



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:25 AM UTC

PDB ID : 8A0L / pdb_00008a0l
Title : Tubulin-CW1-complex
Authors : Protá, A.E.; Díaz, J.F.; Steinmetz, M.O.; Oliva, M.A.
Deposited on : 2022-05-28
Resolution : 2.00 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:

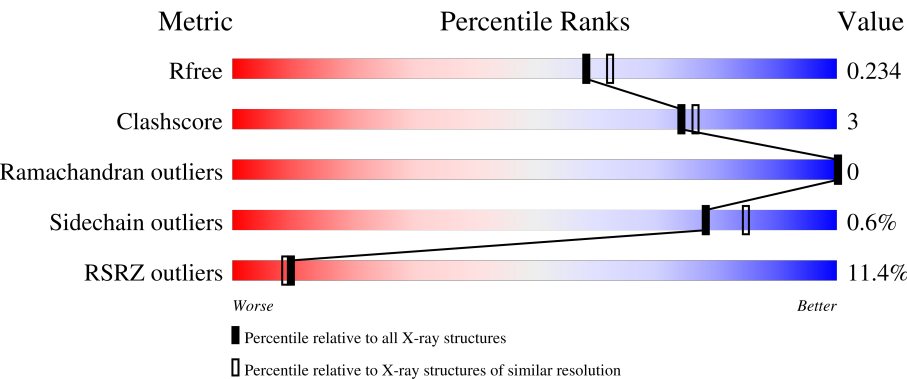
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	49% 80% 9% 11%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18367 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	5	0
			3437	2180	582	652	23			
1	C	440	Total	C	N	O	S	0	7	0
			3465	2196	585	660	24			

- 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	9	0
			3398	2137	580	653	28			
2	D	427	Total	C	N	O	S	0	8	0
			3394	2136	576	652	30			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	632	185	204	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

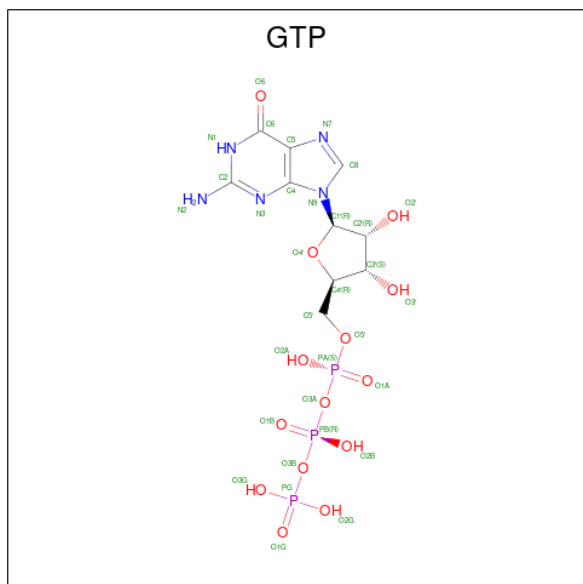
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	343	Total	C	N	O	S	0	2	0
			2814	1805	479	516	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	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		

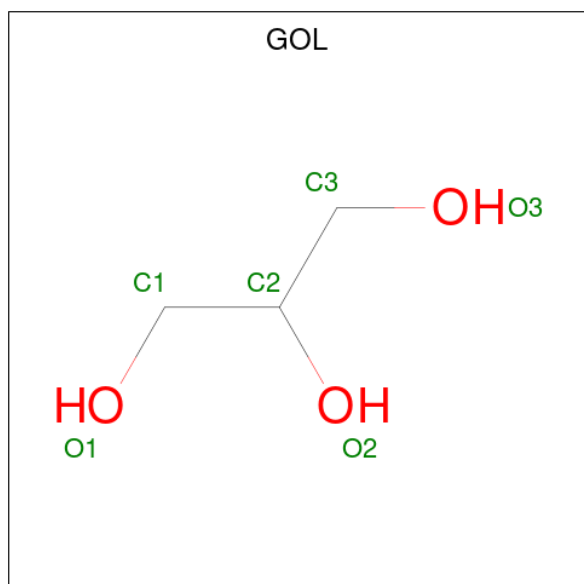
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

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

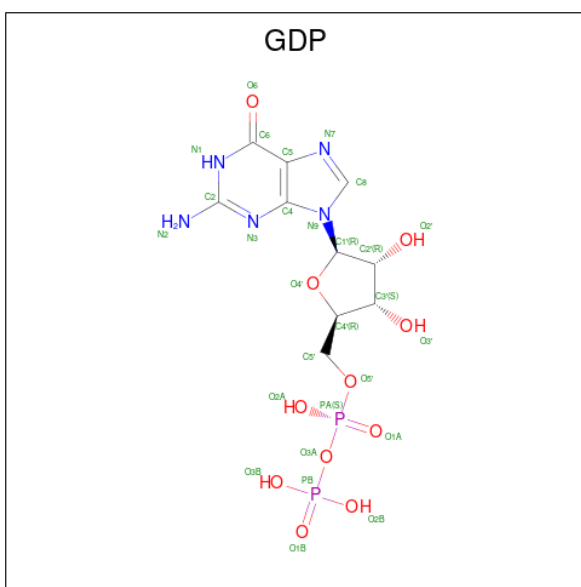
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



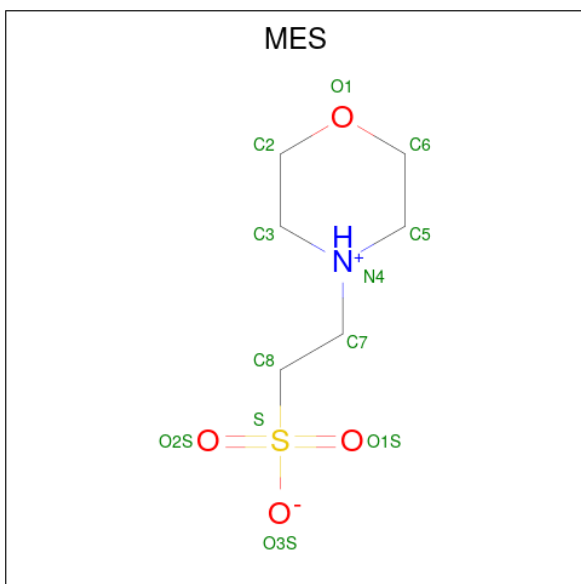
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



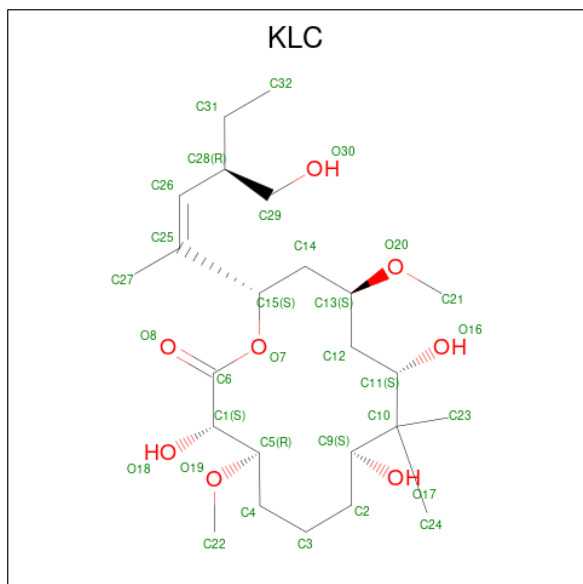
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



