



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:27 am BST

PDB ID : 5XKH
Title : Crystal structure of T2R-TTL-CF1 complex
Authors : Wang, Y.; Yang, J.; Wang, T.; Chen, L.
Deposited on : 2017-05-07
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

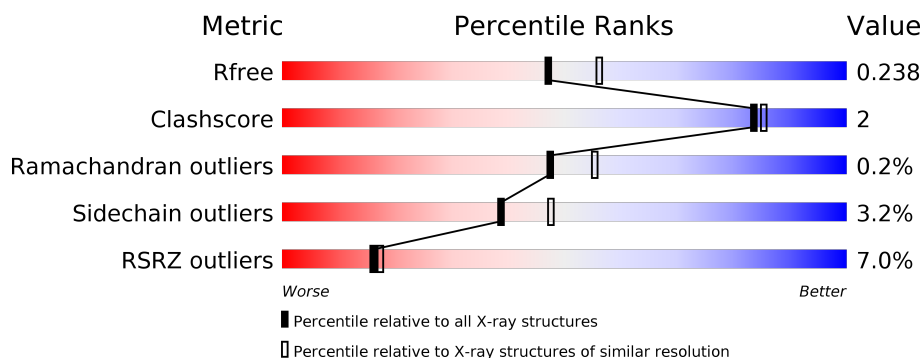
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 ≥ 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></div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div> </div>
1	C	451	<div> <div></div> <div> <div></div> <div>89%</div> <div>8%</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>12%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
3	E	143	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>15%</div> </div> </div>
4	F	384	<div> <div>16%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 18138 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	1	0
			3443	2178	585	657	23			

- 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
			3377	2119	579	652	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLY	GLU	conflict	UNP F2Z5B2
B	441	GLU	GLY	conflict	UNP F2Z5B2
D	440	GLY	GLU	conflict	UNP F2Z5B2
D	441	GLU	GLY	conflict	UNP F2Z5B2

- 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

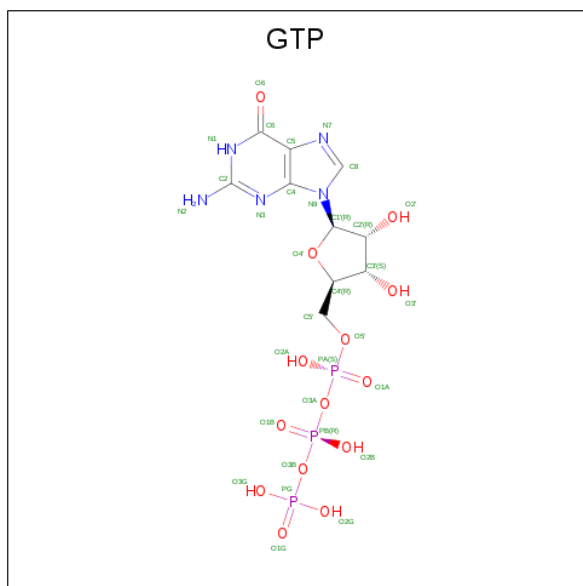
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	333	Total	C	N	O	S	0	0	0
			2737	1757	469	497	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		

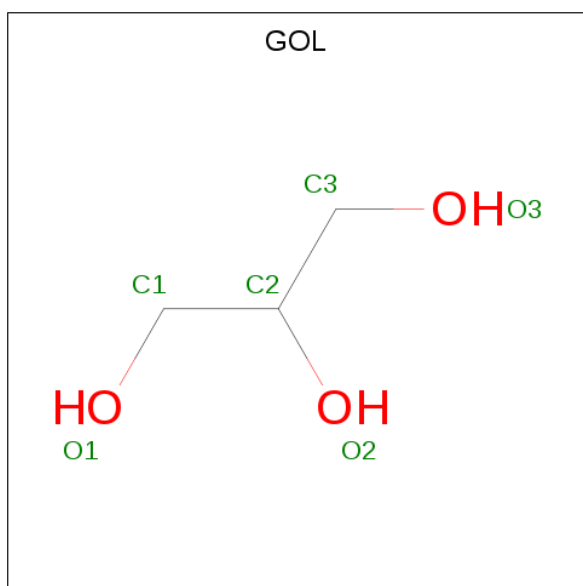
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

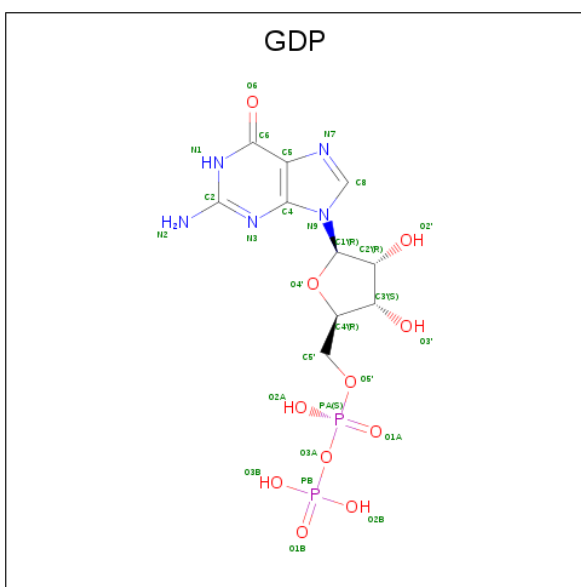
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



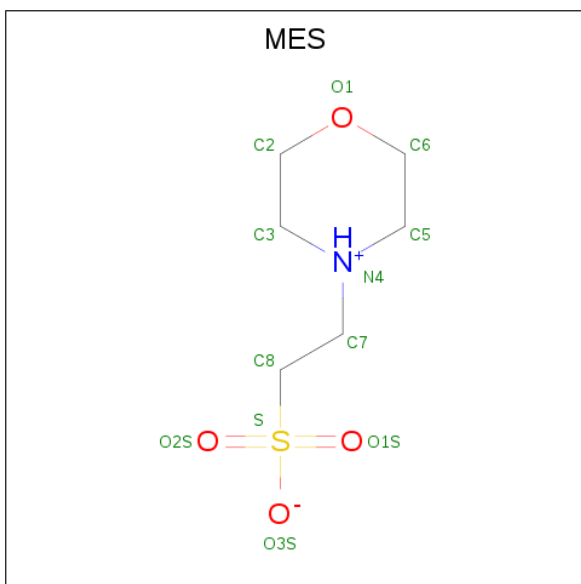
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



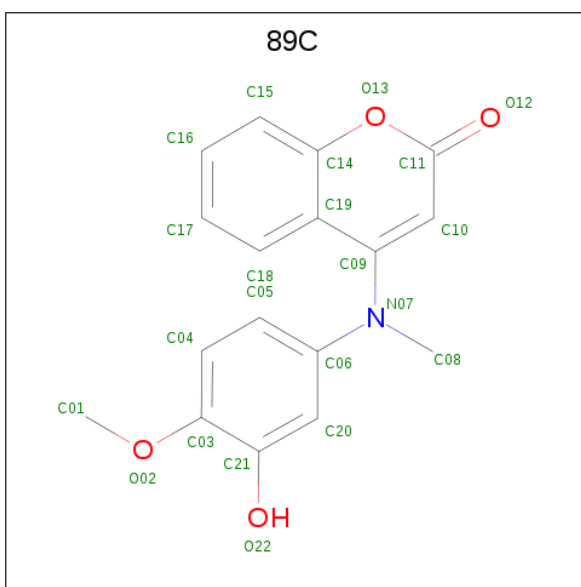
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	
			28	10	5	11	2	

- 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	
			12	6	1	4	1	

- Molecule 11 is 4-[(4-methoxy-3-oxidanyl-phenyl)-methyl-amino]chromen-2-one (three-letter code: 89C) (formula: $C_{17}H_{15}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			22	17	1	4		
11	C	1	Total	C	N	O	0	0
			22	17	1	4		

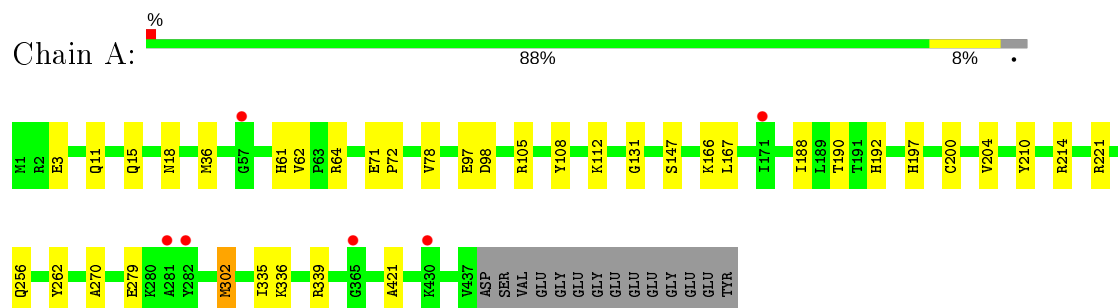
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	163	Total	O	0	0
			163	163		
12	B	107	Total	O	0	0
			107	107		
12	C	246	Total	O	0	0
			246	246		
12	D	62	Total	O	0	0
			62	62		
12	E	34	Total	O	0	0
			34	34		
12	F	52	Total	O	0	0
			52	52		

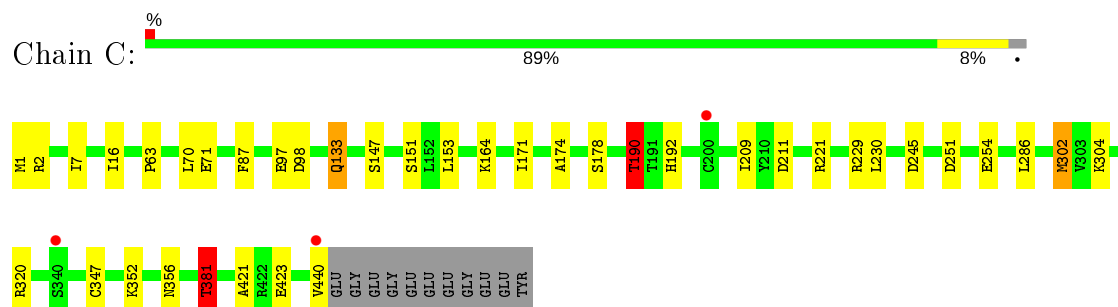
3 Residue-property plots [i](#)

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.

