



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:43 pm BST

PDB ID : 5XAF
Title : Crystal structure of tubulin-stathmin-TTL-Compound Z1 complex
Authors : Zhang, H.; Luo, C.; Wang, Y.
Deposited on : 2017-03-12
Resolution : 2.55 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

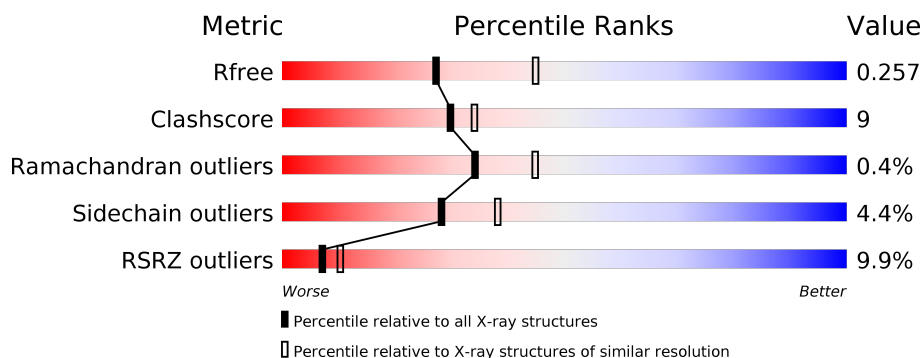
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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>3%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>• •</div> </div> </div>
1	C	451	<div> <div></div> <div> <div>79%</div> <div>18%</div> <div>• •</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• 5%</div> </div> </div>
2	D	445	<div> <div>11%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• 5%</div> </div> </div>
3	E	189	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>12%</div> <div>• 36%</div> </div> </div>
4	F	378	<div> <div>32%</div> <div> <div></div> <div>60%</div> <div>22%</div> <div>• 16%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ACP	F	402	-	-	-	X
7	GOL	B	504	-	-	-	X
7	GOL	B	505	-	-	X	X
7	GOL	D	503	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18303 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	438	Total	C	N	O	S	0	10	0
			3468	2203	583	657	25			
1	C	440	Total	C	N	O	S	0	11	0
			3489	2209	588	668	24			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	7	0
			3355	2111	567	650	27			
2	D	421	Total	C	N	O	S	0	3	0
			3323	2092	562	641	28			

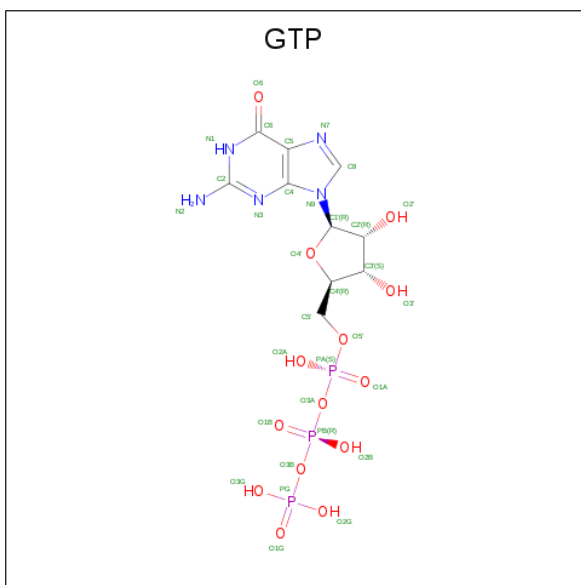
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1011	624	183	199	5			

- Molecule 4 is a protein called TTL Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	3	0
			2608	1688	434	472	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- 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
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

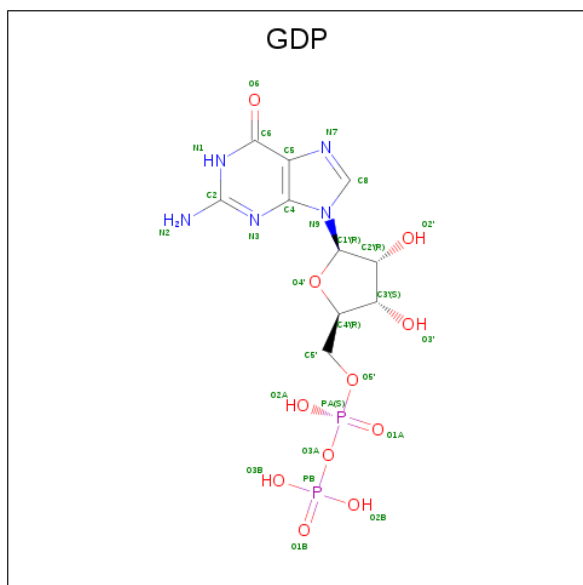


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

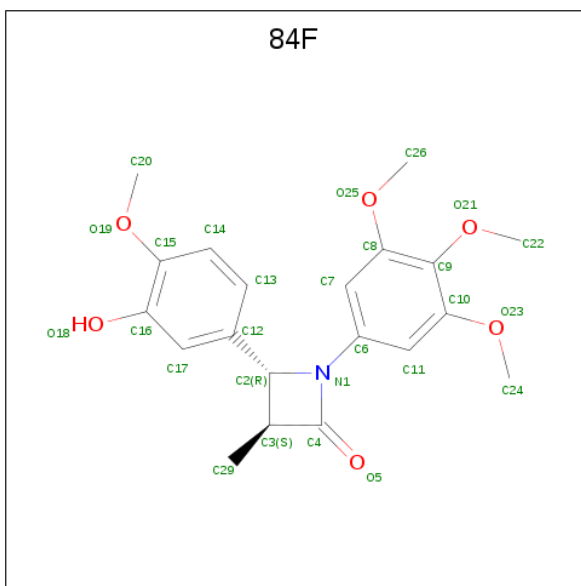
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





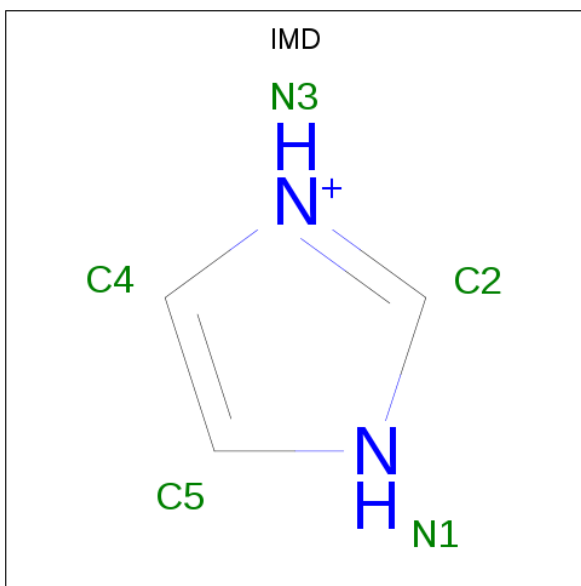
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3S,4R)-4-(3-hydroxy-4-methoxyphenyl)-3-methyl-1-(3,4,5-trimethoxyphenyl)azetidin-2-one (three-letter code: 84F) (formula: C₂₀H₂₃NO₆).



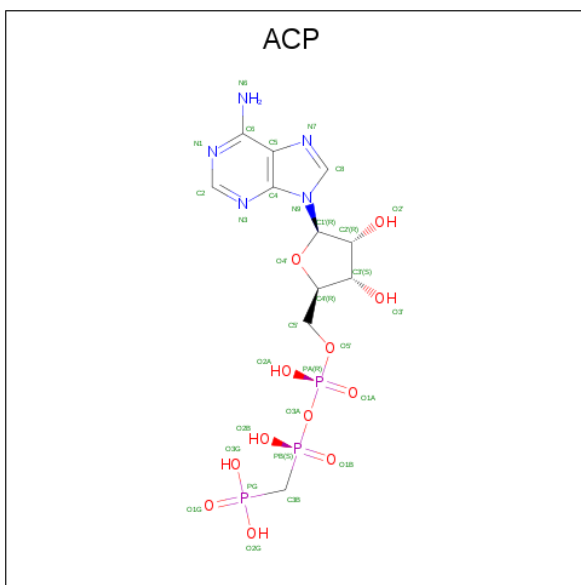
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	20	1	6		
11	D	1	Total	C	N	O	0	0
			27	20	1	6		

- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	N	0	0
			5	3	2		
12	C	1	Total	C	N	0	0
			5	3	2		
12	E	1	Total	C	N	0	0
			5	3	2		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

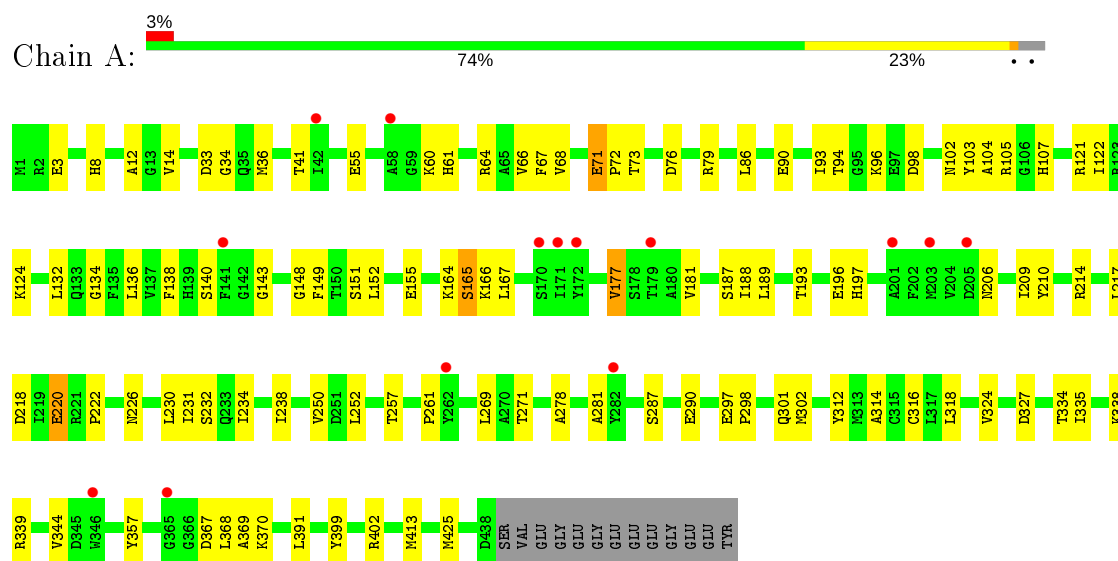
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	131	Total	O	0	0
			131	131		
14	B	136	Total	O	0	0
			136	136		
14	C	211	Total	O	0	0
			211	211		
14	D	99	Total	O	0	0
			99	99		
14	E	59	Total	O	0	0
			59	59		
14	F	101	Total	O	0	0
			101	101		

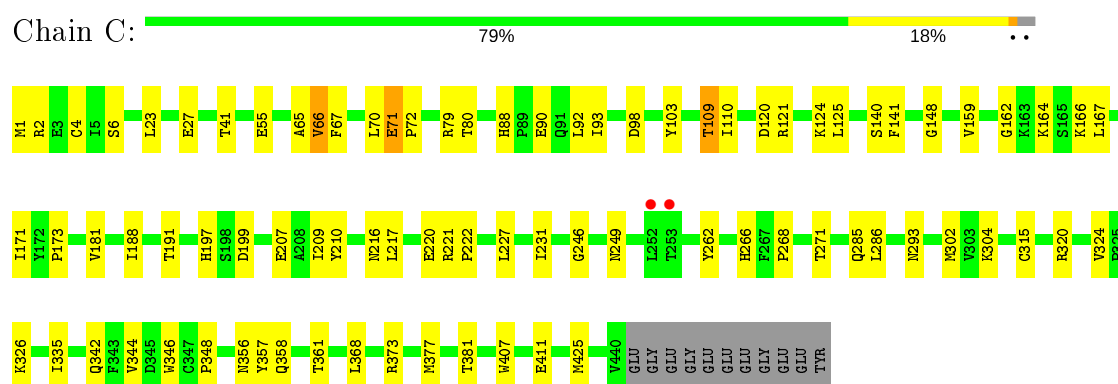
3 Residue-property plots [i](#)

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.

