



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:38 PM UTC

PDB ID : 5M7G / pdb_00005m7g
Title : Tubulin-MTD147 complex
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Deposited on : 2016-10-27
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

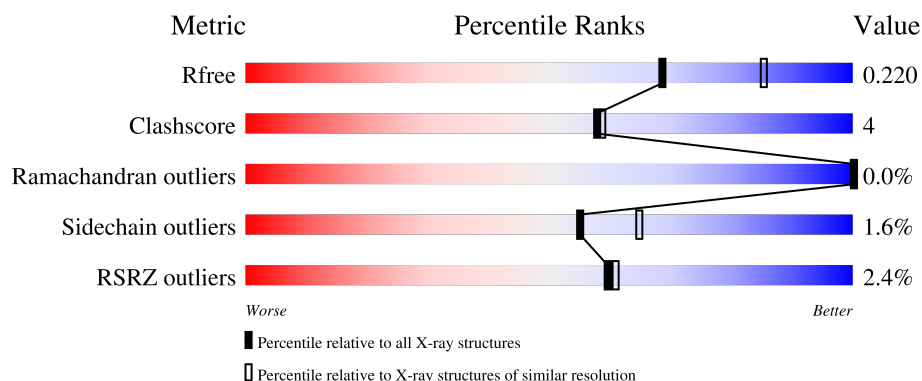
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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 of 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	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	5% 74% 10% 15%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17780 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	436	Total	C	N	O	S	0	0	0
			3409	2158	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3325	2091	567	641	26			
2	D	418	Total	C	N	O	S	0	0	0
			3284	2065	557	636	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

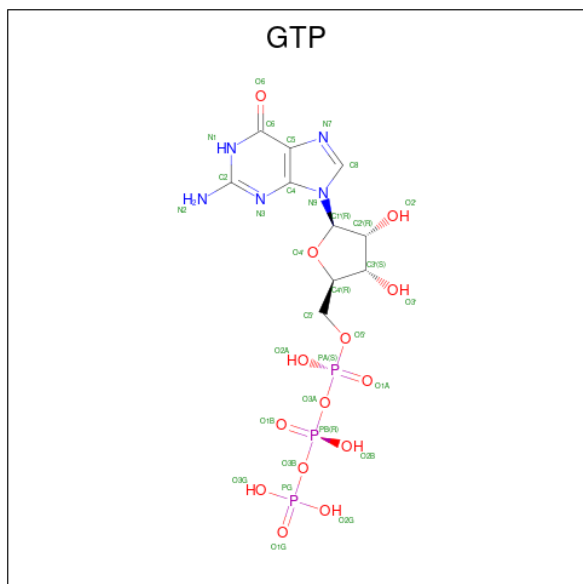
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	326	Total	C	N	O	S	0	0	0
			2647	1707	444	482	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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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 (CCD ID: MG) (formula: Mg).

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

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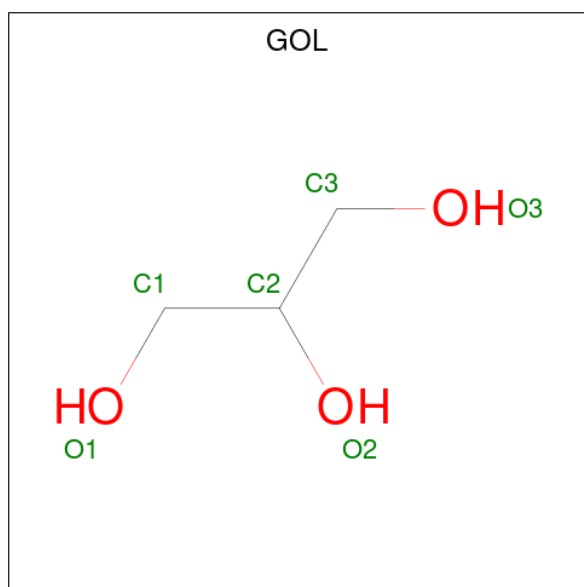
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

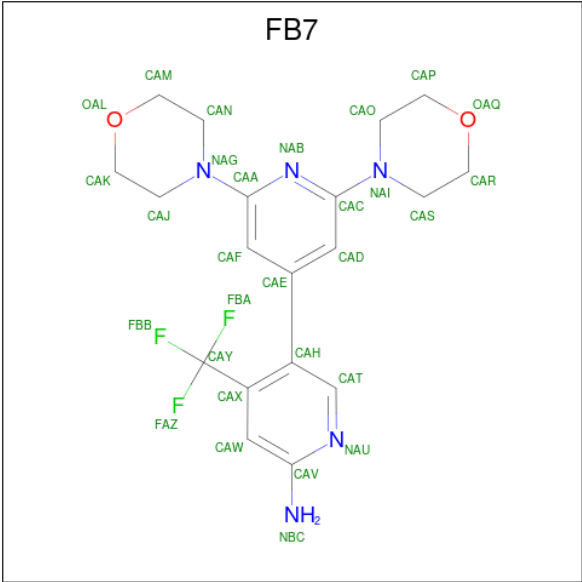
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	2	Total	Ca	0	0
			2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



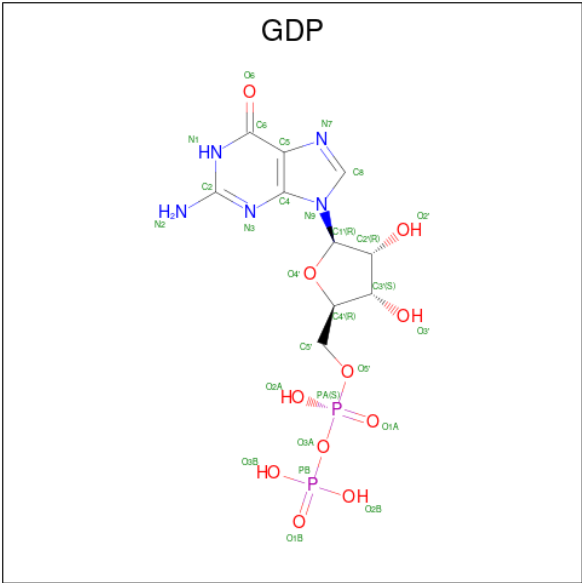
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 5-(2,6-dimorpholin-4-ylpyridin-4-yl)-4-(trifluoromethyl)pyridin-2-amine (CCD ID: FB7) (formula: C₁₉H₂₂F₃N₅O₂).



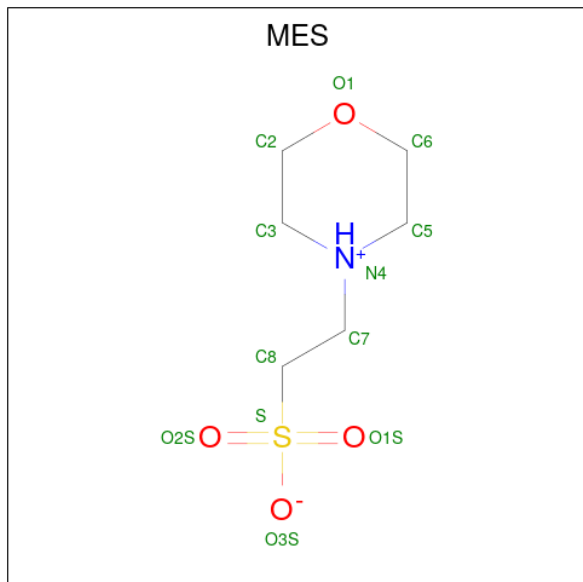
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	F	N	O	0	0
			29	19	3	5	2		
9	D	1	Total	C	F	N	O	0	0
			29	19	3	5	2		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



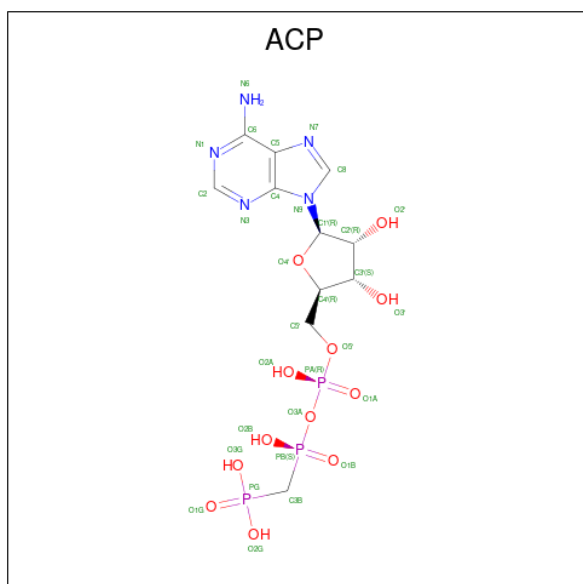
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
10	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

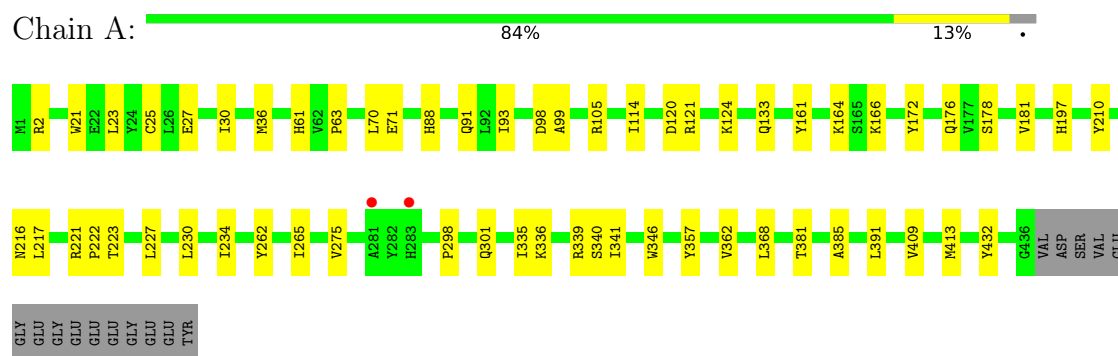
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	82	Total 82	O 82	0	0
13	B	76	Total 76	O 76	0	0
13	C	175	Total 175	O 175	0	0
13	D	45	Total 45	O 45	0	0
13	E	15	Total 15	O 15	0	0
13	F	28	Total 28	O 28	0	0