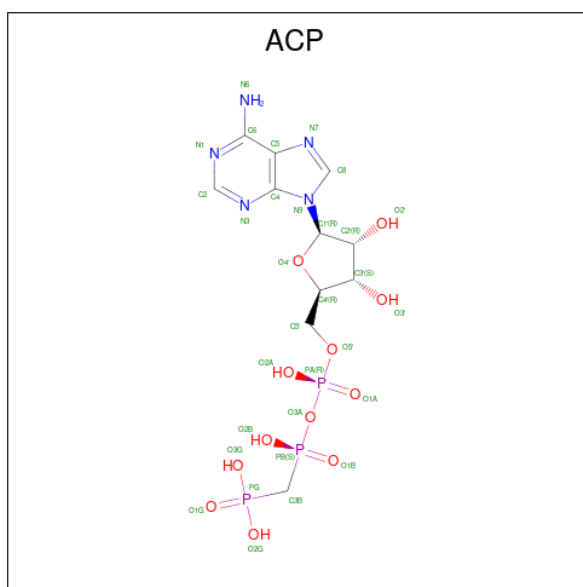
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3 {S},4 {R},8 {S},10 {S},12 {S},14 {S})-14-[({Z},4 {R})-4-(hydroxymethyl)hex-2-en-2-yl]-4,12-dimethoxy-9,9-dimethyl-3,8,10-tris(oxidanyl)-1-oxacyclotetradecan-2-one (CCD ID: KLC) (formula: $C_{24}H_{44}O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			32	24	8		

- 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		

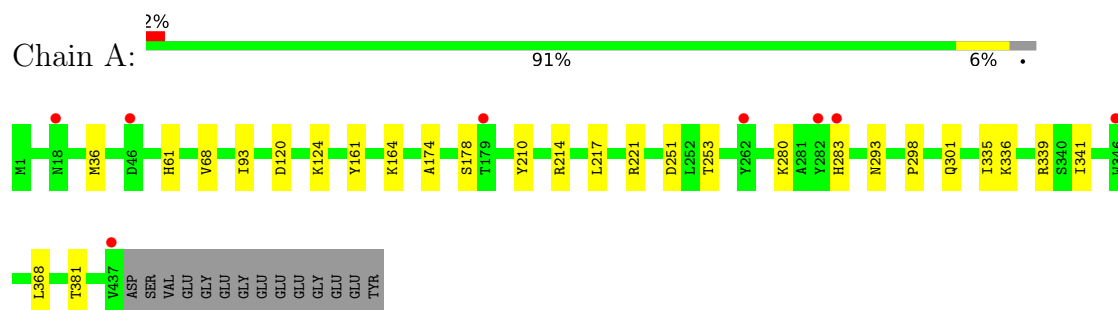
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	138	Total	O	0	0
			138	138		
13	B	129	Total	O	0	0
			129	129		
13	C	233	Total	O	0	0
			233	233		
13	D	68	Total	O	0	0
			68	68		
13	E	32	Total	O	0	0
			32	32		
13	F	18	Total	O	0	0
			18	18		

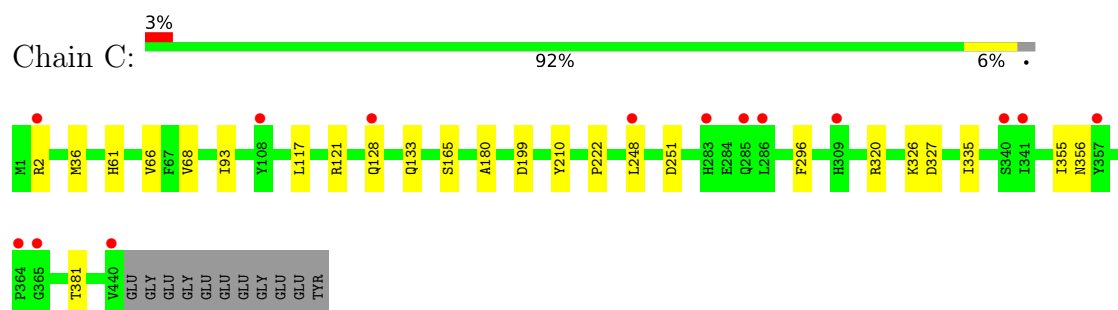
3 Residue-property plots [i](#)

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

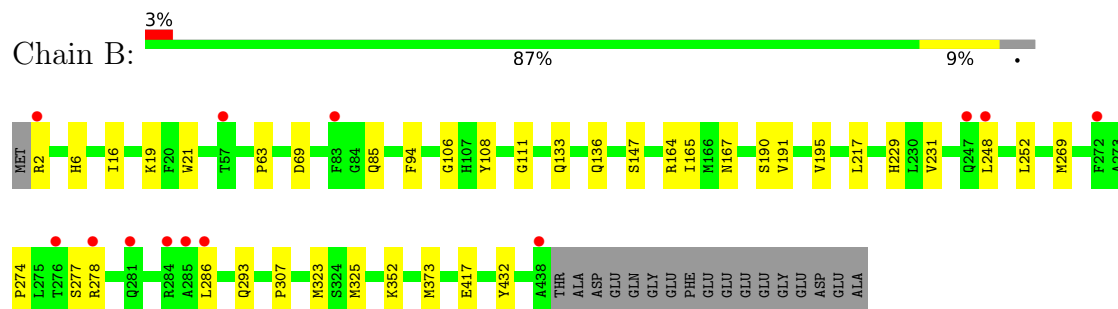
- Molecule 1: Tubulin alpha-1B chain



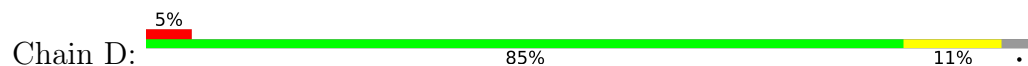
- Molecule 1: Tubulin alpha-1B chain

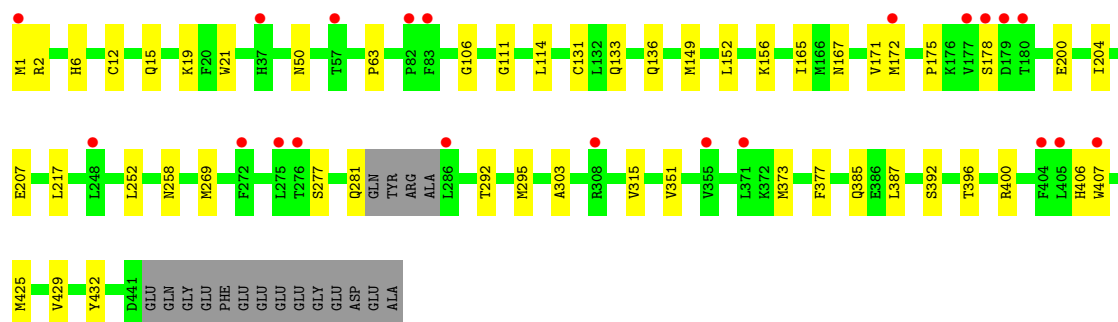


- Molecule 2: Tubulin beta-2B chain

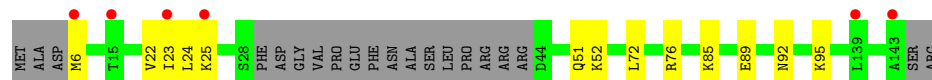
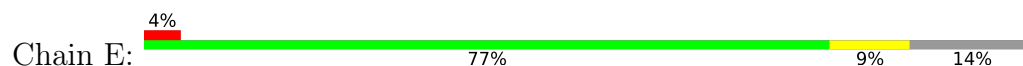