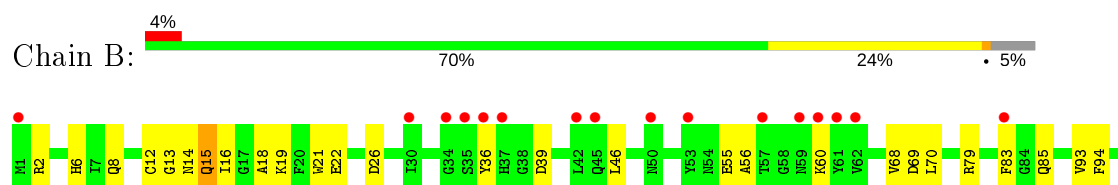
• Molecule 1: Tubulin alpha-1B chain

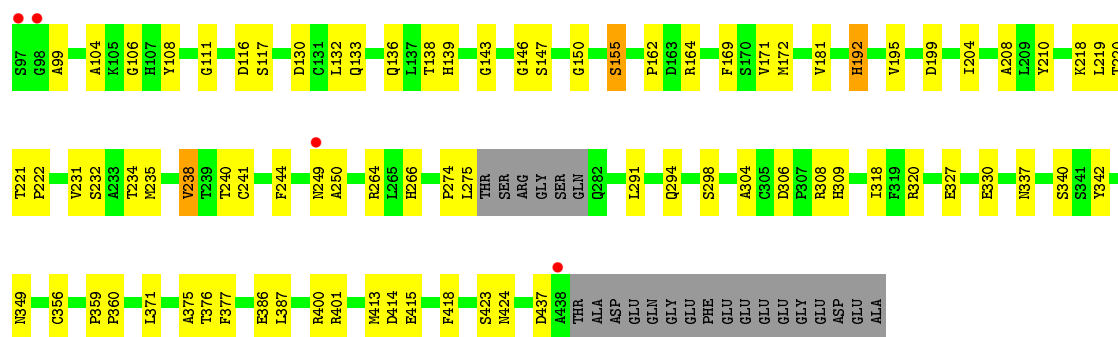


• Molecule 1: Tubulin alpha-1B chain

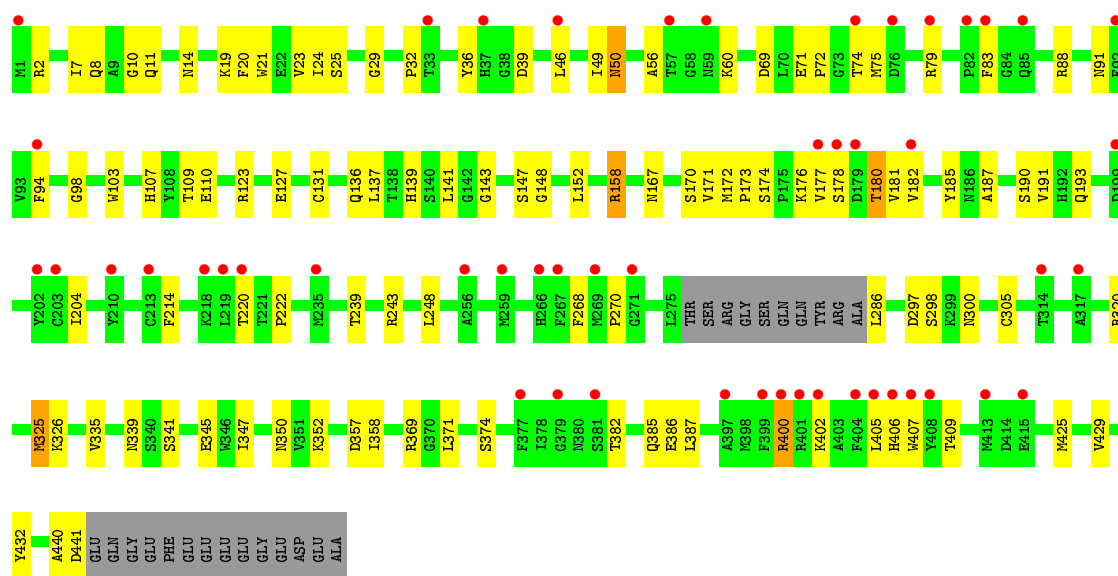


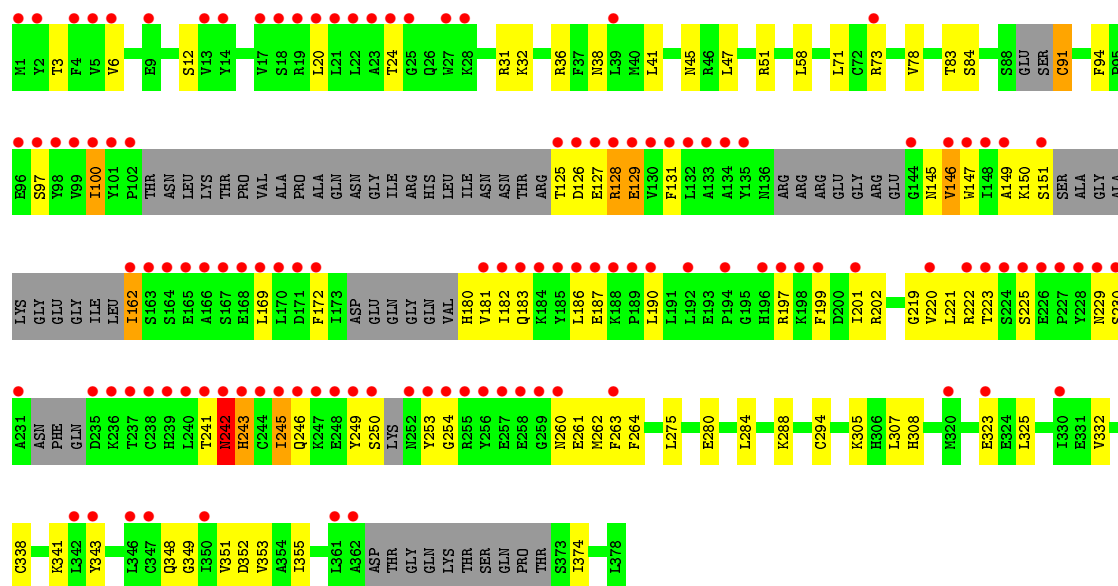
• Molecule 2: Tubulin beta-2B chain





• Molecule 2: Tubulin beta-2B chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.57Å 156.51Å 182.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.77 – 2.55 49.77 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.77-2.55) 99.9 (49.77-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.206 , 0.257 0.206 , 0.257	Depositor DCC
R_{free} test set	1999 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.9	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	0.95	EDS
Total number of atoms	18303	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, IMD, CA, GTP, 84F, ACP, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/3576	0.57	0/4855
1	C	0.51	0/3597	0.63	1/4885 (0.0%)
2	B	0.46	0/3447	0.60	0/4669
2	D	0.40	0/3405	0.55	0/4614
3	E	0.40	0/1025	0.55	0/1360
4	F	0.40	1/2673 (0.0%)	0.54	0/3608
All	All	0.44	1/17723 (0.0%)	0.58	1/23991 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	47	LEU	C-N	7.89	1.49	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	PRO	C-N-CA	5.16	134.61	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	3468	0	3413	63	0
1	C	3489	0	3413	54	0
2	B	3355	0	3237	72	0
2	D	3323	0	3216	67	0
3	E	1011	0	1032	21	0
4	F	2608	0	2597	60	0
5	A	32	0	12	1	0
5	C	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
6	F	1	0	0	0	0
7	A	18	0	24	0	0
7	B	18	0	24	7	0
7	C	24	0	32	1	0
7	D	12	0	15	4	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	12	0	12	0	0
11	B	27	0	0	0	0
11	D	27	0	0	0	0
12	C	10	0	10	4	0
12	E	5	0	4	1	0
13	F	31	0	14	1	0
14	A	131	0	0	2	0
14	B	136	0	0	15	1
14	C	211	0	0	3	1
14	D	99	0	0	10	0
14	E	59	0	0	6	0
14	F	101	0	0	10	0
All	All	18303	0	17091	325	1

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 9.