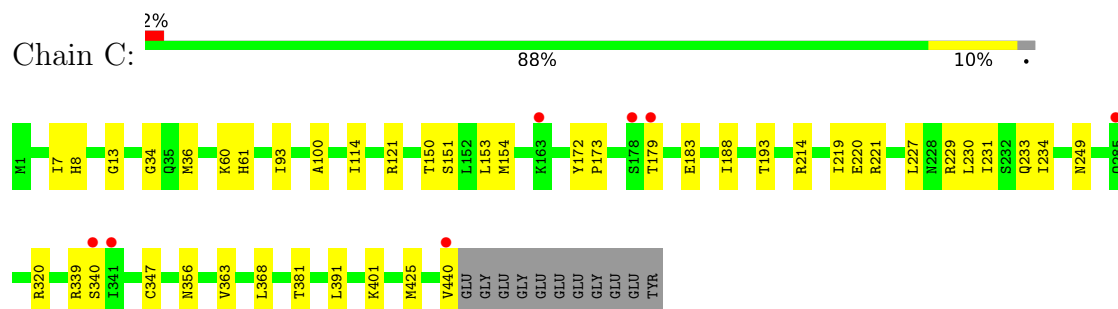
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

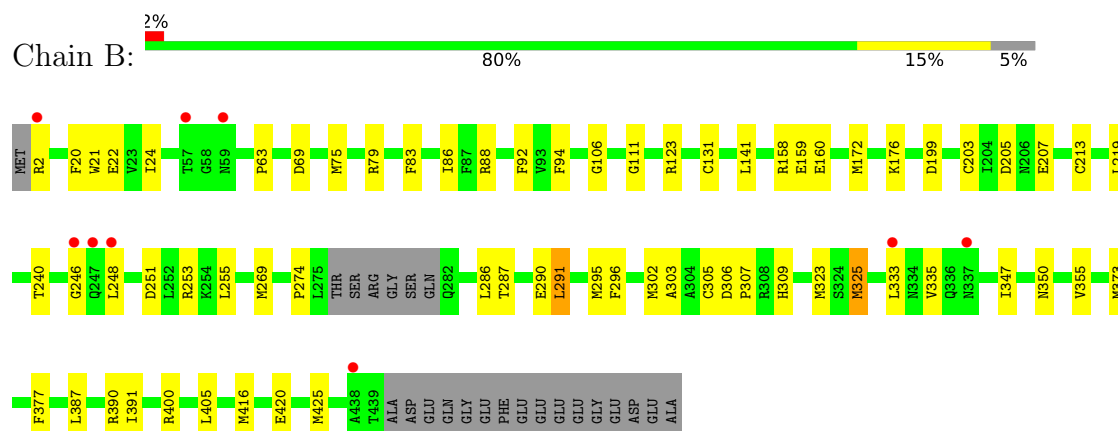
• Molecule 1: Tubulin alpha-1B chain



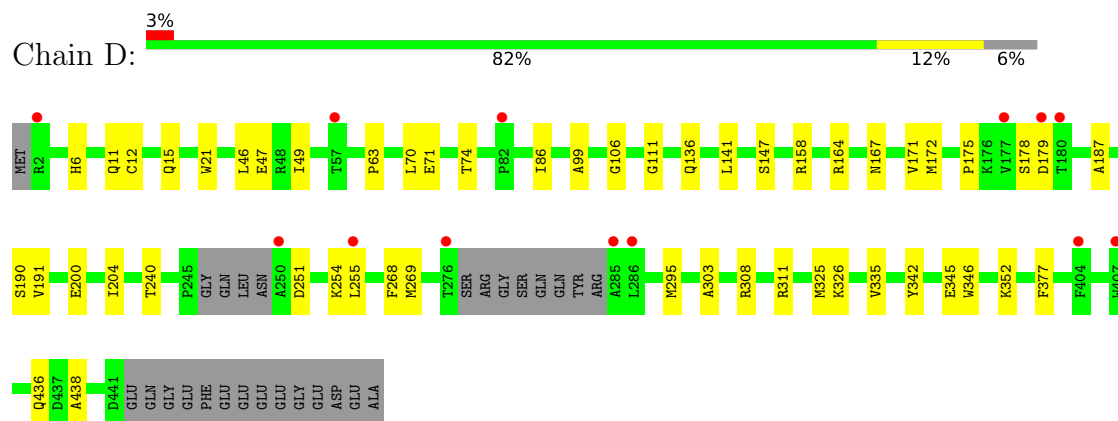
• Molecule 1: Tubulin alpha-1B chain



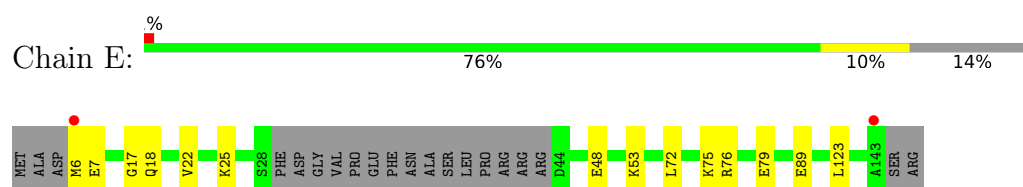
• Molecule 2: Tubulin beta-2B chain



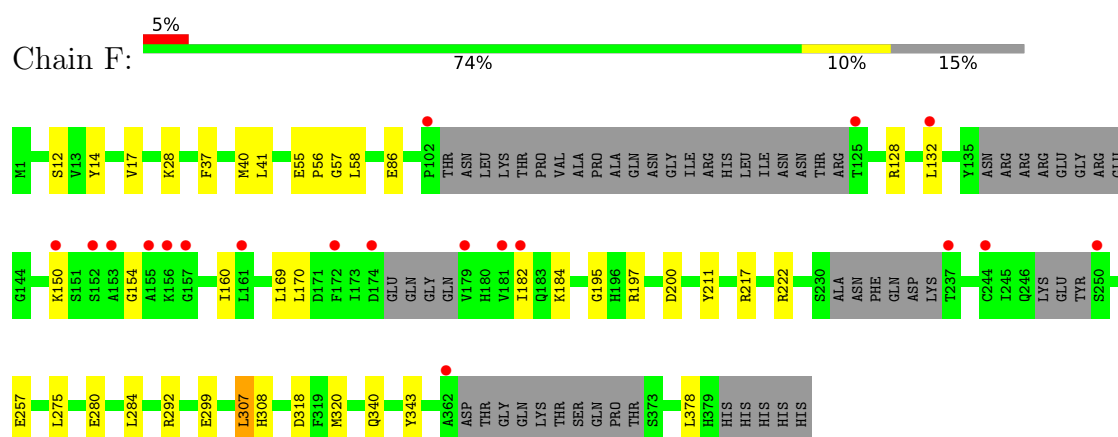
- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.08Å 156.86Å 179.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.72 – 2.25 46.72 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.72-2.25) 99.1 (46.72-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.172 , 0.217 0.176 , 0.220	Depositor DCC
R_{free} test set	6944 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17780	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FB7, MG, ACP, GDP, MES, GOL, CA, GTP

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	0.34	0/3487	0.50	0/4733
1	C	0.41	0/3515	0.59	0/4772
2	B	0.37	0/3399	0.54	0/4604
2	D	0.29	0/3356	0.46	0/4546
3	E	0.33	0/1022	0.45	0/1356
4	F	0.26	0/2705	0.45	0/3653
All	All	0.34	0/17484	0.51	0/23664

