



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:00 am BST

PDB ID : 5MF4  
Title : Tubulin-Dictyostatin complex  
Authors : Trigili, C.; Barasoain, I.; Sanchez-Murcia, P.A.; Bargsten, K.; Redondo-Horcajo, M.; Nogales, A.; Gardner, N.M.; Meyer, A.; Naylor, G.J.; Gomez-Rubio, E.; Gago, F.; Steinmetz, M.O.; Paterson, I.; Protá, A.E.; Diaz, J.F.  
Deposited on : 2016-11-17  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

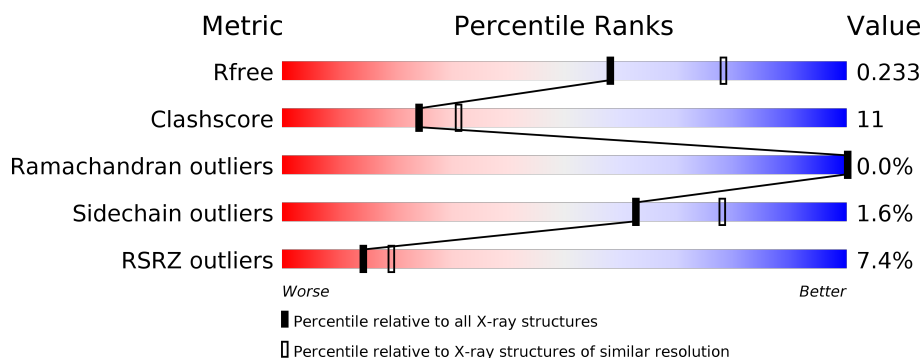
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	451	<div> <div></div> <div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>•</div> </div> </div>
2	D	445	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>•</div> </div> </div>
3	E	143	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>15%</div> </div> </div>
4	F	384	<div> <div>27%</div> <div> <div></div> <div>62%</div> <div>22%</div> <div>• 15%</div> </div> </div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17747 atoms, of which 117 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	435	Total	C	N	O	S	0	0	0
			3399	2150	579	649	21			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3356	2106	574	650	26			
2	D	425	Total	C	N	O	S	0	1	0
			3338	2095	569	647	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	0	0
			1009	622	182	200	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

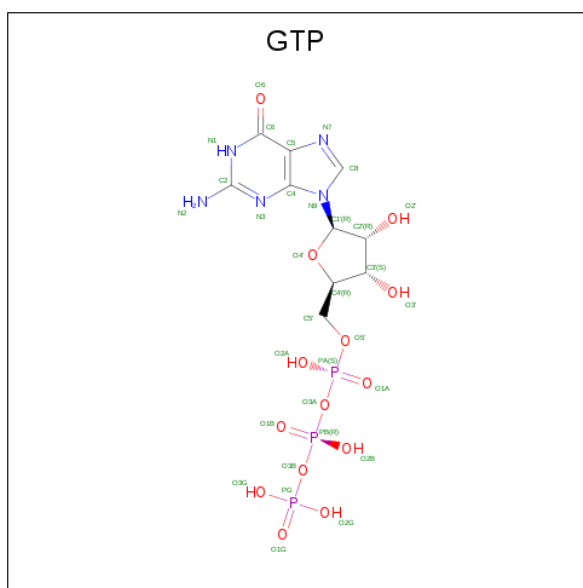
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	326	Total	C	N	O	S	0	0	0
			2678	1725	458	481	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		

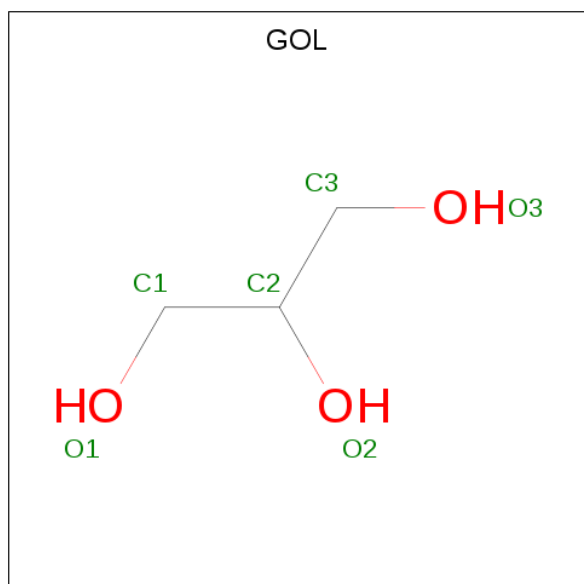
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

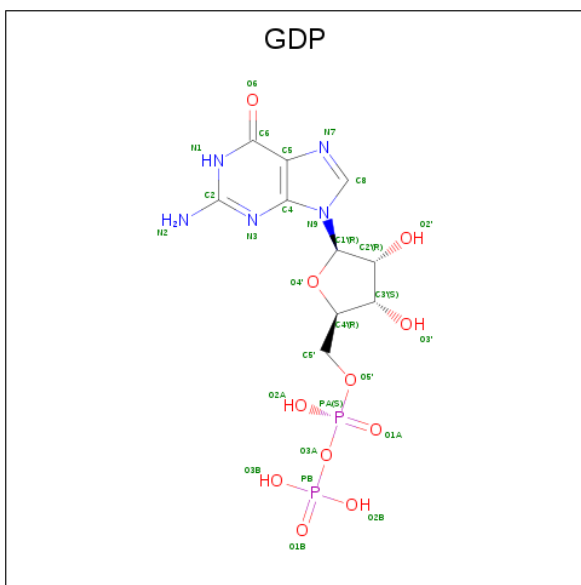
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	F	1	Total	Ca	0	0
			1	1		

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



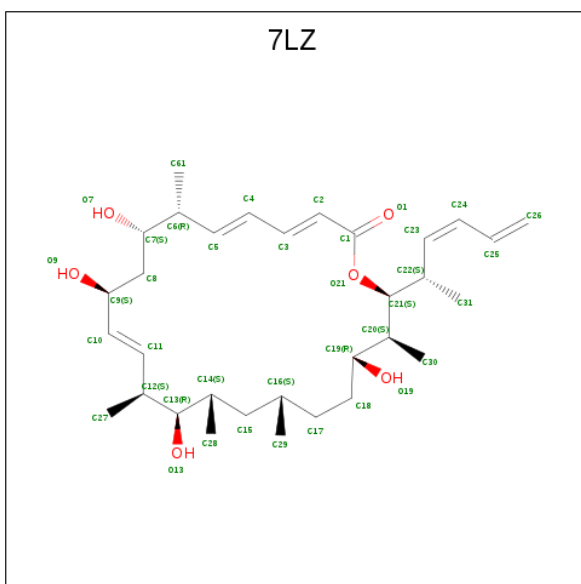
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

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



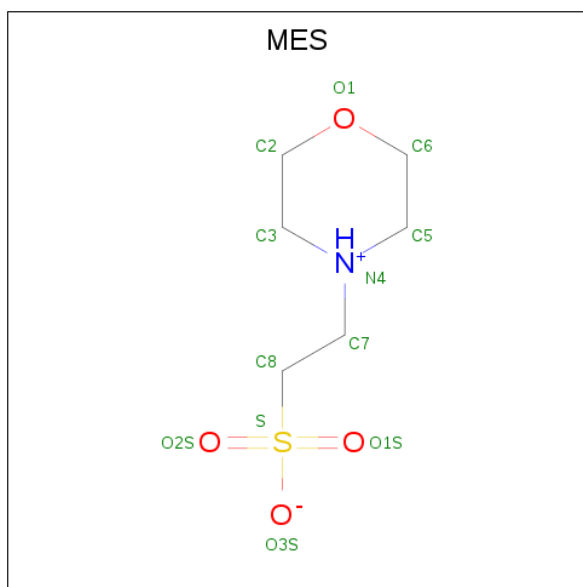
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is (3 {Z},5 {E},7 {R},8 {S},10 {S},11 {Z},13 {S},14 {R},15 {S},17 {S},20 {R},21 {S},22 {S})-22-[(2 {S},3 {Z})-hexa-3,5-dien-2-yl]-7,13,15,17,21-pentamethyl-8,10,14,20-tetrakis(oxidanyl)-1-oxacyclodocosa-3,5,11-trien-2-one (three-letter code: 7LZ) (formula: C<sub>32</sub>H<sub>52</sub>O<sub>6</sub>).



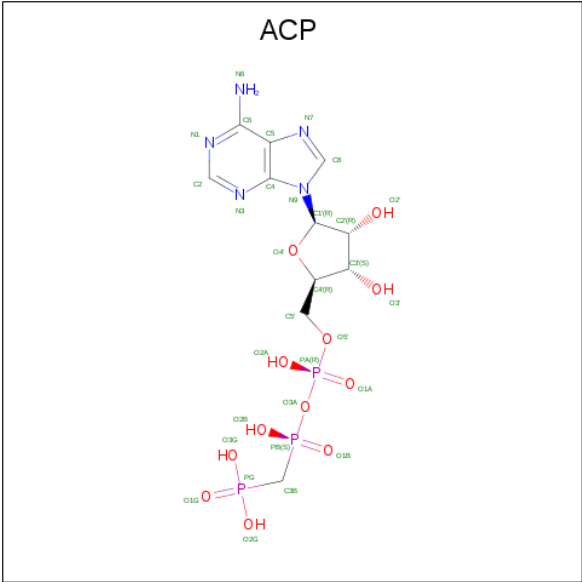
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			90	32	52	6		
10	D	1	Total	C	H	O	0	0
			90	32	52	6		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
11	D	1	Total	C	H	N	O	S	0
			25	6	13	1	4	1	

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).

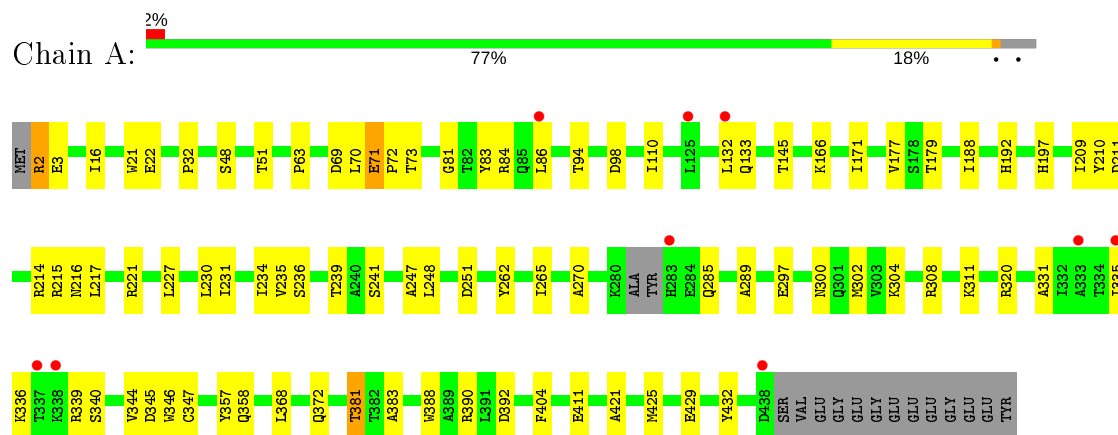




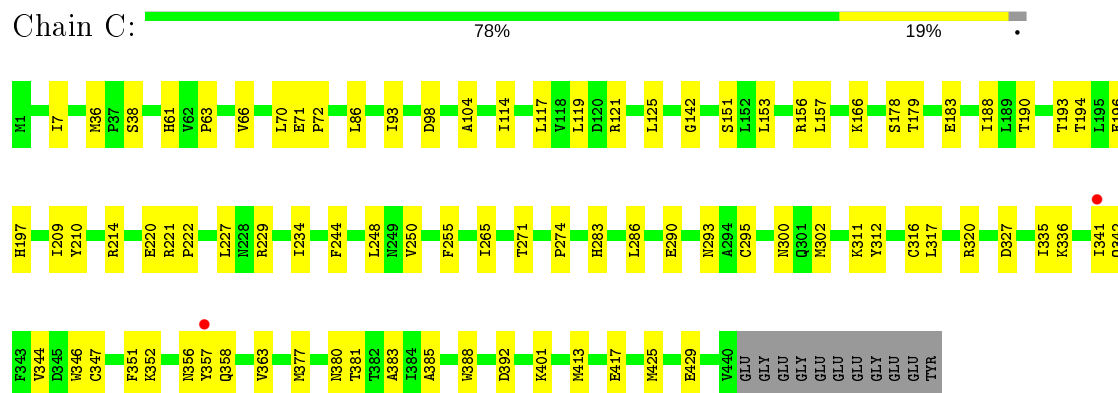
### 3 Residue-property plots [i](#)

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.