All (325) 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:19:LYS:N	14:B:601:HOH:O	1.93	1.00
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.57	0.86
2:D:103:TRP:HD1	2:D:147:SER:HG	1.24	0.85
2:D:10:GLY:O	2:D:14:ASN:ND2	2.12	0.81
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.62	0.81
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.54	0.81
2:B:221:THR:O	14:B:602:HOH:O	1.99	0.79
2:B:401:ARG:HE	7:B:503:GOL:H2	1.49	0.78
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.18	0.77
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.66	0.74
3:E:6:MET:N	14:E:302:HOH:O	2.19	0.74
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.05	0.73
1:A:214:ARG:NH1	1:A:220:GLU:O	2.24	0.71
3:E:140:LYS:O	14:E:301:HOH:O	2.08	0.70
2:D:286:LEU:N	14:D:605:HOH:O	2.23	0.70
4:F:323:GLU:O	14:F:501:HOH:O	2.10	0.69
4:F:151:SER:HB2	4:F:180:HIS:HA	1.75	0.69
2:B:294:GLN:NE2	14:B:610:HOH:O	2.26	0.69
4:F:305:LYS:NZ	14:F:505:HOH:O	2.26	0.69
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.75	0.69
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.74	0.69
2:B:249:ASN:N	14:B:609:HOH:O	2.26	0.68
4:F:31:ARG:HE	4:F:32:LYS:H	1.41	0.66
2:B:162:PRO:O	14:B:603:HOH:O	2.12	0.66
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.30	0.66
4:F:128:ARG:N	14:F:506:HOH:O	2.26	0.66
2:B:337:ASN:HD21	4:F:36:ARG:HH21	1.43	0.66
4:F:201:ILE:HG13	4:F:221:LEU:HD21	1.77	0.66
1:A:90:GLU:OE1	14:A:601:HOH:O	2.14	0.66
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.31	0.65
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.77	0.65
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.79	0.65
2:D:180:THR:O	14:D:602:HOH:O	2.14	0.65
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.79	0.65
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.78	0.64
2:D:75:MET:O	14:D:601:HOH:O	2.14	0.64
2:B:2:ARG:HH21	2:B:133:GLN:HA	1.63	0.64
2:B:309:HIS:ND1	2:B:386:GLU:OE1	2.31	0.63
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.81	0.63
2:D:123:ARG:O	2:D:127:GLU:HG2	1.99	0.63
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.65	0.62
2:D:136:GLN:HA	2:D:167:ASN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:164:LYS:NZ	2.32	0.62
1:C:41:THR:OG1	1:C:41:THR:O	2.15	0.62
1:A:166:LYS:HE2	1:A:197:HIS:O	1.98	0.62
4:F:145:ASN:HB3	4:F:147:TRP:HE1	1.65	0.61
2:D:325:MET:HG3	14:D:626:HOH:O	2.00	0.61
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.81	0.61
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.34	0.61
4:F:261:GLU:O	14:F:503:HOH:O	2.17	0.60
2:D:11:GLN:HB3	9:D:501:GDP:O2A	2.02	0.60
2:D:46:LEU:HA	2:D:49:ILE:HB	1.83	0.60
1:C:166:LYS:HE2	1:C:197:HIS:O	2.02	0.60
2:B:304:ALA:O	14:B:604:HOH:O	2.16	0.59
1:C:286:LEU:O	1:C:373:ARG:NH1	2.35	0.59
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.85	0.58
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.38	0.58
1:C:293[A]:ASN:HA	1:C:335:ILE:HD11	1.86	0.58
4:F:197:ARG:HD2	4:F:225:SER:HA	1.84	0.58
2:B:376:THR:OG1	7:B:505:GOL:H32	2.02	0.58
1:C:1:MET:O	14:C:601:HOH:O	2.17	0.58
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.86	0.57
2:D:21:TRP:O	2:D:25:SER:OG	2.14	0.57
2:D:369:ARG:NH1	14:D:612:HOH:O	2.37	0.57
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.39	0.57
2:D:158:ARG:NH1	14:D:611:HOH:O	2.37	0.57
1:C:293[B]:ASN:HA	1:C:335:ILE:HD11	1.87	0.57
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.33	0.57
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.87	0.56
3:E:6:MET:N	14:E:303:HOH:O	2.37	0.56
1:C:159:VAL:HA	3:E:94:ILE:HG23	1.86	0.56
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.89	0.55
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.40	0.55
1:C:324:VAL:HG22	14:C:631:HOH:O	2.06	0.55
1:A:196:GLU:HG3	1:A:197:HIS:CD2	2.42	0.55
4:F:246:GLN:HG2	4:F:250:SER:HB3	1.87	0.55
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.14	0.55
2:D:222:PRO:O	7:D:503:GOL:O2	2.25	0.55
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.39	0.54
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.43	0.54
1:A:234:ILE:O	1:A:238:ILE:HG13	2.06	0.54
2:B:308:ARG:HG2	2:B:342:TYR:CE2	2.42	0.54
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:201:ILE:HG13	4:F:221:LEU:CD2	2.37	0.54
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.88	0.54
2:D:400:ARG:HG3	14:D:628:HOH:O	2.07	0.54
2:D:103:TRP:HD1	2:D:147:SER:OG	1.88	0.54
2:D:71:GLU:HB3	2:D:98:GLY:HA2	1.90	0.54
2:D:19:LYS:O	2:D:23:VAL:HG23	2.08	0.54
1:C:377:MET:HE2	14:C:668:HOH:O	2.07	0.53
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.88	0.53
2:B:320:ARG:HD3	7:B:505:GOL:H2	1.90	0.53
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.91	0.53
2:B:218:LYS:N	14:B:613:HOH:O	2.34	0.52
2:B:155[B]:SER:OG	3:E:76:ARG:NH2	2.41	0.52
2:B:15:GLN:O	14:B:601:HOH:O	2.19	0.52
2:B:400:ARG:NH2	14:B:620:HOH:O	2.41	0.52
2:D:180:THR:HG22	2:D:181:VAL:H	1.75	0.52
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.91	0.52
4:F:131:PHE:HE2	4:F:182:ILE:HG21	1.74	0.52
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.44	0.52
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.92	0.52
2:D:385:GLN:OE1	14:D:603:HOH:O	2.19	0.52
4:F:351:VAL:HA	4:F:355:ILE:HB	1.92	0.52
2:B:291:LEU:HD13	2:B:375:ALA:HB2	1.92	0.51
1:A:338:LYS:HE2	1:A:339:ARG:HG2	1.92	0.51
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.45	0.51
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.29	0.51
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.44	0.51
1:C:27:GLU:HG2	1:C:361:THR:HG22	1.93	0.51
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.51
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.27	0.51
2:D:177:VAL:HG13	7:D:503:GOL:H2	1.93	0.51
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.46	0.51
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.92	0.51
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.94	0.50
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.76	0.50
4:F:100:ILE:HD12	4:F:128:ARG:HG3	1.91	0.50
2:D:7:ILE:O	2:D:137:LEU:HA	2.11	0.50
2:D:320:ARG:NH1	14:D:617:HOH:O	2.44	0.50
1:A:96:LYS:NZ	2:B:130:ASP:O	2.45	0.50
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.47	0.50
2:B:16:ILE:C	14:B:601:HOH:O	2.50	0.49
1:C:79:ARG:HG2	1:C:92:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.46	0.49
1:A:68[A]:VAL:HG11	1:A:149:PHE:CE2	2.47	0.49
2:B:401:ARG:HE	7:B:503:GOL:C2	2.24	0.49
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.94	0.49
4:F:186:LEU:HB3	13:F:402:ACP:H2	1.94	0.49
4:F:146:VAL:HG13	4:F:187:GLU:OE2	2.10	0.49
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.53	0.49
2:B:132:LEU:HB3	2:B:164:ARG:NH1	2.27	0.49
2:B:69:ASP:O	2:B:94:PHE:HA	2.13	0.49
1:C:262:TYR:CB	12:C:508:IMD:H5	2.43	0.49
1:C:167:LEU:HD13	12:C:509:IMD:H2	1.94	0.49
2:B:195:VAL:HG13	2:B:264:ARG:HG2	1.95	0.49
3:E:83:ILE:O	3:E:87:ILE:HG13	2.12	0.49
4:F:3:THR:HB	4:F:38:ASN:H	1.77	0.49
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.36	0.48
1:A:151:SER:HB2	1:A:193:THR:HG22	1.94	0.48
2:B:221:THR:HG21	1:C:326:LYS:HA	1.95	0.48
2:D:345:GLU:OE2	2:D:440:ALA:N	2.46	0.48
4:F:31:ARG:HE	4:F:32:LYS:HG3	1.77	0.48
4:F:263:PHE:CG	4:F:341:LYS:HE2	2.48	0.48
4:F:6:VAL:HG22	4:F:41:LEU:HD12	1.96	0.48
1:A:104:ALA:HB2	1:A:413:MET:SD	2.53	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.48
4:F:219:GLY:N	14:F:504:HOH:O	2.45	0.48
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.48
2:B:371:LEU:HA	2:B:371:LEU:HD23	1.72	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.48
3:E:141:GLU:HB3	14:E:332:HOH:O	2.12	0.48
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.94	0.48
2:D:109:THR:HG22	2:D:110:GLU:HG2	1.96	0.48
2:D:405:LEU:O	2:D:409:THR:HG22	2.13	0.48
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.48
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.32	0.47
2:D:79:ARG:HB2	14:D:601:HOH:O	2.13	0.47
2:B:415:GLU:HG3	14:B:685:HOH:O	2.13	0.47
4:F:242:ASN:O	4:F:246:GLN:HB2	2.14	0.47
4:F:71:LEU:HD23	4:F:332:VAL:HG11	1.97	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.54	0.47
2:D:335:VAL:O	2:D:339:ASN:HB2	2.14	0.47
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.97	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.96	0.47
1:C:262:TYR:CG	12:C:508:IMD:H5	2.49	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.47
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.96	0.47
2:D:305:CYS:HA	2:D:386:GLU:OE2	2.15	0.46
4:F:126:ASP:HB2	14:F:506:HOH:O	2.14	0.46
4:F:202:ARG:HB3	4:F:220:VAL:HG12	1.96	0.46
4:F:275:LEU:HA	4:F:275:LEU:HD13	1.80	0.46
2:D:358:ILE:HD12	2:D:358:ILE:H	1.80	0.46
2:B:275:LEU:O	14:B:605:HOH:O	2.20	0.46
2:D:352:LYS:HD2	2:D:352:LYS:HA	1.78	0.46
1:A:196:GLU:HG3	1:A:197:HIS:HD2	1.80	0.46
1:A:3:GLU:HG2	1:A:64:ARG:NH1	2.30	0.46
2:B:199:ASP:O	2:B:266:HIS:HB2	2.16	0.46
1:A:68[A]:VAL:HG11	1:A:149:PHE:HE2	1.81	0.46
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.40	0.46
1:A:55:GLU:HA	1:A:60:LYS:O	2.16	0.46
2:B:234:THR:O	2:B:238:VAL:HB	2.15	0.46
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.96	0.46
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.80	0.46
2:D:72:PRO:HB3	2:D:94:PHE:CD1	2.50	0.46
3:E:140:LYS:HD2	3:E:140:LYS:HA	1.61	0.46
4:F:150:LYS:HZ3	4:F:162:ILE:N	2.14	0.46
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.16	0.46
2:B:8:GLN:NE2	2:B:14:ASN:HA	2.31	0.46
1:C:207:GLU:HG2	1:C:304:LYS:HD2	1.97	0.46
2:D:50:ASN:N	2:D:50:ASN:OD1	2.43	0.46
2:B:210:TYR:CE1	2:B:222:PRO:HD2	2.51	0.46
4:F:97:SER:OG	4:F:183:GLN:HG2	2.15	0.46
2:B:360:PRO:HG3	7:B:505:GOL:O2	2.16	0.45
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.51	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45
1:C:407:TRP:HZ3	7:D:504:GOL:H11	1.81	0.45
4:F:129:GLU:HG3	4:F:129:GLU:H	1.46	0.45
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.51	0.45
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.97	0.45
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.82	0.45
2:D:239:THR:O	2:D:243:ARG:HG3	2.17	0.45
1:C:266:HIS:O	1:C:268:PRO:HD3	2.16	0.45
2:B:18:ALA:N	14:B:601:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:223:THR:O	4:F:260:ASN:ND2	2.44	0.45
3:E:92:ASN:O	3:E:96:MET:HG2	2.16	0.45
1:A:324:VAL:HG22	1:A:327:ASP:OD2	2.17	0.45
2:B:274:PRO:HA	14:B:610:HOH:O	2.16	0.45
1:C:220:GLU:CD	2:D:326:LYS:HD3	2.38	0.45
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.44
1:A:76:ASP:HA	1:A:79:ARG:HD2	1.99	0.44
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.74	0.44
1:A:102:ASN:HB3	1:A:105:ARG:HB3	1.98	0.44
1:C:41:THR:OG1	1:C:55:GLU:OE2	2.36	0.44
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.52	0.44
2:D:173:PRO:HG3	2:D:187:ALA:HB2	1.98	0.44
2:B:56:ALA:HB3	2:B:60:LYS:H	1.82	0.44
4:F:126:ASP:OD1	4:F:128:ARG:NH2	2.50	0.44
4:F:78:VAL:HG22	4:F:94:PHE:HE2	1.81	0.44
1:C:4:CYS:SG	12:C:509:IMD:H5	2.58	0.44
4:F:221:LEU:HD23	4:F:221:LEU:HA	1.63	0.44
4:F:58:LEU:HA	4:F:58:LEU:HD23	1.59	0.44
1:A:370:LYS:HE2	1:A:370:LYS:HB3	1.74	0.44
2:D:191:VAL:HG11	2:D:425:MET:HG3	2.00	0.44
4:F:128:ARG:O	4:F:131:PHE:HB3	2.18	0.44
4:F:349:GLY:O	4:F:353[B]:VAL:HG23	2.17	0.44
4:F:127:GLU:N	14:F:506:HOH:O	2.50	0.44
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.83	0.44
2:B:235:MET:HB3	2:B:235:MET:HE2	1.85	0.44
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.52	0.44
4:F:149:ALA:HB3	4:F:169:LEU:HD13	1.99	0.44
1:A:312:TYR:O	1:A:344:VAL:HG13	2.18	0.43
1:A:66[B]:VAL:HG11	1:A:122:ILE:HG12	2.00	0.43
2:B:146:GLY:O	2:B:150:GLY:HA3	2.16	0.43
4:F:221:LEU:HB2	4:F:262:MET:O	2.17	0.43
1:C:1:MET:O	1:C:2:ARG:HG2	2.18	0.43
1:C:199:ASP:OD1	7:C:506:GOL:H32	2.17	0.43
1:C:6:SER:O	1:C:65:ALA:HA	2.18	0.43
2:D:176:LYS:HG2	2:D:176:LYS:H	1.60	0.43
4:F:288:LYS:HE2	4:F:288:LYS:HB2	1.79	0.43
4:F:51:ARG:HD3	14:F:544:HOH:O	2.18	0.43
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.59	0.43
2:B:13:GLY:CA	2:B:138[B]:THR:HG22	2.47	0.43
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.43
1:A:287:SER:OG	1:A:290:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ALA:HB2	2:B:413:MET:SD	2.59	0.43
2:B:320:ARG:HD3	7:B:505:GOL:C3	2.48	0.43
2:B:327:GLU:HA	2:B:330:GLU:HB2	2.00	0.43
2:D:268:PHE:O	2:D:270:PRO:HD3	2.18	0.43
4:F:91:CYS:SG	14:F:512:HOH:O	2.61	0.43
1:A:93:ILE:HD11	1:A:121:ARG:HG3	2.01	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.43
4:F:245:ILE:HG23	4:F:249:TYR:HD2	1.84	0.43
2:D:297:ASP:OD1	2:D:298:SER:N	2.52	0.42
4:F:222:ARG:HA	4:F:260:ASN:O	2.18	0.42
2:B:241:CYS:O	2:B:250:ALA:HB3	2.19	0.42
1:C:71:GLU:HG2	1:C:72:PRO:N	2.33	0.42
2:D:174:SER:O	2:D:178:SER:HB2	2.19	0.42
2:D:182:VAL:O	2:D:185:TYR:HB2	2.19	0.42
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.88	0.42
2:D:214:PHE:CD1	2:D:220:THR:HA	2.54	0.42
2:B:136:GLN:HG3	2:B:169:PHE:HE1	1.83	0.42
1:C:246:GLY:H	1:C:249:ASN:HB2	1.84	0.42
2:D:29:GLY:O	2:D:36:TYR:HA	2.20	0.42
4:F:254:GLY:HA2	14:F:552:HOH:O	2.19	0.42
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.55	0.42
3:E:51:GLN:HA	14:E:318:HOH:O	2.20	0.42
3:E:47:LEU:O	3:E:51:GLN:HG2	2.20	0.42
2:B:26:ASP:HA	14:B:623:HOH:O	2.20	0.42
2:B:413:MET:HE2	2:B:418:PHE:CE1	2.55	0.42
3:E:132:GLU:O	3:E:136:ASN:HB2	2.20	0.42
4:F:242:ASN:HB3	4:F:243:HIS:H	1.48	0.42
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.42
1:A:399:TYR:O	1:A:402:ARG:NH1	2.53	0.42
2:B:240:THR:HG23	2:B:244:PHE:HD2	1.85	0.42
2:B:320:ARG:HG2	2:B:356:CYS:HB3	2.02	0.42
4:F:131:PHE:CE2	4:F:182:ILE:HG21	2.54	0.42
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.42
4:F:263:PHE:CD2	4:F:341:LYS:HE2	2.54	0.42
1:A:214:ARG:NH2	14:A:615:HOH:O	2.51	0.41
1:C:141:PHE:HE1	1:C:191:THR:OG1	2.03	0.41
3:E:128:LYS:HB2	3:E:128:LYS:HE2	1.84	0.41
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.54	0.41
2:B:359:PRO:HB2	2:B:371:LEU:O	2.20	0.41
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.02	0.41
2:B:16:ILE:HD12	2:B:231:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:LYS:O	2:B:219:LEU:HD23	2.19	0.41
4:F:190:LEU:HD23	4:F:199:PHE:HZ	1.86	0.41
2:D:103:TRP:CD1	2:D:148:GLY:HA2	2.55	0.41
1:C:411:GLU:O	3:E:108[A]:ASN:ND2	2.52	0.41
2:D:326:LYS:HB3	2:D:326:LYS:HE2	1.78	0.41
1:A:8:HIS:HD1	1:A:138:PHE:HB2	1.85	0.41
1:A:72:PRO:HA	1:A:94:THR:HG21	2.03	0.41
2:B:132:LEU:HB3	2:B:164:ARG:HH11	1.85	0.41
2:B:320:ARG:HD3	7:B:505:GOL:C2	2.51	0.41
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.56	0.41
1:C:27:GLU:HG2	1:C:361:THR:CG2	2.50	0.41
2:D:107:HIS:ND1	2:D:152:LEU:HB2	2.35	0.41
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.20	0.41
1:A:71:GLU:HB3	1:A:98:ASP:HB3	2.02	0.41
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.56	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.03	0.41
2:B:349:ASN:HD22	2:B:349:ASN:HA	1.73	0.41
1:C:216:ASN:O	1:C:217:LEU:HD23	2.21	0.41
2:D:371:LEU:HD23	2:D:371:LEU:HA	1.87	0.41
2:B:68:VAL:HA	2:B:93:VAL:O	2.21	0.41
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.56	0.41
1:C:70:LEU:HA	1:C:70:LEU:HD23	1.77	0.40
4:F:229:ASN:CG	4:F:230:SER:H	2.25	0.40
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.95	0.40
2:D:382:THR:HA	2:D:432:TYR:CD1	2.56	0.40
3:E:112:ARG:NH1	14:E:305:HOH:O	2.44	0.40
3:E:131:GLU:OE2	3:E:134:ARG:NH2	2.53	0.40
1:A:107:HIS:ND1	1:A:152:LEU:HB2	2.35	0.40
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.40	0.40
2:D:103:TRP:NE1	2:D:148:GLY:HA2	2.36	0.40
2:D:147:SER:HB2	2:D:190:SER:OG	2.20	0.40
1:A:177:VAL:HG11	1:A:206:ASN:HB3	2.04	0.40
1:C:209:ILE:HG23	1:C:209:ILE:HD12	1.79	0.40
1:C:221:ARG:HA	1:C:221:ARG:HD2	1.88	0.40
7:D:504:GOL:H2	12:E:201:IMD:C2	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:621:HOH:O	14:C:605:HOH:O[4_545]	2.08	0.12