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

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	3409	0	3322	36	0
1	C	3437	0	3348	25	0
2	B	3325	0	3203	43	0
2	D	3284	0	3160	32	0
3	E	1014	0	1029	6	0
4	F	2647	0	2627	23	0
5	A	32	0	12	0	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
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
8	A	6	0	8	1	0
8	F	6	0	8	0	0
9	B	29	0	0	0	0
9	D	29	0	0	2	0
10	B	28	0	12	0	0
10	D	28	0	12	2	0
11	B	12	0	12	3	0
12	F	31	0	14	2	0
13	A	82	0	0	1	0
13	B	76	0	0	2	0
13	C	175	0	0	1	0
13	D	45	0	0	3	0
13	E	15	0	0	0	0
13	F	28	0	0	1	0
All	All	17780	0	16779	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (152) 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:253:ARG:NH1	11:B:505:MES:O2S	2.11	0.82
4:F:318:ASP:OD2	12:F:403:ACP:O3G	2.00	0.80
2:B:88:ARG:NH1	13:B:601:HOH:O	2.18	0.75
1:A:221:ARG:HD3	2:B:325:MET:HG3	1.70	0.74
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.71	0.70
2:B:323:MET:HB3	2:B:373:MET:HE1	1.71	0.70
2:D:164:ARG:NH1	13:D:602:HOH:O	2.22	0.70
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.74	0.69
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.74	0.69
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:154:GLY:O	13:F:501:HOH:O	2.12	0.68
2:D:311:ARG:NH1	2:D:436:GLN:O	2.27	0.66
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.29	0.64
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.31	0.63
2:B:416:MET:HE3	2:B:420:GLU:HG3	1.81	0.62
2:D:175:PRO:HA	2:D:178:SER:HB2	1.83	0.61
2:B:400:ARG:NH2	1:C:440:VAL:O	2.33	0.61
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.61
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.82	0.60
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.82	0.60
4:F:150:LYS:HG2	4:F:160:ILE:HG12	1.82	0.59
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.84	0.59
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.85	0.58
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.85	0.57
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.19	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.56
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.56
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.87	0.56
1:C:220:GLU:HG2	2:D:326:LYS:HD2	1.87	0.55
1:A:216:ASN:ND2	8:A:505:GOL:H2	2.21	0.55
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.89	0.54
2:D:11:GLN:HA	2:D:74:THR:HG21	1.90	0.54
4:F:169:LEU:HD13	4:F:182:ILE:HD11	1.90	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.54
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.43	0.53
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.27	0.52
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.89	0.52
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.91	0.52
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.44	0.52
2:B:323:MET:HE2	2:B:373:MET:HE2	1.91	0.52
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.51
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.93	0.51
2:B:323:MET:HB3	2:B:373:MET:CE	2.40	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.93	0.51
2:B:391:ILE:HG22	2:B:425:MET:HE1	1.93	0.51
1:C:401:LYS:HE3	2:D:438:ALA:HB1	1.93	0.50
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.92	0.50
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.94	0.49
1:A:23:LEU:O	1:A:27:GLU:HG3	2.13	0.49
4:F:128:ARG:O	4:F:132:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.49
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.94	0.49
2:B:213:CYS:HB3	2:B:219:LEU:HD12	1.94	0.49
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.95	0.49
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.45	0.48
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.79	0.48
1:A:336:LYS:HE3	1:A:341:ILE:HB	1.96	0.48
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.41	0.48
2:D:141:LEU:HD12	2:D:172:MET:SD	2.54	0.48
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.45	0.48
2:B:199:ASP:OD2	11:B:505:MES:H52	2.15	0.47
1:C:339:ARG:O	13:C:601:HOH:O	2.20	0.47
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.15	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.47
2:B:141:LEU:HD12	2:B:172:MET:SD	2.55	0.46
4:F:14:TYR:HA	4:F:17:VAL:HB	1.96	0.46
2:B:325:MET:H	2:B:325:MET:HG2	1.32	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.46
1:C:150:THR:O	1:C:154:MET:HG2	2.16	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.46
2:D:179:ASP:OD2	13:D:601:HOH:O	2.21	0.46
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.50	0.46
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.50	0.45
4:F:211:TYR:CE2	4:F:299:GLU:HB2	2.51	0.45
1:A:25:CYS:HB3	1:A:30:ILE:O	2.16	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45
3:E:7:GLU:O	3:E:22:VAL:HA	2.16	0.45
1:A:166:LYS:HE2	1:A:197:HIS:O	2.17	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.45
2:B:158:ARG:CZ	11:B:505:MES:H21	2.47	0.45
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.51	0.45
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.99	0.45
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.99	0.45
1:A:340:SER:HA	13:A:655:HOH:O	2.17	0.44
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.52	0.44
4:F:128:ARG:HH11	4:F:170:LEU:HD13	1.82	0.44
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.44
2:B:246:GLY:C	2:B:248:LEU:H	2.25	0.44
1:A:71:GLU:HB3	2:B:2:ARG:NH2	2.32	0.44
1:A:99:ALA:HA	1:A:105:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.53	0.44
2:D:187:ALA:O	2:D:191:VAL:HG23	2.18	0.44
2:D:46:LEU:HA	2:D:49:ILE:HB	1.99	0.44
2:D:15:GLN:NE2	10:D:501:GDP:O6	2.51	0.44
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.43
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.18	0.43
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.53	0.43
2:B:251:ASP:O	2:B:255:LEU:HG	2.18	0.43
2:D:200:GLU:HB3	2:D:268:PHE:CE2	2.53	0.43
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.43
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.99	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.54	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.01	0.43
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.54	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.19	0.42
1:A:176:GLN:HG3	4:F:56:PRO:HB3	2.02	0.42
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.54	0.42
2:B:159:GLU:OE2	13:B:602:HOH:O	2.21	0.42
1:C:8:HIS:HB3	1:C:13:GLY:O	2.19	0.42
4:F:320:MET:HE3	4:F:320:MET:HB3	1.95	0.42
1:C:229:ARG:NE	1:C:363:VAL:HG21	2.34	0.42
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.54	0.42
1:A:230:LEU:O	1:A:234:ILE:HD12	2.20	0.42
2:B:2:ARG:HG2	2:B:131:CYS:O	2.20	0.42
2:B:106:GLY:O	2:B:111:GLY:HA3	2.20	0.42
1:A:223:THR:O	1:A:227:LEU:HG	2.20	0.42
1:A:362:VAL:HG11	1:A:368:LEU:O	2.19	0.42
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.20	0.42
1:C:221:ARG:HG2	2:D:325:MET:HG2	2.00	0.42
2:B:333:LEU:HD13	4:F:57:GLY:HA3	2.02	0.42
1:C:179:THR:HB	9:D:500:FB7:CAP	2.50	0.42
4:F:150:LYS:HE3	12:F:403:ACP:H8	2.01	0.42
1:C:151:SER:HB2	1:C:193:THR:CG2	2.50	0.42
4:F:292:ARG:HD3	4:F:378:LEU:HB3	2.02	0.42
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.50	0.41
4:F:184:LYS:HE2	4:F:184:LYS:HB3	1.91	0.41
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.02	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.85	0.41
1:A:262:TYR:CE2	1:A:346:TRP:CH2	3.08	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.87	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HE3	2:B:203:CYS:SG	2.61	0.41
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.55	0.41
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	0.41
2:B:269:MET:HE1	2:B:307:PRO:HG3	2.01	0.41
4:F:28:LYS:HA	4:F:28:LYS:HD3	1.92	0.41
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.82	0.41
2:D:255:LEU:HD22	9:D:500:FB7:CAT	2.51	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.56	0.41
2:D:251:ASP:O	2:D:255:LEU:HG	2.21	0.41
3:E:72:LEU:O	3:E:76:ARG:HG2	2.20	0.41
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.56	0.40
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.56	0.40
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.89	0.40
2:D:141:LEU:HD22	2:D:190:SER:HB3	2.02	0.40
2:B:205:ASP:CG	2:B:390:ARG:HH21	2.29	0.40
2:B:303:ALA:O	2:B:305:CYS:N	2.49	0.40
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.02	0.40
4:F:55:GLU:HB3	4:F:58:LEU:HD12	2.02	0.40
2:D:352:LYS:HD2	13:D:643:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/451 (96%)	426 (98%)	7 (2%)	1 (0%)	43	48
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	418/445 (94%)	407 (97%)	11 (3%)	0	100	100
2	D	412/445 (93%)	405 (98%)	7 (2%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	312/384 (81%)	307 (98%)	5 (2%)	0	100	100
All	All	2133/2319 (92%)	2093 (98%)	39 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/379 (97%)	364 (99%)	3 (1%)	73	80
1	C	371/379 (98%)	367 (99%)	4 (1%)	65	74
2	B	365/383 (95%)	359 (98%)	6 (2%)	55	65
2	D	361/383 (94%)	355 (98%)	6 (2%)	53	63
3	E	110/127 (87%)	105 (96%)	5 (4%)	24	26
4	F	291/342 (85%)	285 (98%)	6 (2%)	47	56
All	All	1865/1993 (94%)	1835 (98%)	30 (2%)	55	65

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

Mol	Chain	Res	Type
1	A	114	ILE
1	A	181	VAL
1	A	381	THR
2	B	79	ARG
2	B	86	ILE
2	B	240	THR
2	B	291	LEU
2	B	302	MET
2	B	325	MET
1	C	114	ILE

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Mol	Chain	Res	Type
1	C	340	SER
1	C	347	CYS
1	C	381	THR
2	D	47	GLU
2	D	71	GLU
2	D	86	ILE
2	D	240	THR
2	D	335	VAL
2	D	345	GLU
3	E	6	MET
3	E	25	LYS
3	E	48	GLU
3	E	53	LYS
3	E	89	GLU
4	F	12	SER
4	F	86	GLU
4	F	217	ARG
4	F	257	GLU
4	F	275	LEU
4	F	307	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	91	ASN
2	B	336	GLN
2	B	394	GLN
1	C	15	GLN
1	C	372	GLN
1	C	393	HIS
2	D	8	GLN
2	D	14	ASN
2	D	136	GLN
3	E	84	GLN
4	F	196	HIS
4	F	239	HIS
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GTP	C	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.60	11 (22%)
8	GOL	A	505	-	5,5,5	0.35	0	5,5,5	0.61	0
10	GDP	D	501	6	29,30,30	1.25	5 (17%)	45,47,47	1.82	8 (17%)
10	GDP	B	502	6	29,30,30	1.27	4 (13%)	45,47,47	1.87	9 (20%)
8	GOL	F	401	-	5,5,5	0.41	0	5,5,5	0.47	0
5	GTP	A	501	6	33,34,34	0.84	0	50,54,54	1.47	8 (16%)
11	MES	B	505	-	12,12,12	2.38	1 (8%)	15,16,16	2.48	4 (26%)
12	ACP	F	403	6	31,33,33	2.16	11 (35%)	47,52,52	1.81	9 (19%)
9	FB7	D	500	-	32,32,32	1.82	4 (12%)	44,46,46	2.07	12 (27%)
9	FB7	B	501	-	32,32,32	1.70	4 (12%)	44,46,46	1.99	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
8	GOL	A	505	-	-	4/4/4/4	-
10	GDP	D	501	6	-	5/16/32/32	0/3/3/3
10	GDP	B	502	6	-	5/16/32/32	0/3/3/3
8	GOL	F	401	-	-	0/4/4/4	-
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
11	MES	B	505	-	-	5/6/14/14	0/1/1/1
12	ACP	F	403	6	-	6/19/38/38	0/3/3/3
9	FB7	D	500	-	-	2/18/34/34	0/4/4/4
9	FB7	B	501	-	-	0/18/34/34	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	MES	C8-S	-8.02	1.66	1.77
9	D	500	FB7	CAH-CAE	-6.12	1.38	1.49
12	F	403	ACP	PG-O1G	5.66	1.61	1.50
9	B	501	FB7	CAH-CAE	-4.99	1.40	1.49
12	F	403	ACP	C5-C4	4.75	1.47	1.39
9	B	501	FB7	CAY-CAX	-4.59	1.40	1.50
12	F	403	ACP	PB-O1B	4.43	1.62	1.51
9	D	500	FB7	CAY-CAX	-4.30	1.41	1.50
9	D	500	FB7	FBA-CAY	-3.89	1.19	1.33
9	B	501	FB7	FBA-CAY	-3.89	1.19	1.33
9	D	500	FB7	FBB-CAY	-3.74	1.19	1.33
9	B	501	FB7	FBB-CAY	-3.55	1.20	1.33
12	F	403	ACP	PB-O3A	3.42	1.62	1.58
10	B	502	GDP	PA-O3A	2.92	1.62	1.59
12	F	403	ACP	PB-O2B	-2.91	1.49	1.56
10	D	501	GDP	PA-O3A	2.87	1.62	1.59
12	F	403	ACP	C5-C6	2.80	1.48	1.41
10	B	502	GDP	C5-C4	2.79	1.46	1.38
10	D	501	GDP	C5-C4	2.72	1.46	1.38
12	F	403	ACP	PA-O3A	2.66	1.62	1.59
10	B	502	GDP	C6-N1	-2.64	1.33	1.38
12	F	403	ACP	PG-O2G	-2.57	1.49	1.55
5	C	501	GTP	PA-O3A	2.53	1.62	1.59
10	D	501	GDP	C6-N1	-2.45	1.34	1.38
12	F	403	ACP	PG-O3G	2.42	1.60	1.55
12	F	403	ACP	C8-N7	2.34	1.36	1.31
5	C	501	GTP	C2-N3	2.29	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	501	GDP	C4-N9	-2.23	1.32	1.38
12	F	403	ACP	C5-N7	-2.20	1.35	1.39
10	D	501	GDP	C5-N7	-2.08	1.34	1.39
10	B	502	GDP	C4-N9	-2.07	1.32	1.38

