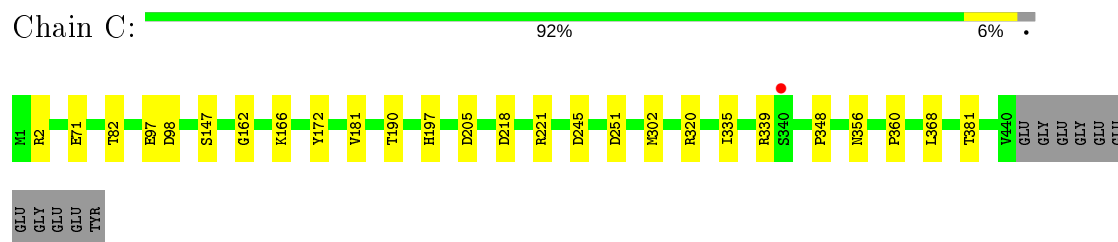
### 3 Residue-property plots [i](#)

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.

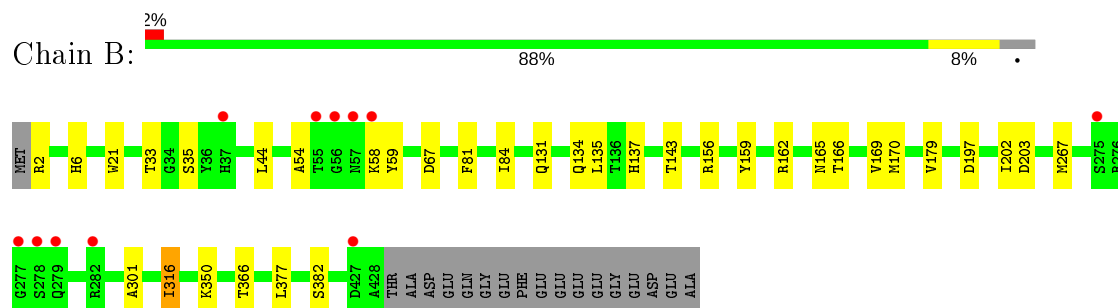
- Molecule 1: Tubulin alpha-1B chain



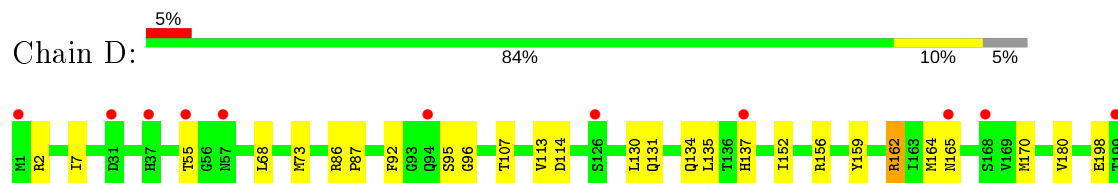
- Molecule 1: Tubulin alpha-1B chain

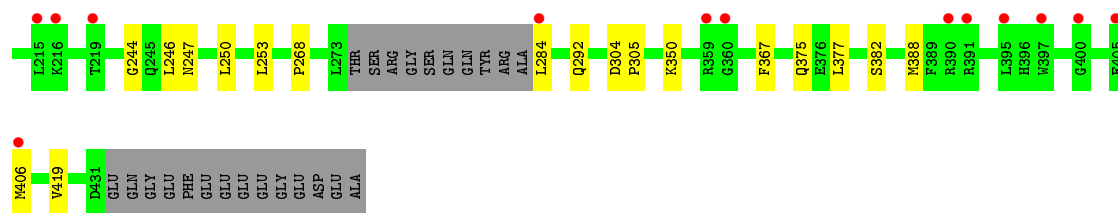


- Molecule 2: Tubulin beta chain

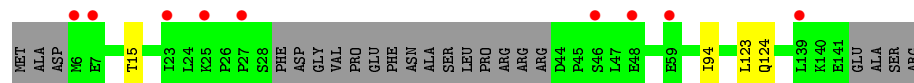
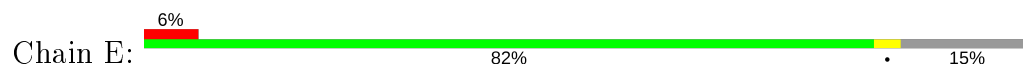


- Molecule 2: Tubulin beta chain

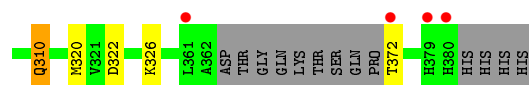
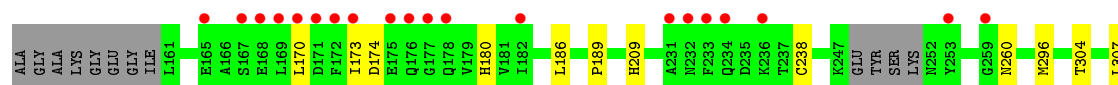
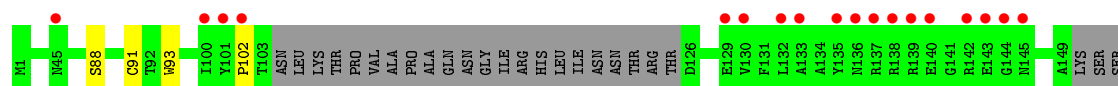
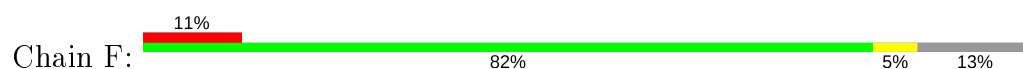




● Molecule 3: Stathmin-4



● 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, $\alpha$ , $\beta$ , $\gamma$	105.62Å 158.57Å 182.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 2.80 39.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.88-2.80) 99.9 (39.88-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.209 , 0.259 0.209 , 0.259	Depositor DCC
$R_{free}$ test set	3827 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.2	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	0.93	EDS
Total number of atoms	17488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, GOL, MG, 88U, CA, 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	0.41	0/3494	0.59	0/4743
1	C	0.41	0/3515	0.61	0/4772
2	B	0.40	0/3436	0.58	0/4654
2	D	0.41	0/3382	0.60	1/4581 (0.0%)
3	E	0.36	0/1008	0.57	0/1337
4	F	0.45	0/2806	0.60	0/3791
All	All	0.41	0/17641	0.60	1/23878 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	246	LEU	CA-CB-CG	5.09	127.00	115.30

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	3416	0	3331	8	0
1	C	3437	0	3348	9	0
2	B	3361	0	3238	20	0
2	D	3309	0	3189	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1000	0	1018	2	0
4	F	2744	0	2709	7	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	2	0
11	B	21	0	0	0	0
11	D	21	0	0	1	0
12	A	4	0	0	0	0
12	B	11	0	0	0	0
12	C	11	0	0	0	0
12	D	4	0	0	0	0
12	E	1	0	0	0	0
All	All	17488	0	16902	61	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 2.