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	446/451 (99%)	419 (94%)	23 (5%)	4 (1%)	17	24
1	C	449/451 (100%)	432 (96%)	16 (4%)	1 (0%)	47	58
2	B	425/445 (96%)	400 (94%)	25 (6%)	0	100	100
2	D	420/445 (94%)	392 (93%)	27 (6%)	1 (0%)	47	58
3	E	119/189 (63%)	114 (96%)	4 (3%)	1 (1%)	19	27
4	F	302/378 (80%)	270 (89%)	31 (10%)	1 (0%)	41	50
All	All	2161/2359 (92%)	2027 (94%)	126 (6%)	8 (0%)	34	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
3	E	140	LYS
4	F	242	ASN
1	A	314	ALA
2	D	143	GLY
1	A	281	ALA
1	C	109	THR
1	A	261	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/379 (100%)	367 (97%)	12 (3%)	39	51
1	C	382/379 (101%)	368 (96%)	14 (4%)	34	45
2	B	371/383 (97%)	350 (94%)	21 (6%)	20	27
2	D	367/383 (96%)	353 (96%)	14 (4%)	33	44
3	E	111/171 (65%)	108 (97%)	3 (3%)	44	58
4	F	289/336 (86%)	268 (93%)	21 (7%)	14	18
All	All	1899/2031 (94%)	1814 (96%)	85 (4%)	28	37

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	41	THR
1	A	71	GLU
1	A	165	SER
1	A	181	VAL
1	A	218	ASP
1	A	220	GLU
1	A	232	SER
1	A	250	VAL
1	A	257	THR
1	A	271	THR
1	A	334	THR
2	B	15	GLN
2	B	39	ASP
2	B	55	GLU
2	B	79	ARG
2	B	85	GLN
2	B	116	ASP
2	B	117	SER
2	B	139	HIS
2	B	155[A]	SER
2	B	155[B]	SER
2	B	192	HIS
2	B	220	THR
2	B	232	SER
2	B	238	VAL
2	B	298	SER

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Mol	Chain	Res	Type
2	B	318	ILE
2	B	340	SER
2	B	377	PHE
2	B	414	ASP
2	B	423	SER
2	B	437	ASP
1	C	66	VAL
1	C	67	PHE
1	C	71	GLU
1	C	80	THR
1	C	181	VAL
1	C	285	GLN
1	C	315[A]	CYS
1	C	315[B]	CYS
1	C	342	GLN
1	C	357	TYR
1	C	358[A]	GLN
1	C	358[B]	GLN
1	C	368	LEU
1	C	381	THR
2	D	8	GLN
2	D	39	ASP
2	D	50	ASN
2	D	139	HIS
2	D	158	ARG
2	D	180	THR
2	D	248	LEU
2	D	300	ASN
2	D	325	MET
2	D	341	SER
2	D	357	ASP
2	D	374	SER
2	D	400	ARG
2	D	441	ASP
3	E	22	VAL
3	E	59	GLU
3	E	101	LEU
4	F	12	SER
4	F	45	ASN
4	F	73	ARG
4	F	83	THR
4	F	84	SER

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Mol	Chain	Res	Type
4	F	91	CYS
4	F	100	ILE
4	F	125	THR
4	F	128	ARG
4	F	129	GLU
4	F	146	VAL
4	F	162	ILE
4	F	172	PHE
4	F	181	VAL
4	F	241	THR
4	F	242	ASN
4	F	243	HIS
4	F	245	ILE
4	F	253	TYR
4	F	264	PHE
4	F	374	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	F	229	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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
7	GOL	D	504	12	5,5,5	0.41	0	5,5,5	0.34	0
13	ACP	F	402	-	27,33,33	2.55	10 (37%)	32,52,52	1.70	4 (12%)
7	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.71	0
12	IMD	E	201	7	3,5,5	0.40	0	4,5,5	0.45	0
7	GOL	D	503	-	5,5,5	0.36	0	5,5,5	0.31	0
9	GDP	B	501	6	24,30,30	1.02	1 (4%)	31,47,47	2.00	8 (25%)
7	GOL	B	504	-	5,5,5	0.44	0	5,5,5	0.50	0
7	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.47	0
11	84F	B	508	-	28,29,29	6.06	11 (39%)	38,42,42	4.14	13 (34%)
10	MES	B	507	-	12,12,12	2.05	1 (8%)	14,16,16	2.17	6 (42%)
12	IMD	C	508	-	3,5,5	0.43	0	4,5,5	0.50	0
7	GOL	A	503	-	5,5,5	0.32	0	5,5,5	0.23	0
11	84F	D	505	-	28,29,29	6.19	10 (35%)	38,42,42	4.30	15 (39%)
5	GTP	A	501	6	26,34,34	1.21	1 (3%)	33,54,54	1.81	8 (24%)
7	GOL	C	506	-	5,5,5	0.50	0	5,5,5	0.56	0
5	GTP	C	502	6	26,34,34	1.11	1 (3%)	33,54,54	1.87	6 (18%)
12	IMD	C	509	-	3,5,5	0.45	0	4,5,5	0.48	0
7	GOL	C	504	-	5,5,5	0.35	0	5,5,5	0.25	0
7	GOL	B	503	-	5,5,5	0.24	0	5,5,5	0.69	0
9	GDP	D	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.75	7 (22%)
7	GOL	C	501	-	5,5,5	0.40	0	5,5,5	0.23	0
7	GOL	C	505	-	5,5,5	0.37	0	5,5,5	0.27	0
7	GOL	B	505	-	5,5,5	0.42	0	5,5,5	0.48	0

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
7	GOL	D	504	12	-	4/4/4/4	-
13	ACP	F	402	-	-	6/15/38/38	0/3/3/3
7	GOL	A	504	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	D	503	-	-	2/4/4/4	-
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
7	GOL	B	504	-	-	2/4/4/4	-
7	GOL	A	506	-	-	3/4/4/4	-
11	84F	B	508	-	-	2/16/32/32	0/3/3/3
10	MES	B	507	-	-	1/6/14/14	0/1/1/1
7	GOL	C	504	-	-	2/4/4/4	-
7	GOL	A	503	-	-	2/4/4/4	-
11	84F	D	505	-	-	6/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
7	GOL	C	506	-	-	4/4/4/4	-
5	GTP	C	502	6	-	7/18/38/38	0/3/3/3
12	IMD	C	509	-	-	-	0/1/1/1
12	IMD	E	201	7	-	-	0/1/1/1
7	GOL	B	503	-	-	2/4/4/4	-
9	GDP	D	501	6	-	4/12/32/32	0/3/3/3
7	GOL	C	501	-	-	2/4/4/4	-
7	GOL	C	505	-	-	0/4/4/4	-
12	IMD	C	508	-	-	-	0/1/1/1
7	GOL	B	505	-	-	2/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	505	84F	C4-N1	24.64	1.75	1.37
11	B	508	84F	C4-N1	24.32	1.75	1.37
11	D	505	84F	C3-C2	-19.19	1.35	1.57
11	B	508	84F	C3-C2	-18.93	1.35	1.57
13	F	402	ACP	PB-O3A	7.46	1.66	1.58
10	B	507	MES	C8-S	-6.80	1.67	1.77
13	F	402	ACP	O4'-C1'	5.94	1.49	1.41
11	D	505	84F	C12-C2	4.75	1.58	1.51
11	D	505	84F	C29-C3	4.12	1.62	1.53
11	B	508	84F	C12-C2	4.06	1.57	1.51
5	A	501	GTP	C6-N1	3.79	1.39	1.33
11	B	508	84F	C29-C3	3.63	1.61	1.53
9	D	501	GDP	C6-C5	3.56	1.47	1.41
13	F	402	ACP	C6-N6	3.55	1.47	1.34
13	F	402	ACP	C2'-C1'	-3.53	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	508	84F	O23-C10	3.49	1.42	1.37
11	D	505	84F	O19-C15	3.48	1.42	1.37
5	C	502	GTP	C6-N1	3.27	1.38	1.33
11	D	505	84F	C2-N1	3.21	1.51	1.48
9	B	501	GDP	C6-C5	3.03	1.46	1.41
13	F	402	ACP	C4-N3	-3.02	1.31	1.35
13	F	402	ACP	C2'-C3'	-2.99	1.45	1.53
11	D	505	84F	O25-C8	2.61	1.41	1.37
13	F	402	ACP	PB-O2B	-2.57	1.50	1.56
11	D	505	84F	O23-C10	2.48	1.41	1.37
11	D	505	84F	O21-C9	2.44	1.42	1.38
11	B	508	84F	C2-N1	2.43	1.50	1.48
11	B	508	84F	O19-C15	2.39	1.41	1.37
9	D	501	GDP	C5-C4	2.33	1.47	1.40
13	F	402	ACP	C5-N7	2.32	1.48	1.39
11	B	508	84F	O25-C8	2.28	1.40	1.37
13	F	402	ACP	O3'-C3'	-2.26	1.37	1.43
11	B	508	84F	O18-C16	2.19	1.40	1.36
11	D	505	84F	C6-N1	2.13	1.46	1.43
11	B	508	84F	O21-C9	2.07	1.42	1.38
13	F	402	ACP	PA-O5'	2.05	1.67	1.59
11	B	508	84F	O5-C4	-2.01	1.18	1.22