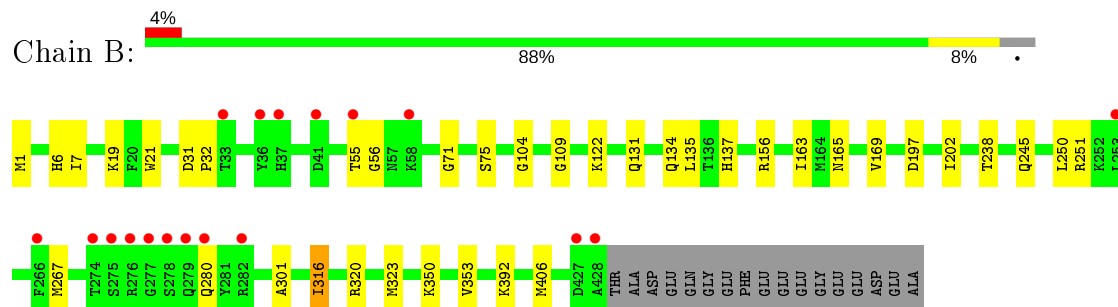
- Molecule 1: Tubulin alpha-1B chain



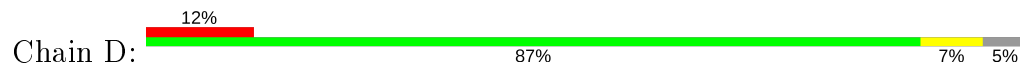
- Molecule 1: Tubulin alpha-1B chain

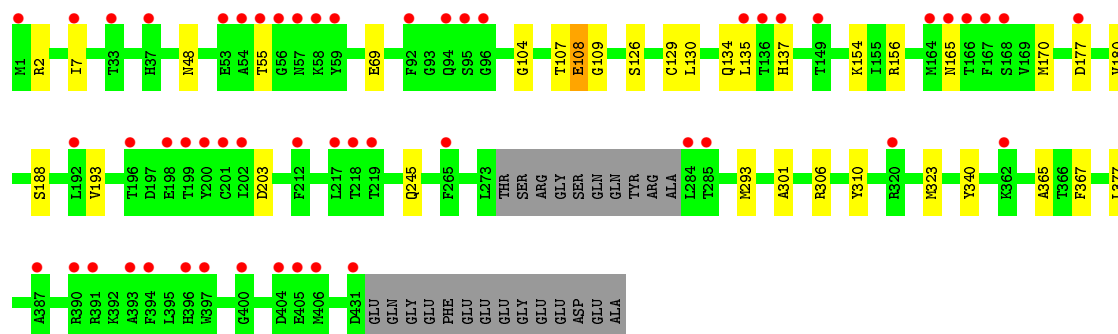


- Molecule 2: Tubulin beta chain

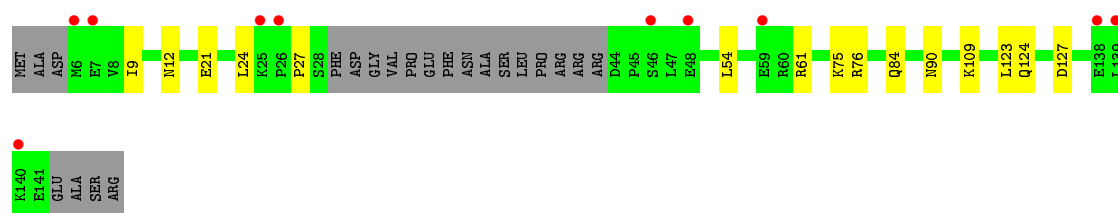


- Molecule 2: Tubulin beta chain

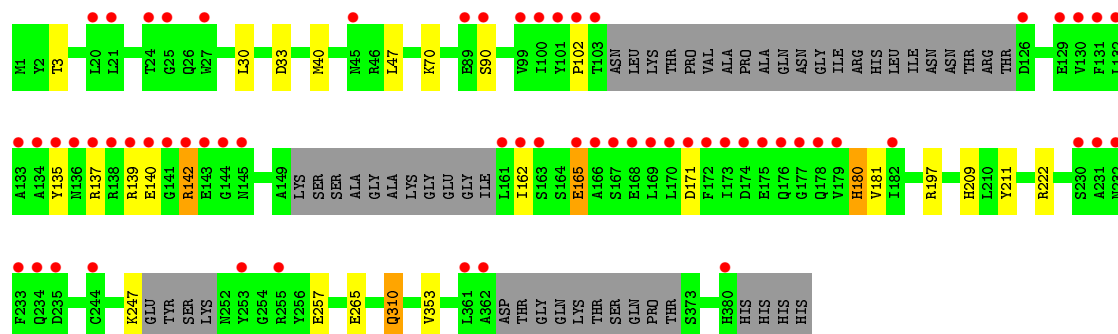
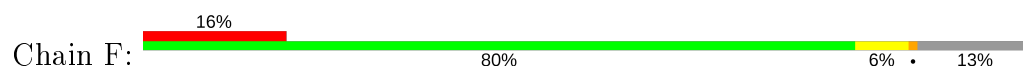




• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.52Å 158.44Å 180.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 40.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.25) 99.7 (40.16-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.195 , 0.240 0.194 , 0.238	Depositor DCC
R_{free} test set	7623 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18138	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, CA, GTP, 89C, 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	0.57	0/3494	0.70	0/4743
1	C	0.65	0/3521	0.76	3/4780 (0.1%)
2	B	0.60	0/3452	0.69	0/4675
2	D	0.52	0/3382	0.69	0/4581
3	E	0.52	0/1008	0.69	1/1337 (0.1%)
4	F	0.52	0/2799	0.69	0/3781
All	All	0.57	0/17656	0.71	4/23897 (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	C	381	THR	CB-CA-C	-6.45	94.19	111.60
1	C	190	THR	CB-CA-C	-5.42	96.96	111.60
3	E	61	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	190	THR	N-CA-CB	5.03	119.85	110.30