- Molecule 2: Tubulin beta-2B chain

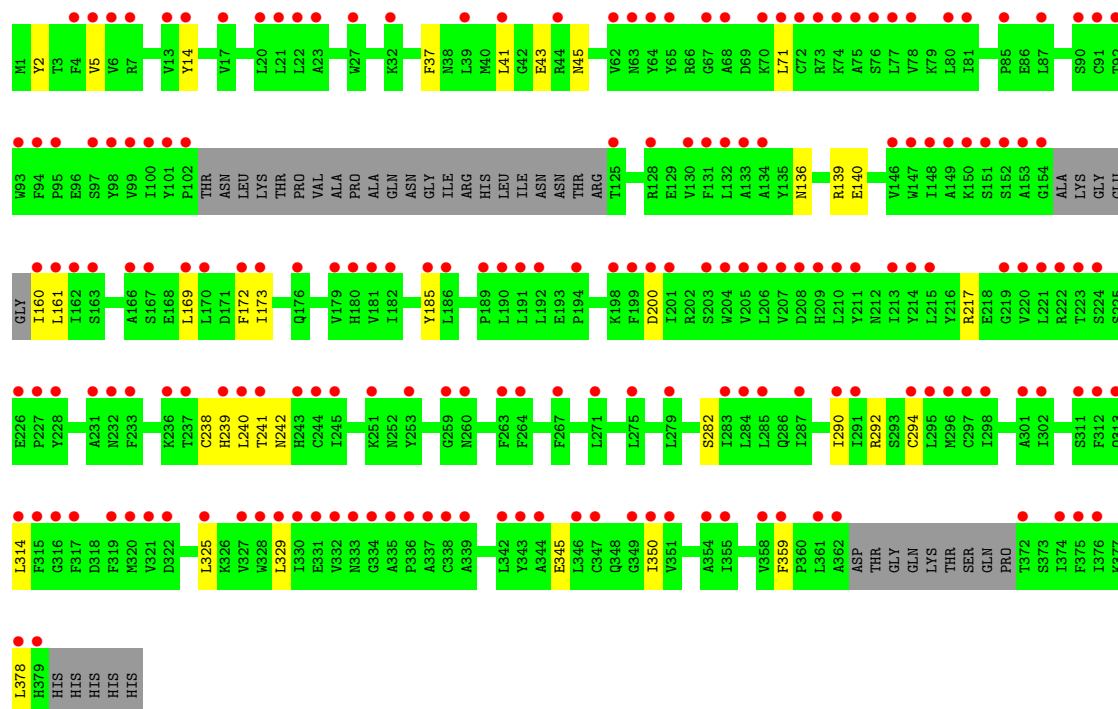
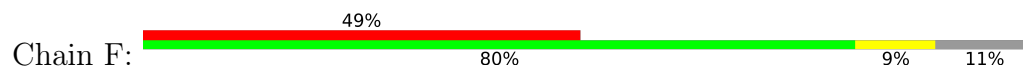




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.63Å 156.56Å 179.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 2.00 47.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.51-2.00) 99.9 (47.51-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.188 , 0.226 0.197 , 0.234	Depositor DCC
R_{free} test set	9918 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18367	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 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.20	0/3530	0.40	0/4793
1	C	0.25	0/3564	0.46	0/4841
2	B	0.23	0/3500	0.43	0/4740
2	D	0.17	0/3493	0.36	0/4730
3	E	0.19	0/1037	0.32	0/1376
4	F	0.14	0/2883	0.32	0/3894
All	All	0.20	0/18007	0.40	0/24374

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	3437	0	3368	14	0
1	C	3465	0	3393	15	0
2	B	3398	0	3302	26	0
2	D	3394	0	3295	31	0
3	E	1026	0	1041	6	0
4	F	2814	0	2788	17	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
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	12	0	16	1	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	12	2	0
11	B	32	0	0	1	0
12	F	31	0	14	1	0
13	A	138	0	0	0	0
13	B	129	0	0	1	0
13	C	233	0	0	4	0
13	D	68	0	0	2	0
13	E	32	0	0	0	0
13	F	18	0	0	0	0
All	All	18367	0	17277	108	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 3.