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	505	84F	C2-C3-C4	13.52	98.49	85.82
11	B	508	84F	C2-C3-C4	13.04	98.04	85.82
11	B	508	84F	C2-N1-C4	-12.61	83.01	95.27
11	D	505	84F	C2-N1-C4	-12.28	83.33	95.27
11	D	505	84F	C3-C4-N1	-11.25	81.43	92.76
11	B	508	84F	C3-C4-N1	-10.78	81.90	92.76
11	B	508	84F	C6-N1-C2	7.88	142.94	130.29
11	D	505	84F	C6-N1-C2	7.51	142.34	130.29
13	F	402	ACP	O3'-C3'-C4'	5.89	128.09	111.05
5	C	502	GTP	N3-C2-N1	-5.71	119.60	127.22
11	D	505	84F	O23-C10-C9	5.59	124.99	115.16
11	D	505	84F	O23-C10-C11	-5.57	114.53	124.12
9	B	501	GDP	C2-N3-C4	5.44	121.57	115.36
11	B	508	84F	O23-C10-C9	5.34	124.55	115.16
5	C	502	GTP	C2-N3-C4	5.17	121.26	115.36
5	A	501	GTP	N3-C2-N1	-5.05	120.48	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	505	84F	O25-C8-C7	-5.04	115.45	124.12
11	D	505	84F	O25-C8-C9	5.03	124.00	115.16
11	B	508	84F	O25-C8-C7	-4.64	116.13	124.12
9	B	501	GDP	C6-C5-C4	-4.53	116.47	120.80
11	B	508	84F	O23-C10-C11	-4.25	116.81	124.12
11	B	508	84F	O25-C8-C9	4.13	122.41	115.16
5	A	501	GTP	C2-N3-C4	4.11	120.05	115.36
13	F	402	ACP	C3'-C2'-C1'	4.05	107.08	100.98
13	F	402	ACP	N3-C2-N1	-4.04	122.36	128.68
9	D	501	GDP	C2-N3-C4	4.00	119.92	115.36
10	B	507	MES	O1S-S-C8	3.98	111.70	106.92
9	B	501	GDP	N3-C2-N1	-3.96	121.94	127.22
11	D	505	84F	C24-O23-C10	-3.93	111.59	117.53
9	D	501	GDP	C6-N1-C2	3.82	121.99	115.93
9	D	501	GDP	C5-C6-N1	-3.72	118.34	123.43
9	B	501	GDP	C6-N1-C2	3.69	121.80	115.93
9	D	501	GDP	C6-C5-C4	-3.66	117.30	120.80
11	B	508	84F	O5-C4-N1	3.65	136.94	131.80
10	B	507	MES	C5-N4-C3	3.59	116.91	108.83
11	D	505	84F	C26-O25-C8	-3.54	112.19	117.53
10	B	507	MES	O3S-S-C8	3.51	111.45	105.77
5	C	502	GTP	C4-C5-N7	-3.44	105.81	109.40
11	D	505	84F	O5-C4-N1	3.30	136.46	131.80
9	B	501	GDP	C5-C6-N1	-3.28	118.95	123.43
5	A	501	GTP	C5-C6-N1	-3.05	119.26	123.43
11	B	508	84F	C12-C2-C3	-2.99	114.72	118.28
5	C	502	GTP	N2-C2-N1	2.87	121.72	117.25
9	D	501	GDP	N3-C2-N1	-2.87	123.40	127.22
11	D	505	84F	C7-C6-N1	2.74	122.41	119.47
11	B	508	84F	O19-C15-C16	2.71	118.50	114.57
11	D	505	84F	C11-C6-N1	-2.65	116.62	119.47
5	A	501	GTP	O3'-C3'-C4'	-2.64	103.40	111.05
5	A	501	GTP	O3G-PG-O3B	2.58	113.30	104.64
9	B	501	GDP	N2-C2-N1	2.47	121.09	117.25
9	B	501	GDP	O5'-PA-O1A	2.43	118.58	109.07
5	A	501	GTP	C6-N1-C2	2.43	119.79	115.93
9	D	501	GDP	PA-O3A-PB	-2.37	124.69	132.83
9	D	501	GDP	C2'-C3'-C4'	2.37	107.25	102.64
5	C	502	GTP	C5-C6-N1	-2.30	120.29	123.43
10	B	507	MES	C7-N4-C5	2.29	117.09	111.23
13	F	402	ACP	C4-C5-N7	-2.24	107.06	109.40
11	B	508	84F	C26-O25-C8	-2.23	114.16	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	507	MES	C6-C5-N4	-2.20	106.77	110.10
11	D	505	84F	C12-C2-C3	-2.20	115.66	118.28
11	B	508	84F	O19-C15-C14	-2.15	120.69	124.37
5	C	502	GTP	C1'-N9-C4	-2.09	122.96	126.64
9	B	501	GDP	C4-C5-N7	-2.08	107.23	109.40
5	A	501	GTP	PB-O3B-PG	-2.07	125.71	132.83
5	A	501	GTP	C4-C5-N7	-2.05	107.26	109.40
10	B	507	MES	O3S-S-O1S	-2.03	106.32	111.27
11	D	505	84F	O19-C15-C16	2.00	117.47	114.57

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	F	402	ACP	C5'-O5'-PA-O3A
7	A	504	GOL	O1-C1-C2-C3
7	D	503	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
7	B	504	GOL	O1-C1-C2-O2
7	A	506	GOL	C1-C2-C3-O3
7	A	503	GOL	O1-C1-C2-C3
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
7	C	506	GOL	C1-C2-C3-O3
5	C	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
7	C	504	GOL	O1-C1-C2-C3
7	B	503	GOL	O1-C1-C2-C3
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
11	D	505	84F	C9-C10-O23-C24
13	F	402	ACP	C3'-C4'-C5'-O5'
11	D	505	84F	C11-C10-O23-C24
7	D	504	GOL	O2-C2-C3-O3
7	C	504	GOL	O1-C1-C2-O2
11	D	505	84F	C9-C8-O25-C26
7	D	504	GOL	O1-C1-C2-C3
7	D	504	GOL	C1-C2-C3-O3
7	A	504	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	B	504	GOL	O1-C1-C2-C3
7	A	506	GOL	O1-C1-C2-C3
7	C	506	GOL	O1-C1-C2-C3
7	C	501	GOL	O1-C1-C2-C3
7	B	505	GOL	O1-C1-C2-C3
7	D	504	GOL	O1-C1-C2-O2
7	A	506	GOL	O2-C2-C3-O3
7	C	506	GOL	O2-C2-C3-O3
7	B	503	GOL	O1-C1-C2-O2
7	C	501	GOL	O1-C1-C2-O2
11	D	505	84F	C7-C8-O25-C26
13	F	402	ACP	O4'-C4'-C5'-O5'
7	A	504	GOL	O1-C1-C2-O2
7	D	503	GOL	O1-C1-C2-O2
7	A	503	GOL	O1-C1-C2-O2
7	B	505	GOL	O1-C1-C2-O2
11	B	508	84F	C8-C9-O21-C22
7	C	506	GOL	O1-C1-C2-O2
5	A	501	GTP	PB-O3B-PG-O1G
13	F	402	ACP	C5'-O5'-PA-O1A
13	F	402	ACP	PG-C3B-PB-O2B
11	B	508	84F	C10-C9-O21-C22
11	D	505	84F	C8-C9-O21-C22
9	D	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	502	GTP	C4'-C5'-O5'-PA
10	B	507	MES	C7-C8-S-O3S
13	F	402	ACP	PG-C3B-PB-O1B
5	C	502	GTP	PB-O3B-PG-O1G
5	C	502	GTP	PB-O3B-PG-O2G
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
11	D	505	84F	C10-C9-O21-C22

There are no ring outliers.

12 monomers are involved in 20 short contacts:

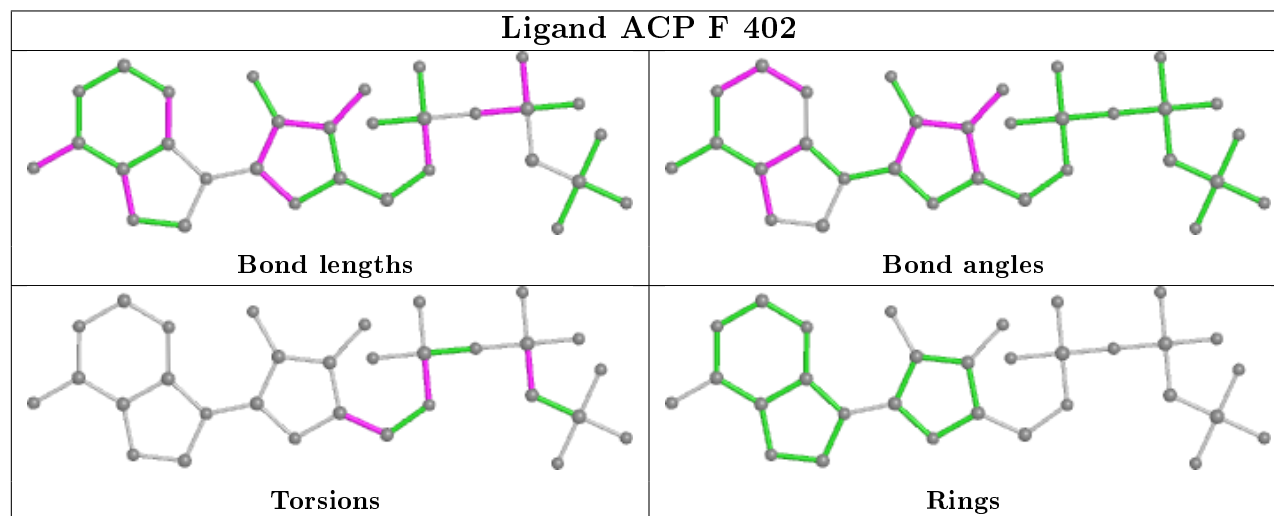
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	504	GOL	2	0
13	F	402	ACP	1	0