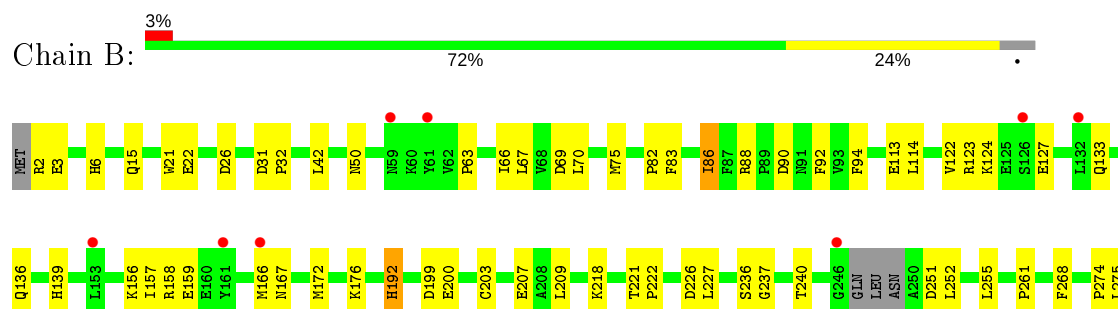
- Molecule 1: Tubulin alpha-1B chain

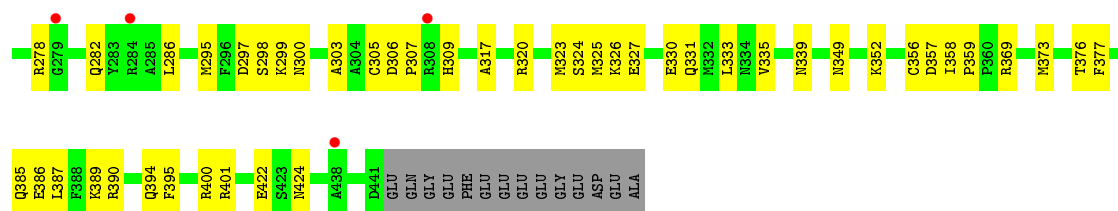


- Molecule 1: Tubulin alpha-1B chain

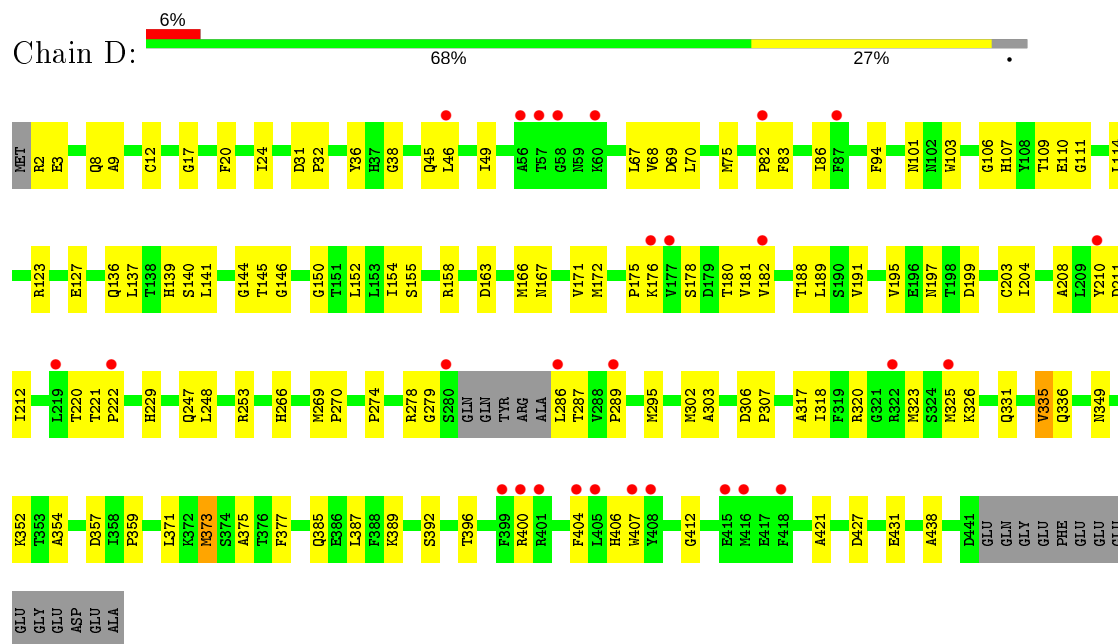


- Molecule 2: Tubulin beta-2B chain

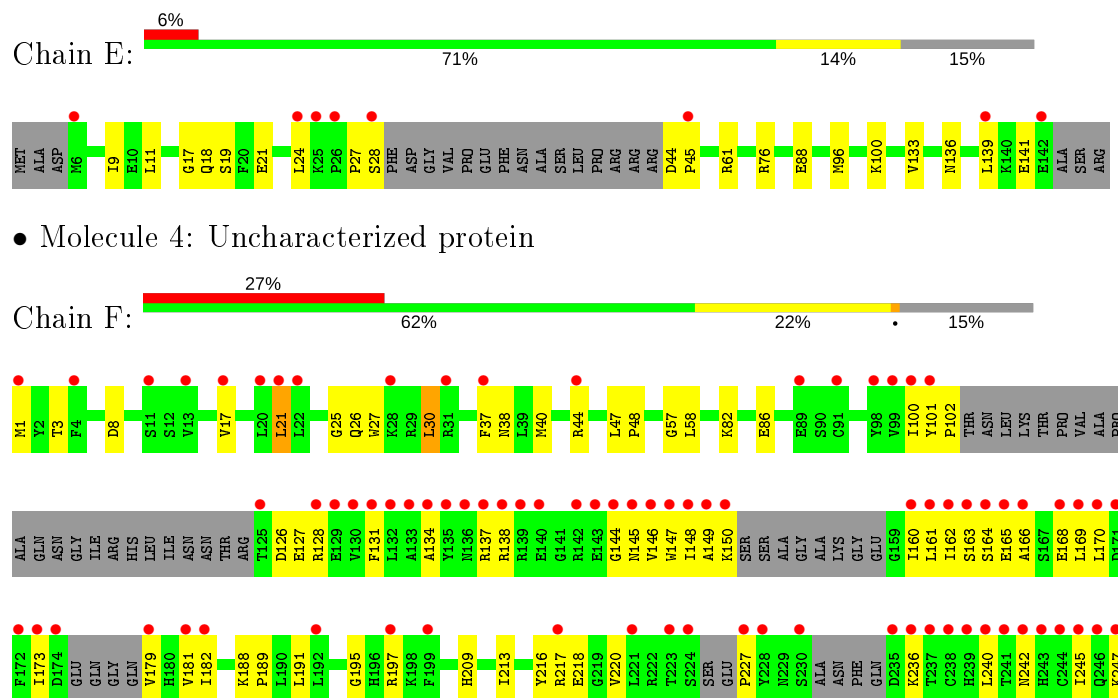


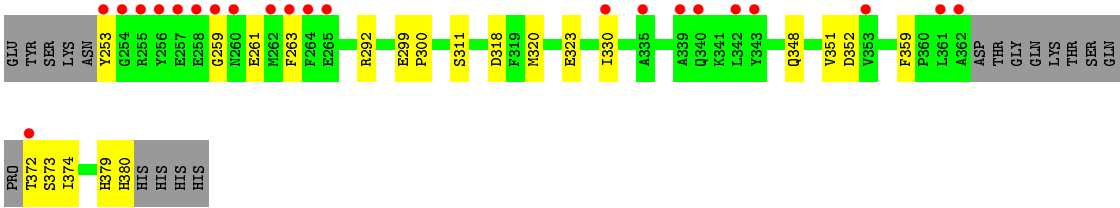


• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.01Å 156.51Å 179.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.85 – 2.30 67.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.85-2.30) 99.9 (67.85-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.183 , 0.233 0.184 , 0.233	Depositor DCC
$R_{free}$ test set	6488 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, CA, 7LZ, GTP, 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	0.43	0/3475	0.56	0/4716
1	C	0.50	0/3515	0.60	0/4772
2	B	0.43	0/3430	0.57	0/4645
2	D	0.37	0/3414	0.53	0/4624
3	E	0.41	0/1017	0.49	0/1349
4	F	0.35	0/2736	0.52	0/3690
All	All	0.42	0/17587	0.56	0/23796

There are no bond length outliers.

There are no bond angle outliers.

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	3399	0	3308	74	0
1	C	3437	0	3349	59	1
2	B	3356	0	3228	99	1
2	D	3338	0	3215	85	0
3	E	1009	0	1024	19	0
4	F	2678	0	2664	63	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
8	A	12	0	14	1	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	38	52	0	2	0
10	D	38	52	0	0	0
11	B	12	0	13	3	0
11	D	12	13	13	1	0
12	F	31	0	14	2	0
13	A	31	0	0	1	0
13	B	27	0	0	1	0
13	C	57	0	0	3	0
13	D	12	0	0	0	0
13	E	9	0	0	1	0
13	F	7	0	0	0	0
All	All	17630	117	16890	377	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 11.