All (108) 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:269:MET:HE1	2:B:307:PRO:HG3	1.67	0.76
2:B:229:HIS:HB2	2:B:278:ARG:HE	1.53	0.73
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.69	0.73
2:D:2:ARG:HB3	2:D:133:GLN:HG3	1.76	0.67
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.78	0.66
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.44	0.65
2:B:432:TYR:OH	13:B:601:HOH:O	2.11	0.65
2:D:175:PRO:HA	2:D:178:SER:HB2	1.78	0.64
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.80	0.64
1:C:128:GLN:NE2	13:C:602:HOH:O	2.21	0.62
1:C:2:ARG:NH2	1:C:251:ASP:OD2	2.32	0.62
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.15	0.61
2:D:281:GLN:NE2	13:D:602:HOH:O	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:185:TYR:OH	4:F:239:HIS:ND1	2.29	0.57
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.40	0.56
2:D:432:TYR:OH	13:D:601:HOH:O	2.17	0.55
2:D:2:ARG:NH1	2:D:131:CYS:O	2.39	0.55
1:A:251:ASP:OD1	1:A:253:THR:OG1	2.24	0.54
1:A:221:ARG:HG3	2:B:325:MET:HG2	1.89	0.54
2:D:136:GLN:HA	2:D:167:ASN:O	2.08	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.54
2:B:293:GLN:NE2	11:B:505:KLC:O16	2.40	0.54
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.89	0.53
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.91	0.53
2:B:16[A]:ILE:HD13	2:B:231:VAL:HG11	1.91	0.53
2:D:1:MET:SD	2:D:50:ASN:HB2	2.50	0.52
2:B:69:ASP:O	2:B:94:PHE:HA	2.09	0.52
1:A:336:LYS:NZ	1:A:341:ILE:O	2.42	0.52
4:F:136:ASN:O	4:F:140:GLU:HG2	2.10	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.51
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.92	0.51
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.45	0.51
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.92	0.50
1:C:327:ASP:OD2	13:C:601:HOH:O	2.19	0.50
1:C:66:VAL:HG12	1:C:68[B]:VAL:HG23	1.93	0.50
1:A:280:LYS:O	1:A:283:HIS:NE2	2.45	0.50
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.95	0.49
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.95	0.49
2:B:229:HIS:HB2	2:B:278:ARG:NE	2.25	0.49
1:C:133:GLN:NE2	13:C:608:HOH:O	2.46	0.49
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.94	0.49
2:D:1:MET:HE3	2:D:50:ASN:ND2	2.27	0.49
2:B:323:MET:HB3	2:B:373:MET:HE1	1.94	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.94	0.48
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.94	0.48
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.32	0.47
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.30	0.47
2:D:106:GLY:O	2:D:111:GLY:HA3	2.14	0.47
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.97	0.46
1:A:68[B]:VAL:HG12	1:A:93:ILE:HB	1.98	0.46
2:D:392:SER:HB2	2:D:425:MET:HE3	1.97	0.46
3:E:24:LEU:O	3:E:25:LYS:HD2	2.16	0.46
3:E:72:LEU:O	3:E:76:ARG:HG2	2.16	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:43:GLU:HG3	4:F:45:ASN:O	2.15	0.45
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.99	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.45
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.45
2:B:373:MET:HB3	2:B:373:MET:HE2	1.49	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.52	0.44
2:D:1:MET:HE3	2:D:50:ASN:HD22	1.81	0.44
2:D:217:LEU:HA	2:D:277:SER:HB3	2.00	0.44
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.99	0.44
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.99	0.44
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.44
3:E:85:LYS:NZ	3:E:89:GLU:OE2	2.49	0.44
4:F:242:ASN:ND2	12:F:401:ACP:H3B1	2.31	0.44
1:A:174:ALA:O	1:A:178:SER:HB3	2.18	0.43
2:B:136:GLN:HA	2:B:167:ASN:O	2.18	0.43
2:B:191:VAL:O	2:B:195[A]:VAL:HG23	2.18	0.43
4:F:161:LEU:HD22	4:F:172:PHE:CG	2.53	0.43
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.47	0.43
2:B:19:LYS:HE2	2:B:278:ARG:NH2	2.33	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.43
2:D:295[B]:MET:HG2	2:D:377:PHE:HB2	2.01	0.43
3:E:95:LYS:HE2	3:E:95:LYS:HB3	1.88	0.43
3:E:6:MET:HE3	3:E:22:VAL:HG11	2.01	0.43
2:B:2:ARG:N	2:B:133:GLN:HG2	2.34	0.42
4:F:5:VAL:HG13	4:F:37:PHE:HB3	2.01	0.42
2:B:323:MET:HE2	2:B:373:MET:HE2	2.01	0.42
2:D:295[B]:MET:CG	2:D:377:PHE:HB2	2.48	0.42
3:E:6:MET:HA	3:E:23:ILE:O	2.19	0.42
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.54	0.42
2:D:406:HIS:CD2	2:D:407[B]:TRP:HD1	2.37	0.42
4:F:160:ILE:HD12	4:F:240:LEU:HD13	2.02	0.42
2:D:114:LEU:HD23	2:D:149:MET:HE1	2.01	0.42
4:F:290:ILE:HG21	4:F:329:LEU:HB2	2.02	0.42
1:C:326:LYS:NZ	13:C:613:HOH:O	2.53	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.20	0.42
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.37	0.42
2:B:217:LEU:HD13	2:B:277:SER:HB3	2.01	0.42
2:D:19:LYS:HA	2:D:19:LYS:HD3	1.90	0.41
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.53	0.41
1:A:293:ASN:ND2	1:A:339:ARG:HH21	2.18	0.41
2:D:396:THR:O	2:D:400:ARG:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:THR:O	2:D:295[A]:MET:HG2	2.21	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.56	0.41
4:F:292:ARG:HD3	4:F:378:LEU:HB3	2.03	0.41
2:B:164:ARG:O	10:B:504:MES:H52	2.20	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.46	0.41
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.56	0.41
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.41
2:D:373:MET:HE2	2:D:373:MET:HB3	1.91	0.41
1:C:296:PHE:CD1	1:C:335:ILE:HD13	2.57	0.40
4:F:169:LEU:O	4:F:173:ILE:HG13	2.22	0.40
8:A:505:GOL:H11	10:B:504:MES:O1S	2.21	0.40
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.57	0.40
2:D:152:LEU:O	2:D:156:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

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	440/451 (98%)	436 (99%)	4 (1%)	0	100	100
1	C	445/451 (99%)	435 (98%)	10 (2%)	0	100	100
2	B	434/445 (98%)	427 (98%)	7 (2%)	0	100	100
2	D	431/445 (97%)	424 (98%)	7 (2%)	0	100	100
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100
4	F	337/384 (88%)	324 (96%)	13 (4%)	0	100	100
All	All	2208/2319 (95%)	2166 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	373/379 (98%)	372 (100%)	1 (0%)	86	91
1	C	378/379 (100%)	377 (100%)	1 (0%)	86	91
2	B	378/383 (99%)	377 (100%)	1 (0%)	86	91
2	D	377/383 (98%)	374 (99%)	3 (1%)	73	80
3	E	112/127 (88%)	109 (97%)	3 (3%)	39	42
4	F	310/342 (91%)	308 (99%)	2 (1%)	78	85
All	All	1928/1993 (97%)	1917 (99%)	11 (1%)	78	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	THR
2	B	85	GLN
1	C	381	THR
2	D	15	GLN
2	D	200	GLU
2	D	207	GLU
3	E	51	GLN
3	E	52	LYS
3	E	92	ASN
4	F	139	ARG
4	F	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	393	HIS
2	B	294	GLN
2	B	331	GLN
2	B	339	ASN
2	B	349	ASN

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Mol	Chain	Res	Type
1	C	15	GLN
2	D	8	GLN
2	D	14	ASN
2	D	50	ASN
2	D	136	GLN
2	D	193	GLN
2	D	247	GLN
2	D	331	GLN
4	F	196	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 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\# Z > 2$
9	GDP	B	501	6	29,30,30	1.13	3 (10%)	45,47,47	1.75	8 (17%)
5	GTP	A	501	6	33,34,34	0.86	1 (3%)	50,54,54	1.45	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	KLC	B	505	-	32,32,32	0.93	1 (3%)	32,44,44	1.63	3 (9%)
9	GDP	D	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.68	5 (11%)
8	GOL	A	505	-	5,5,5	1.04	0	5,5,5	0.90	0
10	MES	B	504	-	12,12,12	2.39	1 (8%)	15,16,16	1.90	6 (40%)
8	GOL	A	506	-	5,5,5	0.82	0	5,5,5	1.22	1 (20%)
12	ACP	F	401	-	31,33,33	2.55	9 (29%)	47,52,52	1.81	9 (19%)
5	GTP	C	501	6	33,34,34	0.92	2 (6%)	50,54,54	1.46	9 (18%)