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	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3443	0	3352	20	0
2	B	3377	0	3255	18	0
2	D	3309	0	3189	14	0
3	E	1000	0	1018	6	0
4	F	2737	0	2702	9	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	5	0
11	B	22	0	0	1	0
11	C	22	0	0	0	0
12	A	163	0	0	2	0
12	B	107	0	0	2	0
12	C	246	0	0	3	0
12	D	62	0	0	1	0
12	E	34	0	0	0	0
12	F	52	0	0	0	0
All	All	18138	0	16916	84	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 (84) 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)
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.66	0.77
2:B:197:ASP:OD2	10:B:503:MES:H52	1.87	0.75
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.68	0.73
2:B:197:ASP:OD1	10:B:503:MES:H32	1.88	0.73
1:A:3:GLU:OE1	12:A:601:HOH:O	2.07	0.72
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.72	0.71
1:C:221:ARG:HG3	2:D:323:MET:HG2	1.75	0.69
2:B:156:ARG:HG3	10:B:503:MES:H62	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:SER:O	1:C:190:THR:HG23	1.93	0.67
1:C:381:THR:HG23	12:C:628:HOH:O	1.94	0.66
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.82	0.62
1:A:131:GLY:C	12:A:601:HOH:O	2.41	0.57
2:B:104:GLY:O	2:B:109:GLY:HA3	2.05	0.57
2:D:134:GLN:HA	2:D:165:ASN:O	2.05	0.56
2:B:1:MET:SD	2:B:251:ARG:NH1	2.78	0.56
2:B:1:MET:HG2	2:B:131:GLN:HA	1.88	0.56
1:A:204:VAL:HG22	1:A:302:MET:HG3	1.87	0.56
1:A:147:SER:HB2	1:A:190:THR:HB	1.89	0.54
4:F:180:HIS:HD2	4:F:181:VAL:H	1.56	0.54
2:B:156:ARG:CZ	10:B:503:MES:H21	2.37	0.54
4:F:180:HIS:CD2	4:F:181:VAL:H	2.26	0.52
4:F:40:MET:HE1	4:F:47:LEU:HG	1.92	0.52
1:C:381:THR:CG2	12:C:628:HOH:O	2.54	0.51
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.46	0.50
2:D:104:GLY:O	2:D:109:GLY:HA3	2.12	0.50
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.41	0.50
1:C:209:ILE:HD11	1:C:302:MET:HG3	1.93	0.50
1:C:151:SER:HB3	1:C:190:THR:HG22	1.94	0.50
4:F:139:ARG:HA	4:F:142:ARG:HA	1.94	0.50
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.94	0.49
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.44	0.49
12:B:628:HOH:O	3:E:76:ARG:HG3	2.12	0.49
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.95	0.48
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.96	0.48
2:D:203:ASP:HB3	2:D:301:ALA:HA	1.95	0.48
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.96	0.48
1:C:70:LEU:O	1:C:97:GLU:O	2.31	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.31	0.48
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.95	0.47
2:D:107:THR:OG1	12:D:601:HOH:O	2.20	0.47
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.49	0.47
1:C:423:GLU:HG2	12:C:827:HOH:O	2.15	0.47
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.33	0.47
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.97	0.46
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.98	0.46
1:C:1:MET:HB2	1:C:2:ARG:HD2	1.97	0.45
4:F:135:TYR:OH	4:F:165:GLU:HA	2.16	0.45
2:B:134:GLN:HA	2:B:165:ASN:O	2.15	0.45
1:A:112:LYS:HG3	3:E:54:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
4:F:137:ARG:HA	4:F:140:GLU:HG2	1.99	0.44
1:A:270:ALA:HB3	1:A:302:MET:HG2	2.00	0.44
10:B:503:MES:H51	10:B:503:MES:H82	1.86	0.44
2:D:2:ARG:HD2	2:D:129:CYS:HB3	1.99	0.44
2:D:154:LYS:HE2	3:E:127:ASP:OD1	2.18	0.44
1:A:11:GLN:O	1:A:15:GLN:HG3	2.18	0.43
1:C:16:ILE:HD13	1:C:171:ILE:HD11	1.99	0.43
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.01	0.43
3:E:9:ILE:HG13	3:E:21:GLU:HB3	1.99	0.43
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.99	0.43
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.53	0.43
1:C:174:ALA:O	1:C:178:SER:HB3	2.19	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.43
4:F:3:THR:HB	4:F:30:LEU:HD11	2.01	0.42
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.01	0.42
1:A:108:TYR:O	1:A:112:LYS:HB2	2.19	0.42
1:A:97:GLU:HG2	1:A:105:ARG:HH21	1.84	0.42
2:D:7:ILE:O	2:D:135:LEU:HA	2.19	0.42
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.55	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.42
1:C:2:ARG:HB3	1:C:133:GLN:HB2	2.02	0.42
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.20	0.41
1:C:320:ARG:HA	1:C:356:ASN:O	2.19	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.51	0.41
2:D:293:MET:CE	2:D:365:ALA:HB1	2.51	0.41
1:C:211:ASP:OD2	1:C:304:LYS:HE3	2.20	0.41
2:D:108:GLU:HG2	2:D:108:GLU:H	1.69	0.41
2:B:323:MET:HG3	2:B:353:VAL:HG21	2.03	0.41
2:B:7:ILE:O	2:B:135:LEU:HA	2.21	0.40
2:B:169:VAL:HA	2:B:202:ILE:O	2.21	0.40
2:B:165:ASN:ND2	12:B:605:HOH:O	2.54	0.40
11:B:504:89C:C18	11:B:504:89C:C06	3.00	0.40
2:B:238:THR:HG21	2:B:316:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	423 (97%)	12 (3%)	0	100	100
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	427/445 (96%)	415 (97%)	10 (2%)	2 (0%)	29	29
2	D	417/445 (94%)	408 (98%)	9 (2%)	0	100	100
3	E	117/143 (82%)	114 (97%)	2 (2%)	1 (1%)	17	14
4	F	323/384 (84%)	310 (96%)	11 (3%)	2 (1%)	25	25
All	All	2158/2319 (93%)	2097 (97%)	56 (3%)	5 (0%)	47	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	GLY
3	E	27	PRO
4	F	102	PRO
4	F	142	ARG
2	B	71	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	368/379 (97%)	361 (98%)	7 (2%)	57	66
1	C	372/379 (98%)	361 (97%)	11 (3%)	41	50
2	B	371/383 (97%)	359 (97%)	12 (3%)	39	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	364/383 (95%)	352 (97%)	12 (3%)	38	46
3	E	109/127 (86%)	103 (94%)	6 (6%)	21	21
4	F	300/342 (88%)	287 (96%)	13 (4%)	29	33
All	All	1884/1993 (94%)	1823 (97%)	61 (3%)	39	47

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	188	ILE
1	A	221	ARG
1	A	256	GLN
1	A	262	TYR
1	A	279	GLU
1	A	302	MET
2	B	19	LYS
2	B	55	THR
2	B	75	SER
2	B	122	LYS
2	B	137	HIS
2	B	245	GLN
2	B	280	GLN
2	B	316	ILE
2	B	320	ARG
2	B	350	LYS
2	B	392	LYS
2	B	406	MET
1	C	133	GLN
1	C	164	LYS
1	C	190	THR
1	C	229	ARG
1	C	245	ASP
1	C	251	ASP
1	C	286	LEU
1	C	302	MET
1	C	347	CYS
1	C	381	THR
1	C	440	VAL
2	D	48	ASN
2	D	55	THR
2	D	69	GLU

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Mol	Chain	Res	Type
2	D	108	GLU
2	D	126	SER
2	D	130	LEU
2	D	137	HIS
2	D	177	ASP
2	D	180	VAL
2	D	188	SER
2	D	193	VAL
2	D	245	GLN
3	E	12	ASN
3	E	75	LYS
3	E	84	GLN
3	E	90	ASN
3	E	109	LYS
3	E	124	GLN
4	F	33	ASP
4	F	70	LYS
4	F	90	SER
4	F	162	ILE
4	F	165	GLU
4	F	171	ASP
4	F	180	HIS
4	F	211	TYR
4	F	222	ARG
4	F	247	LYS
4	F	265	GLU
4	F	310	GLN
4	F	353	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	292	GLN
4	F	180	HIS

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 carbohydrates 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$
5	GTP	C	501	6	26,34,34	1.19	3 (11%)	33,54,54	2.12	8 (24%)
9	GDP	B	501	6	24,30,30	1.02	2 (8%)	31,47,47	2.10	8 (25%)
11	89C	B	504	-	21,24,24	2.06	9 (42%)	27,34,34	1.29	5 (18%)
10	MES	B	503	-	12,12,12	1.82	1 (8%)	14,16,16	6.13	7 (50%)
5	GTP	D	501	-	26,34,34	1.17	2 (7%)	33,54,54	1.81	7 (21%)
8	GOL	A	504	-	5,5,5	0.31	0	5,5,5	0.28	0
11	89C	C	504	-	21,24,24	2.20	11 (52%)	27,34,34	1.64	4 (14%)
5	GTP	A	501	6	26,34,34	1.24	3 (11%)	33,54,54	2.31	11 (33%)