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	505	MES	C5-N4-C3	7.91	125.88	108.84
9	D	500	FB7	CAE-CAD-CAC	7.23	120.71	118.17
9	B	501	FB7	CAE-CAD-CAC	6.55	120.47	118.17
12	F	403	ACP	C5-C4-N3	-5.88	118.63	126.72
10	B	502	GDP	C5-C4-N3	-5.77	119.20	128.39
10	D	501	GDP	C5-C4-N3	-5.51	119.62	128.39
10	B	502	GDP	C2-N3-C4	5.23	121.30	112.30
10	D	501	GDP	C2-N3-C4	4.95	120.83	112.30
5	C	501	GTP	C2-N3-C4	4.77	120.52	112.30
12	F	403	ACP	N3-C4-N9	4.66	135.09	127.17
9	D	500	FB7	CAT-CAH-CAE	-4.23	113.45	119.56
5	A	501	GTP	C5-C4-N3	-4.18	121.74	128.39
10	B	502	GDP	N9-C4-N3	4.13	134.21	125.95
5	C	501	GTP	C5-C4-N3	-4.12	121.84	128.39
5	A	501	GTP	C2-N3-C4	4.11	119.38	112.30
9	B	501	FB7	CAN-NAG-CAJ	3.98	120.51	111.57
10	D	501	GDP	C6-C5-N7	3.91	137.40	130.29
9	B	501	FB7	CAT-CAH-CAE	-3.87	113.97	119.56
10	B	502	GDP	C6-C5-N7	3.86	137.31	130.29
10	D	501	GDP	N9-C4-N3	3.83	133.61	125.95
9	D	500	FB7	NAB-CAC-NAI	3.79	121.35	116.56
12	F	403	ACP	C2-N3-C4	3.71	120.88	111.83
9	D	500	FB7	CAE-CAF-CAA	3.62	119.44	118.17
9	B	501	FB7	CAE-CAF-CAA	3.61	119.44	118.17
9	B	501	FB7	CAS-NAI-CAO	3.60	119.68	111.57
9	B	501	FB7	CAA-NAB-CAC	3.45	122.90	117.27
5	C	501	GTP	N9-C8-N7	-3.43	107.04	113.40
9	D	500	FB7	CAS-NAI-CAO	3.41	119.23	111.57
12	F	403	ACP	C4-C5-N7	-3.37	106.73	110.58
10	B	502	GDP	O2A-PA-O3A	3.18	115.86	107.27
12	F	403	ACP	N3-C2-N1	-3.07	123.94	128.58
5	A	501	GTP	O2A-PA-O3A	2.93	115.20	107.27
9	D	500	FB7	CAA-NAB-CAC	2.93	122.05	117.27
9	D	500	FB7	CAD-CAC-NAI	-2.91	118.84	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	501	GDP	O4'-C1'-N9	-2.89	101.81	108.36
9	B	501	FB7	FBA-CAY-CAX	-2.84	107.62	112.65
5	C	501	GTP	N9-C4-N3	2.83	131.61	125.95
9	D	500	FB7	CAF-CAE-CAH	2.78	125.27	120.61
5	C	501	GTP	C8-N7-C5	2.77	109.20	104.26
9	D	500	FB7	CAD-CAE-CAH	-2.76	115.97	120.61
10	D	501	GDP	C4-C5-N7	-2.74	106.33	110.67
5	C	501	GTP	N1-C2-N3	-2.69	118.40	123.32
5	C	501	GTP	O2B-PB-O3A	2.66	114.47	107.27
12	F	403	ACP	O2G-PG-C3B	2.66	112.85	106.40
12	F	403	ACP	C4-N9-C8	2.63	108.50	105.74
10	B	502	GDP	C4-C5-N7	-2.63	106.51	110.67
9	D	500	FB7	CAW-CAX-CAH	-2.57	116.83	119.85
9	D	500	FB7	CAN-NAG-CAJ	2.55	117.31	111.57
9	B	501	FB7	CAP-CAO-NAI	2.54	114.74	109.93
5	A	501	GTP	O4'-C1'-N9	-2.54	102.61	108.36
5	A	501	GTP	N9-C8-N7	-2.51	108.74	113.40
12	F	403	ACP	PB-O3A-PA	-2.48	124.29	132.37
11	B	505	MES	O3S-S-C8	2.44	110.78	106.00
5	C	501	GTP	C5-C6-N1	2.41	119.39	113.25
9	B	501	FB7	CAR-CAS-NAI	2.40	114.47	109.93
10	B	502	GDP	O6-C6-C5	-2.38	120.26	126.53
12	F	403	ACP	C5-N7-C8	2.35	107.14	103.45
5	C	501	GTP	O6-C6-C5	-2.32	120.41	126.53
10	B	502	GDP	C5-C6-N1	2.32	119.15	113.25
5	A	501	GTP	C8-N7-C5	2.30	108.35	104.26
9	B	501	FB7	CAD-CAC-NAB	-2.29	118.93	123.34
5	A	501	GTP	N9-C4-N3	2.25	130.46	125.95
9	B	501	FB7	CAE-CAH-CAX	2.21	128.26	124.48
11	B	505	MES	C7-N4-C3	2.15	116.97	111.24
9	D	500	FB7	CAF-CAA-NAB	-2.12	119.25	123.34
9	B	501	FB7	CAK-CAJ-NAG	2.12	113.94	109.93
5	C	501	GTP	N2-C2-N1	2.12	121.23	116.76
11	B	505	MES	C2-C3-N4	2.12	113.34	110.12
10	B	502	GDP	O3'-C3'-C4'	-2.08	105.09	111.08
5	C	501	GTP	C2-N1-C6	-2.08	121.34	125.11
10	D	501	GDP	C5-C6-N1	2.03	118.42	113.25
10	D	501	GDP	C2'-C3'-C4'	2.02	106.52	102.61
5	A	501	GTP	C4-C5-N7	-2.01	107.48	110.67

There are no chirality outliers.

All (42) torsion outliers are listed below:

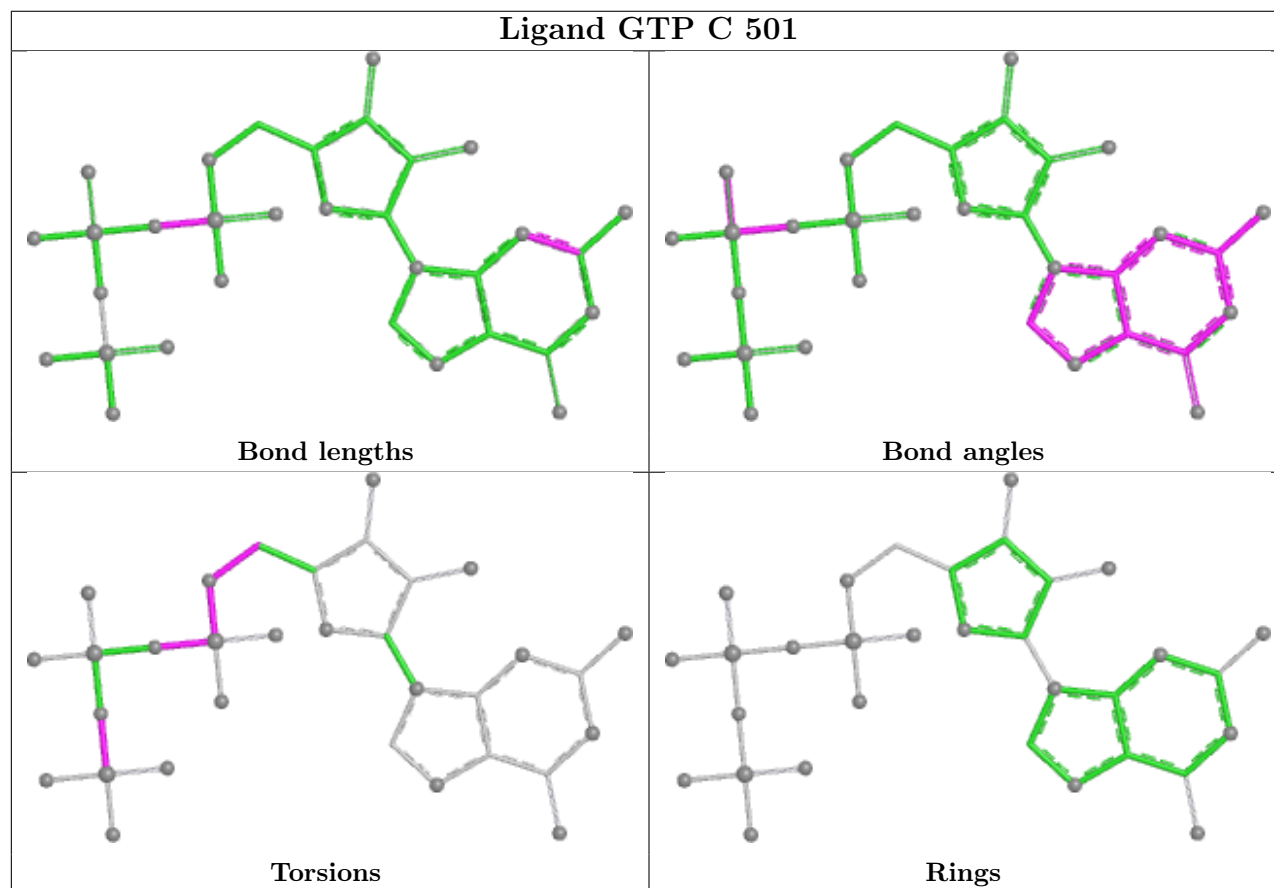
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	505	GOL	O1-C1-C2-C3
10	B	502	GDP	C5'-O5'-PA-O3A
10	B	502	GDP	C5'-O5'-PA-O1A
10	B	502	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O1A
11	B	505	MES	C8-C7-N4-C5
11	B	505	MES	C7-C8-S-O1S
11	B	505	MES	C7-C8-S-O2S
11	B	505	MES	C7-C8-S-O3S
12	F	403	ACP	PB-C3B-PG-O1G
12	F	403	ACP	PB-C3B-PG-O2G
12	F	403	ACP	PB-C3B-PG-O3G
12	F	403	ACP	C5'-O5'-PA-O1A
12	F	403	ACP	C5'-O5'-PA-O3A
8	A	505	GOL	O1-C1-C2-O2
8	A	505	GOL	C1-C2-C3-O3
9	D	500	FB7	CAD-CAC-NAI-CAO
9	D	500	FB7	NAB-CAC-NAI-CAO
5	C	501	GTP	PB-O3B-PG-O3G
10	D	501	GDP	C5'-O5'-PA-O2A
12	F	403	ACP	PG-C3B-PB-O2B
11	B	505	MES	C8-C7-N4-C3
10	B	502	GDP	PB-O3A-PA-O1A
10	B	502	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O1A
10	D	501	GDP	PB-O3A-PA-O2A
8	A	505	GOL	O2-C2-C3-O3
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A