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
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
11	KLC	B	505	-	-	8/54/54/54	0/0/1/1
9	GDP	D	501	6	-	4/16/32/32	0/3/3/3
8	GOL	A	505	-	-	2/4/4/4	-
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
8	GOL	A	506	-	-	3/4/4/4	-
12	ACP	F	401	-	-	0/19/38/38	0/3/3/3
5	GTP	C	501	6	-	5/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.98	1.66	1.77
12	F	401	ACP	PB-O3A	7.37	1.66	1.58
12	F	401	ACP	PA-O3A	7.03	1.67	1.59
12	F	401	ACP	PG-O3G	4.25	1.64	1.55
12	F	401	ACP	C4-N3	4.24	1.42	1.34
12	F	401	ACP	C2-N1	4.10	1.41	1.33
12	F	401	ACP	C8-N7	3.54	1.38	1.31
9	D	501	GDP	C5-C4	2.97	1.46	1.38
9	B	501	GDP	C5-C4	2.75	1.46	1.38
5	C	501	GTP	PA-O3A	2.72	1.62	1.59
12	F	401	ACP	C2-N3	2.63	1.38	1.33
9	D	501	GDP	C6-N1	-2.47	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C6-N1	-2.46	1.34	1.38
12	F	401	ACP	C6-N1	2.34	1.42	1.35
9	D	501	GDP	PA-O3A	2.14	1.61	1.59
5	A	501	GTP	C2-N3	2.12	1.38	1.33
12	F	401	ACP	C5-N7	2.06	1.42	1.39
5	C	501	GTP	C2-N3	2.06	1.38	1.33
11	B	505	KLC	C29-C28	2.02	1.55	1.52
9	B	501	GDP	C5-N7	-2.01	1.35	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	N3-C2-N1	-5.97	119.54	128.58
11	B	505	KLC	C15-O7-C6	5.81	127.02	116.58
9	D	501	GDP	C5-C4-N3	-5.62	119.44	128.39
9	B	501	GDP	C5-C4-N3	-5.52	119.60	128.39
9	B	501	GDP	C2-N3-C4	4.84	120.64	112.30
9	D	501	GDP	C2-N3-C4	4.71	120.42	112.30
5	C	501	GTP	C5-C4-N3	-4.46	121.29	128.39
12	F	401	ACP	C5-C4-N9	4.36	110.56	105.81
5	A	501	GTP	C5-C4-N3	-4.30	121.55	128.39
5	C	501	GTP	C2-N3-C4	4.27	119.66	112.30
5	A	501	GTP	C2-N3-C4	4.27	119.66	112.30
9	B	501	GDP	N9-C4-N3	4.24	134.43	125.95
11	B	505	KLC	O7-C15-C14	4.22	115.48	106.65
9	D	501	GDP	N9-C4-N3	4.11	134.18	125.95
12	F	401	ACP	C5-C4-N3	-3.69	121.64	126.72
9	D	501	GDP	C6-C5-N7	3.55	136.75	130.29
12	F	401	ACP	C4-C5-N7	-3.50	106.58	110.58
10	B	504	MES	C5-N4-C3	3.41	116.19	108.84
12	F	401	ACP	C6-C5-C4	3.38	121.80	117.18
11	B	505	KLC	C24-C10-C23	-3.31	104.82	109.17
9	B	501	GDP	C6-C5-N7	3.30	136.30	130.29
12	F	401	ACP	N9-C8-N7	-3.17	109.43	113.94
5	C	501	GTP	N9-C8-N7	-2.83	108.14	113.40
12	F	401	ACP	C2-N3-C4	2.79	118.64	111.83
9	D	501	GDP	C4-C5-N7	-2.67	106.44	110.67
9	B	501	GDP	O6-C6-C5	-2.66	119.50	126.53
12	F	401	ACP	C5-N7-C8	2.65	107.61	103.45
5	C	501	GTP	N9-C4-N3	2.64	131.24	125.95
5	C	501	GTP	C2-N1-C6	-2.57	120.44	125.11
5	A	501	GTP	N9-C8-N7	-2.55	108.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	C6-O1-C2	2.53	118.05	109.88
10	B	504	MES	C7-N4-C3	2.48	117.86	111.24
5	C	501	GTP	C8-N7-C5	2.45	108.63	104.26
10	B	504	MES	C7-N4-C5	2.42	117.69	111.24
5	A	501	GTP	C2-N1-C6	-2.42	120.73	125.11
12	F	401	ACP	C2-N1-C6	2.40	122.67	118.73
5	A	501	GTP	N2-C2-N1	2.35	121.73	116.76
5	C	501	GTP	C5-C6-N1	2.33	119.19	113.25
5	A	501	GTP	N9-C4-N3	2.29	130.53	125.95
5	A	501	GTP	O6-C6-C5	-2.27	120.54	126.53
9	B	501	GDP	O2B-PB-O3A	2.27	112.23	104.64
10	B	504	MES	C6-C5-N4	-2.23	106.74	110.12
5	A	501	GTP	C8-N7-C5	2.22	108.22	104.26
9	B	501	GDP	C5-C6-N1	2.19	118.84	113.25
5	A	501	GTP	C5-C6-N1	2.18	118.80	113.25
9	B	501	GDP	C4-C5-N7	-2.13	107.29	110.67
8	A	506	GOL	C3-C2-C1	-2.12	104.02	111.80
10	B	504	MES	C2-C3-N4	-2.10	106.92	110.12
5	C	501	GTP	O6-C6-C5	-2.07	121.08	126.53
5	C	501	GTP	O2A-PA-O3A	2.01	112.72	107.27

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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-O2
8	A	505	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
11	B	505	KLC	C3-C4-C5-C1
11	B	505	KLC	C9-C10-C11-O16
11	B	505	KLC	C11-C10-C9-O17