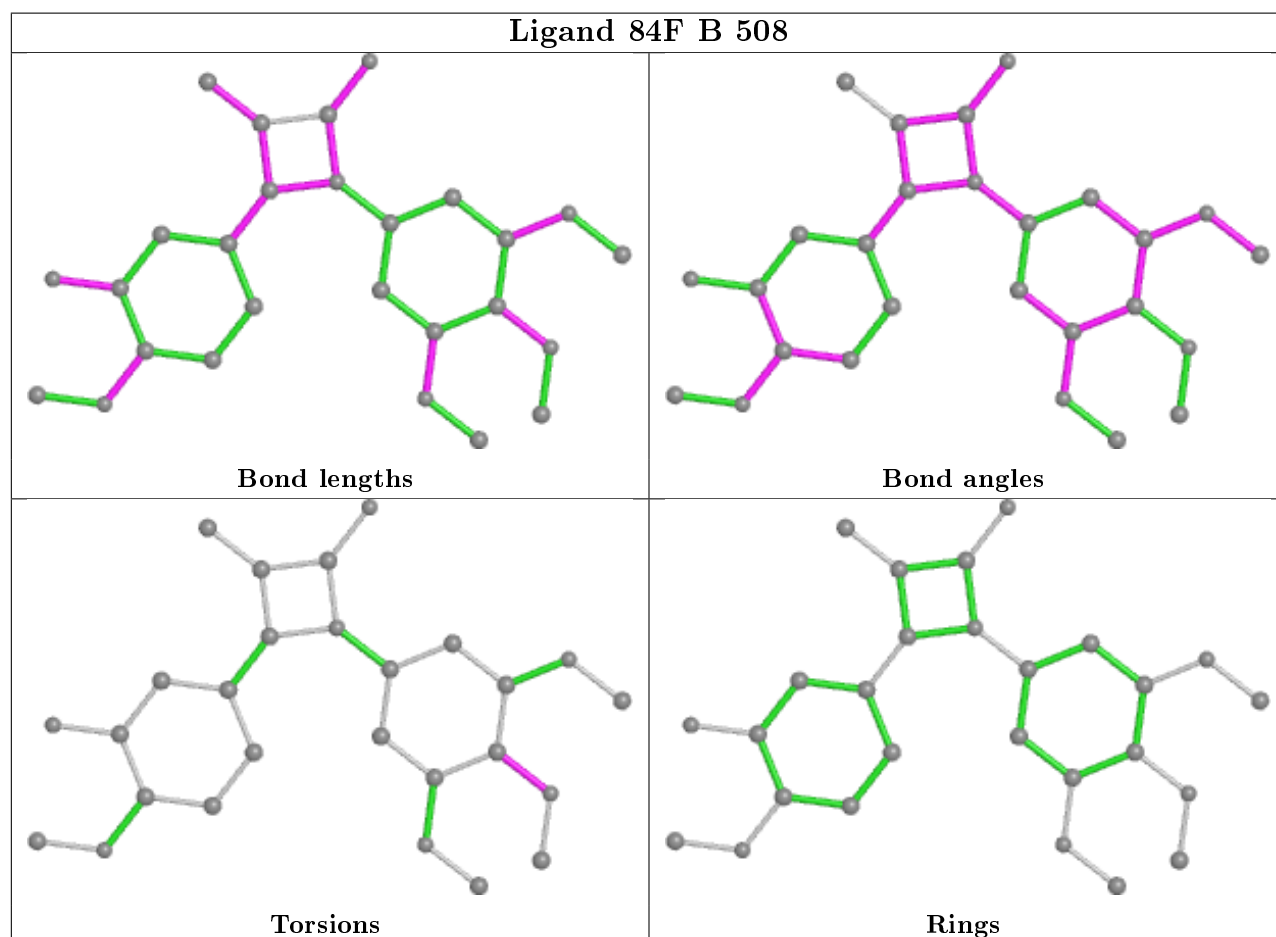
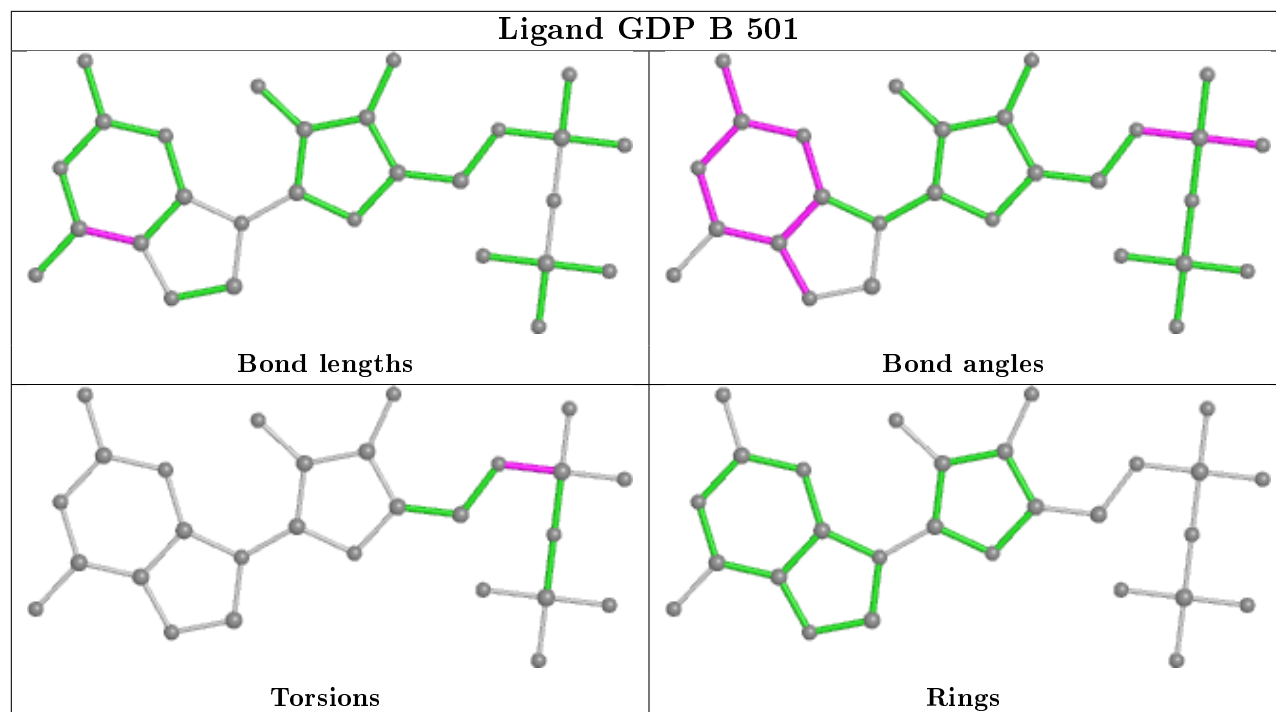
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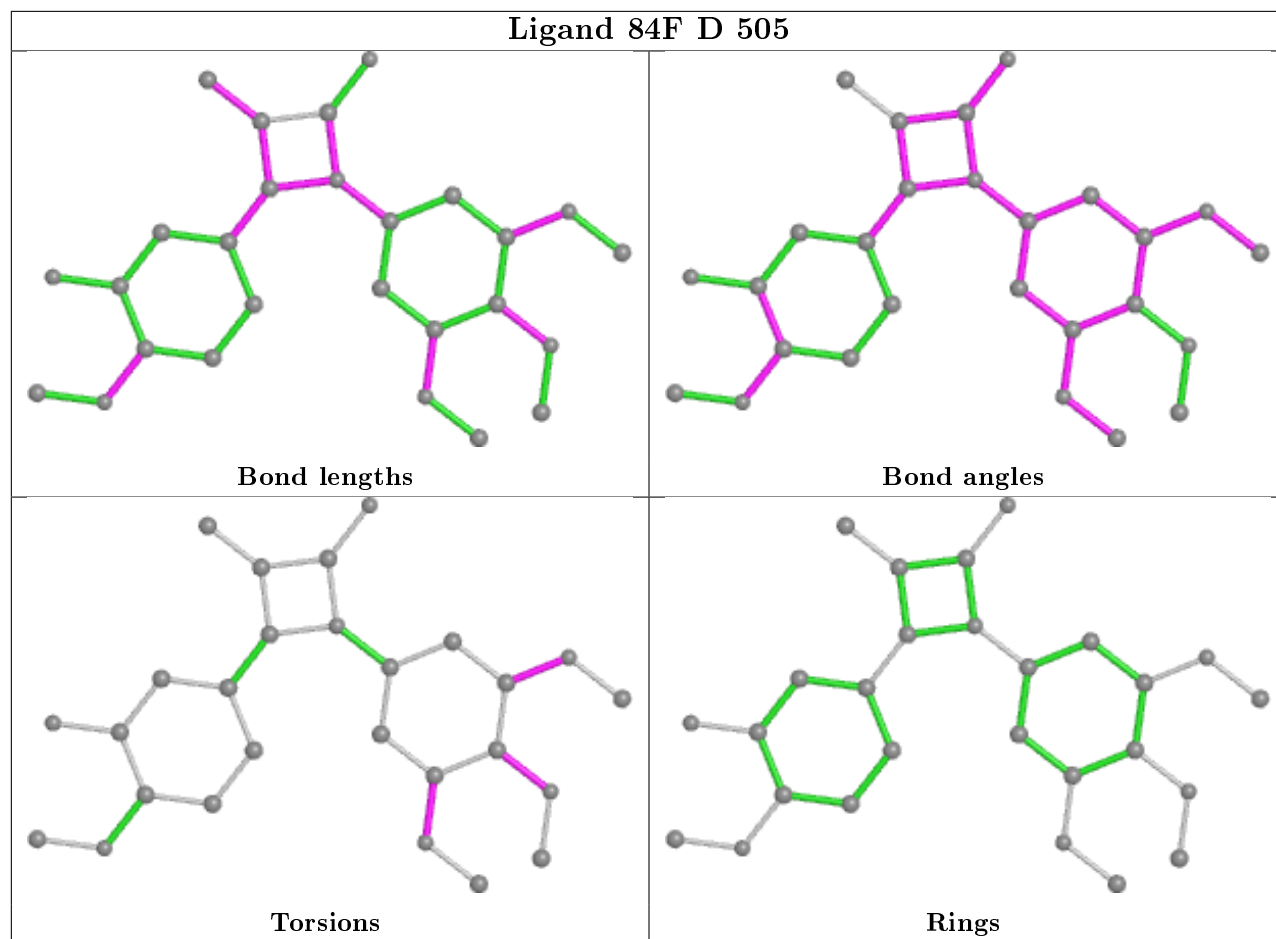
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	201	IMD	1	0
7	D	503	GOL	2	0
9	B	501	GDP	1	0
12	C	508	IMD	2	0
5	A	501	GTP	1	0
7	C	506	GOL	1	0
12	C	509	IMD	2	0
7	B	503	GOL	2	0
9	D	501	GDP	1	0
7	B	505	GOL	5	0

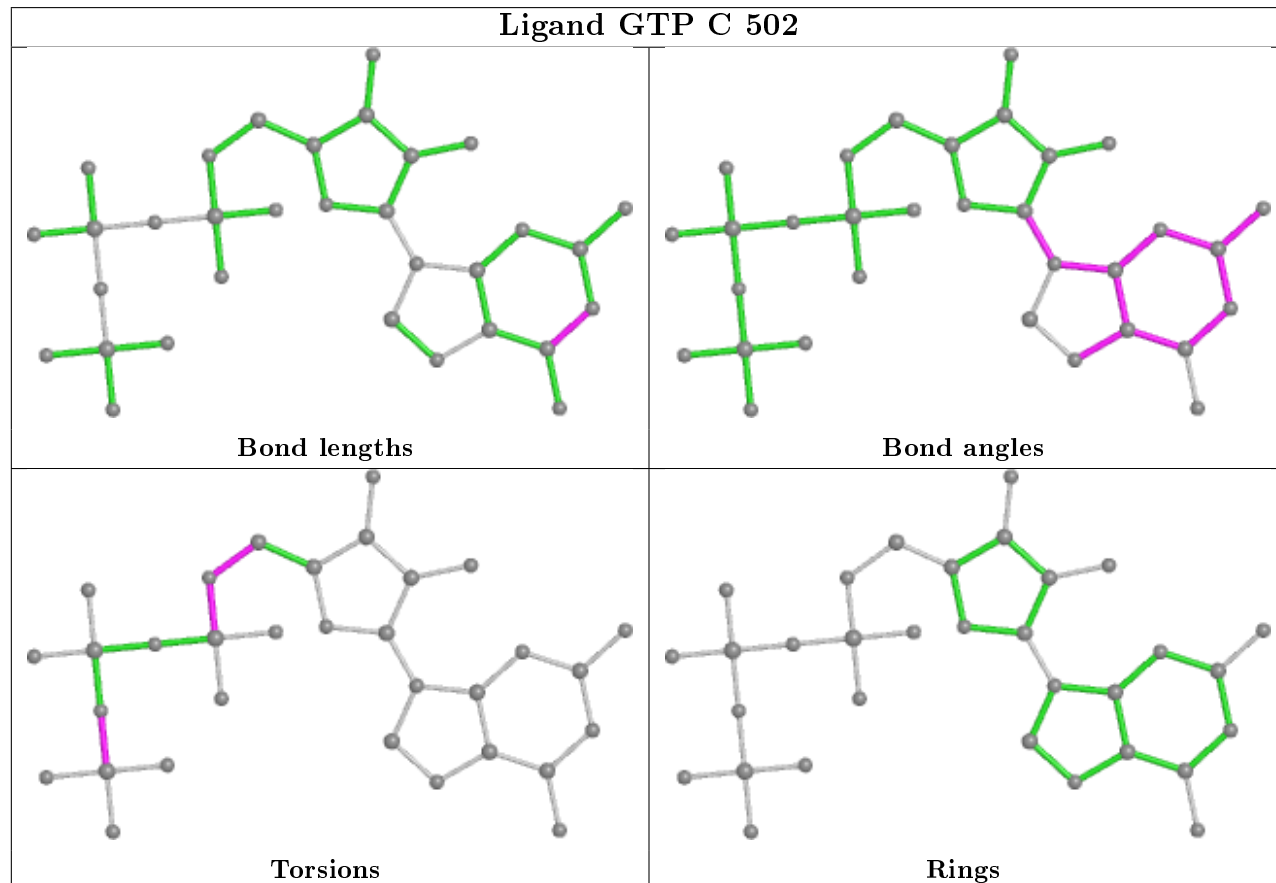
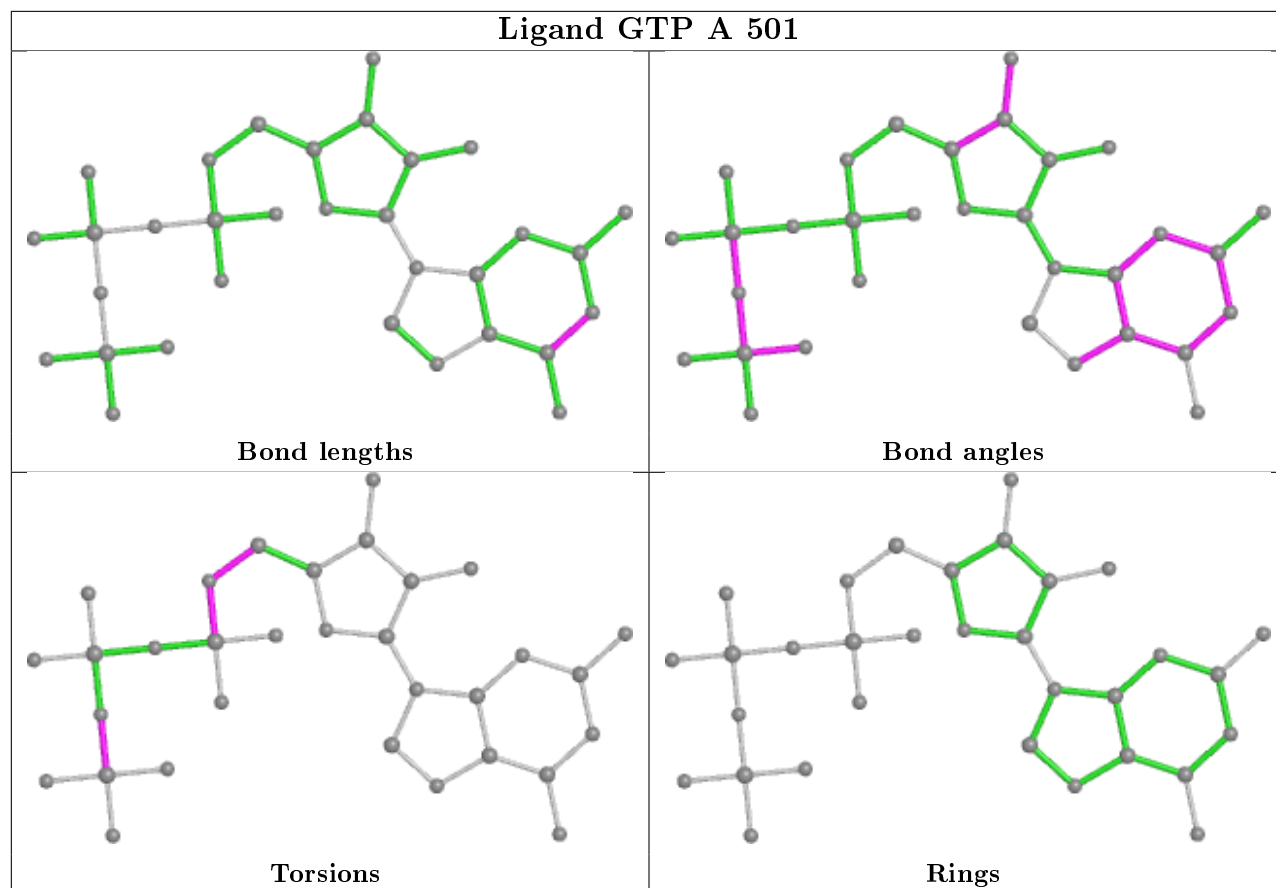
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