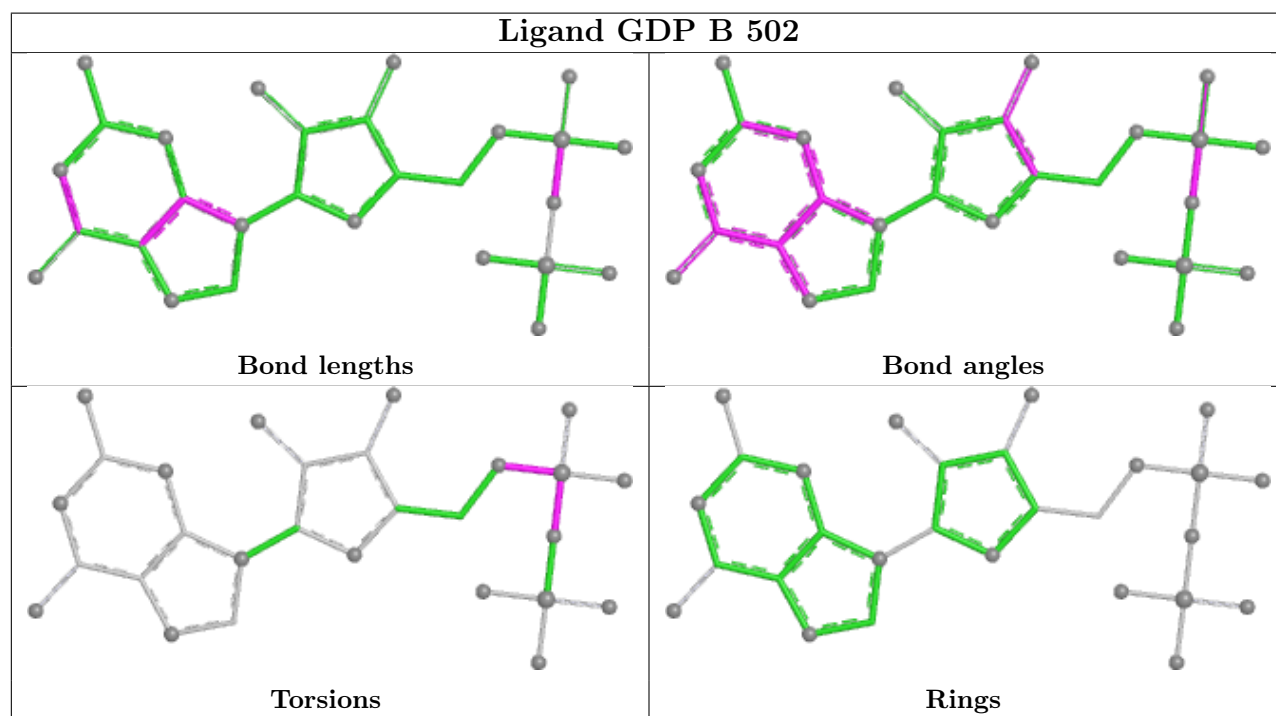
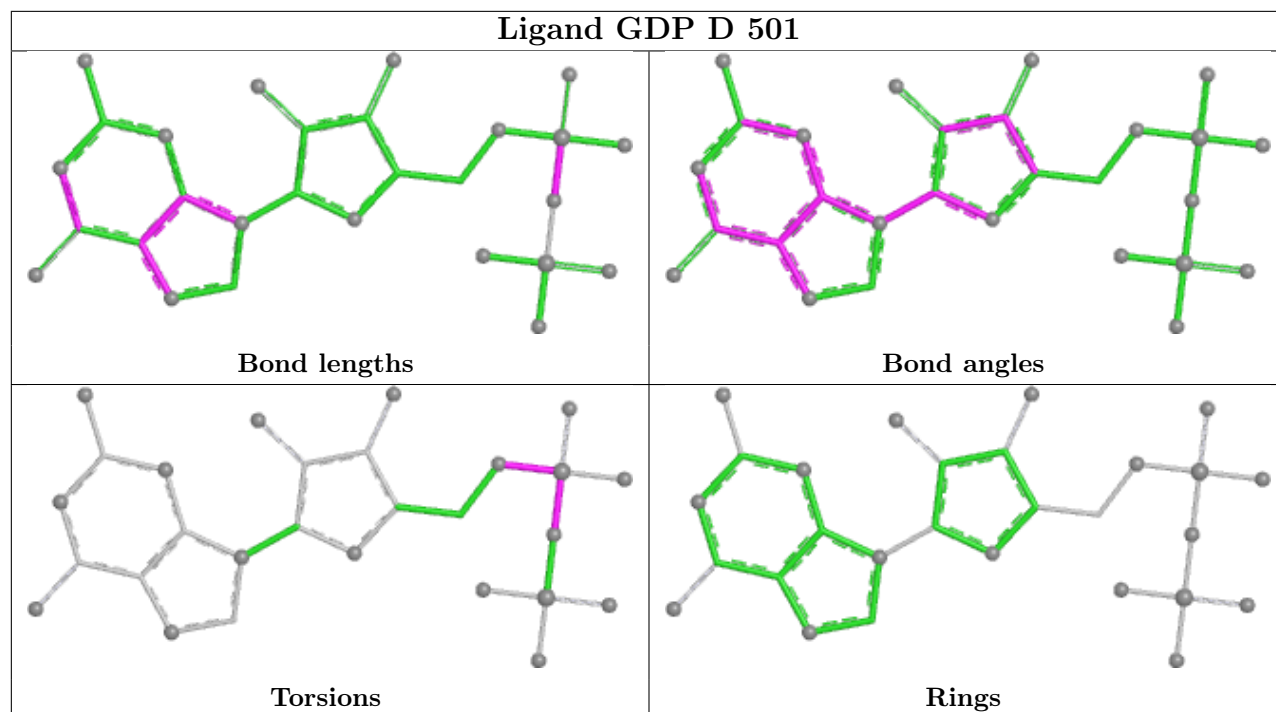
There are no ring outliers.

5 monomers are involved in 10 short contacts:

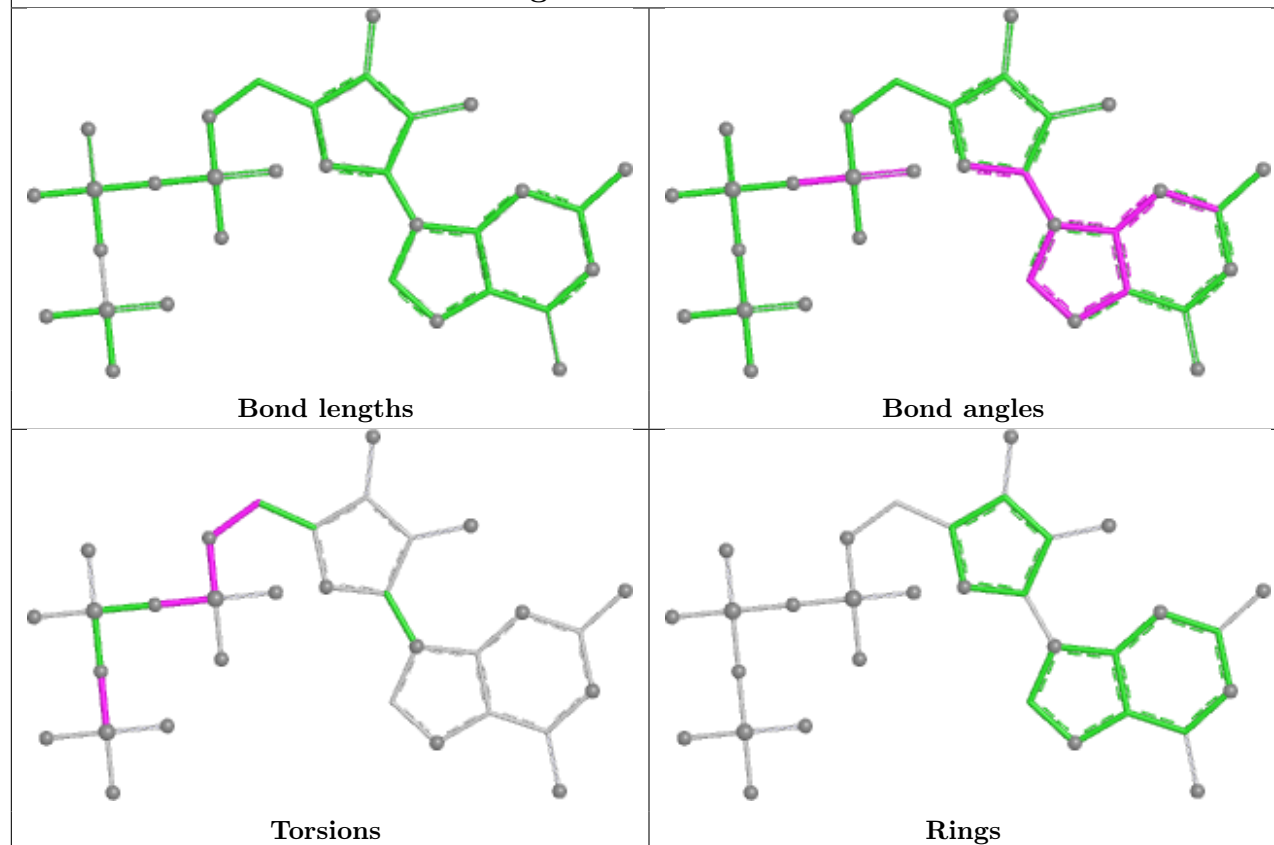
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	505	GOL	1	0
10	D	501	GDP	2	0
11	B	505	MES	3	0
12	F	403	ACP	2	0
9	D	500	FB7	2	0

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.