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
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
11	89C	B	504	-	-	2/10/10/10	0/3/3/3
10	MES	B	503	-	-	5/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	501	-	-	5/18/38/38	0/3/3/3
8	GOL	A	504	-	-	4/4/4/4	-
11	89C	C	504	-	-	2/10/10/10	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-5.61	1.69	1.77
5	D	501	GTP	C6-C5	4.10	1.48	1.41
11	C	504	89C	C06-N07	4.05	1.52	1.42
11	B	504	89C	C19-C14	-3.98	1.36	1.41
5	A	501	GTP	C6-C5	3.90	1.48	1.41
11	C	504	89C	O02-C03	3.45	1.42	1.37
11	B	504	89C	C08-N07	-3.43	1.39	1.46
5	C	501	GTP	C6-C5	3.31	1.47	1.41
11	C	504	89C	C17-C18	3.22	1.44	1.36
11	C	504	89C	C08-N07	-3.15	1.39	1.46
11	B	504	89C	O22-C21	3.01	1.42	1.36
11	B	504	89C	C06-N07	2.90	1.49	1.42
11	B	504	89C	C17-C18	2.88	1.43	1.36
5	A	501	GTP	O4'-C1'	2.71	1.44	1.41
9	B	501	GDP	C6-C5	2.71	1.46	1.41
11	B	504	89C	O02-C03	2.59	1.41	1.37
11	C	504	89C	O22-C21	2.56	1.41	1.36
11	C	504	89C	C19-C14	-2.47	1.38	1.41
11	B	504	89C	C05-C06	2.42	1.44	1.39
11	C	504	89C	C20-C21	2.38	1.42	1.38
5	D	501	GTP	C5-C4	2.35	1.47	1.40
11	C	504	89C	C20-C06	2.34	1.43	1.39
11	B	504	89C	C09-N07	-2.29	1.39	1.44
5	C	501	GTP	C5-C4	2.28	1.47	1.40
11	C	504	89C	C05-C06	2.25	1.43	1.39
9	B	501	GDP	C2'-C1'	-2.24	1.50	1.53
5	C	501	GTP	PG-O3G	-2.17	1.46	1.54
11	C	504	89C	C21-C03	2.17	1.44	1.40
11	C	504	89C	C09-C19	2.15	1.47	1.42
11	B	504	89C	C05-C04	2.14	1.42	1.38
5	A	501	GTP	C5-C4	2.10	1.46	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O3S-S-O1S	-12.27	81.30	111.27
10	B	503	MES	O1S-S-C8	-11.43	93.15	106.92
10	B	503	MES	O2S-S-O1S	-10.44	77.81	113.95
10	B	503	MES	O3S-S-O2S	6.87	128.07	111.27
5	C	501	GTP	C6-N1-C2	6.51	126.27	115.93
5	C	501	GTP	C5-C6-N1	-6.07	115.12	123.43
10	B	503	MES	O3S-S-C8	5.66	114.93	105.77
9	B	501	GDP	C6-C5-C4	-5.47	115.58	120.80
11	C	504	89C	C19-C09-N07	5.40	124.04	118.97
5	A	501	GTP	C2-N3-C4	5.38	121.50	115.36
10	B	503	MES	O2S-S-C8	5.24	113.23	106.92
9	B	501	GDP	C6-N1-C2	4.87	123.66	115.93
5	D	501	GTP	C2-N3-C4	4.83	120.88	115.36
5	A	501	GTP	C6-C5-C4	-4.75	116.26	120.80
5	A	501	GTP	C6-N1-C2	4.53	123.13	115.93
5	A	501	GTP	N3-C2-N1	-4.51	121.20	127.22
9	B	501	GDP	N3-C2-N1	-4.49	121.23	127.22
5	A	501	GTP	C5-C6-N1	-4.18	117.71	123.43
5	C	501	GTP	N3-C2-N1	-4.07	121.79	127.22
9	B	501	GDP	C2-N3-C4	3.96	119.88	115.36
5	D	501	GTP	C5-C6-N1	-3.88	118.13	123.43
5	D	501	GTP	C6-C5-C4	-3.70	117.27	120.80
10	B	503	MES	C6-O1-C2	3.67	122.15	109.89
9	B	501	GDP	C5-C6-N1	-3.64	118.45	123.43
5	D	501	GTP	C6-N1-C2	3.51	121.51	115.93
11	B	504	89C	C19-C09-N07	3.50	122.26	118.97
5	C	501	GTP	C6-C5-C4	-3.49	117.47	120.80
5	A	501	GTP	N2-C2-N1	3.29	122.36	117.25
5	A	501	GTP	C4-C5-N7	-3.20	106.07	109.40
11	C	504	89C	C09-C19-C14	3.10	119.84	116.99
5	C	501	GTP	O3G-PG-O1G	3.08	122.73	110.68
5	A	501	GTP	O3G-PG-O2G	3.02	119.16	107.64
9	B	501	GDP	C1'-N9-C4	-3.00	121.37	126.64
5	D	501	GTP	N3-C2-N1	-2.96	123.27	127.22
5	D	501	GTP	C4-C5-N7	-2.70	106.58	109.40
11	C	504	89C	C01-O02-C03	2.60	121.45	117.53
5	A	501	GTP	C1'-N9-C4	-2.54	122.17	126.64
11	B	504	89C	C18-C19-C14	2.38	119.26	116.50
11	B	504	89C	C06-N07-C09	2.37	123.05	119.91
5	D	501	GTP	PA-O3A-PB	-2.33	124.84	132.83
5	C	501	GTP	C1'-N9-C4	-2.32	122.56	126.64
5	A	501	GTP	O2G-PG-O3B	-2.26	97.06	104.64
9	B	501	GDP	N2-C2-N1	2.23	120.73	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	O3'-C3'-C4'	-2.23	104.61	111.05
5	C	501	GTP	C2-N3-C4	2.13	117.79	115.36
11	B	504	89C	C09-C19-C14	2.09	118.92	116.99
11	C	504	89C	C06-C20-C21	-2.08	119.52	121.28
11	B	504	89C	C06-C20-C21	-2.03	119.56	121.28
5	A	501	GTP	PB-O3B-PG	-2.03	125.85	132.83
5	C	501	GTP	PB-O3B-PG	-2.02	125.89	132.83

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	C7-C8-S-O1S
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O1A
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	C1-C2-C3-O3
8	A	504	GOL	O2-C2-C3-O3
5	A	501	GTP	C5'-O5'-PA-O1A
10	B	503	MES	C7-C8-S-O3S
11	C	504	89C	C10-C09-N07-C08
8	A	504	GOL	O1-C1-C2-O2
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
11	B	504	89C	C10-C09-N07-C08
10	B	503	MES	N4-C7-C8-S
11	B	504	89C	C19-C09-N07-C06
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O3A

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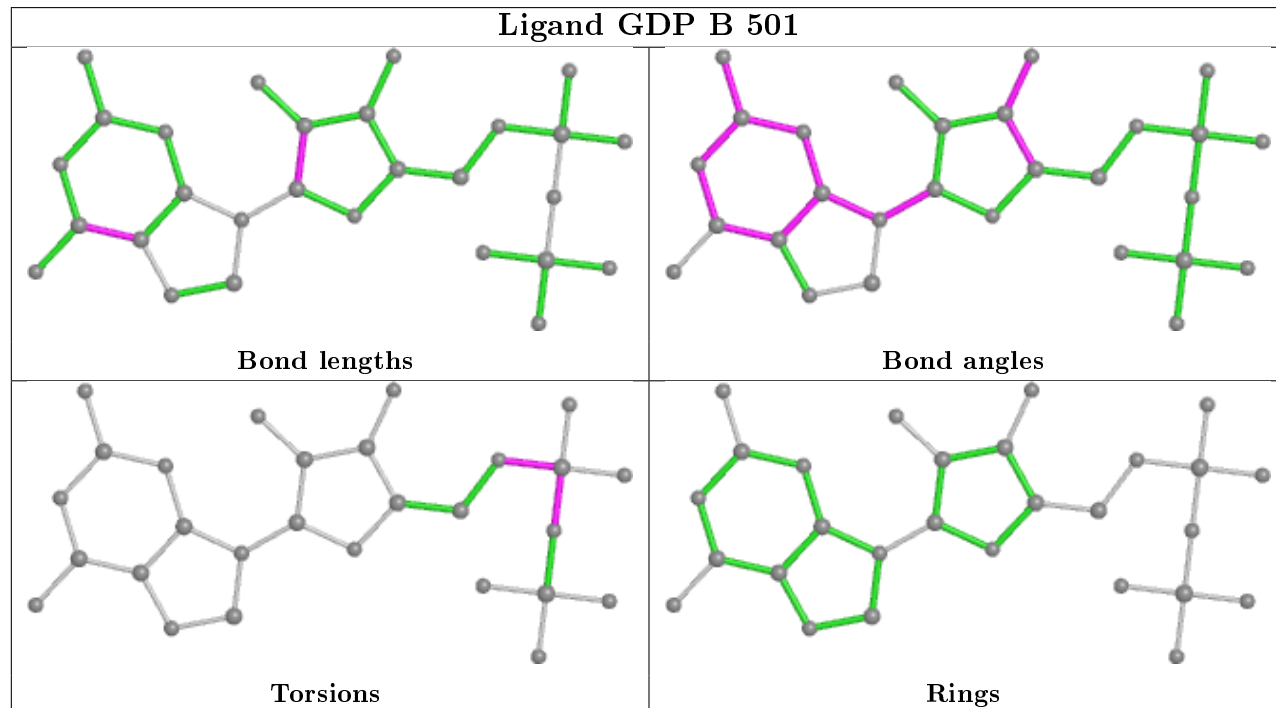
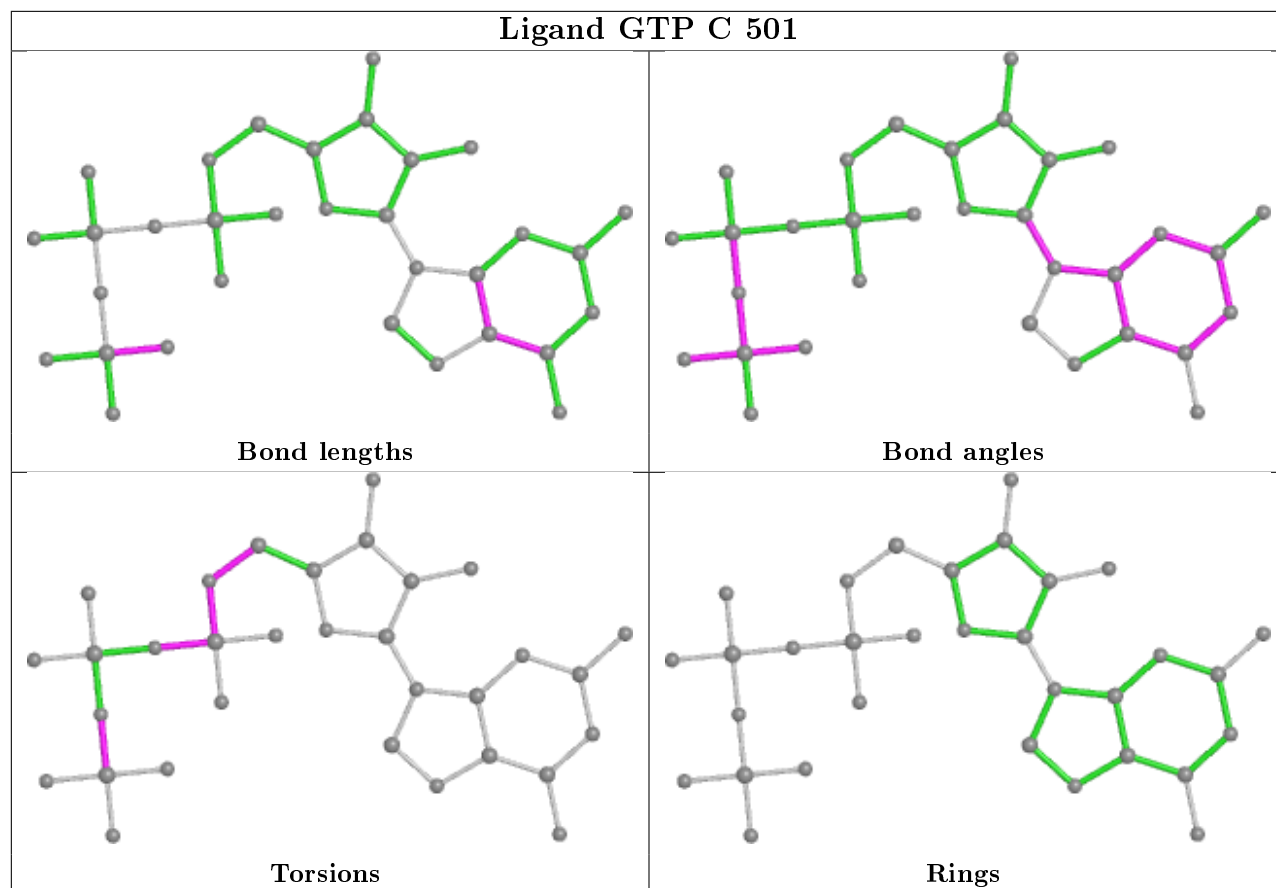
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
11	C	504	89C	C19-C09-N07-C06