All (377) 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:C:381:THR:HG22	1:C:383:ALA:H	1.24	1.01
2:B:2:ARG:HD3	2:B:50:ASN:ND2	1.79	0.97
1:A:221:ARG:HG2	2:B:325:MET:HG2	1.47	0.95
4:F:240:LEU:HD23	4:F:245:ILE:HD13	1.49	0.93
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.53	0.88
3:E:141:GLU:O	13:E:201:HOH:O	1.88	0.88
1:C:327:ASP:OD2	13:C:601:HOH:O	1.94	0.85
2:D:331:GLN:O	2:D:335:VAL:HG12	1.81	0.79
2:B:199:ASP:OD2	11:B:504:MES:H52	1.82	0.79
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.64	0.79
2:B:2:ARG:HD2	2:B:3:GLU:OE1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HD23	4:F:57:GLY:HA3	1.65	0.78
1:A:210:TYR:OH	1:A:221:ARG:HD3	1.83	0.78
2:D:83:PHE:O	2:D:86:ILE:HG22	1.84	0.78
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.64	0.78
2:B:2:ARG:HD3	2:B:50:ASN:HD22	1.44	0.77
1:C:271:THR:HA	1:C:302:MET:HE1	1.68	0.75
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.22	0.74
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.70	0.74
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.69	0.73
2:D:191:VAL:O	2:D:195:VAL:HG23	1.88	0.73
2:D:82:PRO:O	2:D:83:PHE:HB2	1.88	0.72
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.70	0.71
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.25	0.71
1:C:286:LEU:HA	1:C:290:GLU:OE1	1.90	0.70
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.73	0.70
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.72	0.70
1:C:142:GLY:CA	1:C:183:GLU:HG2	2.22	0.70
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.71	0.69
4:F:146:VAL:HG22	4:F:164:SER:HB2	1.73	0.69
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.28	0.68
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.75	0.68
2:D:400:ARG:NH1	2:D:400:ARG:O	2.26	0.68
2:B:88:ARG:HE	2:B:124:LYS:NZ	1.92	0.68
1:A:285:GLN:HE22	1:A:372:GLN:H	1.41	0.67
2:B:158:ARG:CZ	11:B:504:MES:H21	2.26	0.66
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.30	0.66
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.77	0.66
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.77	0.66
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.76	0.66
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.78	0.65
1:A:411:GLU:OE2	8:A:504:GOL:H31	1.95	0.65
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.65
2:B:172:MET:HE2	2:B:203:CYS:CB	2.27	0.64
1:C:179:THR:HG21	2:D:247:GLN:HE21	1.62	0.64
1:C:320:ARG:HA	1:C:356:ASN:O	1.98	0.63
2:D:208:ALA:O	2:D:212:ILE:HG13	1.98	0.63
1:C:142:GLY:HA3	1:C:183:GLU:HG2	1.78	0.63
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.34	0.63
2:B:88:ARG:HE	2:B:124:LYS:HZ2	1.47	0.63
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.27	0.63
2:B:240:THR:HG21	2:B:320:ARG:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:101:TYR:HD2	4:F:179:VAL:HG22	1.63	0.62
4:F:17:VAL:HG13	4:F:351:VAL:CG2	2.30	0.62
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.32	0.62
1:A:381:THR:HG22	1:A:383:ALA:H	1.65	0.61
2:B:26:ASP:OD2	2:B:369:ARG:HD2	1.99	0.61
4:F:138:ARG:HD3	4:F:144:GLY:O	1.99	0.61
1:A:132:LEU:HD12	1:A:133:GLN:N	2.16	0.61
2:D:2:ARG:HD2	2:D:3:GLU:OE1	2.01	0.61
4:F:17:VAL:O	4:F:21:LEU:HD22	2.00	0.61
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.01	0.61
2:B:156:LYS:HE3	3:E:76:ARG:CD	2.31	0.61
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.83	0.61
2:D:385:GLN:O	2:D:389:LYS:HG3	2.01	0.61
2:D:357:ASP:O	2:D:359:PRO:HD3	2.00	0.60
1:C:417:GLU:OE2	13:C:602:HOH:O	2.16	0.60
2:D:392:SER:O	2:D:396:THR:HG22	2.01	0.60
4:F:166:ALA:O	4:F:170:LEU:HG	2.02	0.60
2:B:172:MET:HE2	2:B:203:CYS:HB3	1.84	0.60
4:F:240:LEU:HD23	4:F:245:ILE:CD1	2.27	0.60
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.36	0.60
2:B:295:MET:HE3	2:B:377:PHE:CA	2.32	0.60
2:D:318:ILE:N	2:D:318:ILE:HD12	2.17	0.60
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.02	0.60
2:B:2:ARG:NH1	2:B:2:ARG:HB3	2.16	0.60
4:F:17:VAL:HG13	4:F:351:VAL:HG23	1.83	0.60
1:A:221:ARG:HG2	2:B:325:MET:CG	2.29	0.59
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.38	0.59
1:A:285:GLN:NE2	1:A:372:GLN:H	2.00	0.59
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.33	0.59
2:B:199:ASP:OD1	11:B:504:MES:H32	2.03	0.58
4:F:372:THR:OG1	4:F:373:SER:N	2.36	0.58
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.32	0.58
2:B:306:ASP:HB3	2:B:309:HIS:CG	2.39	0.58
1:C:271:THR:HG23	1:C:300:ASN:O	2.04	0.58
4:F:292:ARG:NH1	4:F:379:HIS:H	2.01	0.58
2:B:386:GLU:HA	2:B:389:LYS:HE2	1.85	0.58
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.84	0.57
4:F:138:ARG:HB3	4:F:145:ASN:ND2	2.19	0.57
2:B:156:LYS:HD3	3:E:76:ARG:CZ	2.34	0.57
4:F:138:ARG:HB3	4:F:145:ASN:CG	2.25	0.57
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HE2	1:A:197:HIS:O	2.05	0.57
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.40	0.57
2:D:67:LEU:N	2:D:67:LEU:HD12	2.20	0.57
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.39	0.57
2:B:42:LEU:HD23	2:B:358:ILE:HD11	1.87	0.57
2:D:210:TYR:CE1	2:D:222:PRO:HG2	2.40	0.57
2:D:2:ARG:CZ	2:D:2:ARG:HB2	2.35	0.57
1:A:404:PHE:CD1	2:B:261:PRO:HA	2.40	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.56
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.41	0.56
4:F:82:LYS:NZ	4:F:127:GLU:OE1	2.39	0.56
4:F:150:LYS:HB3	4:F:160:ILE:HG12	1.88	0.56
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.41	0.56
2:D:175:PRO:HA	2:D:178:SER:HB2	1.87	0.56
1:A:32:PRO:HA	1:A:83:TYR:CD1	2.41	0.56
1:C:341:ILE:HG23	1:C:341:ILE:O	2.06	0.55
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.41	0.55
4:F:163:SER:OG	4:F:168:GLU:OE2	2.12	0.55
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.14	0.55
1:C:244:PHE:CE1	1:C:358:GLN:HG3	2.41	0.55
2:B:2:ARG:HH11	2:B:2:ARG:HB3	1.71	0.55
4:F:320:MET:CG	4:F:330:ILE:HD11	2.33	0.55
2:D:176:LYS:NZ	2:D:211:ASP:OD1	2.34	0.55
2:D:141:LEU:HD12	2:D:172:MET:SD	2.47	0.55
1:C:221:ARG:HG2	2:D:325:MET:HB3	1.89	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.41	0.54
1:C:166:LYS:HE2	1:C:197:HIS:O	2.07	0.54
4:F:149:ALA:HB2	4:F:182:ILE:HG12	1.89	0.54
2:D:412:GLY:O	3:E:133:VAL:HG13	2.07	0.54
2:B:236:SER:O	2:B:240:THR:HG23	2.08	0.54
4:F:195:GLY:O	4:F:227:PRO:HB3	2.08	0.54
1:A:69:ASP:O	1:A:94:THR:HA	2.07	0.54
1:A:311:LYS:HD3	1:A:344:VAL:HA	1.90	0.53
2:D:248:LEU:HB3	2:D:354:ALA:HB2	1.90	0.53
1:C:312:TYR:CE1	1:C:341:ILE:HG13	2.42	0.53
2:B:339:ASN:ND2	13:B:603:HOH:O	2.40	0.53
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.42	0.53
2:D:387:LEU:C	2:D:387:LEU:HD23	2.29	0.53
4:F:318:ASP:OD2	12:F:402:ACP:O2G	2.25	0.53
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.89	0.53
1:A:215:ARG:HB2	1:A:215:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:160:ILE:HG22	4:F:161:LEU:N	2.23	0.53
2:D:9:ALA:HA	2:D:68:VAL:O	2.08	0.53
1:C:190:THR:O	1:C:194:THR:HG23	2.08	0.52
2:D:210:TYR:HE1	2:D:222:PRO:HG2	1.73	0.52
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.91	0.52
2:B:295:MET:HE3	2:B:376:THR:C	2.30	0.52
2:B:385:GLN:O	2:B:389:LYS:HG2	2.09	0.52
2:B:67:LEU:HD12	2:B:67:LEU:N	2.25	0.52
1:A:390:ARG:NH1	13:A:601:HOH:O	2.31	0.52
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.92	0.52
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.90	0.52
1:C:356:ASN:ND2	1:C:358:GLN:HB2	2.24	0.52
2:D:412:GLY:C	3:E:133:VAL:HG13	2.31	0.52
1:A:48:SER:O	1:A:51:THR:HG23	2.10	0.51
2:D:220:THR:O	2:D:222:PRO:HD3	2.10	0.51
2:D:82:PRO:O	2:D:83:PHE:CB	2.58	0.51
4:F:1:MET:HE3	4:F:25:GLY:O	2.09	0.51
1:A:81:GLY:O	1:A:84:ARG:HD3	2.10	0.51
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.93	0.51
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.93	0.51
2:B:303:ALA:O	2:B:305:CYS:N	2.41	0.51
2:B:295:MET:CG	2:B:377:PHE:HB2	2.37	0.51
2:D:163:ASP:O	2:D:253:ARG:NH1	2.44	0.51
2:D:136:GLN:HA	2:D:167:ASN:O	2.10	0.51
4:F:148:ILE:O	4:F:148:ILE:HG23	2.11	0.51
2:D:188:THR:HG22	2:D:421:ALA:HB1	1.93	0.50
2:D:323:MET:HB3	2:D:373:MET:CE	2.41	0.50
2:D:146:GLY:O	2:D:150:GLY:HA3	2.11	0.50
2:D:36:TYR:CE2	2:D:46:LEU:HD11	2.47	0.50
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.45	0.50
1:A:345:ASP:N	1:A:345:ASP:OD1	2.45	0.50
2:B:2:ARG:HD3	2:B:50:ASN:HD21	1.69	0.50
2:B:172:MET:HE2	2:B:203:CYS:HA	1.93	0.50
1:C:311:LYS:HE2	1:C:342:GLN:OE1	2.12	0.50
2:B:222:PRO:HA	2:B:226:ASP:OD2	2.11	0.50
1:C:356:ASN:HD21	1:C:358:GLN:HB2	1.77	0.49
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.44	0.49
2:D:349:ASN:O	2:D:352:LYS:HE2	2.13	0.49
4:F:217:ARG:HB2	4:F:374:ILE:O	2.13	0.49
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.12	0.49
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:ASN:O	2:B:352:LYS:HE2	2.12	0.49
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.12	0.49
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.49
2:B:251:ASP:O	2:B:255:LEU:HG	2.12	0.49
2:B:282:GLN:HB3	10:B:503:7LZ:C31	2.42	0.49
3:E:11:LEU:HD11	3:E:18:GLN:OE1	2.12	0.49
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.94	0.49
1:A:336:LYS:O	1:A:336:LYS:HD2	2.13	0.49
2:B:42:LEU:CD2	2:B:358:ILE:HD11	2.43	0.49
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.95	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.48
2:D:295:MET:CG	2:D:377:PHE:HB2	2.43	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.29	0.48
1:C:220:GLU:OE1	2:D:326:LYS:HD3	2.14	0.48
1:A:247:ALA:HB3	3:E:19:SER:OG	2.14	0.48
2:B:295:MET:HE3	2:B:377:PHE:HA	1.95	0.48
2:B:390:ARG:O	2:B:394:GLN:HG3	2.13	0.48
2:B:69:ASP:OD1	2:B:70:LEU:N	2.45	0.48
2:D:323:MET:HB3	2:D:373:MET:HE1	1.95	0.48
2:B:240:THR:HG21	2:B:320:ARG:CD	2.43	0.48
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.78	0.48
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.48
1:C:317:LEU:HD23	1:C:377:MET:HB2	1.96	0.48
2:D:69:ASP:HA	2:D:145:THR:HG21	1.94	0.48
2:D:221:THR:HG22	2:D:221:THR:O	2.12	0.48
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.44	0.48
2:B:297:ASP:OD2	2:B:299:LYS:NZ	2.41	0.48
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.44	0.48
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.43	0.48
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.47
2:D:109:THR:HG22	2:D:110:GLU:N	2.29	0.47
1:A:227:LEU:O	1:A:231:ILE:HG13	2.13	0.47
2:D:287:THR:CB	2:D:289:PRO:HD2	2.44	0.47
4:F:292:ARG:HH11	4:F:379:HIS:N	2.13	0.47
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.14	0.47
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.95	0.47
4:F:38:ASN:HB3	4:F:359:PHE:CE1	2.50	0.47
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.48	0.47
4:F:245:ILE:HG22	4:F:245:ILE:O	2.15	0.47
4:F:1:MET:HE3	4:F:26:GLN:HA	1.96	0.47
4:F:209:HIS:HA	4:F:311:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ALA:HA	1:A:331:ALA:CB	2.45	0.47
1:C:151:SER:HB3	1:C:193:THR:HG21	1.95	0.47
2:B:333:LEU:CD2	4:F:57:GLY:HA3	2.40	0.47
1:A:3:GLU:O	1:A:133:GLN:HB2	2.14	0.47
2:D:220:THR:C	2:D:222:PRO:HD3	2.35	0.46
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.98	0.46
4:F:292:ARG:HH11	4:F:379:HIS:H	1.62	0.46
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.97	0.46
2:B:386:GLU:HA	2:B:389:LYS:CE	2.45	0.46
1:C:271:THR:CA	1:C:302:MET:HE1	2.43	0.46
2:B:357:ASP:O	2:B:359:PRO:HD3	2.15	0.46
2:D:70:LEU:HD23	2:D:114:LEU:HD22	1.97	0.46
2:B:176:LYS:HD3	2:B:207:GLU:CG	2.44	0.46
2:D:8:GLN:OE1	2:D:17:GLY:HA3	2.15	0.46
4:F:102:PRO:HB3	4:F:173:ILE:O	2.16	0.46
4:F:299:GLU:N	4:F:300:PRO:HD2	2.30	0.46
4:F:3:THR:HB	4:F:30:LEU:HD11	1.96	0.46
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.97	0.46
2:B:172:MET:HE2	2:B:203:CYS:CA	2.46	0.46
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.46	0.46
1:A:210:TYR:OH	1:A:221:ARG:NH2	2.48	0.46
2:B:114:LEU:O	2:B:114:LEU:HG	2.16	0.46
2:B:323:MET:HB3	2:B:373:MET:HE2	1.98	0.46
1:A:345:ASP:O	3:E:28:SER:N	2.47	0.45
2:B:295:MET:CE	2:B:317:ALA:HB1	2.46	0.45
2:B:331:GLN:O	2:B:335:VAL:HG12	2.15	0.45
2:D:172:MET:HE2	2:D:203:CYS:HA	1.99	0.45
4:F:138:ARG:HD2	4:F:145:ASN:OD1	2.16	0.45
4:F:213:ILE:HD12	4:F:380:HIS:HE1	1.80	0.45
1:A:285:GLN:HE22	1:A:372:GLN:N	2.12	0.45
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.35	0.45
2:B:159:GLU:OE1	3:E:76:ARG:NH1	2.45	0.45
2:B:172:MET:CE	2:B:203:CYS:HA	2.46	0.45
2:D:427:ASP:O	2:D:431:GLU:HG3	2.17	0.45
1:C:265:ILE:HG22	1:C:380:ASN:HD21	1.81	0.45
2:B:15:GLN:NE2	9:B:501:GDP:O6	2.49	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.45
2:D:181:VAL:HG21	2:D:404:PHE:CE2	2.52	0.45
2:D:158:ARG:HG3	11:D:504:MES:H22	1.97	0.45
2:D:75:MET:CE	2:D:94:PHE:HD1	2.29	0.45
2:D:123:ARG:O	2:D:127:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HH11	2:B:326:LYS:HA	1.82	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.45
4:F:213:ILE:CD1	4:F:380:HIS:HE1	2.30	0.45
2:B:2:ARG:NH1	2:B:2:ARG:CB	2.80	0.44
1:C:229:ARG:NH1	1:C:363:VAL:HG11	2.32	0.44
1:A:392:ASP:OD2	1:A:429:GLU:OE1	2.35	0.44
1:A:297:GLU:HA	1:A:297:GLU:OE1	2.16	0.44
4:F:100:ILE:HD12	4:F:128:ARG:HG2	1.98	0.44
4:F:149:ALA:HA	4:F:181:VAL:O	2.17	0.44
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.53	0.44
4:F:247:LYS:HD2	4:F:253:TYR:OH	2.18	0.44
2:B:200:GLU:HB3	2:B:268:PHE:HE2	1.83	0.44
4:F:134:ALA:HA	4:F:137:ARG:HD2	2.00	0.44
4:F:188:LYS:HD3	4:F:323:GLU:CD	2.38	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.44
1:A:262:TYR:HE2	1:A:346:TRP:CZ2	2.35	0.44
2:B:156:LYS:HE3	3:E:76:ARG:HD3	1.99	0.44
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.99	0.44
1:C:392:ASP:OD2	1:C:429:GLU:OE1	2.36	0.44
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.52	0.44
1:A:216:ASN:N	1:A:216:ASN:HD22	2.16	0.43
1:A:32:PRO:HA	1:A:83:TYR:CE1	2.53	0.43
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.18	0.43
2:B:275:LEU:HA	10:B:503:7LZ:O19	2.18	0.43
2:D:295:MET:SD	2:D:375:ALA:HB1	2.58	0.43
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.47	0.43
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.99	0.43
1:A:308:ARG:HG2	1:A:340:SER:HB2	2.00	0.43
2:D:199:ASP:O	2:D:266:HIS:HB2	2.19	0.43
2:B:295:MET:HE3	2:B:376:THR:O	2.19	0.43
2:B:295:MET:HE3	2:B:377:PHE:N	2.33	0.43
4:F:160:ILE:CG2	4:F:161:LEU:N	2.82	0.43
1:C:63:PRO:HD3	1:C:86:LEU:HG	1.99	0.43
1:A:234:ILE:N	1:A:234:ILE:HD12	2.33	0.43
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.53	0.43
4:F:131:PHE:HE2	4:F:170:LEU:HD21	1.83	0.43
2:B:324:SER:HB3	2:B:327:GLU:HB2	2.01	0.42
1:C:104:ALA:HB2	1:C:413:MET:SD	2.59	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
3:E:139:LEU:HD23	3:E:139:LEU:C	2.39	0.42
1:A:177:VAL:HG23	1:A:177:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.54	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.42
2:D:306:ASP:OD1	2:D:307:PRO:HD2	2.18	0.42
2:D:317:ALA:C	2:D:318:ILE:HD12	2.40	0.42
2:D:400:ARG:O	2:D:400:ARG:HD2	2.19	0.42
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.42
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.54	0.42
2:D:158:ARG:NH2	2:D:197:ASN:OD1	2.52	0.42
4:F:242:ASN:OD1	12:F:402:ACP:H3B2	2.19	0.42
1:A:297:GLU:HB2	1:A:300:ASN:HD22	1.84	0.42
2:B:123:ARG:O	2:B:127:GLU:HG3	2.19	0.42
2:B:295:MET:CE	2:B:376:THR:O	2.68	0.42
1:A:236:SER:OG	1:A:320:ARG:NH1	2.51	0.42
1:A:262:TYR:CE2	1:A:346:TRP:CH2	3.07	0.42
2:B:298:SER:C	2:B:300:ASN:H	2.22	0.42
3:E:96:MET:CE	3:E:100:LYS:HE3	2.49	0.42
1:A:235:VAL:O	1:A:239:THR:HG23	2.20	0.42
2:B:326:LYS:O	2:B:330:GLU:HG3	2.20	0.42
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.55	0.42
1:A:70:LEU:HD22	1:A:110:ILE:CG2	2.50	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.42
2:B:221:THR:O	2:B:221:THR:HG22	2.20	0.42
1:C:271:THR:HG21	1:C:295:CYS:O	2.20	0.42
1:C:401:LYS:HE3	2:D:438:ALA:HB1	2.02	0.42
2:D:295:MET:HG3	2:D:377:PHE:HB2	2.02	0.42
2:D:320:ARG:O	2:D:323:MET:HE1	2.20	0.41
2:B:305:CYS:O	2:B:307:PRO:HD3	2.20	0.41
2:B:295:MET:HE1	2:B:317:ALA:HB1	2.02	0.41
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.68	0.41
2:D:406:HIS:NE2	2:D:407:TRP:HD1	2.18	0.41
3:E:24:LEU:HD12	3:E:24:LEU:N	2.35	0.41
1:A:411:GLU:O	3:E:61:ARG:HD3	2.20	0.41
2:B:2:ARG:CZ	2:B:2:ARG:CB	2.99	0.41
1:C:153:LEU:O	1:C:157:LEU:HG	2.20	0.41
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.54	0.41
2:B:320:ARG:HA	2:B:356:CYS:O	2.20	0.41
1:C:234:ILE:HD13	1:C:302:MET:SD	2.61	0.41
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.20	0.41
4:F:47:LEU:HD23	4:F:48:PRO:N	2.36	0.41
1:A:70:LEU:HD12	1:A:145:THR:OG1	2.20	0.41
2:B:298:SER:O	2:B:300:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:PRO:HB2	2:D:371:LEU:O	2.21	0.41
2:B:157:ILE:HG21	2:B:166:MET:HE1	2.01	0.41
2:B:218:LYS:HA	2:B:218:LYS:HD3	1.85	0.41
2:D:182:VAL:HG21	2:D:407:TRP:HZ3	1.85	0.41
4:F:8:ASP:OD2	4:F:44:ARG:HG3	2.20	0.41
2:D:352:LYS:HD3	2:D:352:LYS:HA	1.91	0.41
2:D:46:LEU:O	2:D:49:ILE:HG22	2.20	0.41
4:F:27:TRP:HZ2	4:F:359:PHE:HB2	1.86	0.41
1:A:132:LEU:HD12	1:A:133:GLN:H	1.86	0.41
2:B:136:GLN:HA	2:B:167:ASN:O	2.21	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.55	0.41
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.03	0.41
1:C:70:LEU:HA	1:C:70:LEU:HD23	1.77	0.41
1:A:70:LEU:HD22	1:A:110:ILE:HG21	2.03	0.41
1:C:196:GLU:HG2	13:C:633:HOH:O	2.21	0.41
2:D:101:ASN:HA	2:D:144:GLY:N	2.36	0.41
2:D:278:ARG:HA	2:D:279:GLY:HA2	1.71	0.41
4:F:161:LEU:HD12	4:F:236:LYS:NZ	2.36	0.41
4:F:162:ILE:H	4:F:236:LYS:NZ	2.18	0.41
4:F:58:LEU:HA	4:F:58:LEU:HD23	1.88	0.41
1:A:270:ALA:HB3	1:A:302:MET:HG3	2.03	0.41
2:B:192:HIS:ND1	2:B:424:ASN:ND2	2.69	0.41
1:C:336:LYS:HZ3	1:C:351:PHE:HE1	1.63	0.41
1:A:347:CYS:C	3:E:27:PRO:HB3	2.41	0.41
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.52	0.40
2:D:107:HIS:O	2:D:152:LEU:HD22	2.21	0.40
4:F:242:ASN:HD22	4:F:245:ILE:HD11	1.86	0.40
1:C:293:ASN:HA	1:C:335:ILE:HD11	2.03	0.40
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.39	0.40
1:C:36:MET:O	1:C:36:MET:HG2	2.21	0.40
1:A:241:SER:HB2	1:A:248:LEU:O	2.21	0.40
2:B:209:LEU:HB3	2:B:227:LEU:HG	2.03	0.40
2:D:137:LEU:HD23	2:D:154:ILE:HD11	2.03	0.40
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.56	0.40
2:D:75:MET:HE2	2:D:94:PHE:HD1	1.85	0.40
2:B:83:PHE:O	2:B:86:ILE:HG22	2.21	0.40
1:C:151:SER:HB3	1:C:193:THR:CG2	2.52	0.40
4:F:259:GLY:O	4:F:261:GLU:HG3	2.20	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)
2:B:113:GLU:OE1	1:C:283:HIS:NE2[4_555]	2.15	0.05