All (61) 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:35:SER:OG	2:B:58:LYS:HE3	1.88	0.72
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.71	0.72
2:B:156:ARG:HG3	10:B:503:MES:H62	1.75	0.69
2:B:54:ALA:HB3	2:B:58:LYS:O	1.94	0.68
2:B:2:ARG:HD2	2:B:131:GLN:HG2	1.78	0.65
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.79	0.64
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.81	0.61
2:D:244:GLY:H	2:D:247:ASN:HD21	1.49	0.59
2:B:44:LEU:HD22	2:B:59:TYR:OH	2.02	0.59
1:C:147:SER:HB2	1:C:190:THR:OG1	2.04	0.58
4:F:91:CYS:SG	4:F:93:TRP:CE2	2.99	0.56
2:D:2:ARG:HH11	2:D:131:GLN:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLN:HA	2:B:165:ASN:O	2.08	0.53
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.90	0.53
2:D:198:GLU:OE2	2:D:253:LEU:HD23	2.08	0.53
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.90	0.52
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.89	0.52
2:D:134:GLN:HA	2:D:165:ASN:O	2.10	0.52
2:D:159:TYR:HB3	2:D:162:ARG:HG3	1.90	0.51
2:D:68:LEU:HB3	2:D:96:GLY:H	1.76	0.51
2:B:135:LEU:HB3	2:B:166:THR:HG22	1.93	0.51
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.93	0.51
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.94	0.50
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.94	0.49
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.94	0.49
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.48
2:B:316:ILE:HG23	2:B:366:THR:HB	1.93	0.48
2:B:159:TYR:HB3	2:B:162:ARG:HG3	1.95	0.48
1:A:166:LYS:HE2	1:A:197:HIS:O	2.14	0.48
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.95	0.47
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.95	0.47
1:C:166:LYS:HE2	1:C:197:HIS:O	2.15	0.47
4:F:102:PRO:HB3	4:F:174:ASP:HA	1.97	0.47
2:D:284:LEU:HD13	2:D:292:GLN:HE22	1.80	0.47
2:B:197:ASP:OD1	10:B:503:MES:H32	2.16	0.45
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.98	0.45
2:D:350:LYS:HG3	11:D:503:88U:C04	2.47	0.45
1:A:161:TYR:HB3	1:A:164:LYS:HD3	2.00	0.44
2:B:35:SER:OG	2:B:58:LYS:CE	2.61	0.44
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.48	0.44
2:B:81:PHE:O	2:B:84:ILE:HG22	2.18	0.44
4:F:170:LEU:HA	4:F:173:ILE:HD12	1.99	0.43
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.99	0.43
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.00	0.43
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.02	0.42
2:B:170:MET:HB2	2:B:203:ASP:HA	2.02	0.42
1:C:320:ARG:HG3	1:C:360:PRO:HD3	2.02	0.42
2:D:7:ILE:O	2:D:135:LEU:HA	2.19	0.42
2:B:2:ARG:HH11	2:B:131:GLN:HG2	1.84	0.41
2:D:131:GLN:NE2	2:D:250:LEU:H	2.17	0.41
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.02	0.41
1:C:320:ARG:HA	1:C:356:ASN:O	2.21	0.41
4:F:189:PRO:HA	4:F:322:ASP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:VAL:HA	2:B:202:ILE:O	2.21	0.41
2:B:67:ASP:HA	2:B:143:THR:HG21	2.03	0.41
2:D:152:ILE:HG23	2:D:164:MET:HG2	2.03	0.41
2:D:268:PRO:HA	2:D:367:PHE:O	2.21	0.41
2:D:86:ARG:HA	2:D:87:PRO:HD3	1.91	0.40
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.02	0.40
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.03	0.40
2:D:304:ASP:HA	2:D:305:PRO:HD2	1.94	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	435/451 (96%)	424 (98%)	9 (2%)	2 (0%)	29	61
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	417/445 (94%)	410 (98%)	6 (1%)	1 (0%)	47	78
3	E	117/143 (82%)	113 (97%)	4 (3%)	0	100	100
4	F	324/384 (84%)	315 (97%)	8 (2%)	1 (0%)	41	72
All	All	2156/2319 (93%)	2109 (98%)	43 (2%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	88	SER
1	A	282	TYR
2	D	95	SER
1	A	89	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	368/379 (97%)	364 (99%)	4 (1%)	73	92
1	C	371/379 (98%)	360 (97%)	11 (3%)	41	75
2	B	369/383 (96%)	364 (99%)	5 (1%)	67	90
2	D	364/383 (95%)	353 (97%)	11 (3%)	41	75
3	E	109/127 (86%)	107 (98%)	2 (2%)	59	86
4	F	301/342 (88%)	294 (98%)	7 (2%)	50	82
All	All	1882/1993 (94%)	1842 (98%)	40 (2%)	53	84

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	176	GLN
1	A	188	ILE
1	A	279	GLU
2	B	33	THR
2	B	137	HIS
2	B	316	ILE
2	B	350	LYS
2	B	382	SER
1	C	2	ARG
1	C	82	THR
1	C	97	GLU
1	C	181	VAL
1	C	218	ASP
1	C	221	ARG
1	C	245	ASP
1	C	251	ASP
1	C	302	MET
1	C	368	LEU
1	C	381	THR
2	D	55	THR
2	D	107	THR

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Mol	Chain	Res	Type
2	D	113	VAL
2	D	114	ASP
2	D	130	LEU
2	D	137	HIS
2	D	162	ARG
2	D	180	VAL
2	D	382	SER
2	D	388	MET
2	D	406	MET
3	E	15	THR
3	E	124	GLN
4	F	180	HIS
4	F	238	CYS
4	F	260	ASN
4	F	296	MET
4	F	310	GLN
4	F	326	LYS
4	F	372	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
2	B	375	GLN
1	C	11	GLN
1	C	358	GLN
2	D	131	GLN
2	D	247	ASN
2	D	292	GLN
3	E	92	ASN
4	F	260	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 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
11	88U	D	503	-	23,23,23	2.42	9 (39%)	31,32,32	1.59	6 (19%)
5	GTP	C	501	6	26,34,34	1.20	2 (7%)	33,54,54	1.97	7 (21%)
9	GDP	B	501	6	24,30,30	1.29	2 (8%)	31,47,47	1.97	7 (22%)
5	GTP	A	501	6	26,34,34	1.23	2 (7%)	33,54,54	1.96	7 (21%)
5	GTP	D	501	6	26,34,34	1.27	2 (7%)	33,54,54	2.04	10 (30%)
8	GOL	A	504	-	5,5,5	0.26	0	5,5,5	0.38	0
10	MES	B	503	-	12,12,12	2.13	1 (8%)	14,16,16	6.84	6 (42%)
11	88U	B	504	-	23,23,23	2.46	9 (39%)	31,32,32	1.63	7 (22%)