There are no ring outliers.

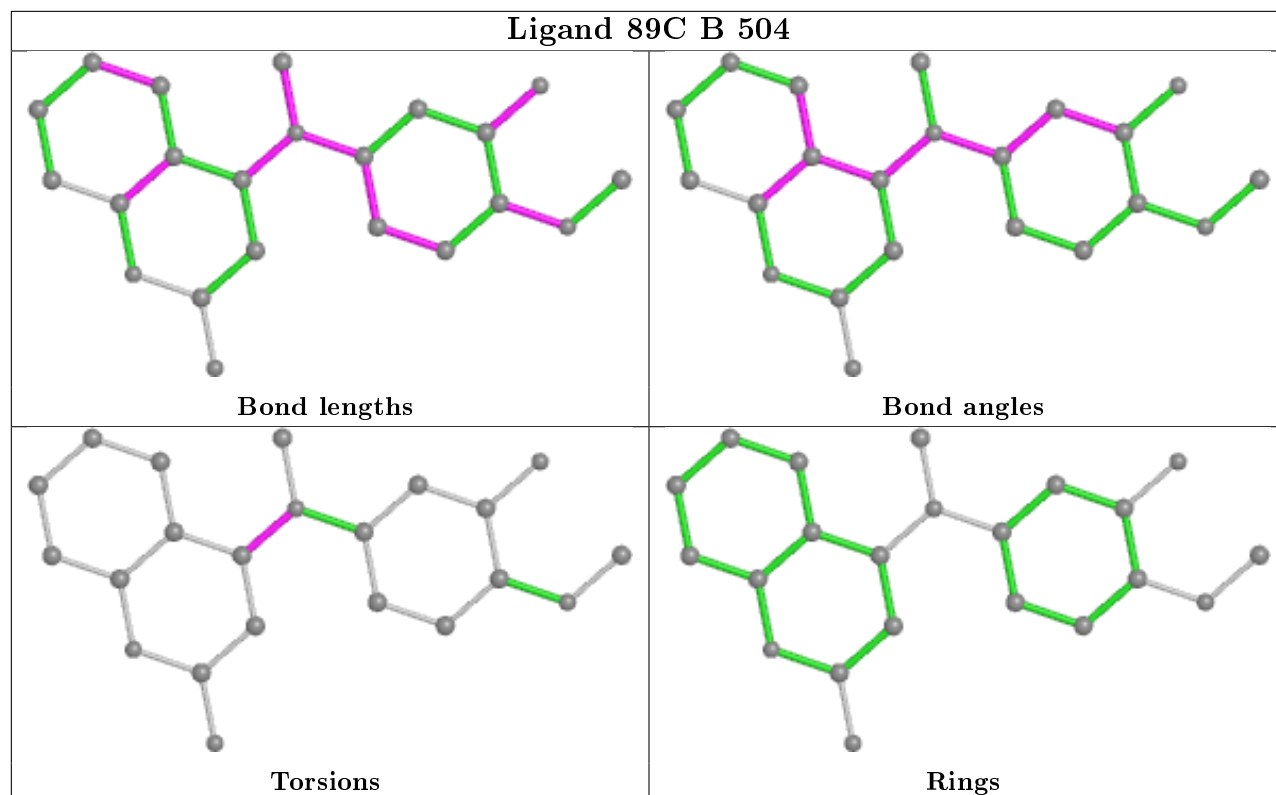
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	504	89C	1	0
10	B	503	MES	5	0

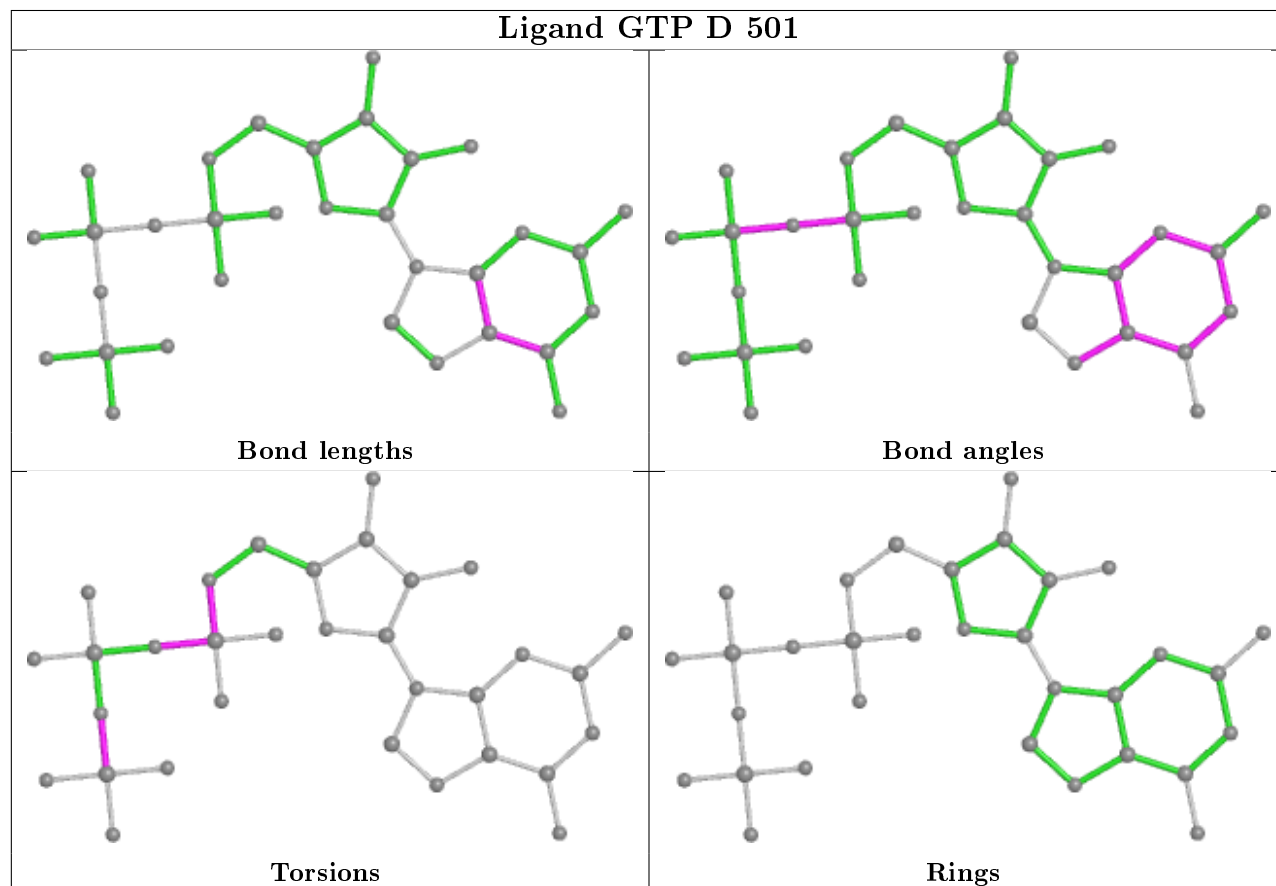
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