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/451 (96%)	421 (98%)	10 (2%)	0	100	100
1	C	438/451 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	423/445 (95%)	410 (97%)	12 (3%)	1 (0%)	47	58
2	D	422/445 (95%)	405 (96%)	17 (4%)	0	100	100
3	E	118/143 (82%)	115 (98%)	3 (2%)	0	100	100
4	F	310/384 (81%)	296 (96%)	14 (4%)	0	100	100
All	All	2142/2319 (92%)	2074 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	82	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/379 (97%)	361 (98%)	6 (2%)	62	78
1	C	371/379 (98%)	366 (99%)	5 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	368/383 (96%)	363 (99%)	5 (1%)	67	81
2	D	368/383 (96%)	361 (98%)	7 (2%)	57	73
3	E	110/127 (87%)	108 (98%)	2 (2%)	59	75
4	F	294/342 (86%)	289 (98%)	5 (2%)	60	76
All	All	1878/1993 (94%)	1848 (98%)	30 (2%)	62	78

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	71	GLU
1	A	179	THR
1	A	251	ASP
1	A	358	GLN
1	A	381	THR
2	B	86	ILE
2	B	90	ASP
2	B	139	HIS
2	B	192	HIS
2	B	278	ARG
1	C	38	SER
1	C	114	ILE
1	C	178	SER
1	C	274	PRO
1	C	347	CYS
2	D	139	HIS
2	D	155	SER
2	D	180	THR
2	D	229	HIS
2	D	335	VAL
2	D	336	GLN
2	D	373	MET
3	E	88	GLU
3	E	136	ASN
4	F	21	LEU
4	F	30	LEU
4	F	86	GLU
4	F	165	GLU
4	F	197	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	300	ASN
1	C	11	GLN
1	C	380	ASN
2	D	247	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	$\# Z  > 2$
10	7LZ	B	503	-	37,38,38	2.23	13 (35%)	42,50,50	1.88	12 (28%)
10	7LZ	D	503	-	37,38,38	2.26	14 (37%)	42,50,50	1.76	10 (23%)
9	GDP	D	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.88	7 (22%)
5	GTP	C	501	6	26,34,34	1.22	3 (11%)	33,54,54	1.84	7 (21%)
9	GDP	B	501	6	24,30,30	1.20	3 (12%)	31,47,47	2.05	9 (29%)
5	GTP	A	501	6	26,34,34	1.06	2 (7%)	33,54,54	2.13	10 (30%)
11	MES	D	504	-	12,12,12	2.35	1 (8%)	14,16,16	1.36	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	GOL	A	505	-	5,5,5	0.31	0	5,5,5	0.51	0
11	MES	B	504	8	12,12,12	2.40	2 (16%)	14,16,16	1.70	2 (14%)
8	GOL	A	504	11	5,5,5	0.43	0	5,5,5	0.87	0
12	ACP	F	402	7	27,33,33	2.06	8 (29%)	32,52,52	1.29	4 (12%)