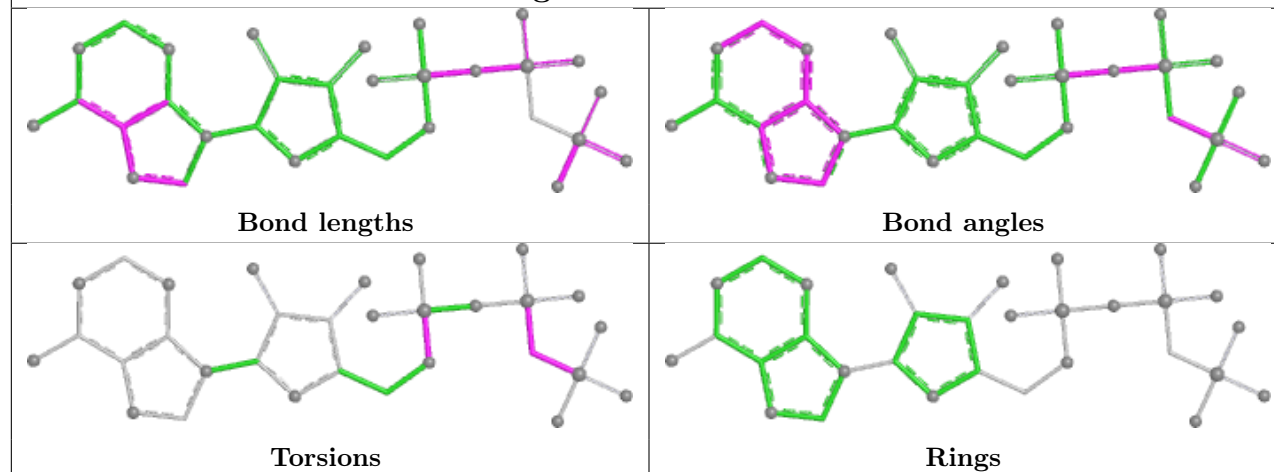




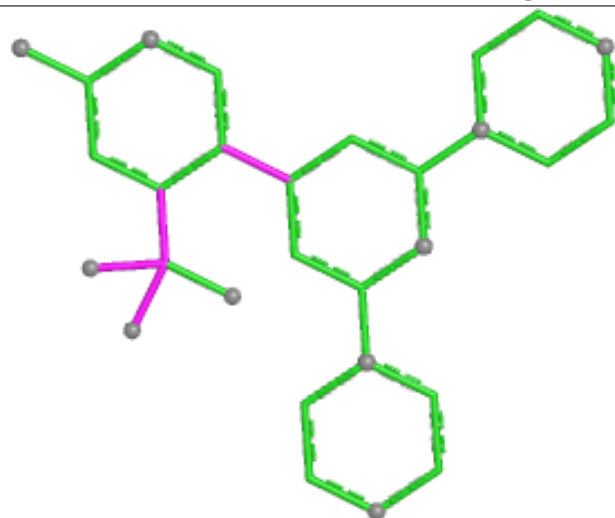
Ligand GTP A 501



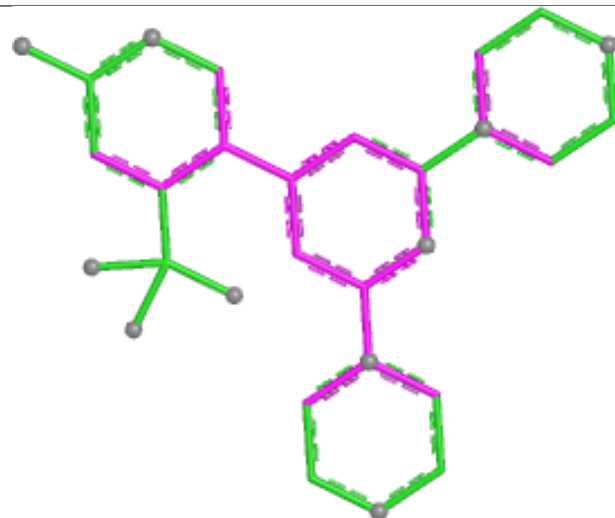
Ligand ACP F 403



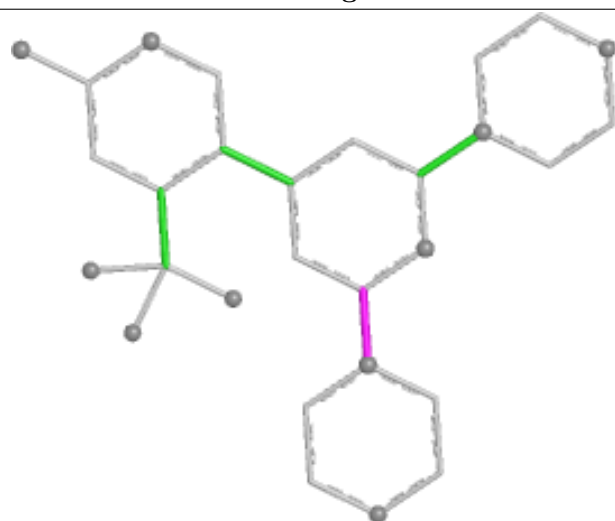
Ligand FB7 D 500



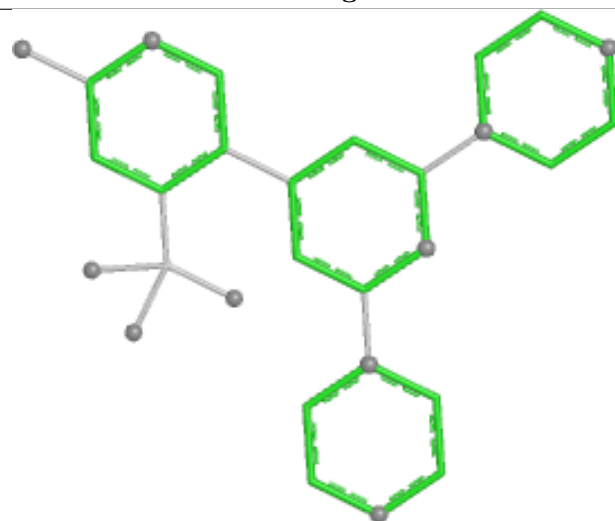
Bond lengths



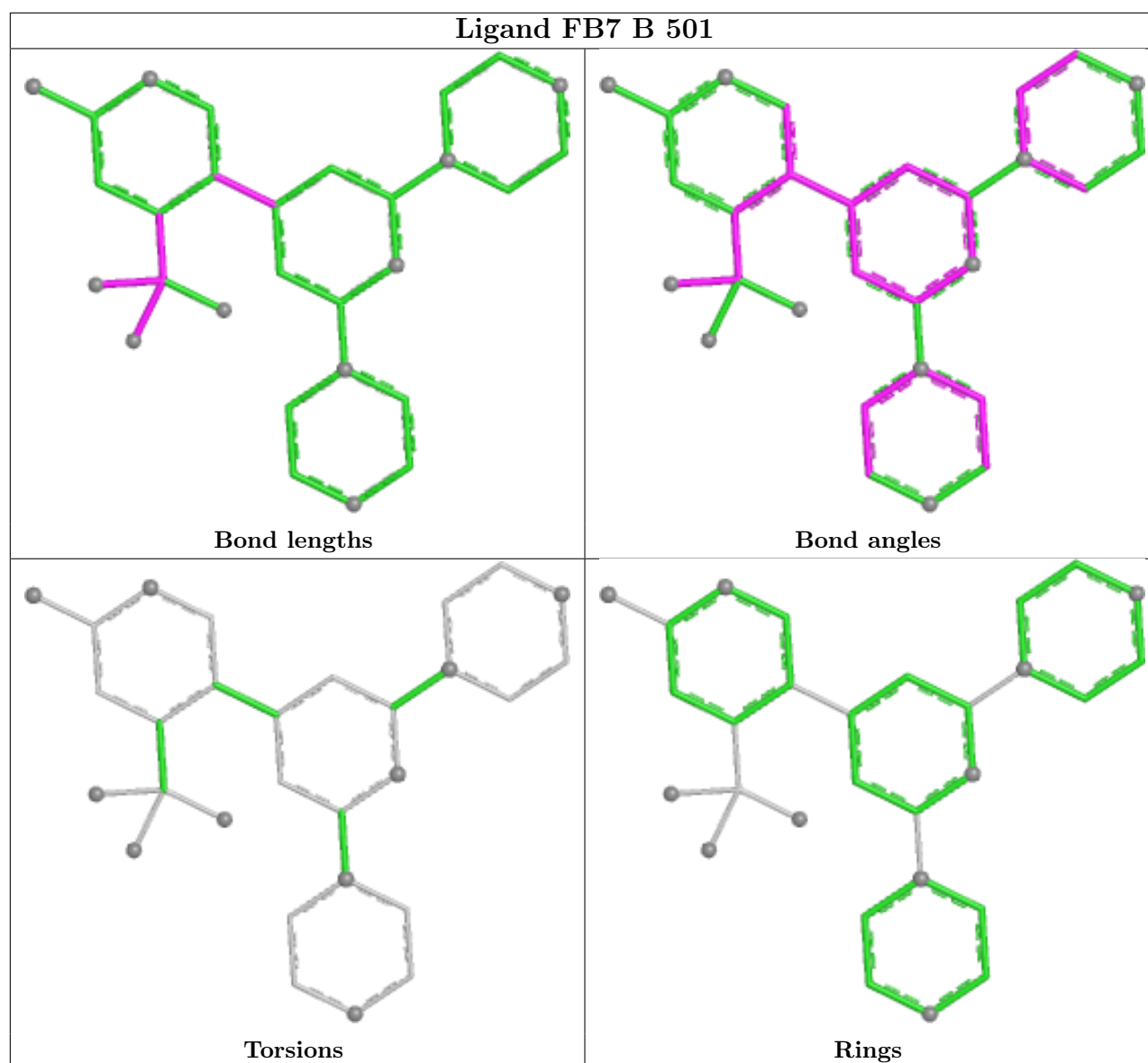
Bond angles



Torsions



Rings



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	436/451 (96%)	-0.22	2 (0%) 87 88	40, 58, 96, 124	0
1	C	440/451 (97%)	-0.37	7 (1%) 70 72	34, 46, 77, 111	1 (0%)
2	B	422/445 (94%)	-0.11	9 (2%) 63 65	35, 56, 96, 139	2 (0%)
2	D	418/445 (93%)	0.07	13 (3%) 51 51	40, 67, 102, 132	5 (1%)
3	E	123/143 (86%)	0.19	2 (1%) 70 72	46, 74, 116, 127	0
4	F	326/384 (84%)	0.33	19 (5%) 29 27	47, 84, 135, 155	0
All	All	2165/2319 (93%)	-0.07	52 (2%) 59 61	34, 61, 111, 155	8 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	THR	5.0
4	F	155	ALA	4.4
4	F	237	THR	4.2
4	F	179	VAL	3.9
3	E	143	ALA	3.9
2	B	248	LEU	3.6
4	F	153	ALA	3.4
4	F	182	ILE	3.3
2	D	250	ALA	3.2
4	F	102	PRO	3.2
2	D	276	THR	3.2
4	F	152	SER	3.2
2	B	438	ALA	3.2
2	D	180	THR	3.2
2	D	2	ARG	3.1
2	B	2	ARG	3.1
2	B	333	LEU	2.9
2	D	177	VAL	2.8
1	C	285	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	6	MET	2.8
2	B	337	ASN	2.7
1	C	440	VAL	2.7
2	B	57	THR	2.7
2	D	57	THR	2.6
2	B	246	GLY	2.6
4	F	250	SER	2.6
2	B	247	GLN	2.6
2	D	179	ASP	2.6
1	C	178	SER	2.6
4	F	181	VAL	2.5
1	C	340	SER	2.5
4	F	150	LYS	2.4
4	F	125	THR	2.4
2	D	285	ALA	2.4
2	D	255	LEU	2.3
1	C	163	LYS	2.3
1	A	283	HIS	2.3
2	B	59	ASN	2.2
2	D	82	PRO	2.2
4	F	157	GLY	2.2
1	A	281	ALA	2.2
2	D	407	TRP	2.2
2	D	286	LEU	2.2
4	F	156	LYS	2.2