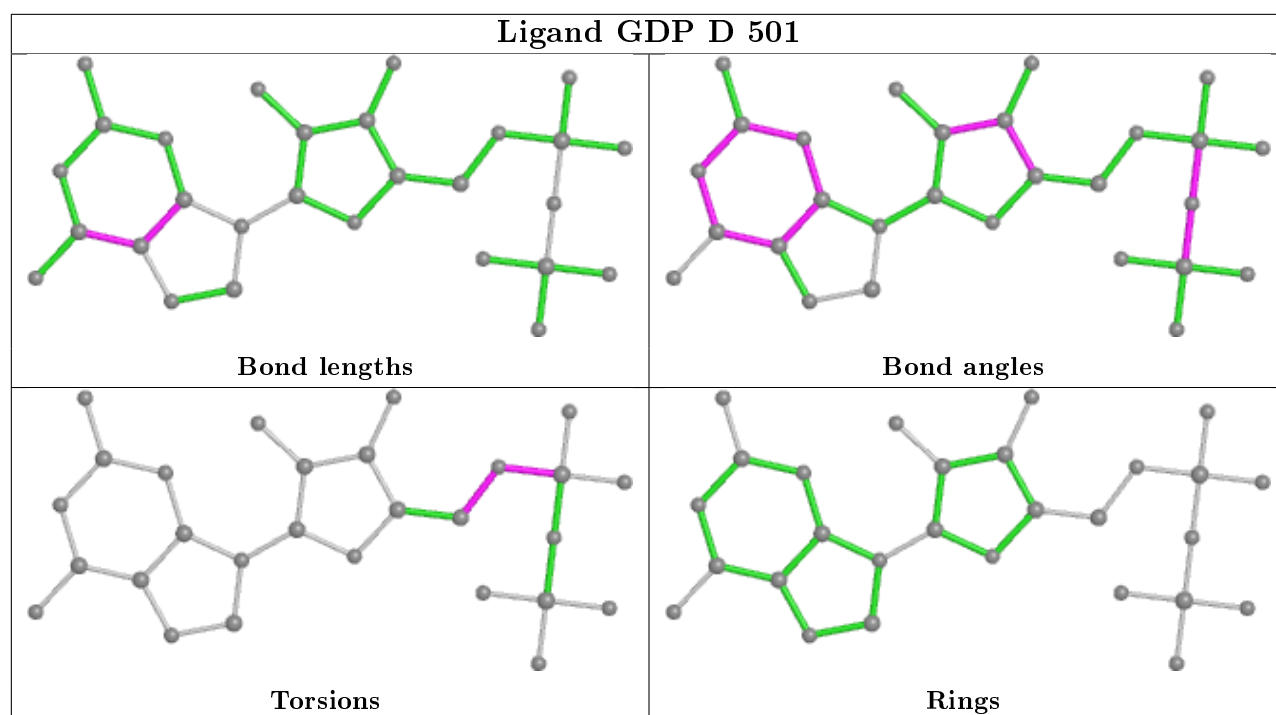




Ligand 84F D 505







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	438/451 (97%)	0.42	14 (3%) 47 57	47, 71, 107, 149	0
1	C	440/451 (97%)	0.05	2 (0%) 91 94	38, 55, 87, 106	0
2	B	422/445 (94%)	0.32	20 (4%) 31 40	41, 63, 105, 186	0
2	D	421/445 (94%)	0.72	50 (11%) 4 6	51, 86, 126, 180	3 (0%)
3	E	121/189 (64%)	0.38	8 (6%) 18 23	48, 83, 120, 171	0
4	F	317/378 (83%)	1.85	120 (37%) 0 0	62, 105, 194, 234	0
All	All	2159/2359 (91%)	0.59	214 (9%) 7 10	38, 74, 130, 234	3 (0%)

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	13.7
4	F	249	TYR	12.9
4	F	256	TYR	10.4
4	F	245	ILE	9.1
4	F	235	ASP	8.9
4	F	240	LEU	8.7
4	F	247	LYS	8.5
4	F	248	GLU	8.5
4	F	238	CYS	8.1
4	F	229	ASN	7.7
4	F	253	TYR	7.6
4	F	239	HIS	7.4
2	D	177	VAL	7.3
4	F	225	SER	7.3
4	F	252	ASN	7.1
4	F	254	GLY	6.6
4	F	361	LEU	6.5
4	F	257	GLU	6.4
4	F	231	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
4	F	250	SER	6.3
4	F	243	HIS	6.3
4	F	241	THR	6.0
4	F	182	ILE	6.0
4	F	134	ALA	5.8
4	F	255	ARG	5.8
4	F	224	SER	5.8
4	F	133	ALA	5.6
4	F	100	ILE	5.5
4	F	230	SER	5.5
4	F	149	ALA	5.4
4	F	237	THR	5.2
2	D	179	ASP	5.2
4	F	125	THR	5.1
4	F	131	PHE	5.0
4	F	147	TRP	5.0
4	F	227	PRO	5.0
4	F	226	GLU	4.9
4	F	102	PRO	4.9
4	F	162	ILE	4.8
4	F	21	LEU	4.7
4	F	236	LYS	4.7
4	F	246	GLN	4.7
4	F	259	GLY	4.7
2	B	59	ASN	4.6
2	D	405	LEU	4.5
4	F	99	VAL	4.5
4	F	98	TYR	4.5
4	F	148	ILE	4.4
4	F	362	ALA	4.4
4	F	168	GLU	4.4
4	F	169	LEU	4.4
4	F	228	TYR	4.4
4	F	132	LEU	4.3
2	B	62	VAL	4.3
4	F	183	GLN	4.3
2	D	399	PHE	4.2
4	F	260	ASN	4.2
2	D	400	ARG	4.1
2	D	219	LEU	4.1
2	B	60	LYS	4.1
2	D	401	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	404	PHE	4.1
2	B	1	MET	4.1
4	F	242	ASN	4.0
4	F	185	TYR	4.0
3	E	27	PRO	4.0
3	E	22	VAL	3.9
4	F	17	VAL	3.9
3	E	141	GLU	3.8
2	B	61	TYR	3.8
4	F	165	GLU	3.7
2	D	408	TYR	3.7
3	E	24	LEU	3.7
4	F	258	GLU	3.6
1	A	42	ILE	3.5
2	D	415	GLU	3.5
2	D	1	MET	3.5
4	F	163	SER	3.5
4	F	184	LYS	3.5
4	F	101	TYR	3.5
4	F	24	THR	3.5
4	F	1	MET	3.5
2	B	37	HIS	3.5
4	F	27	TRP	3.5
2	D	94	PHE	3.4
3	E	133	VAL	3.4
4	F	199	PHE	3.4
4	F	13	VAL	3.4
4	F	171	ASP	3.4
4	F	128	ARG	3.3
4	F	197	ARG	3.3
4	F	144	GLY	3.3
4	F	151	SER	3.3
4	F	181	VAL	3.3
4	F	343	TYR	3.3
4	F	22	LEU	3.2
4	F	5	VAL	3.2
4	F	320	MET	3.2
4	F	97	SER	3.2
4	F	96	GLU	3.2
4	F	346	LEU	3.2
2	D	407	TRP	3.2
4	F	323	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	20	LEU	3.1
4	F	172	PHE	3.1
4	F	129	GLU	3.1
4	F	198	LYS	3.1
2	D	83	PHE	3.1
2	D	57	THR	3.0
4	F	6	VAL	3.0
2	B	57	THR	3.0
2	B	50[A]	ASN	3.0
2	D	85	GLN	3.0
4	F	135	TYR	2.9
4	F	126	ASP	2.9
4	F	4	PHE	2.9
4	F	14	TYR	2.9
2	D	267	PHE	2.9
4	F	9	GLU	2.9
2	D	74	THR	2.9
2	B	83	PHE	2.8
4	F	347	CYS	2.8
2	D	377	PHE	2.8
4	F	220	VAL	2.7
1	A	282	TYR	2.7
2	D	33	THR	2.7
4	F	130	VAL	2.7
4	F	330	ILE	2.7
4	F	263	PHE	2.6
1	A	171	ILE	2.6
4	F	342	LEU	2.6
1	A	346	TRP	2.6
4	F	146	VAL	2.6
2	D	218	LYS	2.6
4	F	186	LEU	2.6
2	D	413	MET	2.6
1	A	201	ALA	2.5
2	B	30	ILE	2.5
4	F	19	ARG	2.5
3	E	26	PRO	2.5
4	F	28	LYS	2.5
4	F	192	LEU	2.5
2	D	92	PHE	2.5
2	D	46	LEU	2.5
4	F	194	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	127	GLU	2.4
2	D	402	LYS	2.4
4	F	188	LYS	2.4
2	D	37	HIS	2.4
4	F	73	ARG	2.4
2	B	35	SER	2.4
4	F	222	ARG	2.4
2	D	269[A]	MET	2.4
2	D	406	HIS	2.4
2	D	314	THR	2.4
4	F	18	SER	2.4
2	D	59	ASN	2.4
1	A	141	PHE	2.4
4	F	2	TYR	2.4
2	D	256	ALA	2.4
2	D	379	GLY	2.4
2	B	36	TYR	2.4
4	F	166	ALA	2.4
2	D	213	CYS	2.4
4	F	39	LEU	2.4
2	D	82	PRO	2.3
4	F	190	LEU	2.3
3	E	7	GLU	2.3
2	D	271	GLY	2.3
4	F	201	ILE	2.3
1	A	262	TYR	2.3
2	D	202	TYR	2.3
2	D	178	SER	2.3
2	D	220	THR	2.3
2	B	98	GLY	2.3
4	F	23	ALA	2.3
4	F	196	HIS	2.3
3	E	139	LEU	2.3
2	D	317	ALA	2.2
1	A	179	THR	2.2
2	B	53	TYR	2.2
2	D	210	TYR	2.2
4	F	187	GLU	2.2
2	B	438	ALA	2.2
2	D	203	CYS	2.2
2	D	235	MET	2.2
4	F	167	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	76	ASP	2.1
2	B	34	GLY	2.1
2	D	182	VAL	2.1
2	B	42	LEU	2.1
1	A	170	SER	2.1
2	D	259	MET	2.1
2	D	199	ASP	2.1
1	A	203	MET	2.1
2	D	79	ARG	2.1
2	B	97	SER	2.1
2	D	266	HIS	2.1
4	F	164	SER	2.1
4	F	170	LEU	2.1
2	B	249	ASN	2.1
1	C	253	THR	2.1
1	A	205	ASP	2.1
4	F	223	THR	2.0
1	A	172	TYR	2.0
2	D	381	SER	2.0
1	C	252	LEU	2.0
4	F	25	GLY	2.0
1	A	58	ALA	2.0
2	D	397	ALA	2.0
4	F	189	PRO	2.0
1	A	365	GLY	2.0
4	F	350	ILE	2.0
2	B	45	GLN	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,