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
11	88U	D	503	-	-	2/10/10/10	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
11	88U	B	504	-	-	0/10/10/10	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	88U	C11-N10	6.84	1.46	1.34
11	D	503	88U	C11-N10	6.77	1.46	1.34
10	B	503	MES	C8-S	-6.62	1.68	1.77
5	D	501	GTP	C6-C5	4.66	1.49	1.41
11	D	503	88U	C14-N13	4.66	1.45	1.37
9	B	501	GDP	C6-C5	4.57	1.49	1.41
5	A	501	GTP	C6-C5	4.54	1.49	1.41
11	B	504	88U	C14-N13	4.50	1.44	1.37
5	C	501	GTP	C6-C5	4.47	1.49	1.41
11	B	504	88U	C16-C15	4.12	1.46	1.36
11	D	503	88U	C16-C15	3.89	1.45	1.36
11	B	504	88U	O02-C03	3.68	1.45	1.37
11	D	503	88U	O02-C03	3.48	1.44	1.37
11	B	504	88U	C17-C18	2.80	1.43	1.36
11	D	503	88U	C17-C18	2.72	1.42	1.36
5	D	501	GTP	C5-C4	2.71	1.48	1.40
11	D	503	88U	C09-N10	2.68	1.36	1.32
9	B	501	GDP	C5-C4	2.64	1.47	1.40
5	A	501	GTP	C5-C4	2.60	1.47	1.40
11	B	504	88U	C09-N10	2.59	1.36	1.32
5	C	501	GTP	C5-C4	2.56	1.47	1.40
11	B	504	88U	C09-C19	2.48	1.49	1.43
11	B	504	88U	C06-N07	2.42	1.48	1.42
11	D	503	88U	C09-C19	2.39	1.48	1.43
11	D	503	88U	C06-N07	2.33	1.47	1.42
11	D	503	88U	C08-N07	-2.26	1.41	1.46
11	B	504	88U	C08-N07	-2.18	1.42	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O3S-S-C8	-13.17	84.48	105.77
10	B	503	MES	O2S-S-C8	11.24	120.45	106.92
10	B	503	MES	O3S-S-O1S	-11.13	84.07	111.27
10	B	503	MES	O3S-S-O2S	-11.12	84.10	111.27
10	B	503	MES	O1S-S-C8	9.52	118.38	106.92
11	B	504	88U	C11-N13-C14	5.95	120.58	116.54
11	D	503	88U	C11-N13-C14	5.77	120.45	116.54
5	D	501	GTP	C2-N3-C4	5.01	121.08	115.36
9	B	501	GDP	C2-N3-C4	4.87	120.92	115.36
5	A	501	GTP	C2-N3-C4	4.86	120.91	115.36
5	C	501	GTP	C5-C6-N1	-4.55	117.20	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C6-N1-C2	4.53	123.13	115.93
9	B	501	GDP	C6-N1-C2	4.43	122.97	115.93
5	C	501	GTP	C2-N3-C4	4.43	120.42	115.36
5	A	501	GTP	C6-N1-C2	4.37	122.88	115.93
5	D	501	GTP	C6-N1-C2	4.35	122.85	115.93
5	D	501	GTP	C6-C5-C4	-4.31	116.69	120.80
5	A	501	GTP	C6-C5-C4	-4.30	116.69	120.80
9	B	501	GDP	C5-C6-N1	-4.24	117.64	123.43
5	A	501	GTP	C5-C6-N1	-4.14	117.77	123.43
5	C	501	GTP	C6-C5-C4	-4.08	116.90	120.80
9	B	501	GDP	C6-C5-C4	-4.05	116.93	120.80
5	D	501	GTP	C5-C6-N1	-3.90	118.10	123.43
5	D	501	GTP	N3-C2-N1	-3.71	122.27	127.22
9	B	501	GDP	N3-C2-N1	-3.64	122.37	127.22
5	A	501	GTP	N3-C2-N1	-3.58	122.44	127.22
5	C	501	GTP	N3-C2-N1	-3.43	122.65	127.22
11	B	504	88U	N13-C11-N10	-3.21	119.87	125.73
11	D	503	88U	N13-C11-N10	-3.19	119.90	125.73
5	A	501	GTP	C4-C5-N7	-2.93	106.35	109.40
5	C	501	GTP	PA-O3A-PB	-2.82	123.15	132.83
5	C	501	GTP	C4-C5-N7	-2.80	106.48	109.40
5	D	501	GTP	PA-O3A-PB	-2.80	123.23	132.83
11	D	503	88U	C11-N10-C09	2.66	123.53	116.99
11	B	504	88U	C11-N10-C09	2.66	123.53	116.99
10	B	503	MES	C5-N4-C3	2.64	114.78	108.83
9	B	501	GDP	C4-C5-N7	-2.60	106.69	109.40
11	D	503	88U	N10-C09-N07	2.55	118.76	116.09
5	D	501	GTP	C4-C5-N7	-2.55	106.75	109.40
5	D	501	GTP	PB-O3B-PG	-2.53	124.14	132.83
11	B	504	88U	C19-C09-N10	-2.51	117.32	122.66
11	B	504	88U	N10-C09-N07	2.47	118.68	116.09
11	D	503	88U	C19-C09-N10	-2.44	117.46	122.66
5	A	501	GTP	PA-O3A-PB	-2.36	124.72	132.83
9	B	501	GDP	PA-O3A-PB	-2.31	124.90	132.83
11	D	503	88U	C12-C11-N13	2.19	120.57	117.16
11	B	504	88U	C12-C11-N13	2.17	120.54	117.16
5	D	501	GTP	C2'-C3'-C4'	2.17	106.85	102.64
11	B	504	88U	C19-C14-N13	-2.08	120.60	122.81
5	D	501	GTP	C3'-C2'-C1'	2.06	104.08	100.98

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O1A
10	B	503	MES	C7-C8-S-O2S
10	B	503	MES	C7-C8-S-O3S
8	A	504	GOL	C1-C2-C3-O3
8	A	504	GOL	O2-C2-C3-O3
10	B	503	MES	N4-C7-C8-S
10	B	503	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
11	D	503	88U	C21-C03-O02-C01
5	D	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C3'-C4'-C5'-O5'
11	D	503	88U	C04-C03-O02-C01
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	C3'-C4'-C5'-O5'

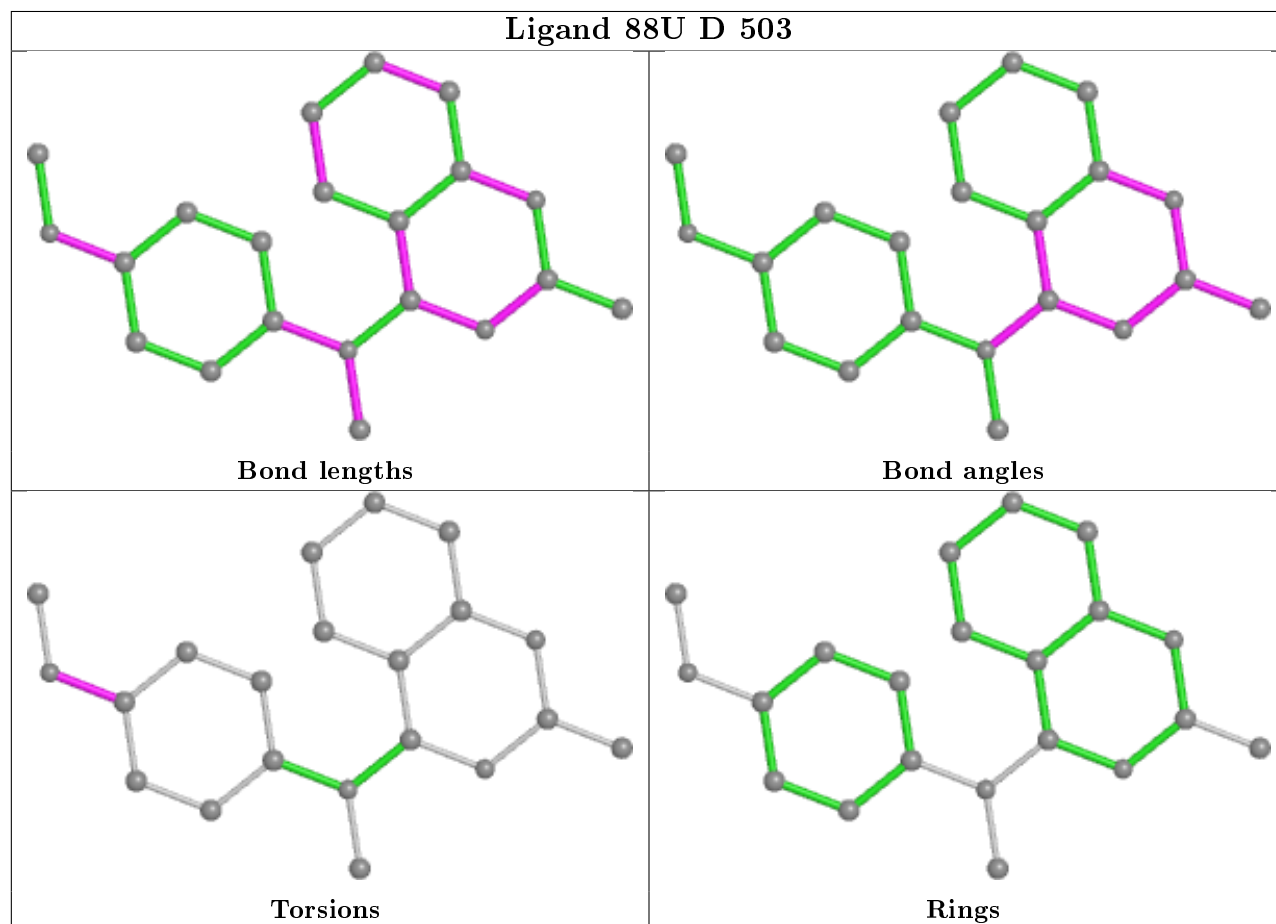
There are no ring outliers.