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
10	7LZ	B	503	-	-	5/57/57/57	0/0/1/1
10	7LZ	D	503	-	-	7/57/57/57	0/0/1/1
9	GDP	D	501	6	-	4/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
11	MES	D	504	-	-	0/6/14/14	0/1/1/1
8	GOL	A	505	-	-	2/4/4/4	-
11	MES	B	504	8	-	5/6/14/14	0/1/1/1
8	GOL	A	504	11	-	2/4/4/4	-
12	ACP	F	402	7	-	7/15/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	504	MES	C8-S	-7.88	1.66	1.77
11	B	504	MES	C8-S	-7.81	1.66	1.77
10	D	503	7LZ	C3-C2	5.87	1.49	1.34
10	B	503	7LZ	C3-C2	5.73	1.49	1.34
12	F	402	ACP	PG-O1G	5.54	1.61	1.50
10	D	503	7LZ	C26-C25	5.02	1.45	1.32
10	B	503	7LZ	C26-C25	4.81	1.44	1.32
10	B	503	7LZ	C24-C23	4.33	1.50	1.33
12	F	402	ACP	PB-O3A	4.24	1.63	1.58
10	D	503	7LZ	C24-C23	4.19	1.50	1.33
12	F	402	ACP	PB-O1B	4.07	1.61	1.51
5	C	501	GTP	C6-N1	3.84	1.39	1.33
9	D	501	GDP	C6-C5	3.81	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C6-C5	3.80	1.47	1.41
10	D	503	7LZ	C11-C10	3.63	1.43	1.32
10	B	503	7LZ	C11-C10	3.58	1.42	1.32
10	D	503	7LZ	C6-C5	3.52	1.60	1.51
10	B	503	7LZ	C6-C5	3.49	1.60	1.51
10	D	503	7LZ	C18-C19	3.27	1.58	1.52
10	B	503	7LZ	C15-C14	3.18	1.59	1.54
10	B	503	7LZ	C18-C19	3.13	1.58	1.52
12	F	402	ACP	PG-O2G	3.01	1.61	1.54
12	F	402	ACP	PB-O2B	-3.01	1.49	1.56
10	B	503	7LZ	C28-C14	2.89	1.60	1.53
5	A	501	GTP	C6-N1	2.87	1.38	1.33
10	D	503	7LZ	C28-C14	2.84	1.60	1.53
10	D	503	7LZ	C8-C9	2.77	1.58	1.52
10	D	503	7LZ	C15-C14	2.71	1.58	1.54
10	B	503	7LZ	C8-C9	2.70	1.58	1.52
12	F	402	ACP	PG-O3G	-2.70	1.48	1.54
12	F	402	ACP	C5-C4	2.54	1.47	1.40
9	B	501	GDP	C2'-C1'	-2.46	1.50	1.53
10	B	503	7LZ	C4-C5	2.36	1.42	1.33
12	F	402	ACP	O4'-C1'	2.36	1.44	1.41
10	D	503	7LZ	C4-C5	2.35	1.42	1.33
9	D	501	GDP	C5-C4	2.34	1.47	1.40
10	D	503	7LZ	C22-C23	-2.28	1.45	1.51
10	D	503	7LZ	C20-C19	2.22	1.58	1.54
5	C	501	GTP	C2'-C1'	-2.22	1.50	1.53
10	B	503	7LZ	C22-C23	-2.19	1.45	1.51
10	D	503	7LZ	O7-C7	2.18	1.48	1.43
5	A	501	GTP	C2'-C1'	-2.17	1.50	1.53
10	B	503	7LZ	O19-C19	2.16	1.47	1.43
11	B	504	MES	O1S-S	2.15	1.51	1.45
9	B	501	GDP	C5-C4	2.09	1.46	1.40
5	C	501	GTP	C6-C5	-2.06	1.37	1.41
10	B	503	7LZ	O7-C7	2.01	1.47	1.43
10	D	503	7LZ	O13-C13	2.00	1.47	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-6.64	118.36	127.22
5	C	501	GTP	N3-C2-N1	-5.75	119.56	127.22
10	B	503	7LZ	O21-C21-C22	4.91	115.30	107.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	MES	O1S-S-C8	4.68	112.56	106.92
9	D	501	GDP	C2-N3-C4	4.53	120.53	115.36
9	D	501	GDP	C5-C6-N1	-4.50	117.28	123.43
10	B	503	7LZ	C30-C20-C21	4.49	119.45	111.40
9	B	501	GDP	C2-N3-C4	4.47	120.46	115.36
10	D	503	7LZ	C21-O21-C1	4.45	124.67	117.47
9	B	501	GDP	C6-C5-C4	-4.41	116.59	120.80
9	B	501	GDP	C6-N1-C2	4.38	122.89	115.93
5	A	501	GTP	C6-N1-C2	4.30	122.76	115.93
5	A	501	GTP	C2-N3-C4	4.20	120.16	115.36
9	D	501	GDP	C6-N1-C2	4.11	122.46	115.93
10	D	503	7LZ	C25-C24-C23	-3.99	116.92	126.33
10	B	503	7LZ	C25-C24-C23	-3.96	116.99	126.33
9	B	501	GDP	N3-C2-N1	-3.88	122.05	127.22
10	D	503	7LZ	O21-C1-C2	3.88	120.18	111.38
5	A	501	GTP	C5-C6-N1	-3.83	118.19	123.43
5	C	501	GTP	C2-N3-C4	3.80	119.70	115.36
9	B	501	GDP	C5-C6-N1	-3.78	118.26	123.43
10	D	503	7LZ	C30-C20-C21	3.71	118.07	111.40
11	D	504	MES	O3S-S-C8	3.47	111.37	105.77
10	D	503	7LZ	O21-C21-C22	3.44	112.83	107.09
9	B	501	GDP	O3'-C3'-C4'	-3.28	101.57	111.05
9	D	501	GDP	C6-C5-C4	-3.26	117.68	120.80
9	D	501	GDP	C4-C5-N7	-3.16	106.10	109.40
10	B	503	7LZ	C21-O21-C1	3.14	122.56	117.47
10	B	503	7LZ	O21-C1-C2	3.12	118.45	111.38
12	F	402	ACP	N3-C2-N1	-3.04	123.93	128.68
5	A	501	GTP	C6-C5-C4	-2.94	117.99	120.80
9	D	501	GDP	N3-C2-N1	-2.93	123.32	127.22
5	C	501	GTP	C6-N1-C2	2.91	120.55	115.93
5	C	501	GTP	C6-C5-C4	-2.82	118.11	120.80
10	B	503	7LZ	C4-C3-C2	2.79	131.65	124.67
5	C	501	GTP	N2-C2-N1	2.78	121.57	117.25
5	C	501	GTP	C5-C6-N1	-2.73	119.70	123.43
12	F	402	ACP	C3'-C2'-C1'	2.71	105.05	100.98
5	A	501	GTP	C1'-N9-C4	-2.67	121.95	126.64
12	F	402	ACP	PA-O3A-PB	-2.66	124.12	132.56
5	A	501	GTP	O2G-PG-O3B	2.65	113.54	104.64
5	C	501	GTP	PA-O3A-PB	-2.61	123.86	132.83
9	D	501	GDP	PA-O3A-PB	-2.61	123.88	132.83
9	B	501	GDP	PA-O3A-PB	-2.55	124.07	132.83
9	B	501	GDP	C4-C5-N7	-2.52	106.77	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	PA-O3A-PB	-2.48	124.32	132.83
10	B	503	7LZ	C12-C13-C14	-2.47	109.81	114.86
9	B	501	GDP	C1'-N9-C4	-2.45	122.34	126.64
5	A	501	GTP	N2-C2-N1	2.38	120.95	117.25
11	B	504	MES	O2S-S-C8	2.37	109.77	106.92
12	F	402	ACP	C4-C5-N7	-2.35	106.95	109.40
10	D	503	7LZ	C13-C12-C11	2.28	116.80	111.42
10	D	503	7LZ	C22-C23-C24	2.27	130.93	126.16
10	D	503	7LZ	C4-C3-C2	2.20	130.16	124.67
10	B	503	7LZ	C13-C12-C11	2.18	116.58	111.42
10	B	503	7LZ	C28-C14-C13	-2.18	107.50	111.54
10	B	503	7LZ	C22-C23-C24	2.16	130.71	126.16
10	B	503	7LZ	C31-C22-C21	2.10	114.99	111.11
10	D	503	7LZ	O1-C1-C2	-2.05	116.43	123.58
5	A	501	GTP	C4-C5-N7	-2.03	107.28	109.40
10	B	503	7LZ	O21-C21-C20	-2.03	102.78	107.50
10	D	503	7LZ	C12-C13-C14	-2.01	110.74	114.86

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	A	505	GOL	O1-C1-C2-C3
11	B	504	MES	C7-C8-S-O1S
8	A	504	GOL	O1-C1-C2-C3
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O2B
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O3A
10	B	503	7LZ	C20-C21-O21-C1
11	B	504	MES	C7-C8-S-O3S
10	B	503	7LZ	C22-C21-O21-C1

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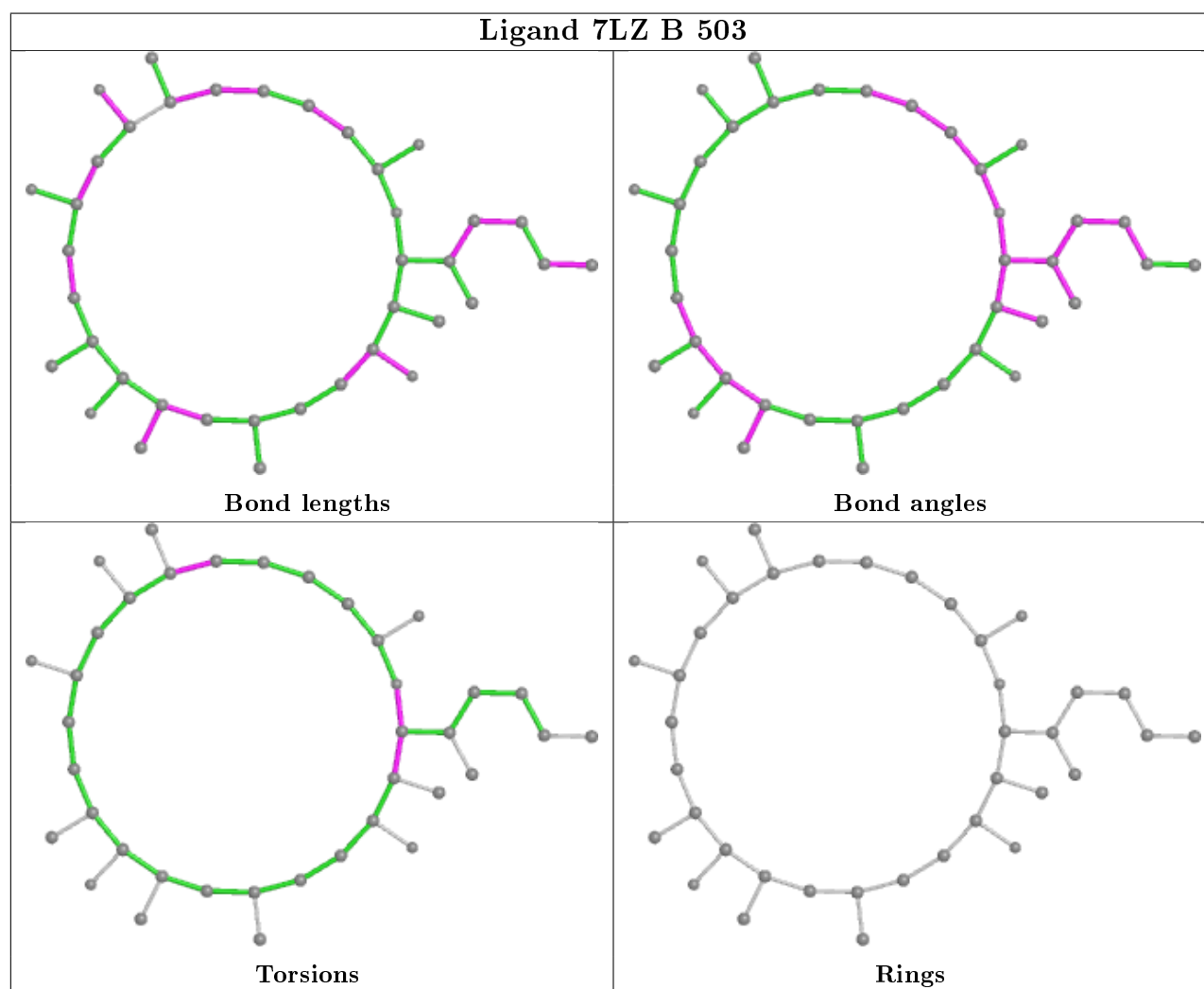
Mol	Chain	Res	Type	Atoms
10	B	503	7LZ	C4-C5-C6-C61
10	D	503	7LZ	C4-C5-C6-C61
8	A	504	GOL	O1-C1-C2-O2
10	D	503	7LZ	C20-C21-O21-C1
8	A	505	GOL	O1-C1-C2-O2
11	B	504	MES	C8-C7-N4-C5
10	D	503	7LZ	C22-C21-O21-C1
5	C	501	GTP	PB-O3B-PG-O1G
10	D	503	7LZ	C4-C5-C6-C7
10	D	503	7LZ	C10-C11-C12-C13
12	F	402	ACP	C5'-O5'-PA-O2A
11	B	504	MES	C7-C8-S-O2S
10	B	503	7LZ	C30-C20-C21-C22
11	B	504	MES	C8-C7-N4-C3
10	D	503	7LZ	C19-C20-C21-C22
10	D	503	7LZ	C30-C20-C21-C22
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3B-PG-O3G
12	F	402	ACP	PB-O3A-PA-O2A
10	B	503	7LZ	C19-C20-C21-C22
9	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
9	D	501	GDP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

8 monomers are involved in 12 short contacts:

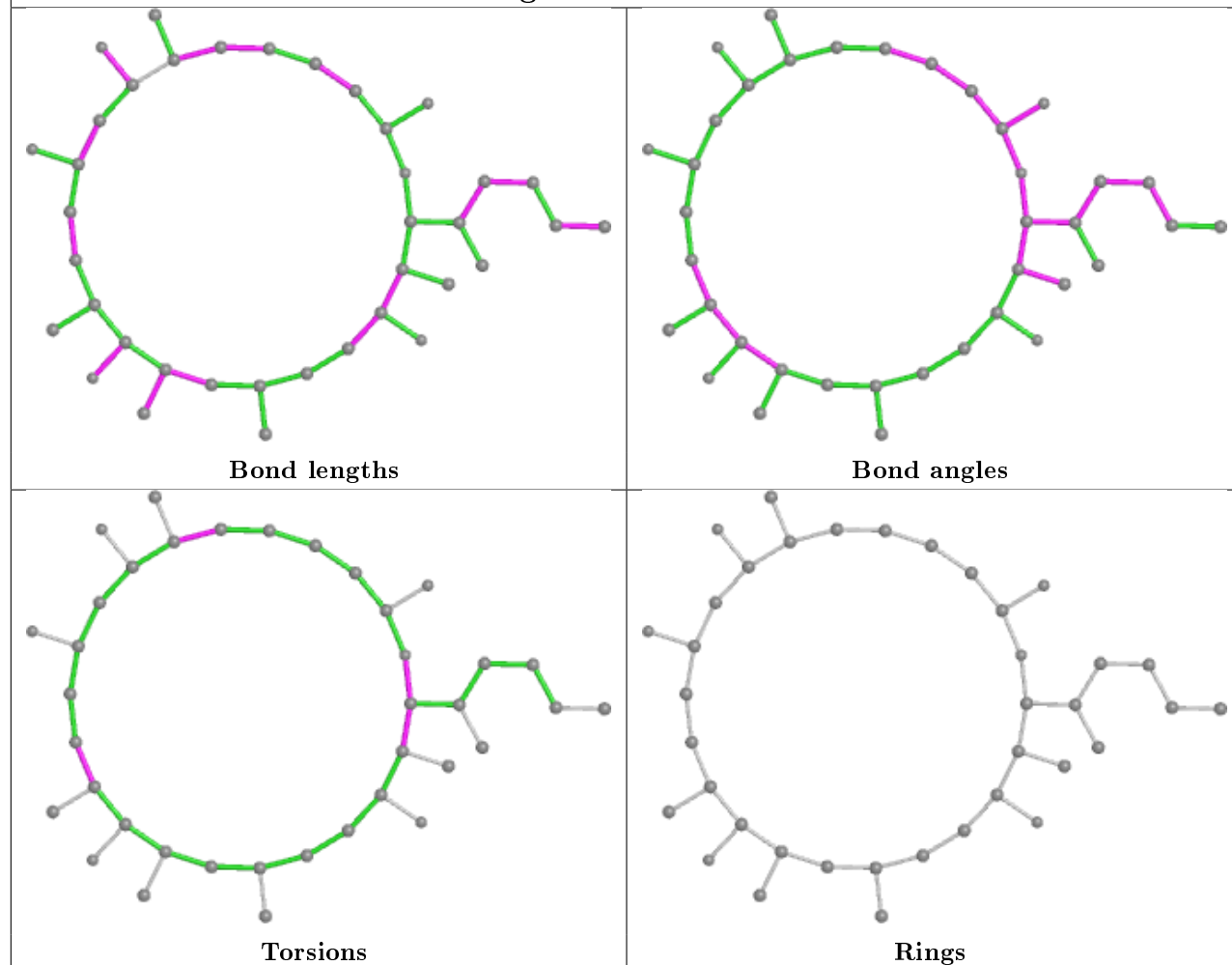
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	7LZ	2	0
9	D	501	GDP	1	0
9	B	501	GDP	1	0
5	A	501	GTP	1	0
11	D	504	MES	1	0
11	B	504	MES	3	0
8	A	504	GOL	1	0
12	F	402	ACP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

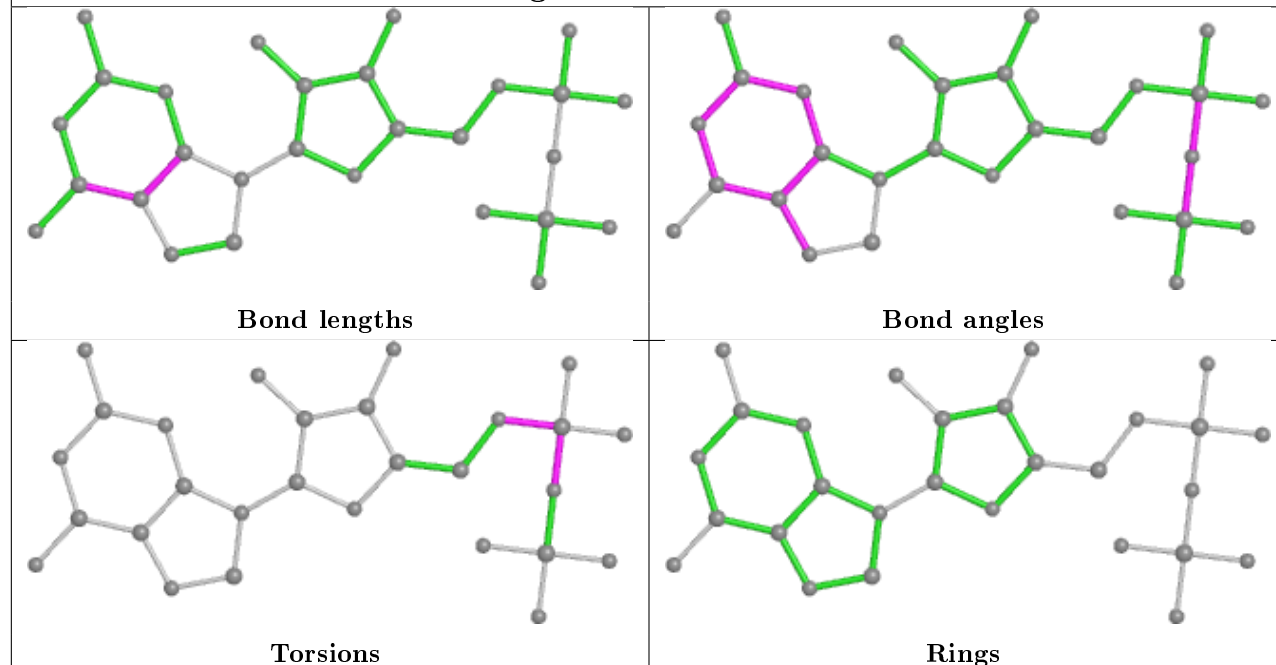


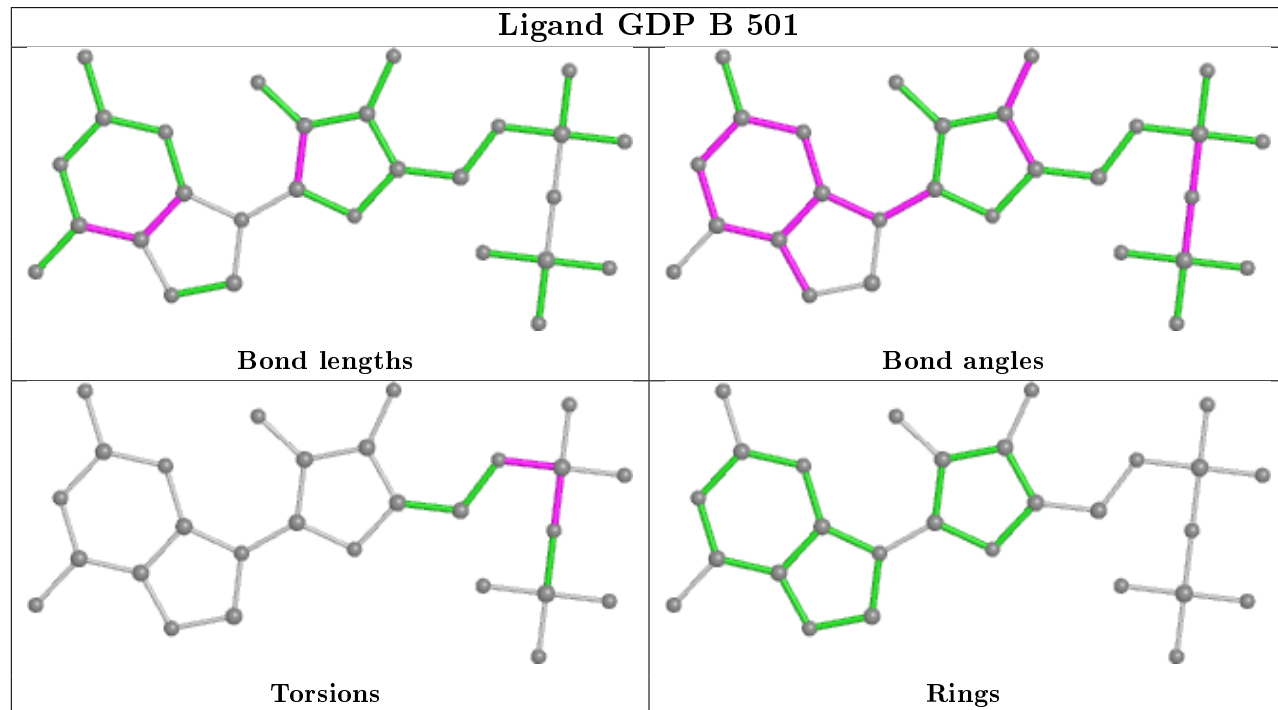
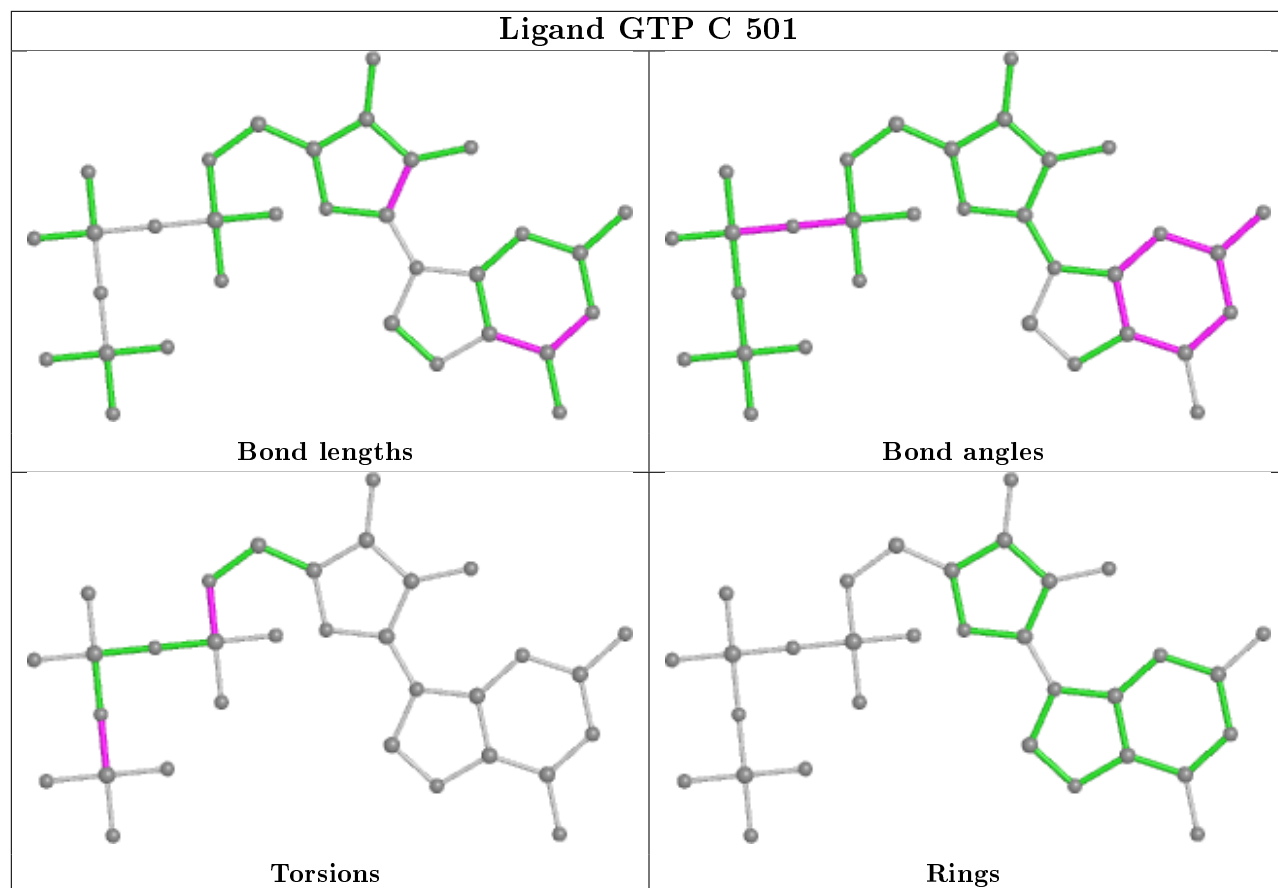