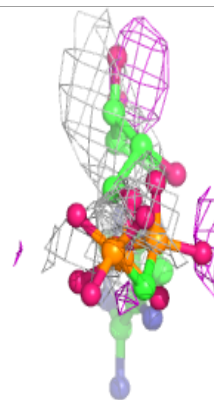
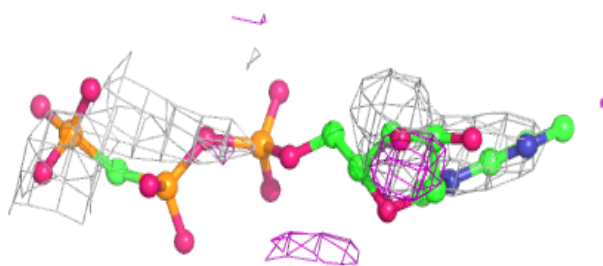
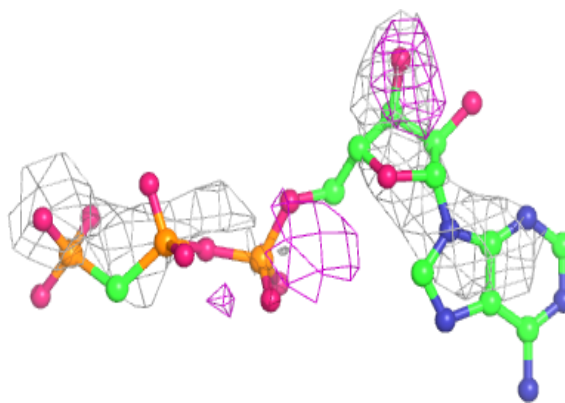
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.48	0.20	97,97,97,97	0
13	ACP	F	402	31/31	0.54	0.70	83,201,241,243	0
7	GOL	B	504	6/6	0.57	0.54	74,115,118,121	0
7	GOL	D	503	6/6	0.67	0.50	150,152,158,158	0
7	GOL	B	505	6/6	0.70	0.85	102,115,129,143	0
7	GOL	A	506	6/6	0.73	0.23	90,98,107,109	0
7	GOL	A	504	6/6	0.78	0.28	106,113,114,117	0
7	GOL	C	505	6/6	0.81	0.39	99,113,123,127	0
6	MG	F	401	1/1	0.81	0.33	162,162,162,162	0
7	GOL	C	504	6/6	0.83	0.21	105,110,112,112	0
7	GOL	C	501	6/6	0.85	0.46	82,100,104,107	0
12	IMD	E	201	5/5	0.85	0.24	130,130,138,138	0
12	IMD	C	509	5/5	0.87	0.43	113,117,121,122	0
7	GOL	C	506	6/6	0.88	0.31	79,94,98,99	0
7	GOL	B	503	6/6	0.88	0.42	88,95,100,115	0
7	GOL	A	503	6/6	0.90	0.35	88,100,107,109	0
12	IMD	C	508	5/5	0.91	0.31	77,78,85,85	0
7	GOL	D	504	6/6	0.91	0.28	89,105,114,118	0
6	MG	B	502	1/1	0.93	0.48	58,58,58,58	0
9	GDP	D	501	28/28	0.93	0.15	65,94,108,113	0
10	MES	B	507	12/12	0.94	0.19	46,75,86,99	0
8	CA	A	505	1/1	0.96	0.07	106,106,106,106	0
8	CA	C	507	1/1	0.97	0.15	135,135,135,135	0
8	CA	B	506	1/1	0.97	0.14	121,121,121,121	0
6	MG	A	502	1/1	0.97	0.73	67,67,67,67	0
11	84F	D	505	27/27	0.97	0.22	49,60,77,91	0
11	84F	B	508	27/27	0.97	0.20	44,59,72,86	0
9	GDP	B	501	28/28	0.98	0.22	35,48,58,60	0
5	GTP	C	502	32/32	0.98	0.17	42,50,56,58	0
5	GTP	A	501	32/32	0.98	0.25	43,51,65,70	0
6	MG	C	503	1/1	0.99	0.18	48,48,48,48	0

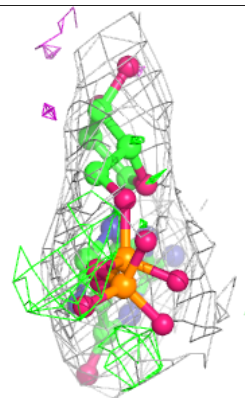
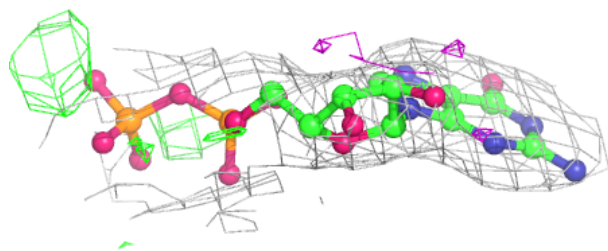
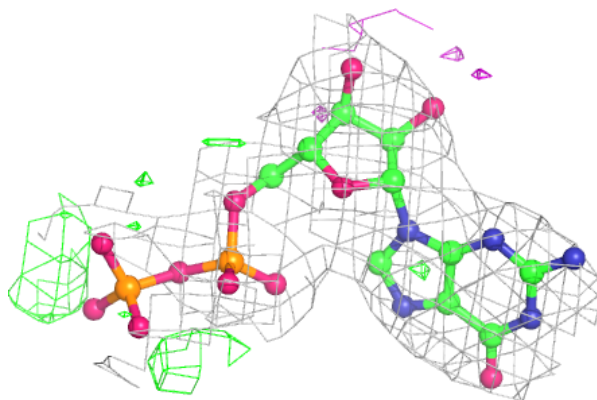
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

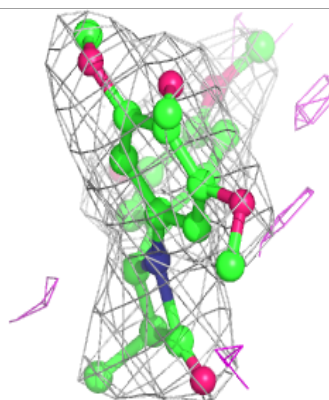
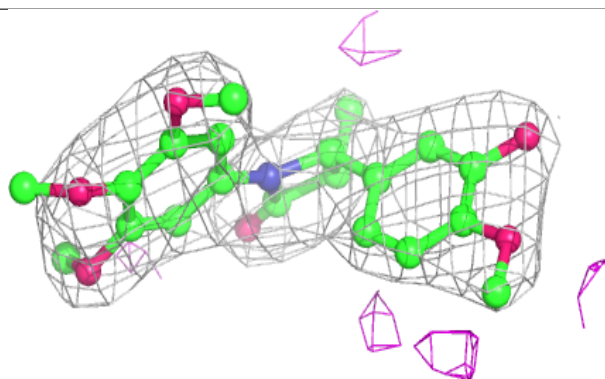
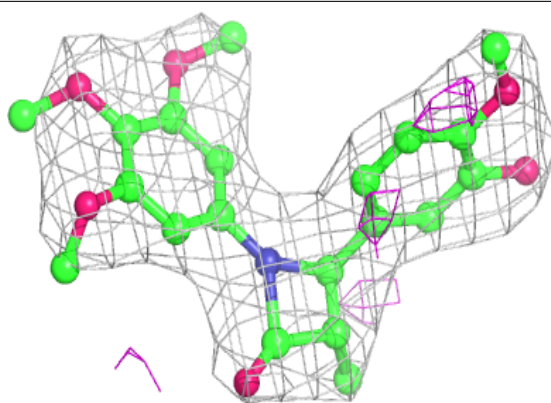
**Electron density around GDP D 501:**

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

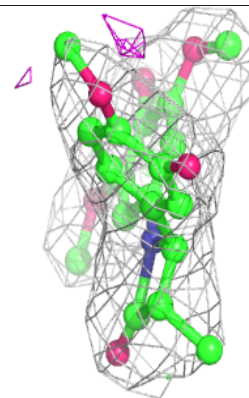
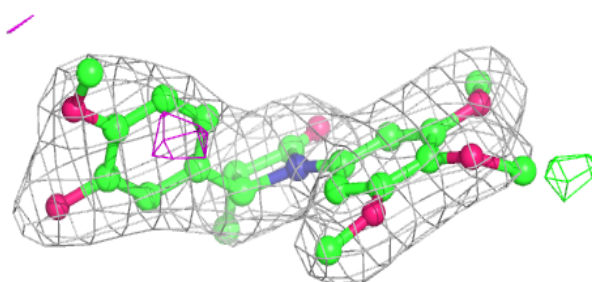
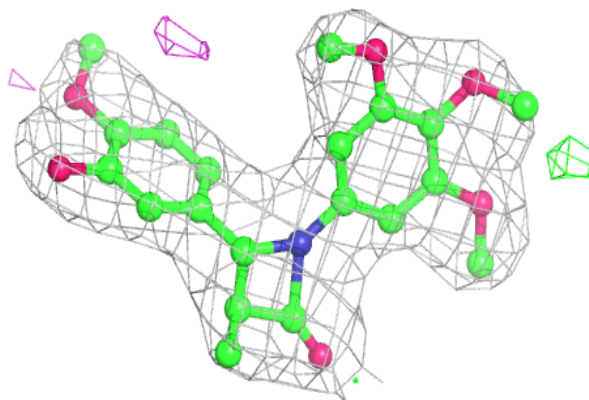


Electron density around 84F D 505:

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

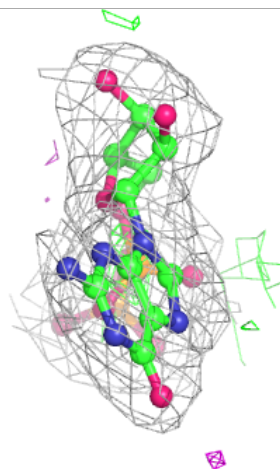
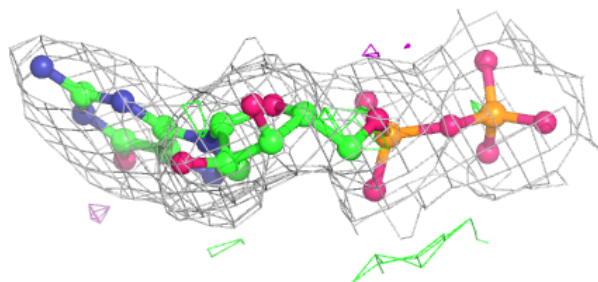
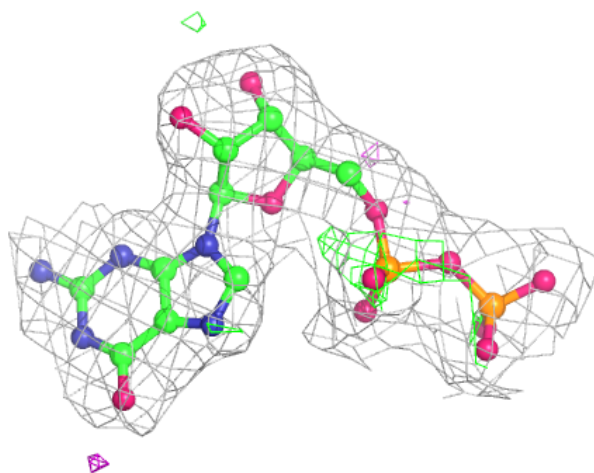
**Electron density around 84F B 508:**

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



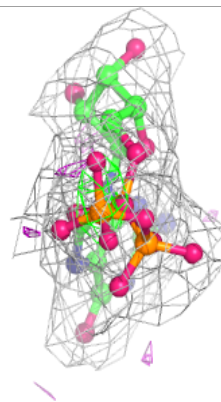
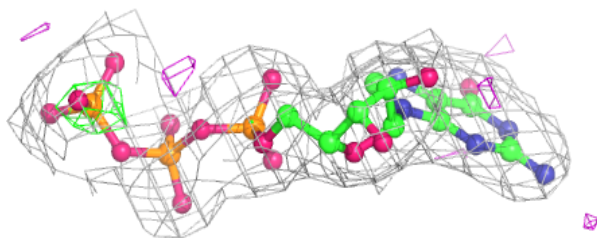
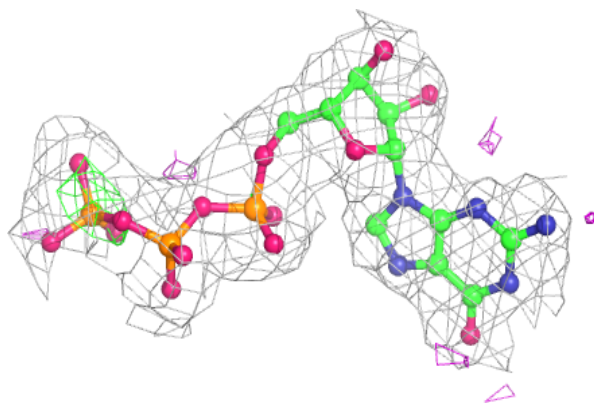
Electron density around GDP B 501:

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

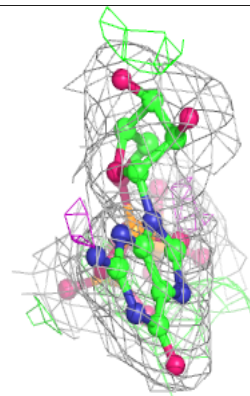
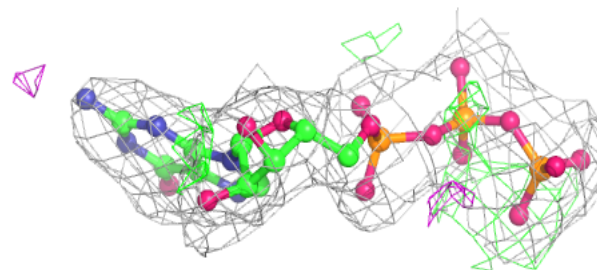
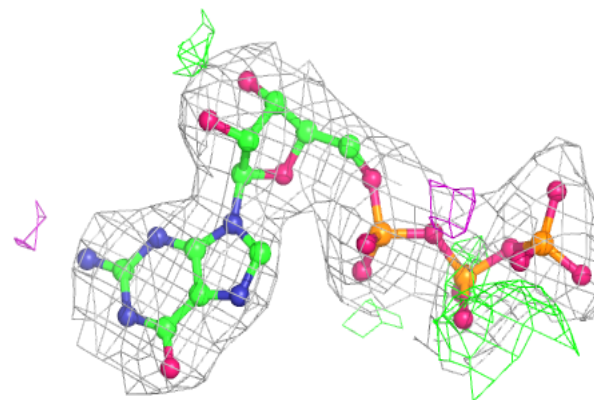


Electron density around GTP C 502:

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

**Electron density around GTP A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.