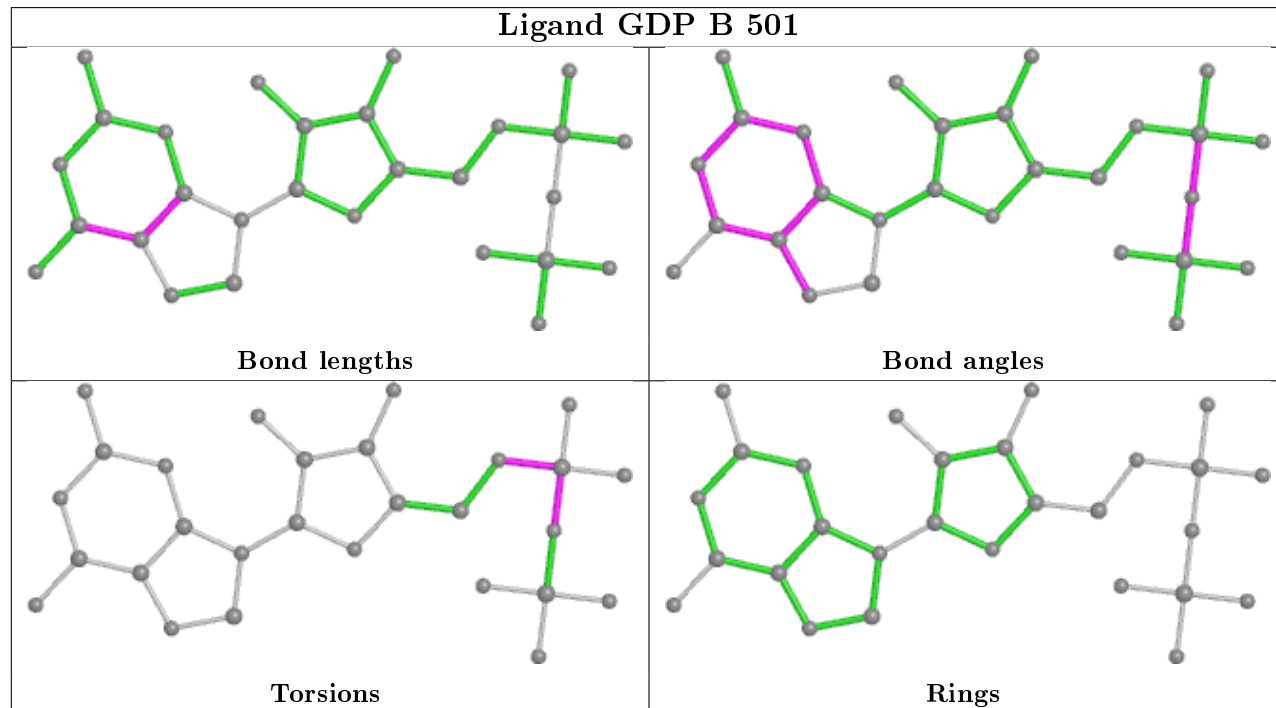
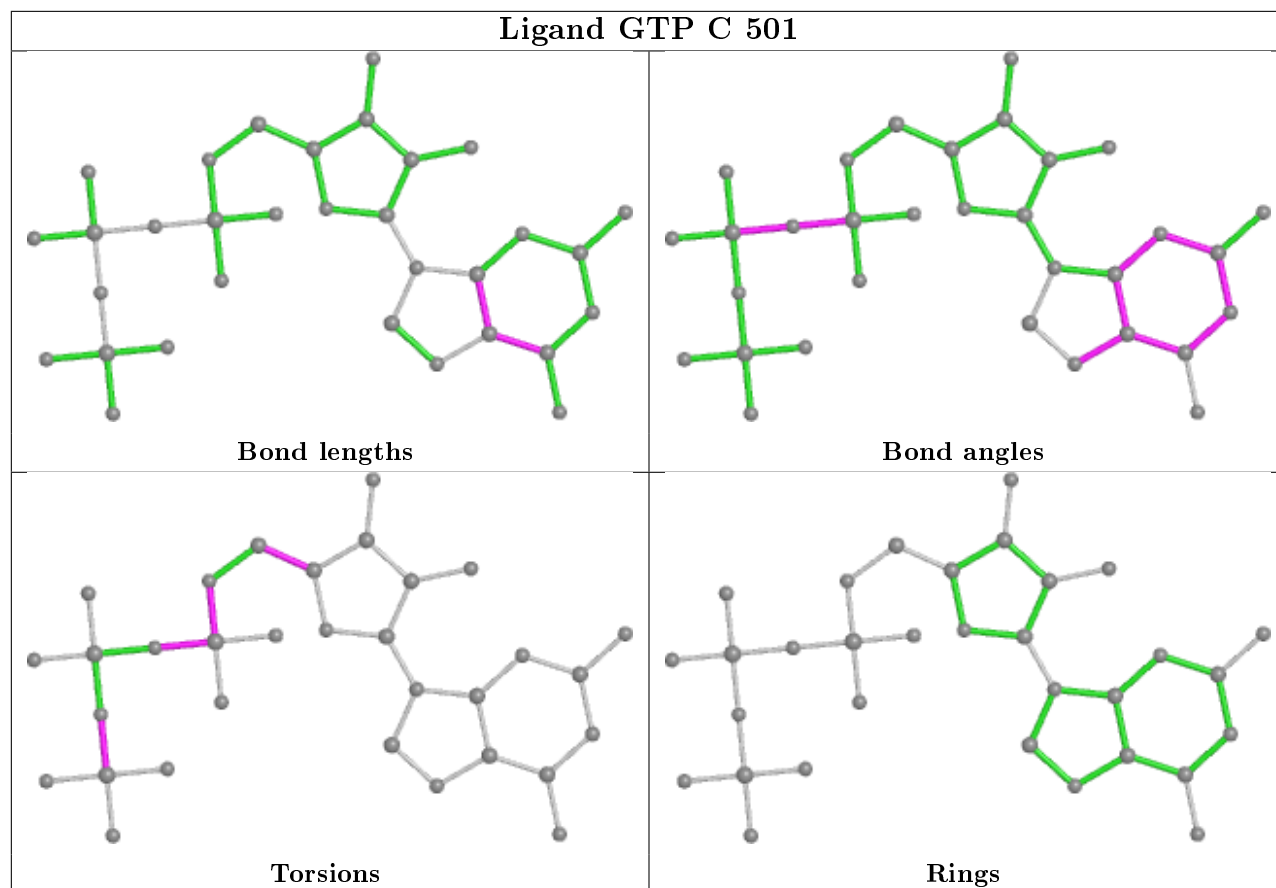
2 monomers are involved in 3 short contacts:

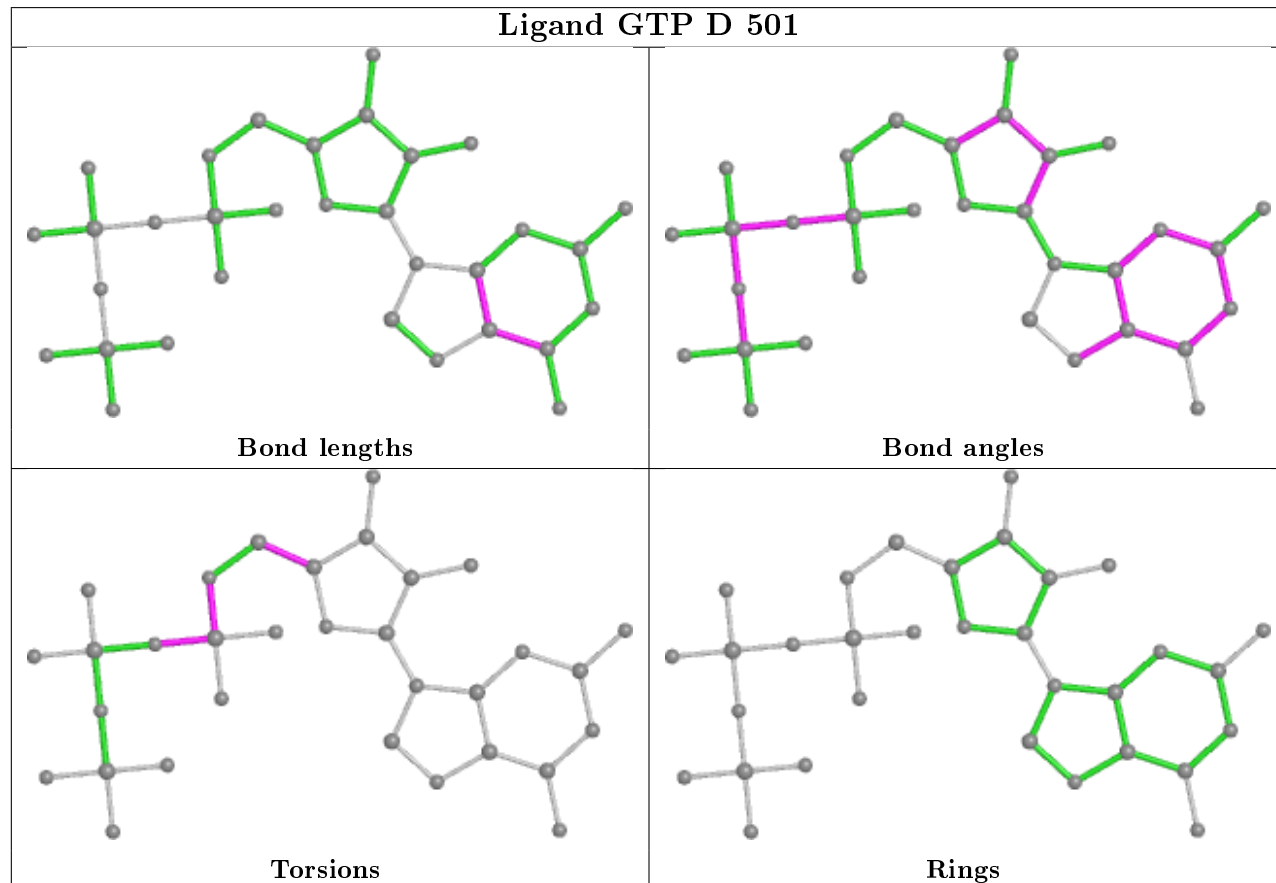
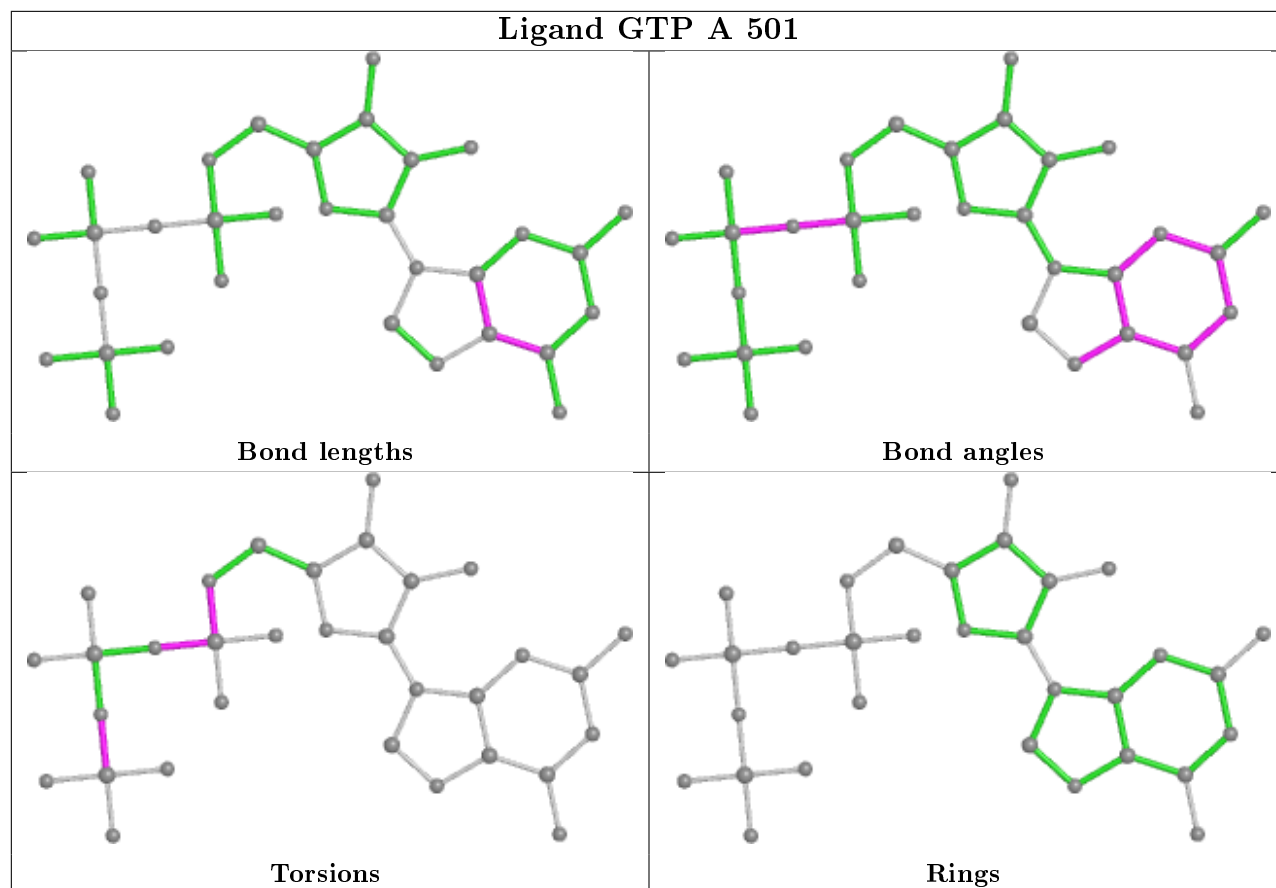
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	503	88U	1	0
10	B	503	MES	2	0