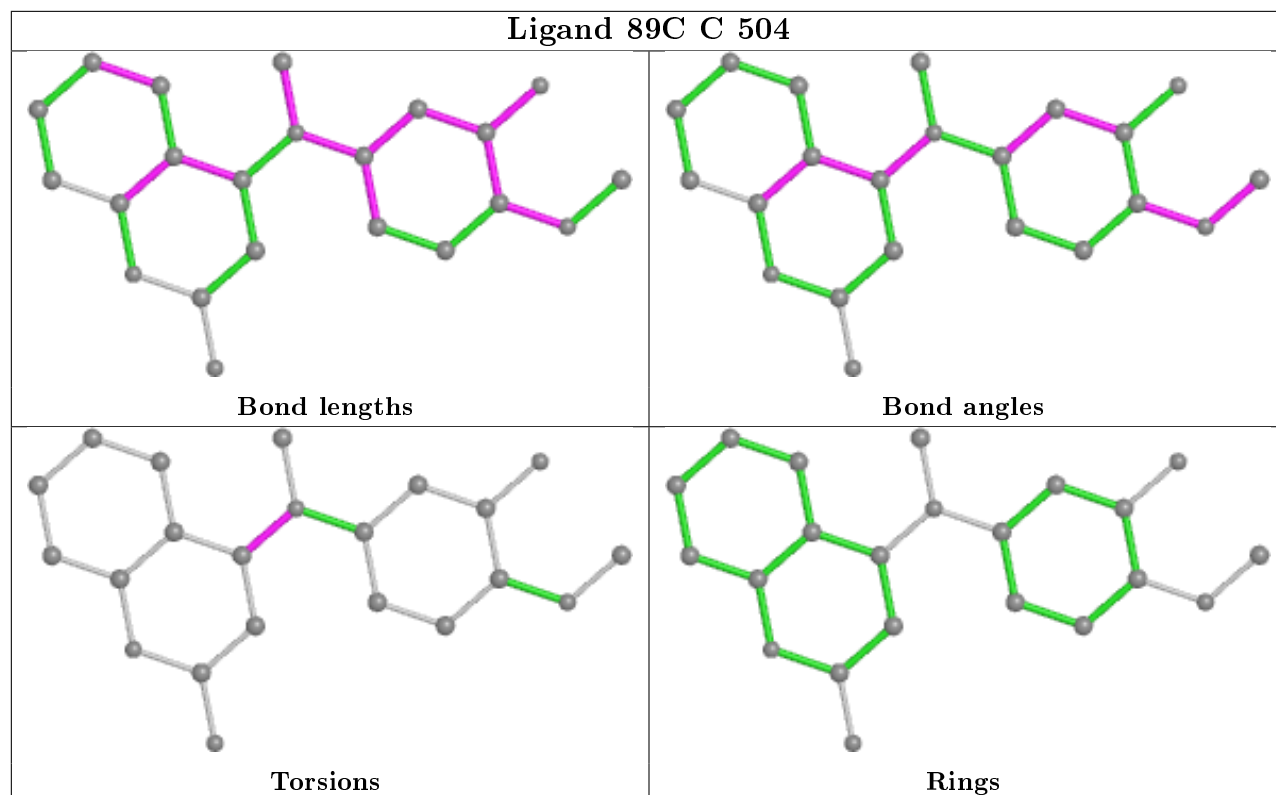
Ligand 89C B 504



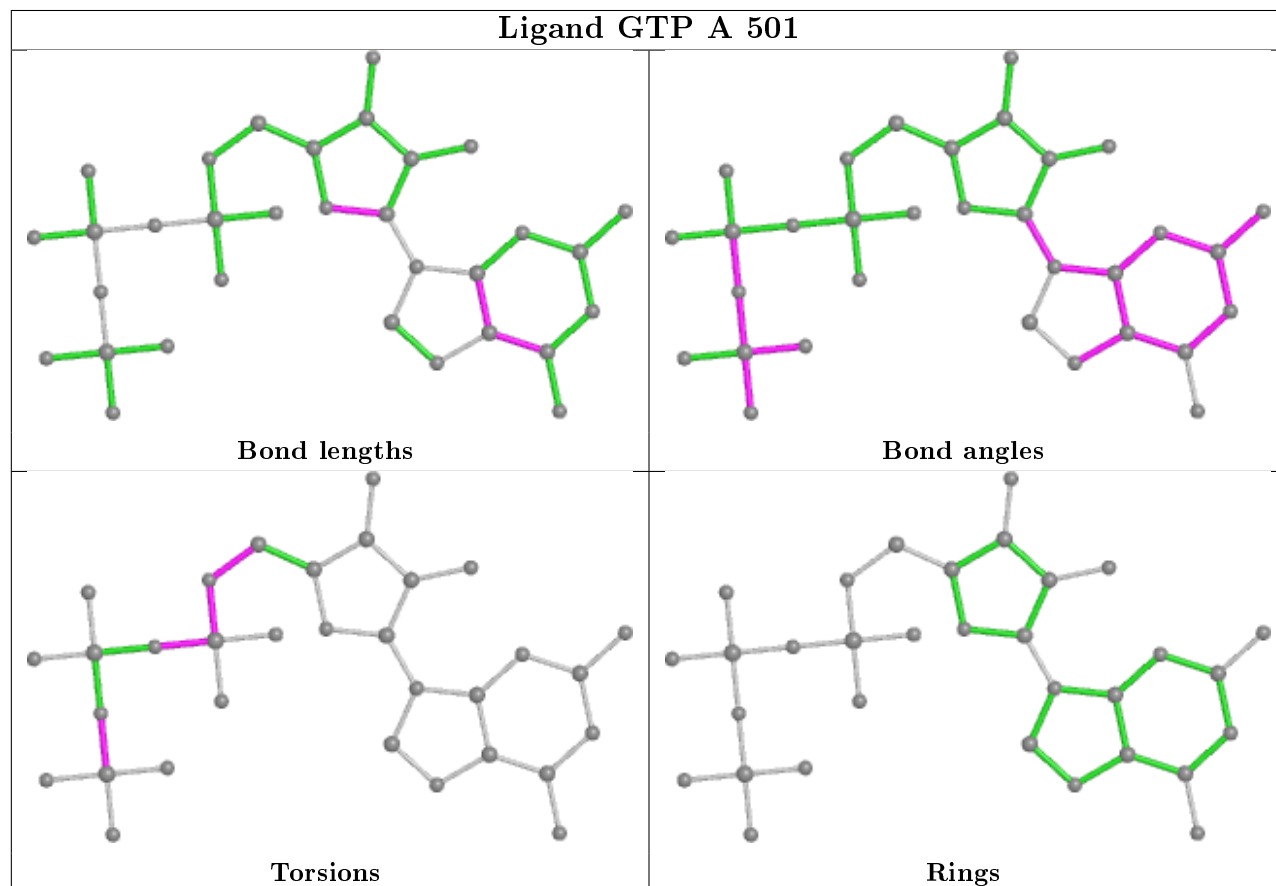
Ligand GTP D 501



Ligand 89C C 504



Ligand GTP A 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	-0.05	6 (1%) 75 77	28, 43, 69, 90	0
1	C	440/451 (97%)	-0.31	3 (0%) 87 88	24, 35, 59, 78	0
2	B	428/445 (96%)	0.08	18 (4%) 36 38	25, 43, 82, 154	0
2	D	421/445 (94%)	0.57	53 (12%) 3 3	31, 60, 99, 113	0
3	E	121/143 (84%)	0.41	10 (8%) 11 12	32, 59, 97, 119	0
4	F	333/384 (86%)	0.62	62 (18%) 1 1	36, 66, 125, 155	0
All	All	2180/2319 (94%)	0.17	152 (6%) 16 17	24, 48, 97, 155	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	141	GLY	10.1
2	B	279	GLN	8.6
2	B	278	SER	7.8
4	F	176	GLN	7.3
4	F	173	ILE	7.2
4	F	177	GLY	6.7
4	F	130	VAL	6.6
2	D	1	MET	6.6
4	F	132	LEU	6.4
4	F	133	ALA	6.0
4	F	169	LEU	5.6
4	F	102	PRO	5.6
3	E	139	LEU	5.3
4	F	231	ALA	5.3
4	F	182	ILE	5.2
4	F	101	TYR	5.1
4	F	170	LEU	5.1
4	F	380	HIS	5.0
4	F	137	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	4.8
2	D	390	ARG	4.5
4	F	234	GLN	4.4
4	F	233	PHE	4.4
4	F	172	PHE	4.4
4	F	103	THR	4.3
1	A	281	ALA	4.3
2	D	135	LEU	4.3
2	B	277	GLY	4.2
4	F	174	ASP	4.2
4	F	179	VAL	4.2
2	D	394	PHE	4.1
1	A	282	TYR	4.1
4	F	131	PHE	4.1
2	D	55	THR	4.1
2	D	284	LEU	4.0
2	D	218	THR	4.0
2	B	55	THR	4.0
4	F	134	ALA	4.0
4	F	45	ASN	3.8
2	D	219	THR	3.8
3	E	7	GLU	3.8
4	F	135	TYR	3.8
2	D	165	ASN	3.7
4	F	100	ILE	3.7
2	B	280	GLN	3.7
3	E	140	LYS	3.6
2	D	95	SER	3.6
2	D	166	THR	3.6
4	F	253	TYR	3.6
4	F	136	ASN	3.6
4	F	361	LEU	3.6
4	F	178	GLN	3.5
4	F	138	ARG	3.5
2	D	199	THR	3.5
2	D	168	SER	3.5
2	B	276	ARG	3.5
2	D	405	GLU	3.5
2	D	94	GLN	3.4
2	D	57	ASN	3.4
4	F	362	ALA	3.4
2	B	282	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	167	SER	3.4
2	B	275	SER	3.3
2	D	167	PHE	3.3
2	D	391	ARG	3.2
2	B	428	ALA	3.2
4	F	162	ILE	3.2
4	F	232	ASN	3.2
2	B	427	ASP	3.2
2	D	200	TYR	3.1
4	F	171	ASP	3.1
4	F	90	SER	3.1
2	D	37	HIS	3.1
2	D	136	THR	3.0
4	F	168	GLU	3.0
3	E	6	MET	2.9
2	D	396	HIS	2.9
2	D	137	HIS	2.9
2	D	397	TRP	2.9
2	B	37	HIS	2.9
1	A	365	GLY	2.9
4	F	126	ASP	2.9
2	D	404	ASP	2.8
2	D	192	LEU	2.8
2	D	387	ALA	2.8
2	B	41	ASP	2.8
4	F	144	GLY	2.7