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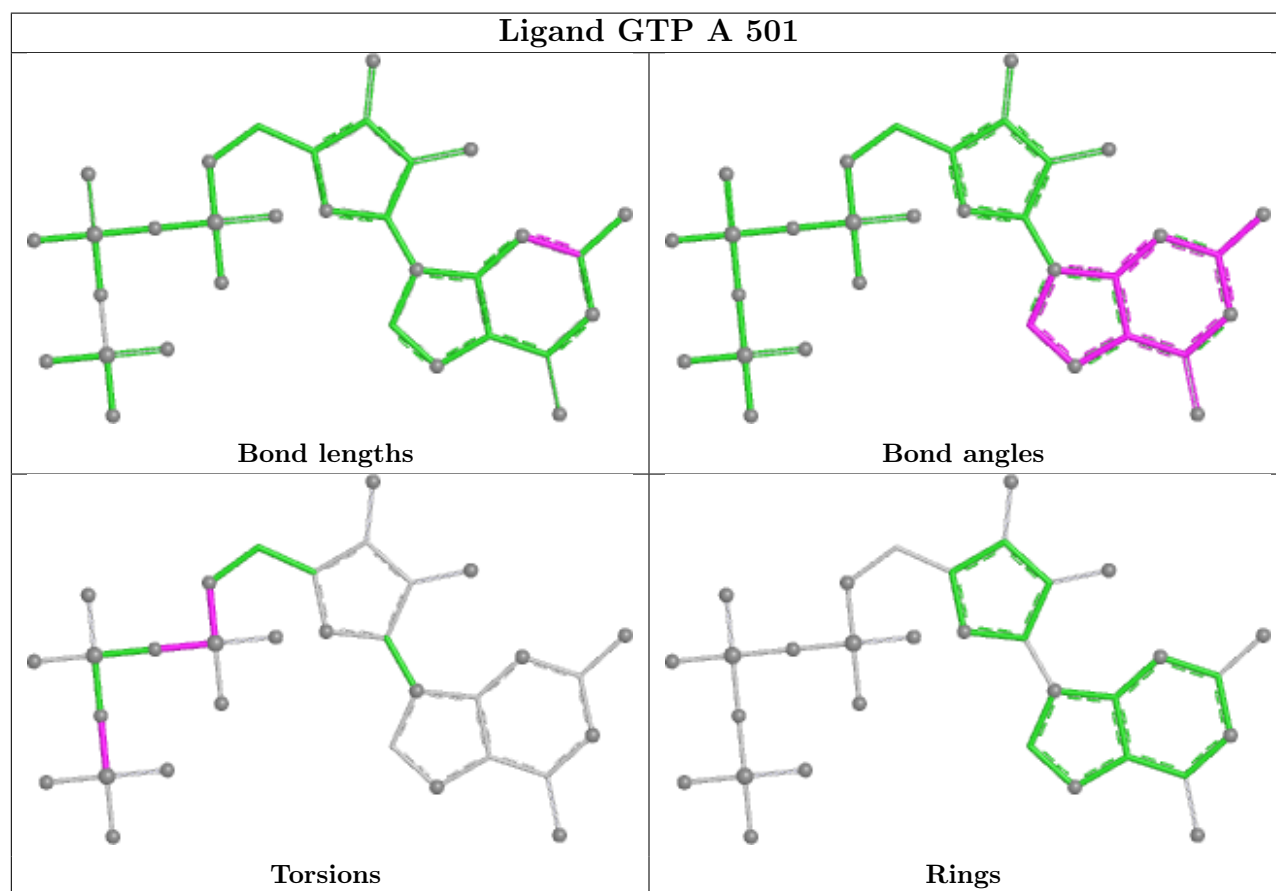
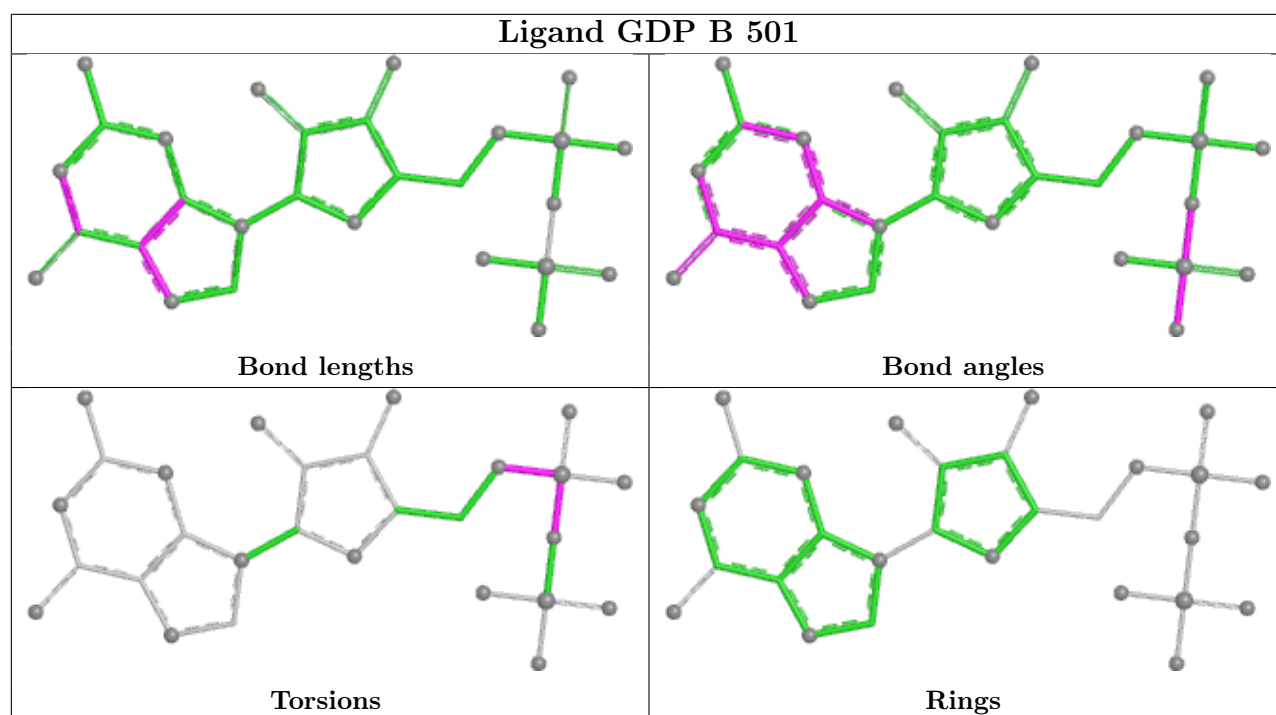
Mol	Chain	Res	Type	Atoms
11	B	505	KLC	C9-C2-C3-C4
11	B	505	KLC	C15-C25-C26-C28
11	B	505	KLC	C27-C25-C26-C28
5	A	501	GTP	PB-O3B-PG-O3G
8	A	506	GOL	C1-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
8	A	506	GOL	O1-C1-C2-C3
9	B	501	GDP	PB-O3A-PA-O2A
11	B	505	KLC	C13-C14-C15-O7
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
10	B	504	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O1A
8	A	506	GOL	O1-C1-C2-O2
11	B	505	KLC	C12-C13-C14-C15
9	D	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

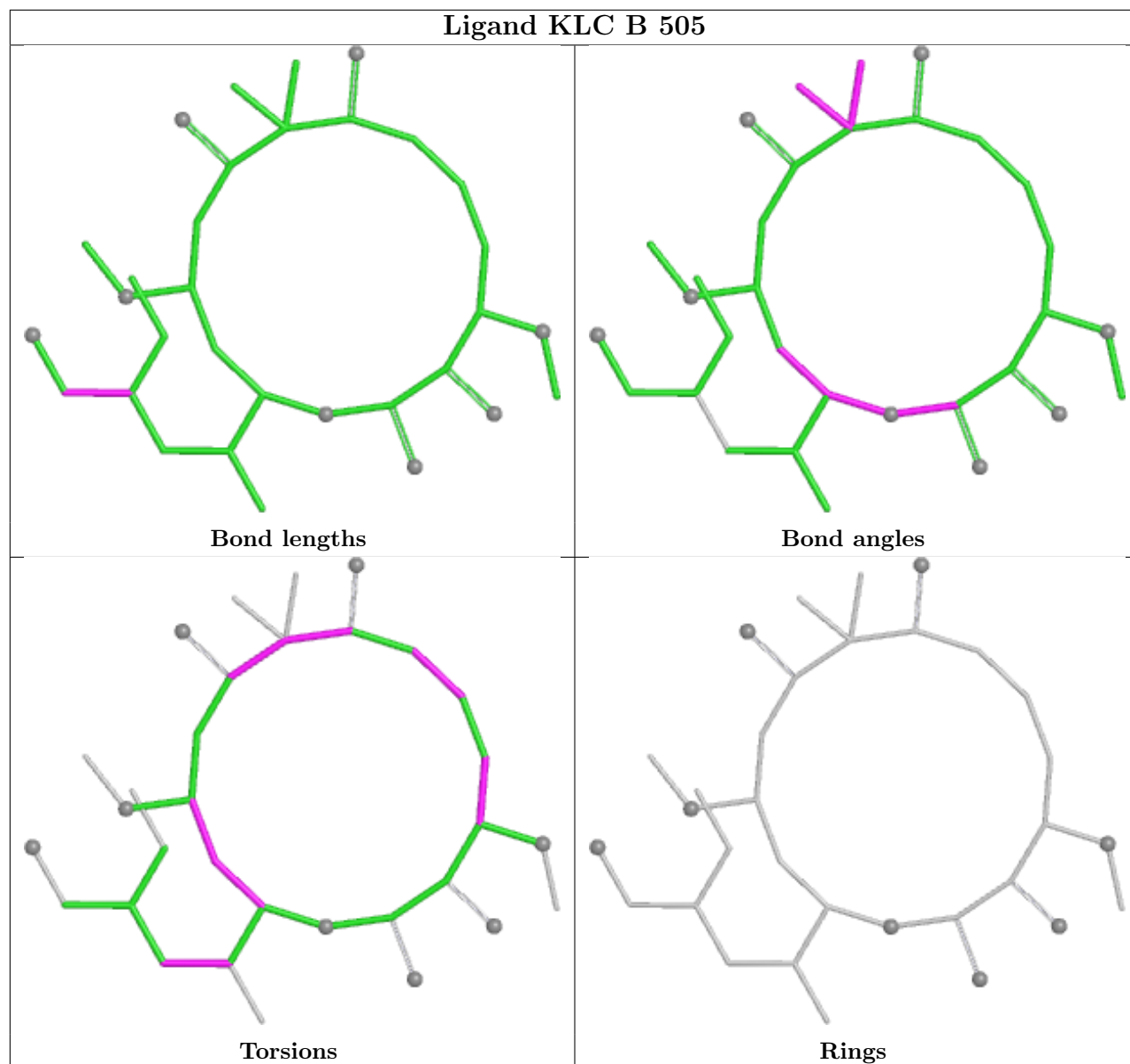
5 monomers are involved in 5 short contacts:

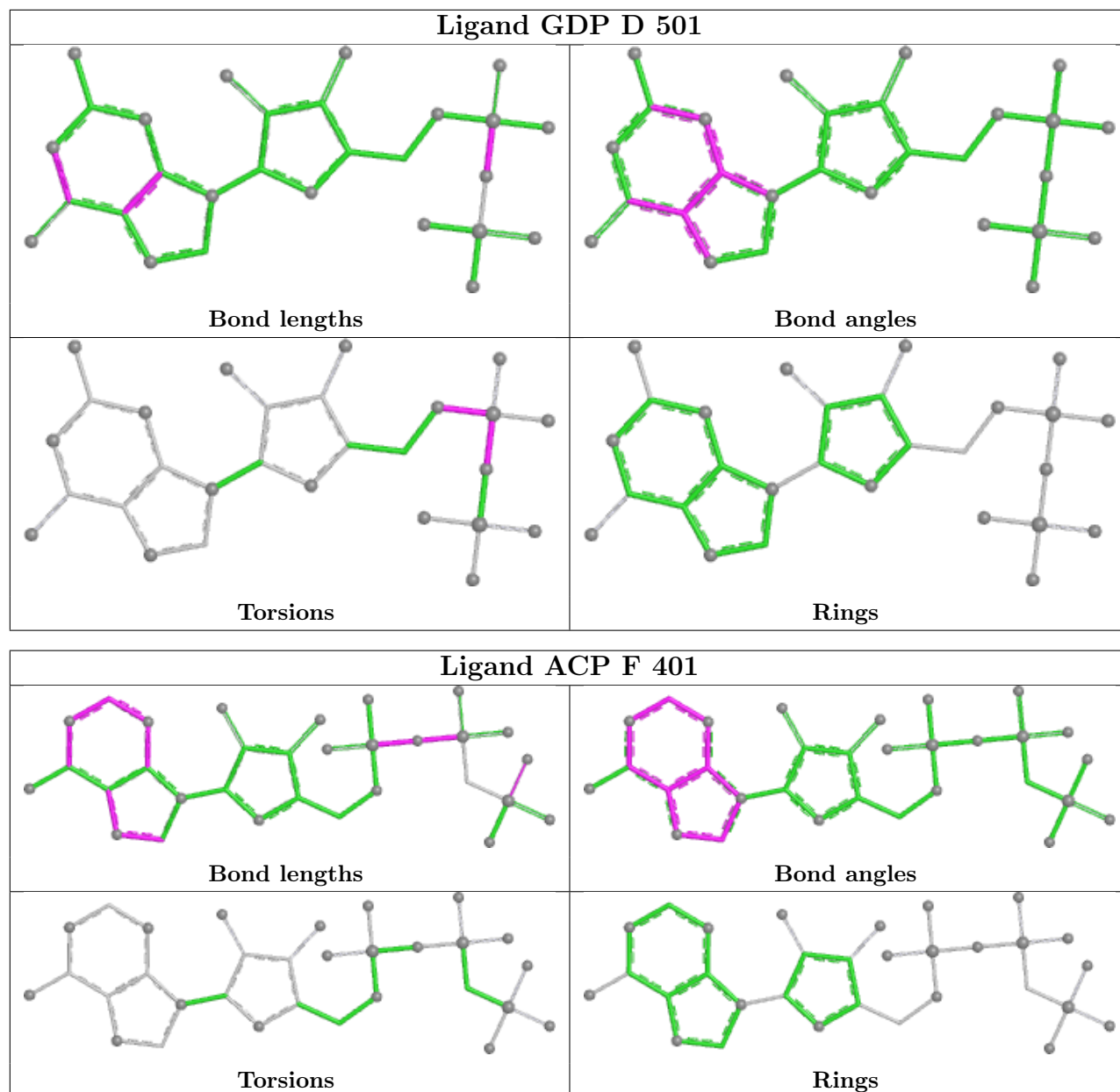
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	505	KLC	1	0
9	D	501	GDP	1	0
8	A	505	GOL	1	0
10	B	504	MES	2	0
12	F	401	ACP	1	0

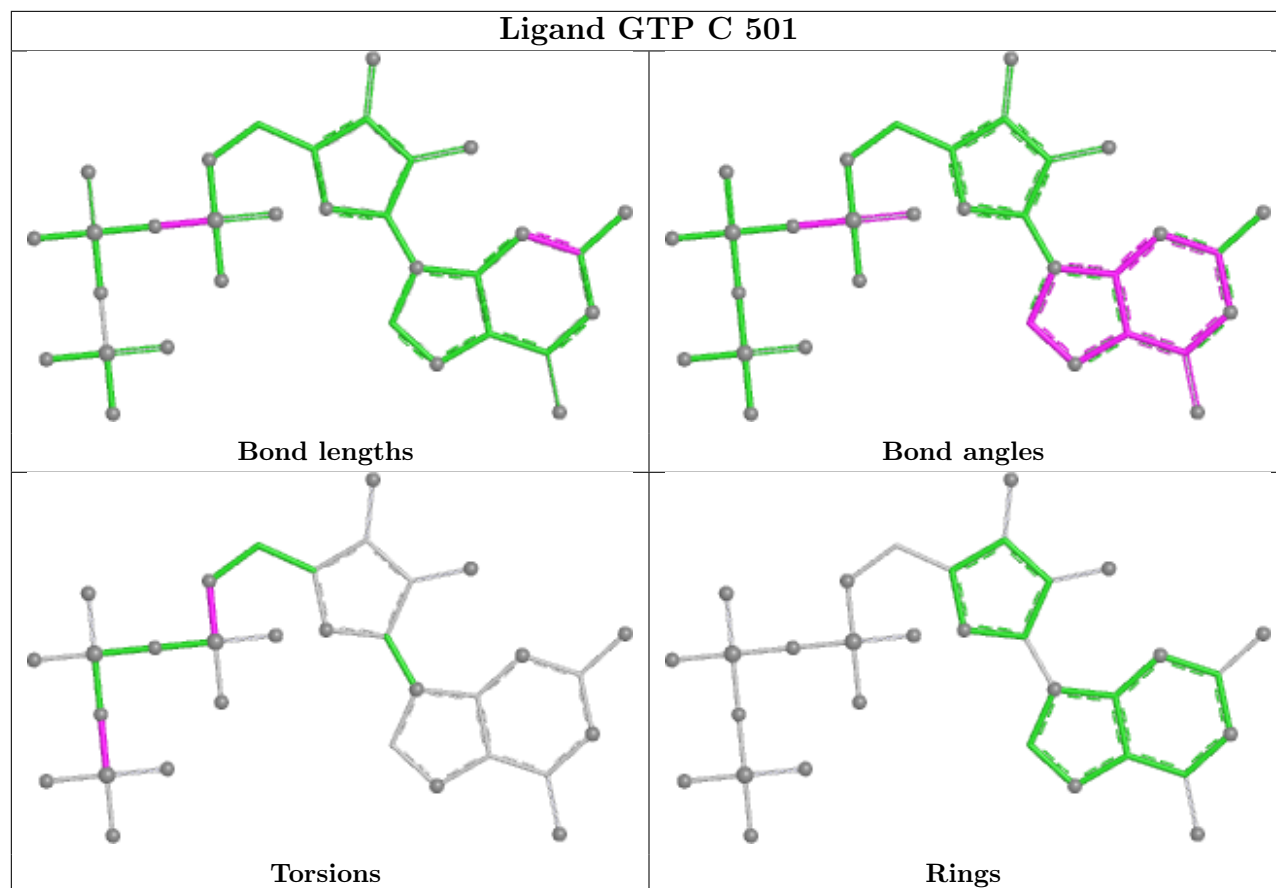
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 KLC B 505