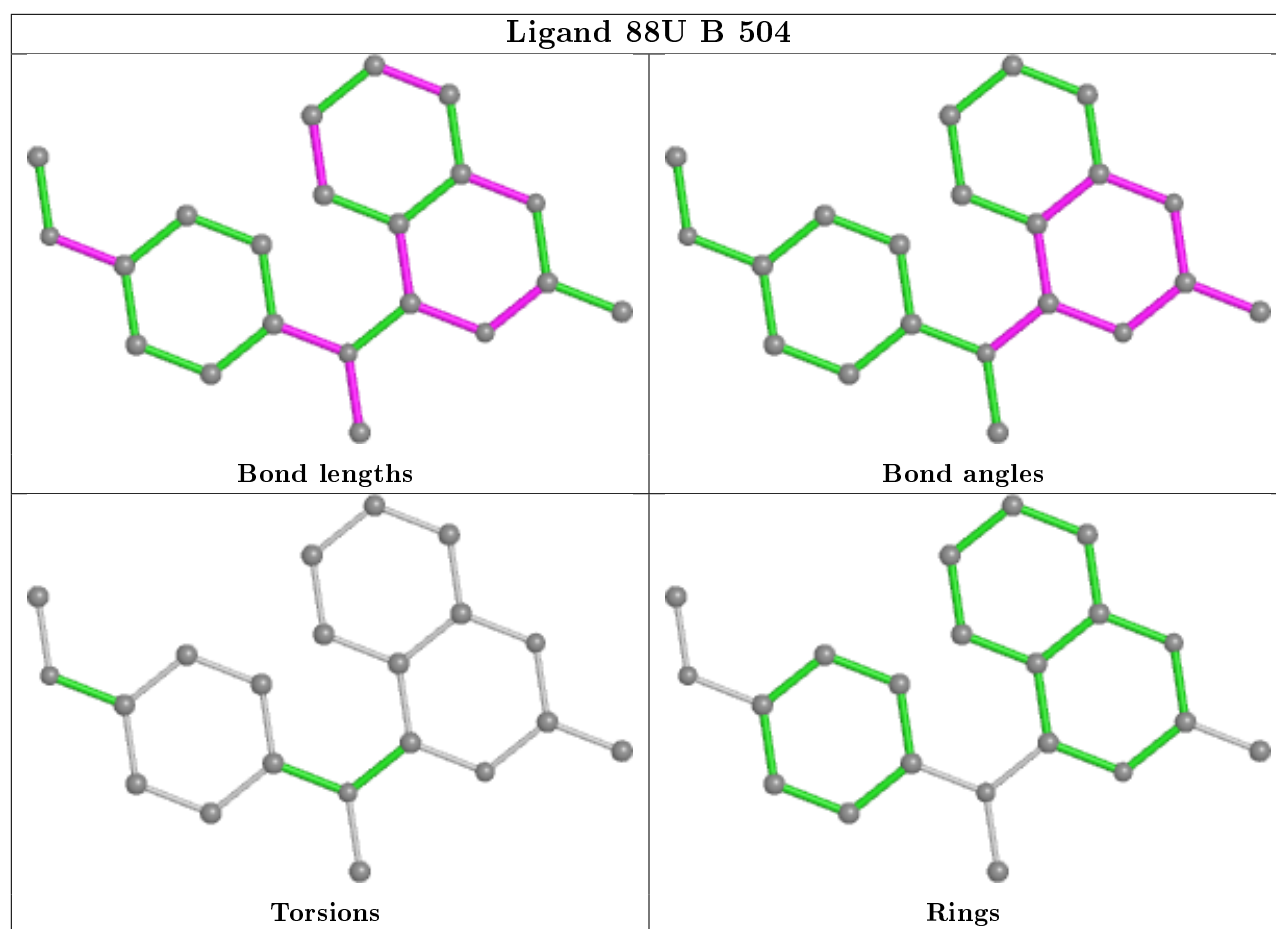
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.









## 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	437/451 (96%)	-0.10	2 (0%) 91 88	35, 53, 80, 105	0
1	C	440/451 (97%)	-0.30	1 (0%) 95 94	29, 44, 68, 87	0
2	B	427/445 (95%)	-0.03	11 (2%) 56 46	31, 54, 88, 123	0
2	D	421/445 (94%)	0.34	24 (5%) 23 15	39, 74, 111, 141	0
3	E	121/143 (84%)	0.50	9 (7%) 14 8	44, 71, 105, 118	0
4	F	334/384 (86%)	0.33	42 (12%) 3 2	42, 74, 134, 147	0
All	All	2180/2319 (94%)	0.06	89 (4%) 37 27	29, 59, 107, 147	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	176	GLN	4.6
2	D	284	LEU	4.5
4	F	173	ILE	4.3
4	F	232	ASN	4.2
2	B	277	GLY	4.0
2	B	279	GLN	3.8
3	E	48	GLU	3.7
4	F	169	LEU	3.7
4	F	140	GLU	3.6
4	F	135	TYR	3.5
2	D	219	THR	3.5
2	D	1	MET	3.5
4	F	182	ILE	3.5
1	C	340	SER	3.5
2	D	37	HIS	3.5
3	E	7	GLU	3.4
2	D	391	ARG	3.4
2	D	94	GLN	3.3
4	F	143	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	3.3
4	F	137	ARG	3.2
2	D	390	ARG	3.2
4	F	380	HIS	3.1
3	E	139	LEU	3.1
4	F	130	VAL	3.1
2	D	55	THR	3.1
4	F	136	ASN	3.0
4	F	101	TYR	2.9
2	D	168	SER	2.9
4	F	234	GLN	2.9
4	F	231	ALA	2.9
3	E	25	LYS	2.9
4	F	133	ALA	2.9
4	F	138	ARG	2.9
4	F	233	PHE	2.9
2	D	216	LYS	2.8
3	E	59	GLU	2.8
4	F	142	ARG	2.8
4	F	102	PRO	2.7
4	F	177	GLY	2.7
4	F	170	LEU	2.7
2	B	58	LYS	2.7
2	B	275	SER	2.7
4	F	178	GLN	2.7
2	B	278	SER	2.6
2	D	405	GLU	2.6
3	E	46	SER	2.6
3	E	27	PRO	2.5
3	E	6	MET	2.5
2	D	359	ARG	2.5
2	B	282	ARG	2.5
4	F	167	SER	2.4
2	D	57	ASN	2.4
4	F	361	LEU	2.4
2	D	395	LEU	2.4
2	D	215	LEU	2.4
2	D	360	GLY	2.4
4	F	236	LYS	2.4
4	F	145	ASN	2.4
3	E	23	ILE	2.3
1	A	345	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	45	ASN	2.3
4	F	100	ILE	2.3
4	F	372	THR	2.3
4	F	259	GLY	2.3
4	F	379	HIS	2.3
1	A	262	TYR	2.2
2	B	57	ASN	2.2
2	D	126	SER	2.2
4	F	172	PHE	2.2
4	F	129	GLU	2.2
2	B	56	GLY	2.2
2	D	165	ASN	2.2
2	D	406	MET	2.2
4	F	175	GLU	2.1
4	F	139	ARG	2.1
2	B	37	HIS	2.1
2	D	397	TRP	2.1
2	B	427	ASP	2.1
2	B	55	THR	2.1
4	F	253	TYR	2.1
4	F	144	GLY	2.1
4	F	165	GLU	2.1
2	D	31	ASP	2.0
2	D	137	HIS	2.0
4	F	168	GLU	2.0
2	D	400	GLY	2.0
4	F	171	ASP	2.0
2	D	199	THR	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.