2	D	406	MET	2.7
2	D	54	ALA	2.7
4	F	140	GLU	2.7
4	F	166	ALA	2.7
4	F	129	GLU	2.7
1	A	171	ILE	2.7
2	B	274	THR	2.7
4	F	21	LEU	2.7
2	D	285	THR	2.6
4	F	244	CYS	2.6
4	F	143	GLU	2.6
2	D	393	ALA	2.6
4	F	27	TRP	2.6
2	D	33	THR	2.6
4	F	165	GLU	2.6
2	D	92	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	58	LYS	2.5
2	D	149	THR	2.5
3	E	138	GLU	2.5
4	F	235	ASP	2.5
4	F	230	SER	2.5
2	B	33	THR	2.5
4	F	24	THR	2.5
3	E	26	PRO	2.5
4	F	25	GLY	2.5
4	F	145	ASN	2.5
2	D	164	MET	2.4
2	D	320	ARG	2.4
2	D	201	CYS	2.4
3	E	48	GLU	2.4
4	F	161	LEU	2.4
2	B	253	LEU	2.4
1	A	430	LYS	2.3
2	D	362	LYS	2.3
2	D	56	GLY	2.3
1	C	440	VAL	2.3
4	F	255	ARG	2.3
1	C	340	SER	2.3
4	F	99	VAL	2.3
2	D	217	LEU	2.3
2	D	7	ILE	2.3
1	C	200	CYS	2.3
2	B	58	LYS	2.3
3	E	59	GLU	2.2
2	D	400	GLY	2.2
2	B	266	PHE	2.2
2	D	212	PHE	2.2
3	E	46	SER	2.2
2	D	196	THR	2.2
3	E	25	LYS	2.2
2	B	36	TYR	2.2
2	D	59	TYR	2.2
2	D	53	GLU	2.2
4	F	175	GLU	2.2
2	D	177	ASP	2.2
4	F	139	ARG	2.1
4	F	89	GLU	2.1
2	D	202	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	20	LEU	2.1
4	F	163	SER	2.1
2	D	265	PHE	2.1
2	D	431	ASP	2.0
2	D	198	GLU	2.0
1	A	57	GLY	2.0
2	D	96	GLY	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.

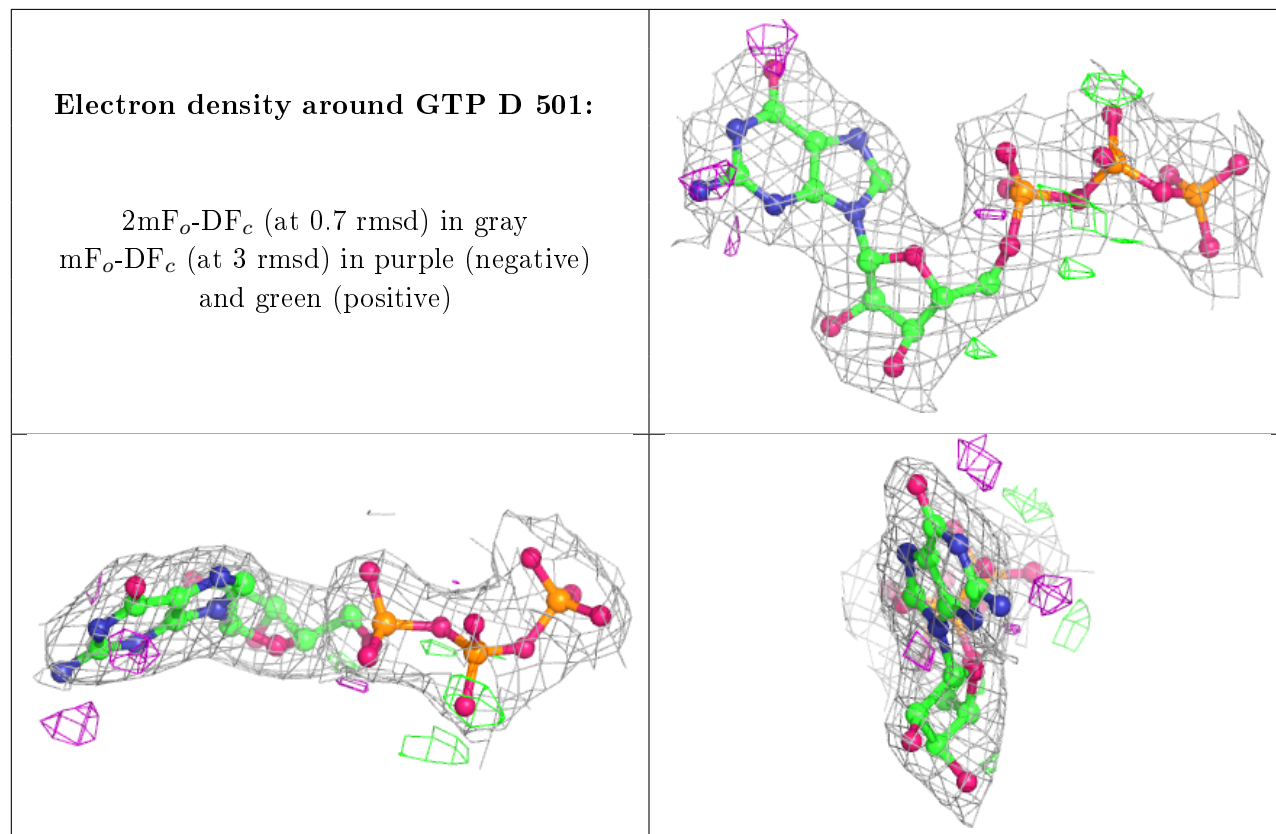
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	502	1/1	0.94	0.12	82,82,82,82	0
10	MES	B	503	12/12	0.94	0.13	44,52,59,60	0
5	GTP	D	501	32/32	0.95	0.10	49,58,70,78	0
7	CA	A	503	1/1	0.96	0.03	56,56,56,56	0
8	GOL	A	504	6/6	0.96	0.12	44,55,57,62	0
11	89C	C	504	22/22	0.96	0.11	33,43,47,48	0
11	89C	B	504	22/22	0.97	0.20	30,34,38,40	0
6	MG	C	502	1/1	0.98	0.13	32,32,32,32	0
6	MG	B	502	1/1	0.98	0.09	29,29,29,29	0
5	GTP	A	501	32/32	0.98	0.17	28,33,36,43	0
5	GTP	C	501	32/32	0.99	0.13	23,28,33,40	0
7	CA	C	503	1/1	0.99	0.03	42,42,42,42	0
9	GDP	B	501	28/28	0.99	0.12	26,31,32,36	0
6	MG	A	502	1/1	0.99	0.16	40,40,40,40	0

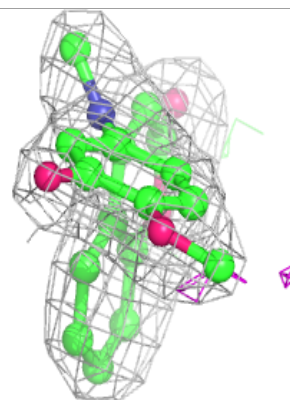
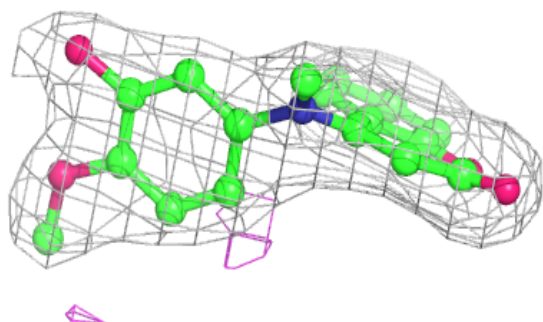
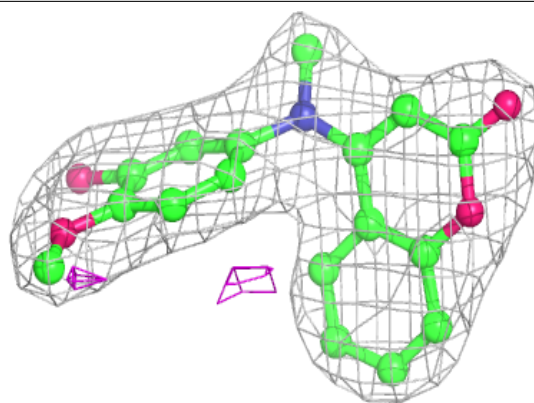
The following is a graphical depiction of the model fit to experimental electron density of all

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.