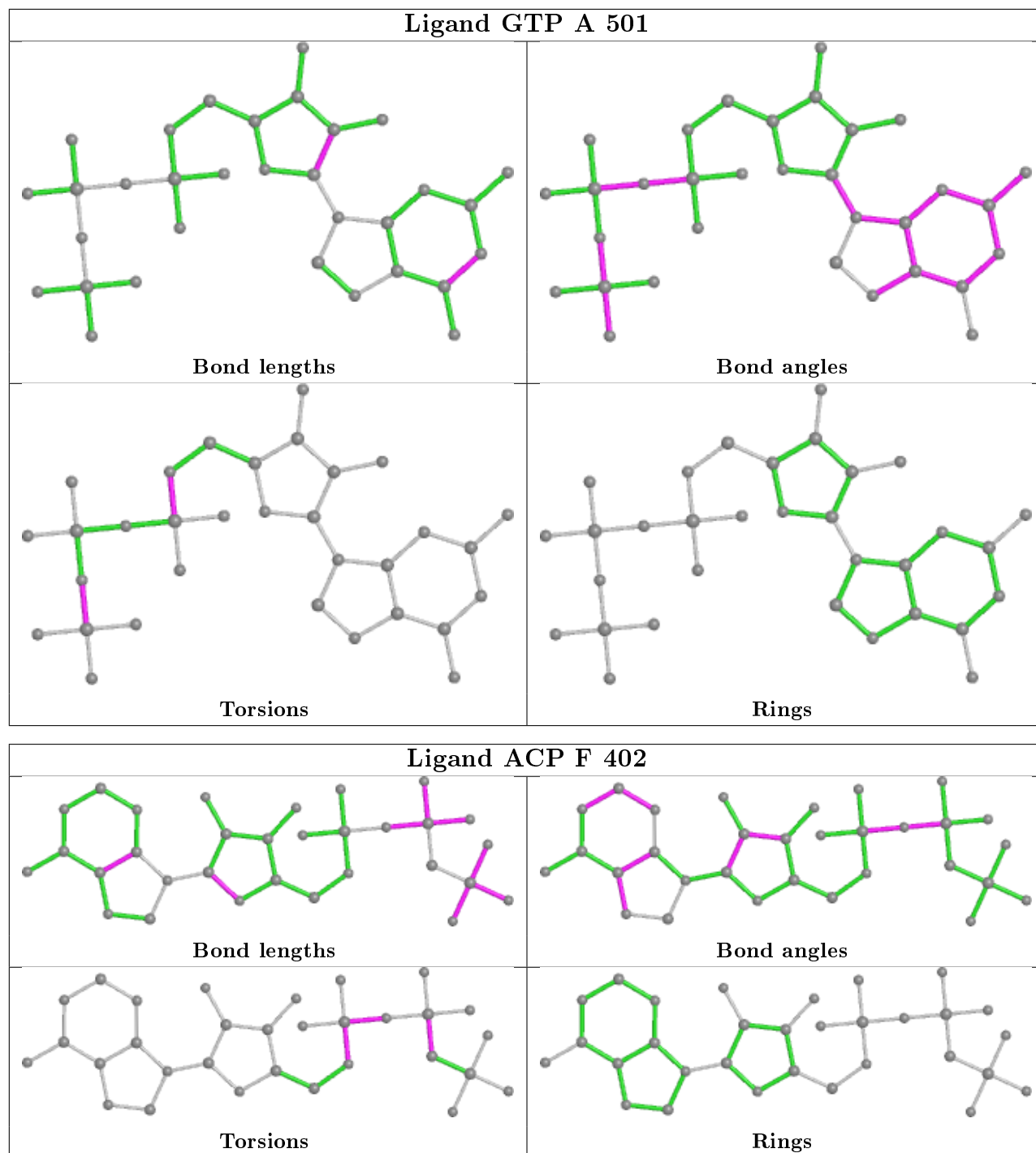
## Ligand 7LZ D 503



## Ligand GDP D 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	435/451 (96%)	0.23	9 (2%) 63 70	47, 71, 108, 143	0
1	C	440/451 (97%)	0.16	2 (0%) 91 94	46, 62, 98, 137	0
2	B	427/445 (95%)	0.54	12 (2%) 53 60	46, 70, 113, 163	2 (0%)
2	D	425/445 (95%)	0.45	28 (6%) 18 23	51, 85, 125, 140	4 (0%)
3	E	122/143 (85%)	0.49	8 (6%) 18 23	54, 83, 127, 151	0
4	F	326/384 (84%)	1.59	103 (31%) 0 0	57, 102, 160, 183	0
All	All	2175/2319 (93%)	0.54	162 (7%) 14 19	46, 77, 129, 183	6 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	13.8
4	F	173	ILE	13.1
4	F	179	VAL	8.0
4	F	245	ILE	8.0
4	F	160	ILE	7.8
4	F	253	TYR	7.6
4	F	161	LEU	7.4
4	F	100	ILE	7.2
4	F	244	CYS	7.2
4	F	172	PHE	6.9
4	F	238	CYS	6.8
4	F	182	ILE	6.7
4	F	131	PHE	6.6
4	F	240	LEU	6.4
4	F	254	GLY	6.3
4	F	236	LYS	6.0
4	F	255	ARG	5.9
4	F	99	VAL	5.8
4	F	256	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	5.8
4	F	136	ASN	5.7
4	F	162	ILE	5.5
4	F	139	ARG	5.1
4	F	132	LEU	5.0
2	B	279	GLY	4.9
4	F	239	HIS	4.9
4	F	166	ALA	4.8
4	F	101	TYR	4.8
4	F	372	THR	4.6
4	F	247	LYS	4.6
4	F	150	LYS	4.5
4	F	192	LEU	4.4
4	F	241	THR	4.4
4	F	259	GLY	4.4
4	F	263	PHE	4.4
4	F	242	ASN	4.4
2	D	405	LEU	4.3
4	F	163	SER	4.3
4	F	17	VAL	4.3
4	F	165	GLU	4.3
4	F	257	GLU	4.2
4	F	258	GLU	4.1
4	F	223	THR	4.1
2	D	286	LEU	4.0
2	D	57	THR	4.0
4	F	181	VAL	4.0
3	E	6	MET	3.9
4	F	174	ASP	3.9
4	F	13	VAL	3.9
4	F	147	TRP	3.8
2	D	401	ARG	3.8
3	E	45	PRO	3.7
4	F	171	ASP	3.7
4	F	21	LEU	3.6
2	D	177	VAL	3.6
4	F	243	HIS	3.6
4	F	246	GLN	3.5
2	D	418	PHE	3.4
2	B	59	ASN	3.4
2	B	438	ALA	3.4
4	F	98	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	170	LEU	3.4
4	F	143	GLU	3.4
2	D	82	PRO	3.4
2	D	404	PHE	3.3
4	F	168	GLU	3.3
2	D	280	SER	3.2
4	F	133	ALA	3.2
4	F	137	ARG	3.1
2	D	222	PRO	3.1
4	F	134	ALA	3.1
1	A	132	LEU	3.1
4	F	260	ASN	3.1
4	F	264	PHE	3.0
4	F	148	ILE	3.0
4	F	235	ASP	3.0
4	F	146	VAL	3.0
4	F	228	TYR	2.9
2	B	284	ARG	2.9
4	F	31	ARG	2.9
4	F	144	GLY	2.9
1	A	283	HIS	2.8
4	F	140	GLU	2.8
4	F	149	ALA	2.8
4	F	28	LYS	2.8
2	D	60	LYS	2.8
2	D	219	LEU	2.8
4	F	199	PHE	2.7
4	F	265	GLU	2.8
3	E	139	LEU	2.7
4	F	129	GLU	2.7
2	B	246	GLY	2.7
4	F	44	ARG	2.7
1	A	333	ALA	2.7
2	B	166	MET	2.7
2	D	416	MET	2.7
4	F	125	THR	2.7
4	F	20	LEU	2.7
4	F	362	ALA	2.7
4	F	145	ASN	2.7
4	F	353	VAL	2.7
4	F	164	SER	2.6
4	F	89	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	224	SER	2.6
4	F	230	SER	2.5
2	D	408	TYR	2.5
4	F	342	LEU	2.5
3	E	28	SER	2.5
4	F	22	LEU	2.4
4	F	361	LEU	2.4
2	D	58	GLY	2.4
1	A	86	LEU	2.4
2	D	415	GLU	2.4
2	D	399	PHE	2.3
4	F	128	ARG	2.3
4	F	237	THR	2.3
4	F	340	GLN	2.3
1	A	337	THR	2.3
4	F	221	LEU	2.3
2	D	176	LYS	2.3
4	F	330	ILE	2.3
4	F	138	ARG	2.3
3	E	142	GLU	2.2
2	D	407	TRP	2.2
2	D	322	ARG	2.2
4	F	1	MET	2.2
2	D	289	PRO	2.2
2	D	87	PHE	2.2
4	F	4	PHE	2.2
4	F	142	ARG	2.2
4	F	135	TYR	2.2
4	F	227	PRO	2.2
2	B	126	SER	2.2
4	F	335	ALA	2.2
1	A	125	LEU	2.2
2	D	46	LEU	2.2
4	F	197	ARG	2.2
4	F	262	MET	2.2
2	D	400	ARG	2.2
2	B	308	ARG	2.1
1	A	438	ASP	2.1
4	F	91	CYS	2.1
3	E	25	LYS	2.1
2	D	210	TYR	2.1
1	A	335	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	56	ALA	2.1
4	F	343	TYR	2.1
4	F	11	SER	2.1
4	F	37	PHE	2.1
3	E	26	PRO	2.1
4	F	339	ALA	2.1
2	D	182	VAL	2.1
1	C	357	TYR	2.1
2	B	161	TYR	2.1
1	A	338	LYS	2.1
2	B	61	TYR	2.1
3	E	24	LEU	2.0
4	F	217	ARG	2.0
2	B	132	LEU	2.0
2	B	153	LEU	2.0
2	D	325	MET	2.0
1	C	341	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	GOL	A	504	6/6	0.70	0.28	85,92,103,103	0
11	MES	D	504	12/12	0.78	0.23	116,132,148,149	0
10	7LZ	B	503	38/38	0.88	0.37	73,115,136,142	0
8	GOL	A	505	6/6	0.90	0.21	97,101,106,112	0
7	CA	F	401	1/1	0.90	0.05	134,134,134,134	0
6	MG	B	502	1/1	0.91	0.24	55,55,55,55	0

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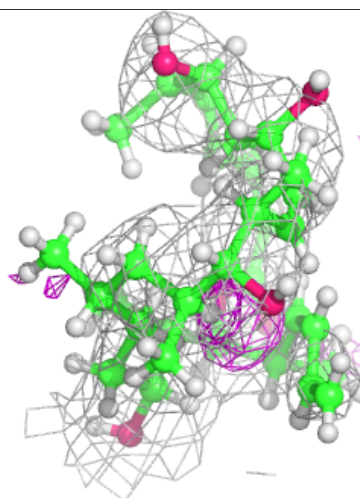
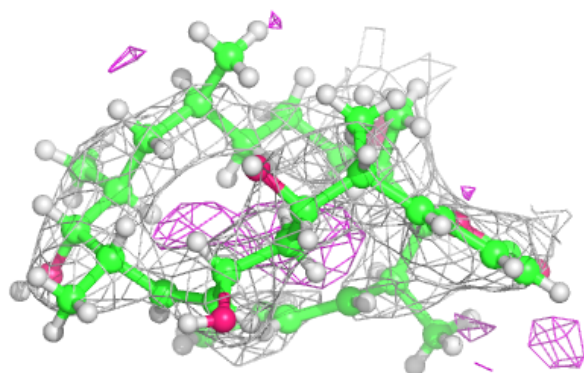
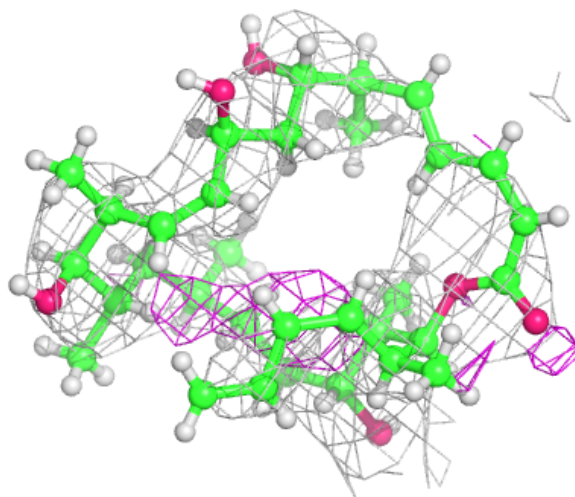
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	502	1/1	0.91	0.04	61,61,61,61	0
6	MG	A	502	1/1	0.92	0.28	61,61,61,61	0
10	7LZ	D	503	38/38	0.93	0.25	83,108,129,135	0
12	ACP	F	402	31/31	0.93	0.13	96,123,162,166	0
7	CA	C	503	1/1	0.95	0.10	79,79,79,79	0
11	MES	B	504	12/12	0.95	0.23	53,63,89,102	0
7	CA	A	503	1/1	0.96	0.05	99,99,99,99	0
9	GDP	D	501	28/28	0.96	0.13	64,75,87,100	0
5	GTP	A	501	32/32	0.97	0.17	45,53,66,75	0
6	MG	C	502	1/1	0.98	0.14	55,55,55,55	0
5	GTP	C	501	32/32	0.99	0.16	40,52,59,61	0
9	GDP	B	501	28/28	0.99	0.18	44,53,58,67	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.