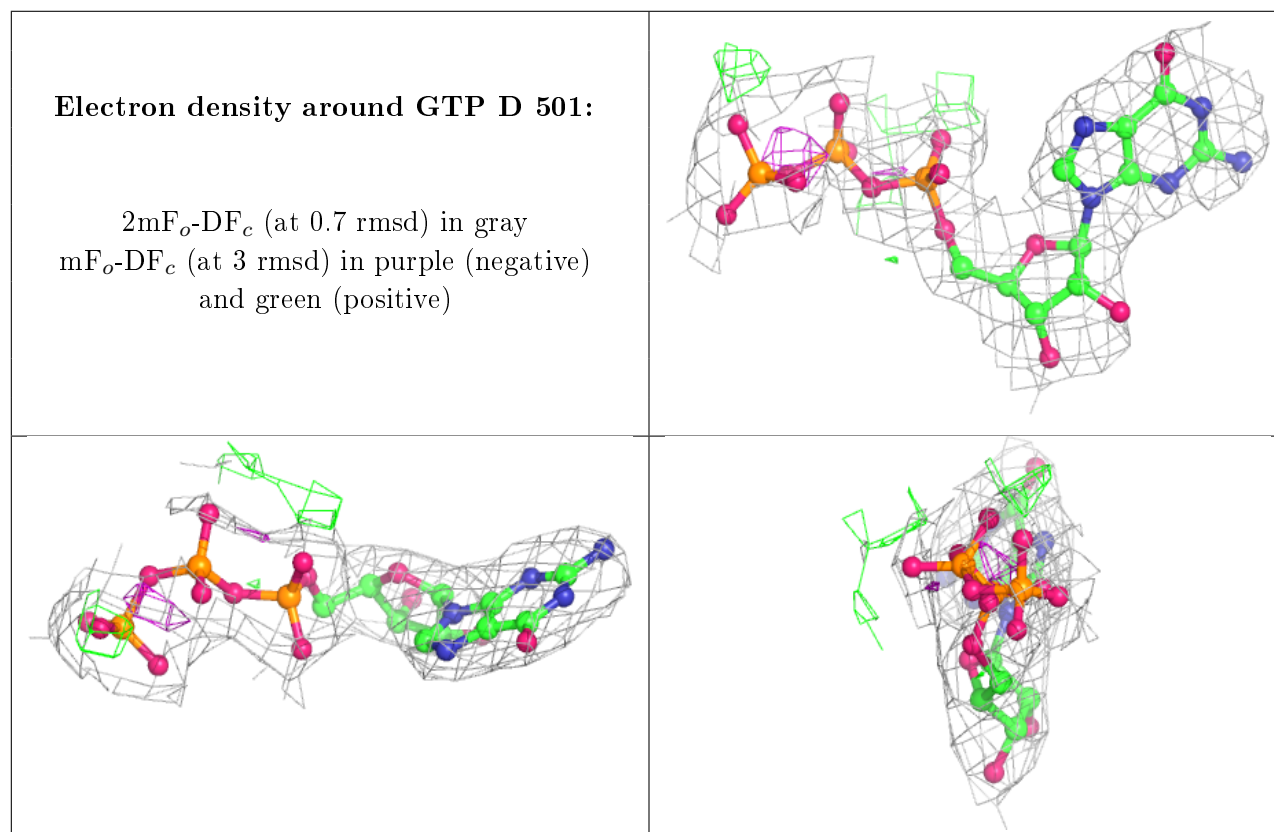
## 6.4 Ligands [i](#)

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.

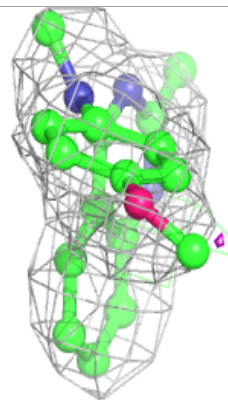
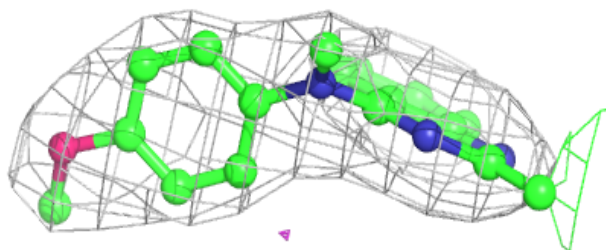
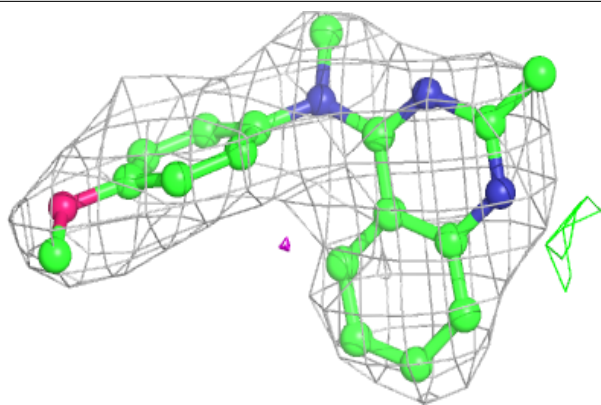
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	CA	A	503	1/1	0.86	0.12	70,70,70,70	0
8	GOL	A	504	6/6	0.87	0.23	71,73,74,75	0
6	MG	D	502	1/1	0.88	0.11	72,72,72,72	0
10	MES	B	503	12/12	0.91	0.23	79,83,87,89	0
7	CA	C	503	1/1	0.91	0.09	62,62,62,62	0
5	GTP	D	501	32/32	0.94	0.16	59,69,88,91	0
11	88U	D	503	21/21	0.97	0.19	49,52,58,58	0
11	88U	B	504	21/21	0.97	0.20	39,41,43,44	0
6	MG	A	502	1/1	0.97	0.12	32,32,32,32	0
9	GDP	B	501	28/28	0.98	0.15	33,37,39,40	0
5	GTP	A	501	32/32	0.98	0.16	39,40,43,44	0
6	MG	B	502	1/1	0.98	0.30	42,42,42,42	0
5	GTP	C	501	32/32	0.99	0.14	33,37,41,42	0
6	MG	C	502	1/1	0.99	0.13	32,32,32,32	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.