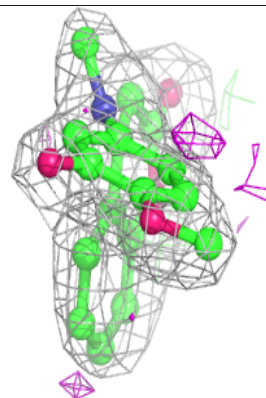
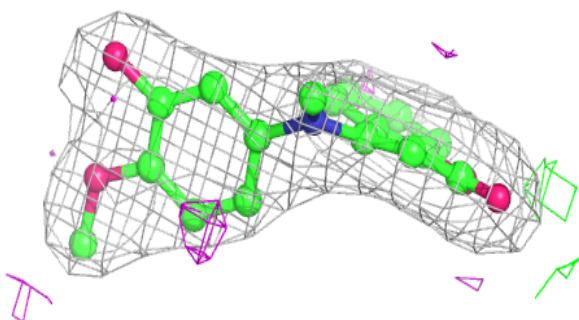
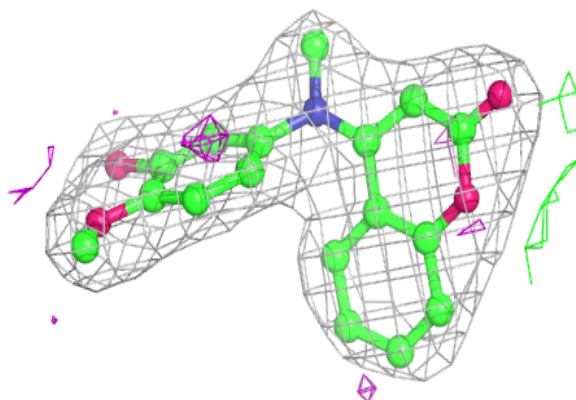


Electron density around 89C C 504:

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

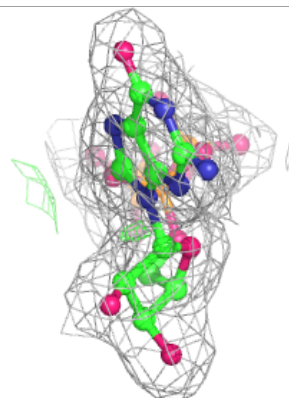
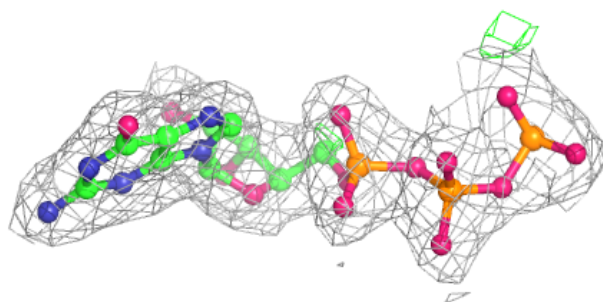
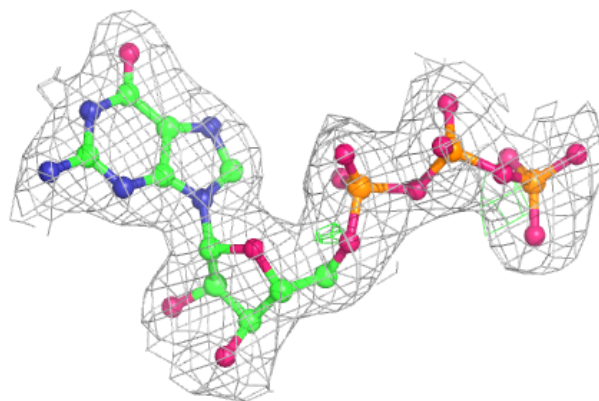
**Electron density around 89C B 504:**

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

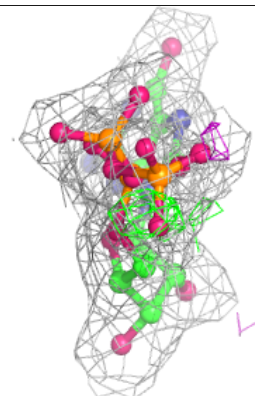
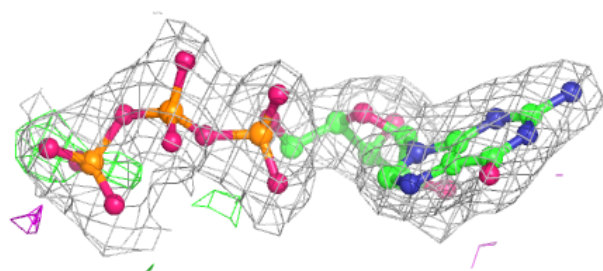
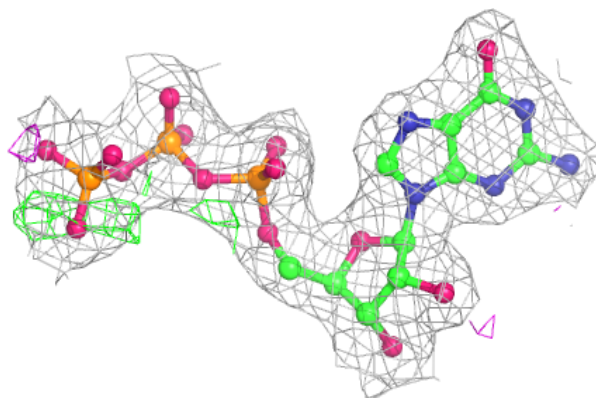


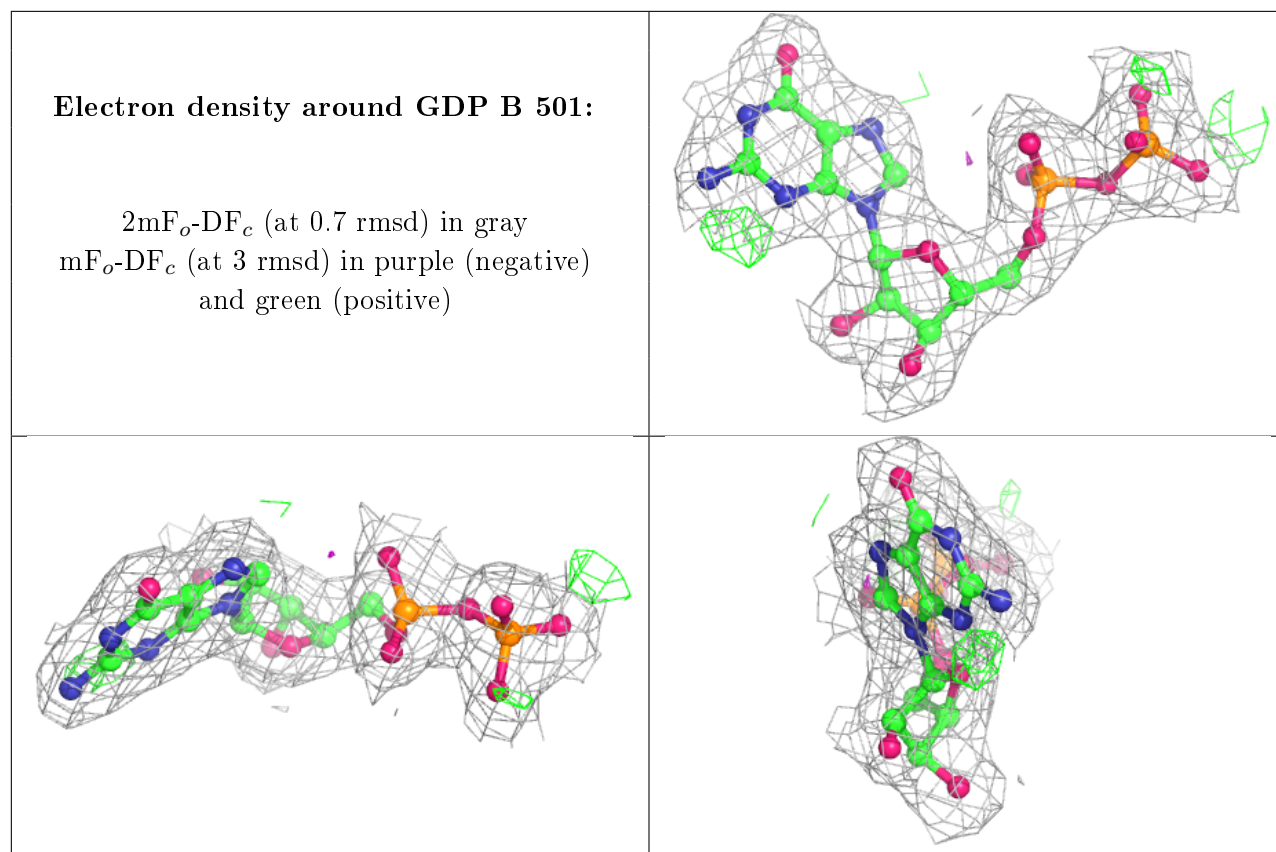
Electron density around GTP A 501:

$2mF_o-DF_c$ (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.