4	F	362	ALA	2.2
4	F	132	LEU	2.1
1	C	341	ILE	2.1
2	D	404	PHE	2.1
4	F	172	PHE	2.0
4	F	244	CYS	2.0
4	F	161	LEU	2.0
4	F	174	ASP	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

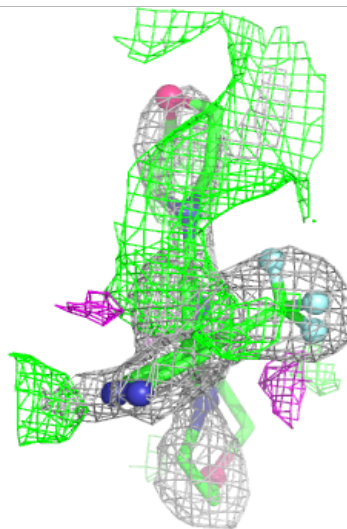
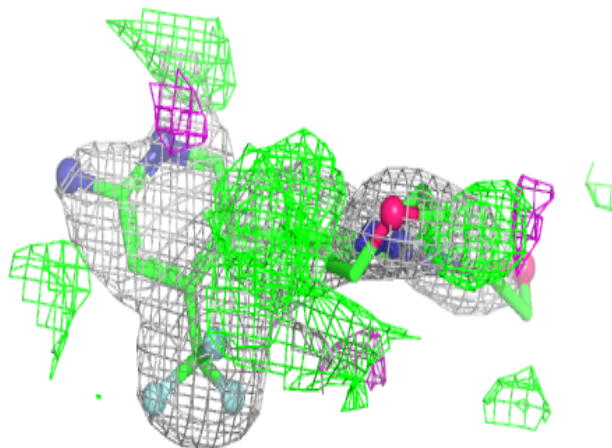
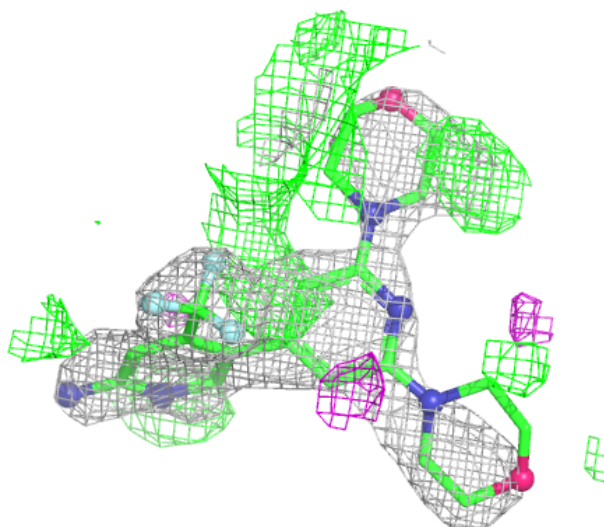
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	FB7	D	500	29/29	0.84	0.23	33,50,65,66	29
8	GOL	A	505	6/6	0.85	0.17	79,83,84,84	0
8	GOL	F	401	6/6	0.86	0.15	76,84,89,94	0
7	CA	C	504	1/1	0.86	0.13	127,127,127,127	0
6	MG	F	402	1/1	0.92	0.13	82,82,82,82	0
12	ACP	F	403	31/31	0.92	0.09	86,97,122,134	0
11	MES	B	505	12/12	0.93	0.10	56,66,84,88	0
10	GDP	D	501	28/28	0.95	0.08	45,59,69,74	0
7	CA	A	504	1/1	0.95	0.10	100,100,100,100	0
7	CA	B	504	1/1	0.95	0.05	83,83,83,83	0
6	MG	D	502	1/1	0.96	0.10	58,58,58,58	0
9	FB7	B	501	29/29	0.96	0.08	35,49,68,70	0
6	MG	B	503	1/1	0.98	0.05	34,34,34,34	0
5	GTP	C	501	32/32	0.99	0.04	32,37,43,51	0
7	CA	C	503	1/1	0.99	0.02	67,67,67,67	0
10	GDP	B	502	28/28	0.99	0.04	29,40,45,50	0
6	MG	A	502	1/1	0.99	0.15	74,74,74,74	0
7	CA	A	503	1/1	0.99	0.03	81,81,81,81	0
5	GTP	A	501	32/32	0.99	0.05	35,43,49,49	0
6	MG	C	502	1/1	1.00	0.03	40,40,40,40	0

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

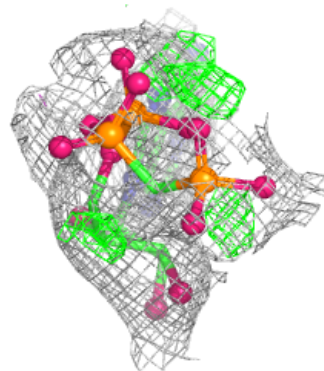
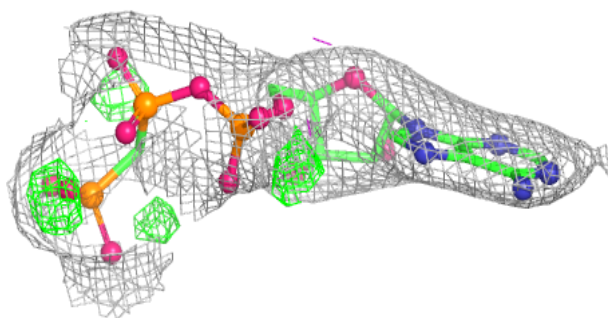
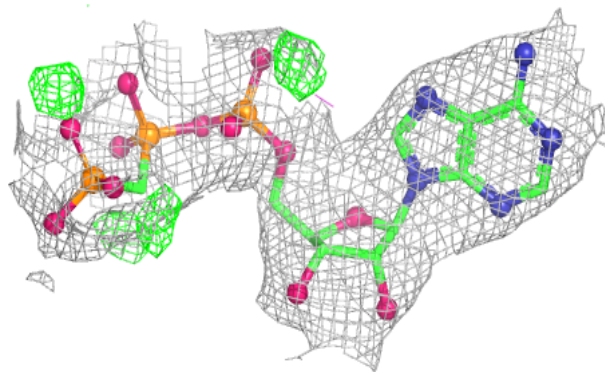
Electron density around FB7 D 500:

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



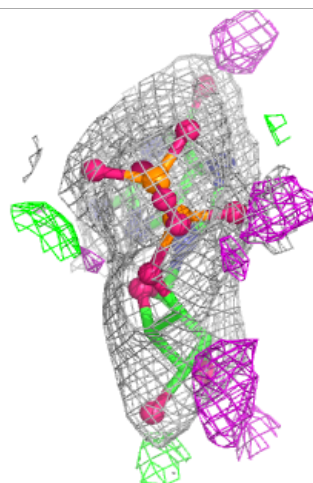
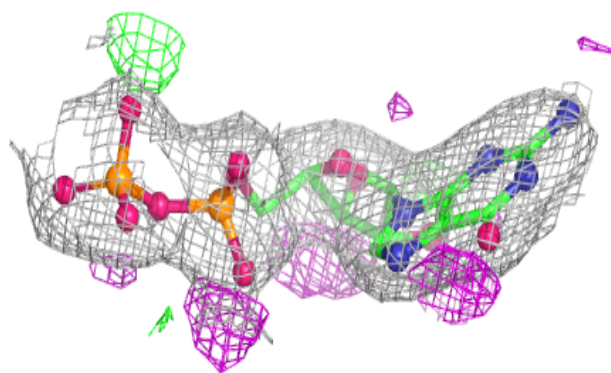
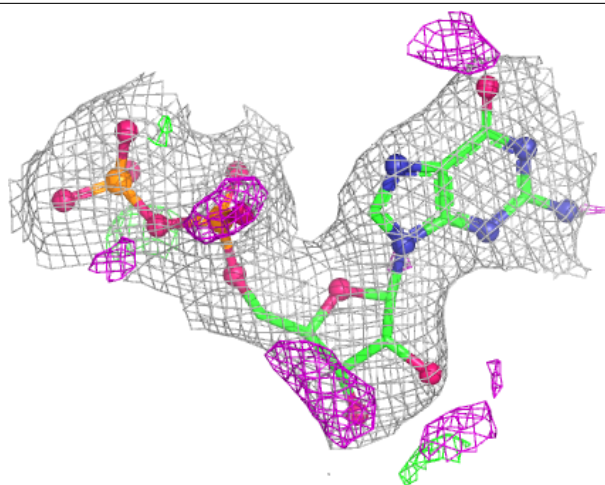
Electron density around ACP F 403:

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



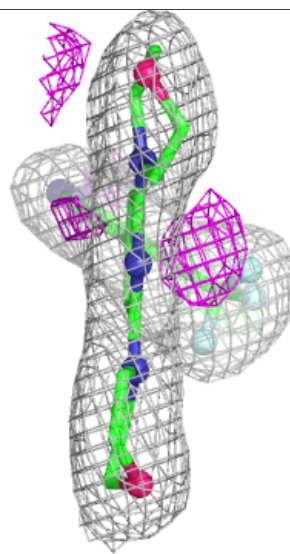
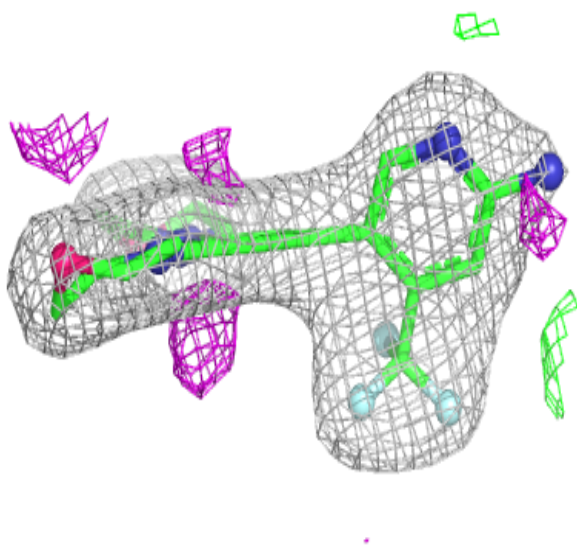
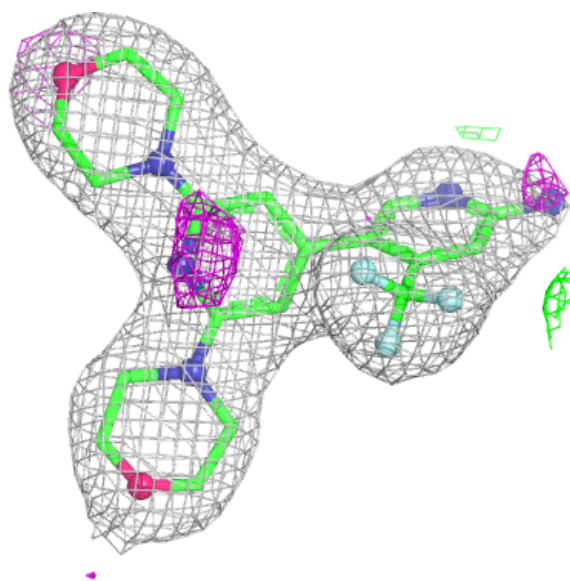
Electron density around GDP D 501:

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



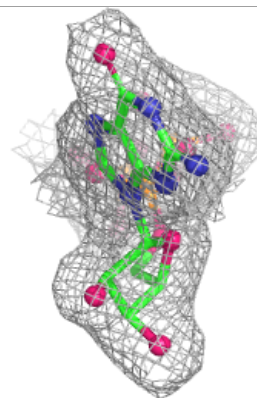
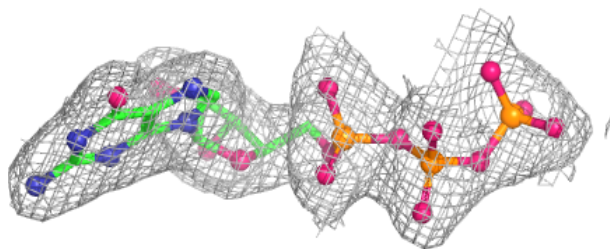
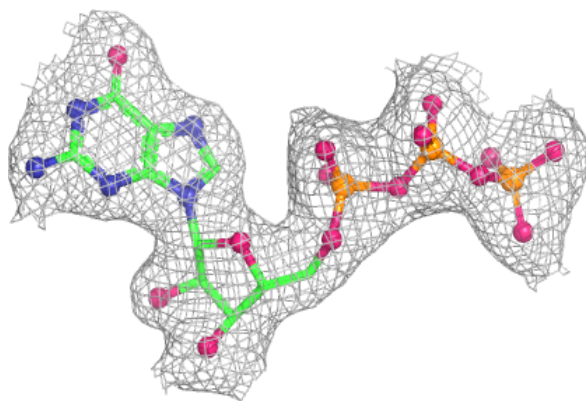
Electron density around FB7 B 501:

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

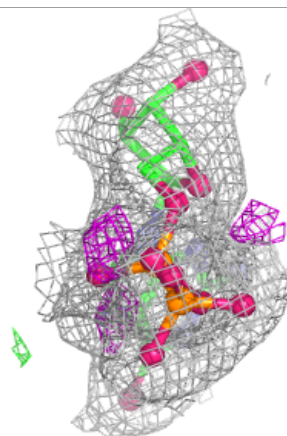
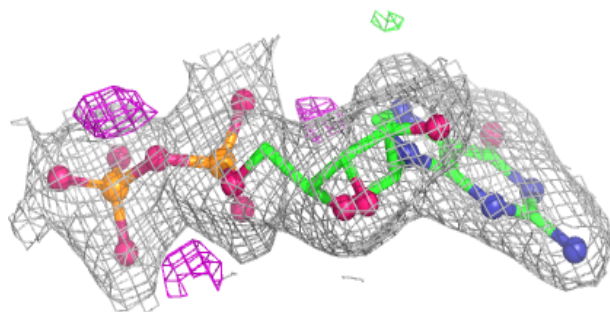
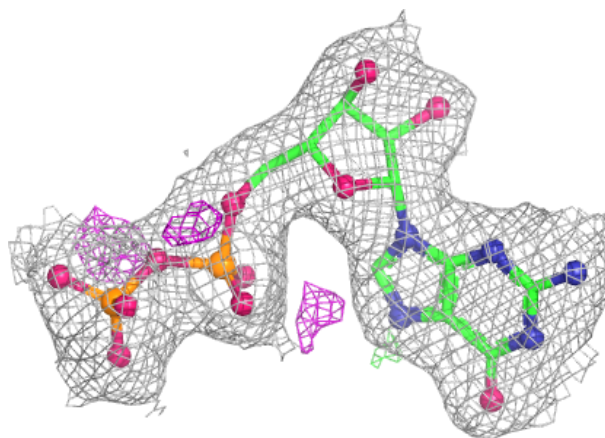


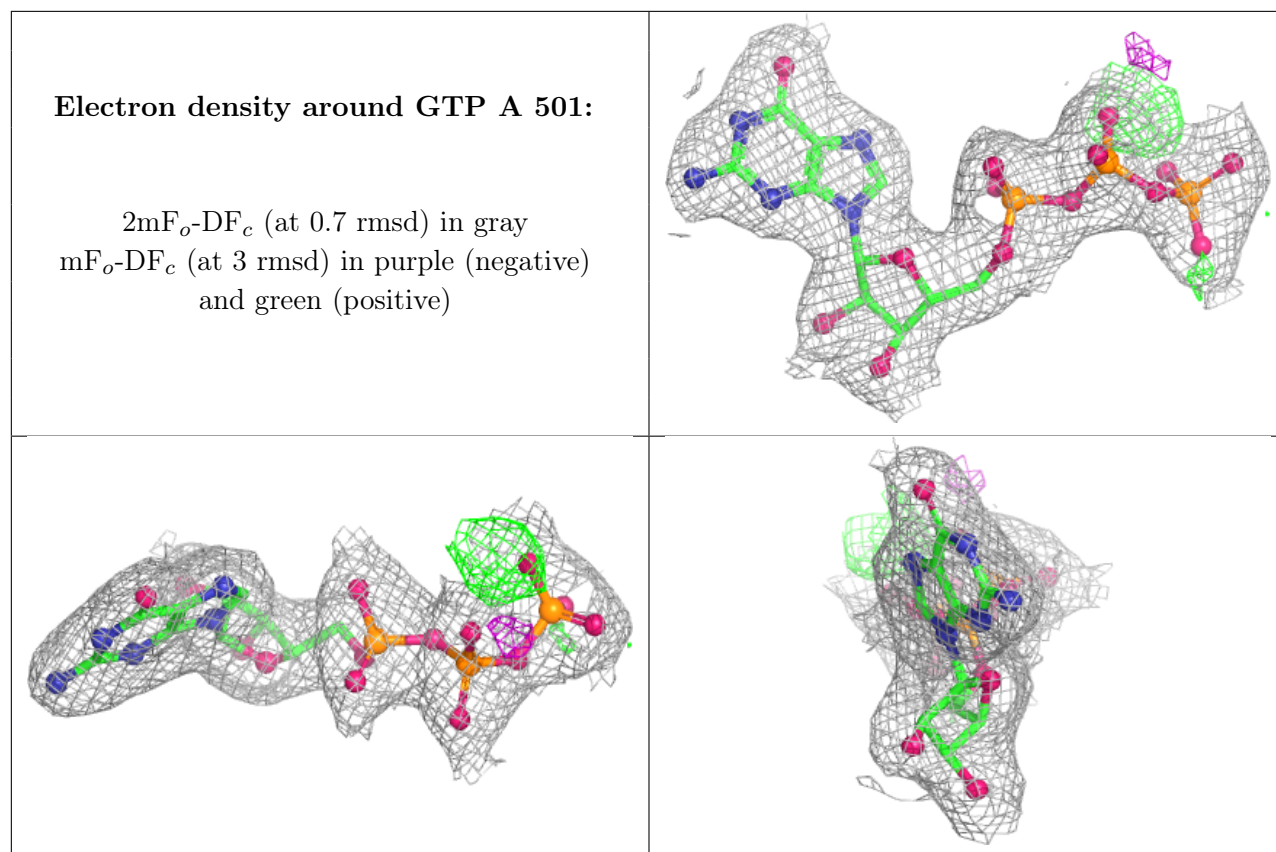
Electron density around GTP C 501:

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

**Electron density around GDP B 502:**

$2mF_o-DF_c$ (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.