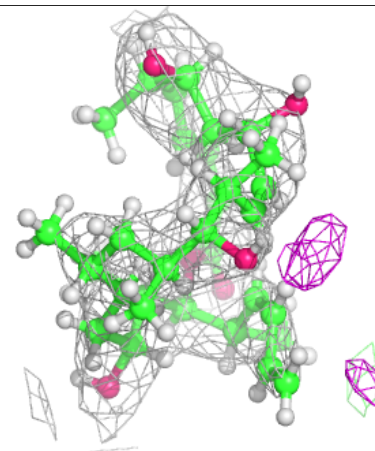
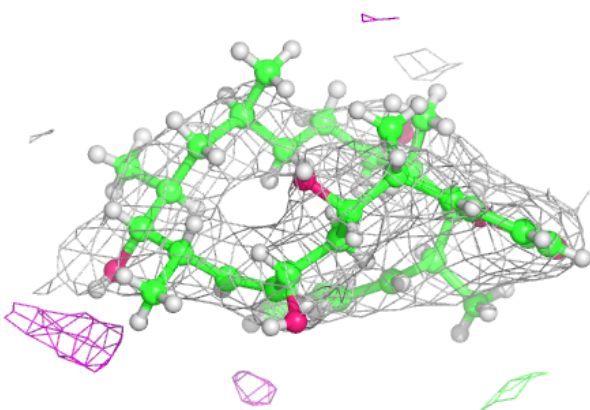
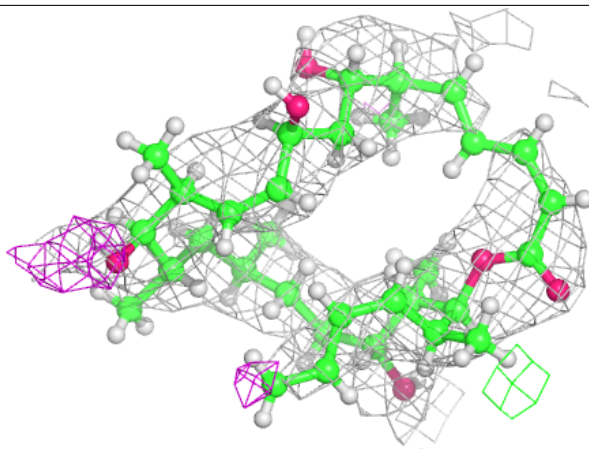
**Electron density around 7LZ B 503:**

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

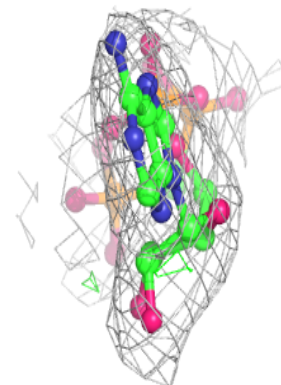
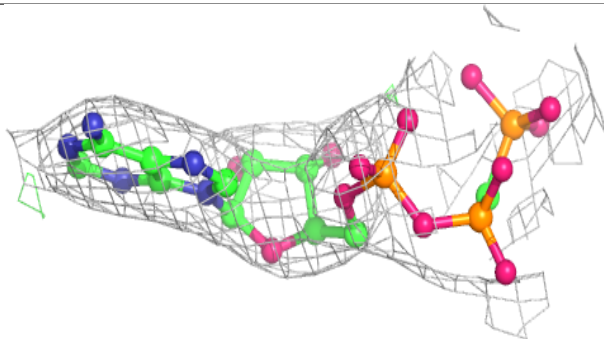
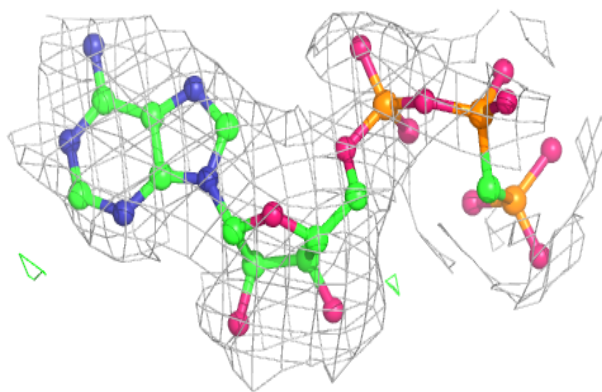


**Electron density around 7LZ D 503:**

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

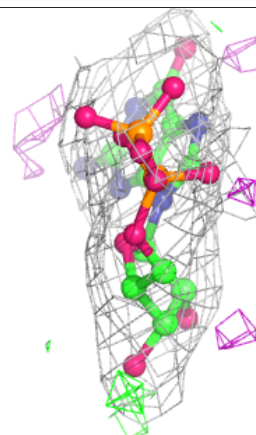
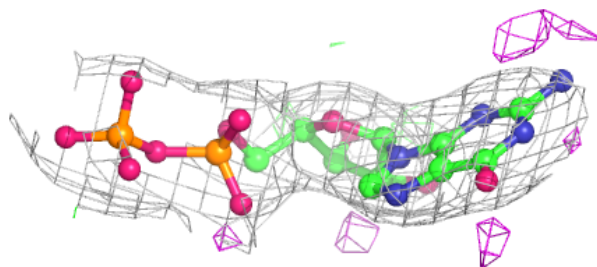
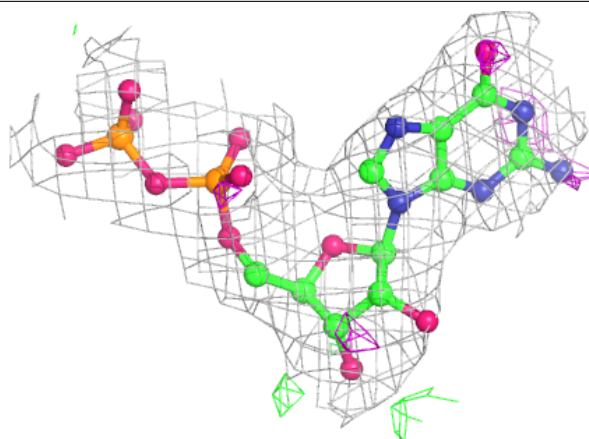
**Electron density around ACP F 402:**

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

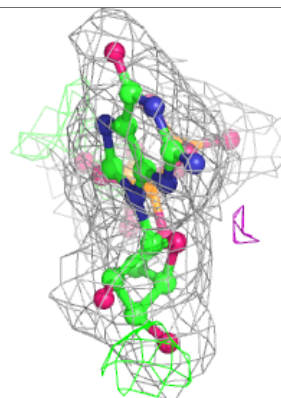
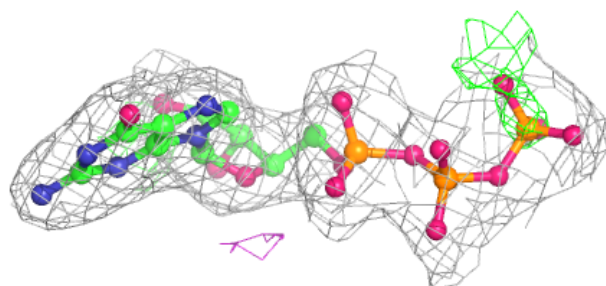
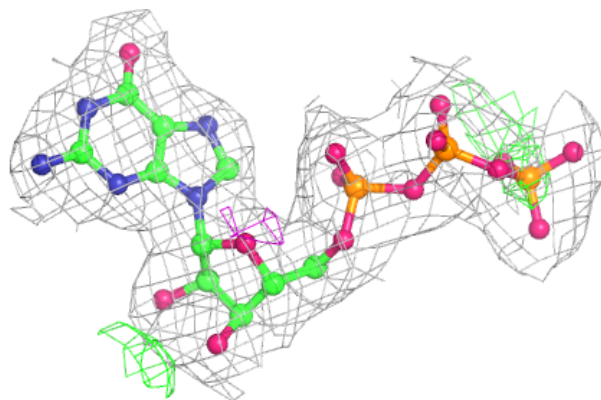


**Electron density around GDP D 501:**

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

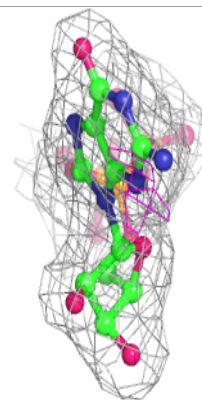
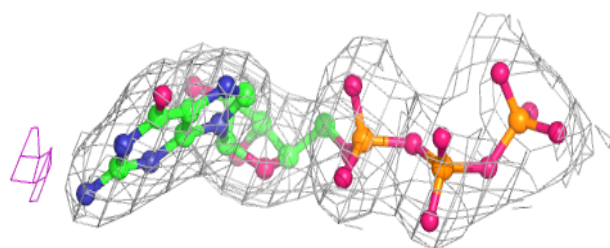
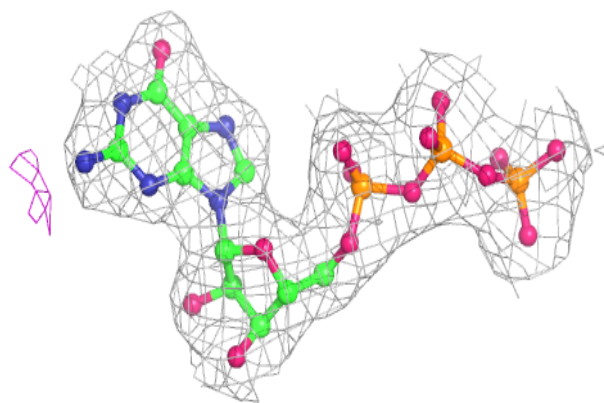
**Electron density around GTP A 501:**

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



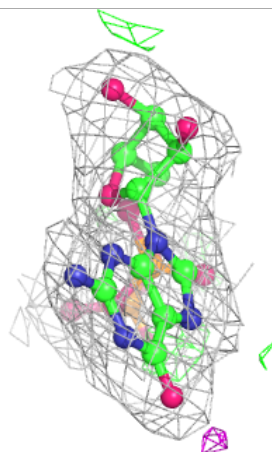
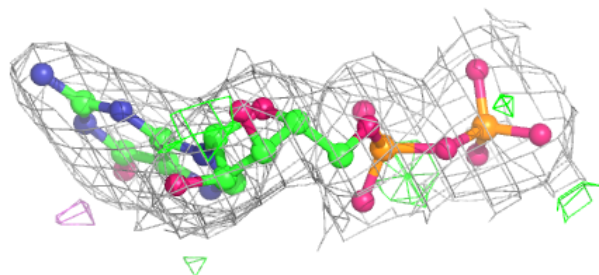
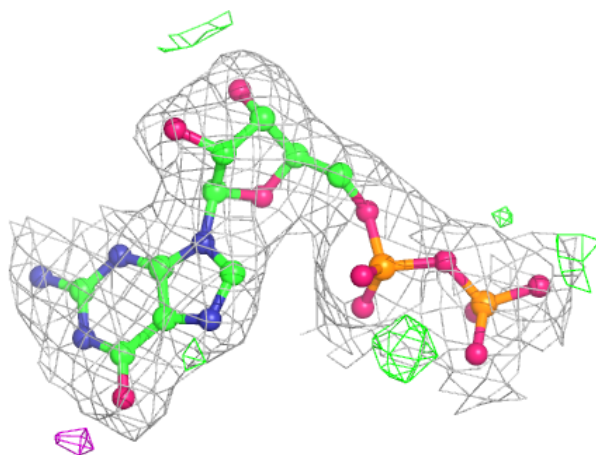
**Electron density around GTP C 501:**

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



**Electron density around GDP B 501:**

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



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.