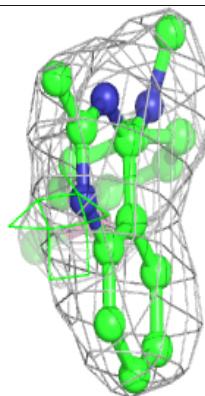
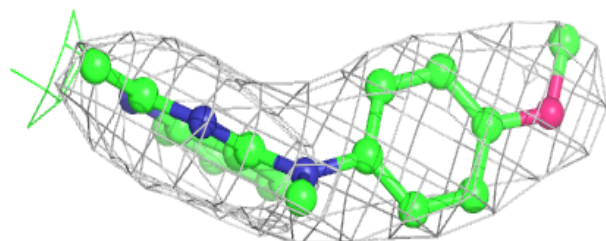
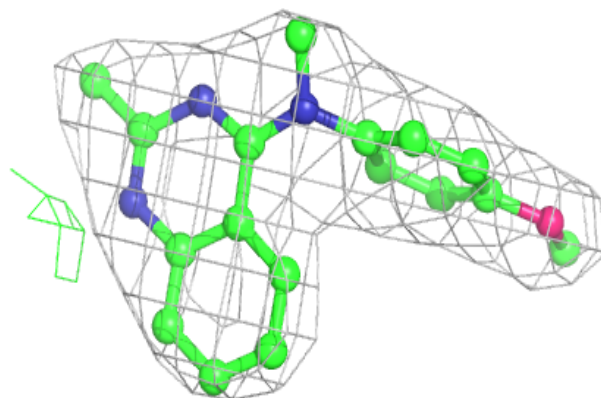


**Electron density around 88U D 503:**

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

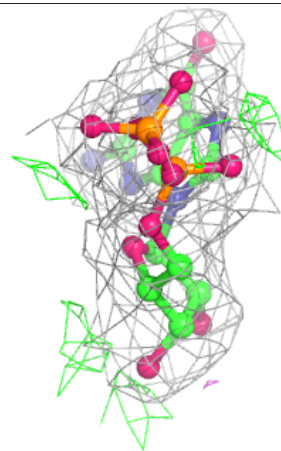
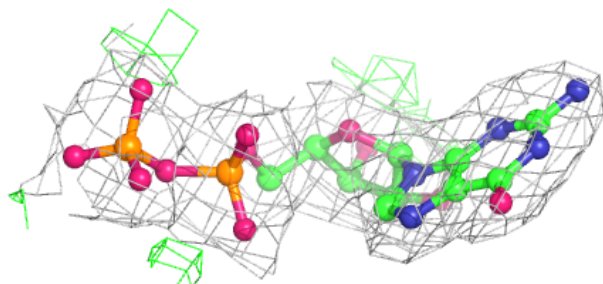
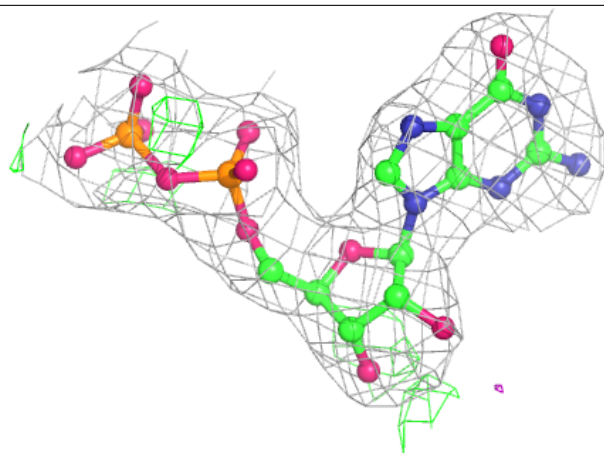
**Electron density around 88U B 504:**

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



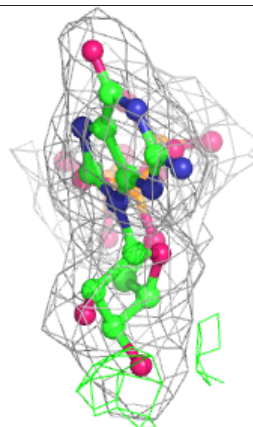
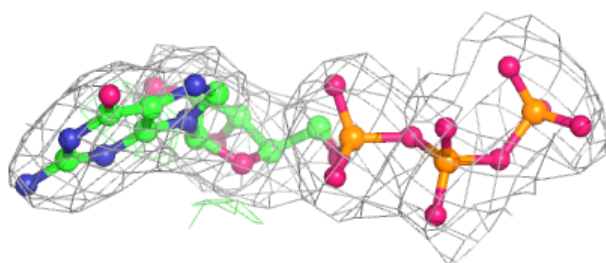
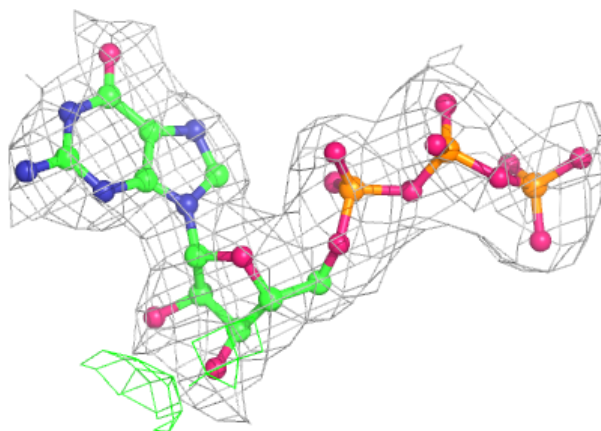
**Electron density around GDP B 501:**

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

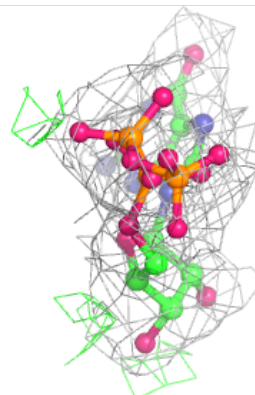
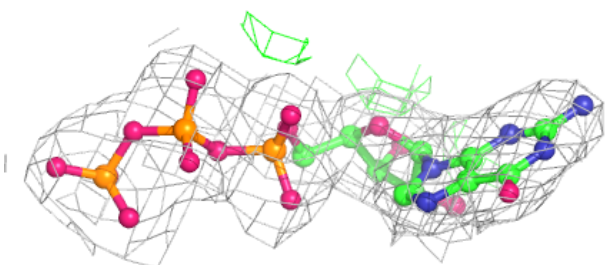
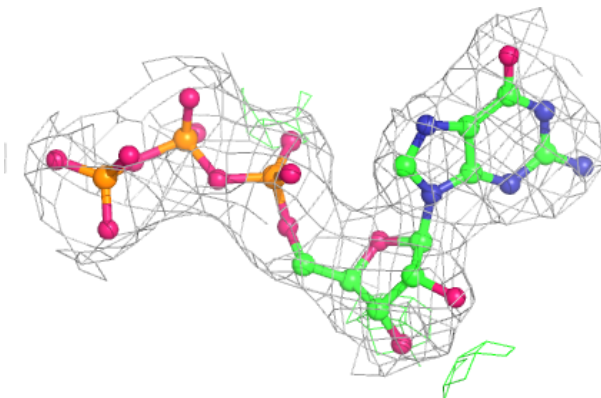


**Electron density around GTP A 501:**

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

**Electron density around 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.