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	0.19	8 (1%) 67 67	27, 54, 87, 163	5 (1%)
1	C	440/451 (97%)	0.08	14 (3%) 50 49	24, 43, 70, 120	7 (1%)
2	B	427/445 (95%)	0.22	13 (3%) 52 51	22, 50, 85, 151	9 (2%)
2	D	427/445 (95%)	0.54	21 (4%) 35 34	31, 64, 98, 128	8 (1%)
3	E	123/143 (86%)	0.56	6 (4%) 35 34	23, 65, 105, 145	2 (1%)
4	F	343/384 (89%)	2.43	189 (55%) 0 0	58, 114, 170, 211	2 (0%)
All	All	2197/2319 (94%)	0.61	251 (11%) 10 9	22, 58, 131, 211	33 (1%)

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	99	VAL	8.0
4	F	71	LEU	7.3
4	F	346	LEU	6.4
4	F	220	VAL	6.4
4	F	169	LEU	6.3
4	F	13	VAL	6.2
4	F	337	ALA	6.2
4	F	186	LEU	6.2
2	D	407[A]	TRP	6.1
4	F	132	LEU	6.1
4	F	154	GLY	5.9
4	F	68	ALA	5.8
4	F	170	LEU	5.7
4	F	317	PHE	5.3
4	F	179	VAL	5.2
4	F	321	VAL	5.2
4	F	161	LEU	5.1
4	F	149	ALA	5.0
4	F	92	THR	5.0

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Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	4.9
4	F	206	LEU	4.9
4	F	64	TYR	4.8
4	F	199	PHE	4.8
4	F	160	ILE	4.8
4	F	207	VAL	4.8
4	F	173	ILE	4.8
4	F	240	LEU	4.8
4	F	283	ILE	4.7
4	F	201	ILE	4.6
4	F	330	ILE	4.6
4	F	350	ILE	4.6
4	F	14	TYR	4.5
4	F	190	LEU	4.5
4	F	344	ALA	4.4
4	F	181	VAL	4.4
4	F	131	PHE	4.3
4	F	172	PHE	4.3
4	F	378	LEU	4.3
3	E	143	ALA	4.3
4	F	329	LEU	4.2
4	F	77	LEU	4.2
4	F	233	PHE	4.2
4	F	290	ILE	4.2
4	F	354	ALA	4.2
4	F	271	LEU	4.2
4	F	224	SER	4.1
4	F	245	ILE	4.1
4	F	361	LEU	4.1
4	F	320	MET	4.1
4	F	17	VAL	4.0
4	F	166	ALA	4.0
4	F	291	ILE	4.0
4	F	241	THR	4.0
4	F	205	VAL	4.0
4	F	162	ILE	3.9
4	F	295	LEU	3.9
4	F	148	ILE	3.8
4	F	376	ILE	3.8
4	F	223	THR	3.8
4	F	182	ILE	3.8
4	F	244	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	6	VAL	3.7
4	F	78	VAL	3.7
4	F	194	PRO	3.7
4	F	338	CYS	3.7
4	F	100	ILE	3.6
2	D	1	MET	3.6
4	F	213	ILE	3.6
2	D	177	VAL	3.6
4	F	189	PRO	3.6
4	F	215	LEU	3.6
4	F	359	PHE	3.6
2	B	248	LEU	3.6
4	F	150	LYS	3.5
4	F	379	HIS	3.5
4	F	27	TRP	3.5
4	F	298	ILE	3.5
4	F	70	LYS	3.5
2	B	57	THR	3.5
2	D	272	PHE	3.4
4	F	200	ASP	3.4
2	B	278	ARG	3.4
4	F	287	ILE	3.4
1	C	440	VAL	3.4
4	F	362	ALA	3.4
4	F	22	LEU	3.4
4	F	151	SER	3.4
1	A	437	VAL	3.4
2	B	285	ALA	3.4
4	F	93	TRP	3.4
2	D	172	MET	3.3
4	F	335	ALA	3.3
4	F	267	PHE	3.3
4	F	319	PHE	3.3
1	C	285	GLN	3.3
1	A	282	TYR	3.3
4	F	355	ILE	3.2
2	B	438	ALA	3.2
1	C	357	TYR	3.2
4	F	75	ALA	3.2
4	F	191	LEU	3.2
4	F	94	PHE	3.2
4	F	185	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	358	VAL	3.2
2	D	286	LEU	3.2
4	F	336	PRO	3.1
1	C	340	SER	3.1
4	F	210	LEU	3.1
4	F	81	ILE	3.1
4	F	343	TYR	3.1
1	C	309	HIS	3.1
4	F	62	VAL	3.1
2	D	180	THR	3.1
2	D	276	THR	3.1
4	F	374	ILE	3.0
4	F	285	LEU	3.0
4	F	312	PHE	3.0
4	F	152	SER	3.0
4	F	133	ALA	3.0
4	F	20	LEU	3.0
4	F	332	VAL	3.0
2	D	83	PHE	3.0
1	C	248	LEU	3.0
4	F	76[A]	SER	3.0
2	D	82	PRO	3.0
4	F	180	HIS	2.9
4	F	315	PHE	2.9
4	F	328	TRP	2.9
4	F	325	LEU	2.9
4	F	90	SER	2.9
3	E	15	THR	2.9
4	F	209	HIS	2.9
1	A	46	ASP	2.9
1	C	341	ILE	2.9
4	F	39	LEU	2.9
4	F	192	LEU	2.9
4	F	327	VAL	2.8
4	F	211	TYR	2.8
4	F	294	CYS	2.8
4	F	331	GLU	2.8
2	D	275	LEU	2.8
3	E	139	LEU	2.8
4	F	80	LEU	2.8
4	F	221	LEU	2.8
4	F	203	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	308	ARG	2.8
3	E	6	MET	2.8
4	F	214	TYR	2.8
4	F	198	LYS	2.8
1	A	179	THR	2.8
2	D	57	THR	2.8
4	F	226	GLU	2.8
4	F	342	LEU	2.8
4	F	372	THR	2.8
4	F	67	GLY	2.7
4	F	227	PRO	2.7
1	A	262	TYR	2.7
4	F	236	LYS	2.7
4	F	297	CYS	2.7
1	C	286	LEU	2.7
2	D	179	ASP	2.6
4	F	73	ARG	2.6
2	B	286	LEU	2.6
4	F	284	LEU	2.6
4	F	316	GLY	2.6
4	F	208	ASP	2.6
2	B	247	GLN	2.6
4	F	125	THR	2.6
2	D	404	PHE	2.6
2	D	355	VAL	2.6
4	F	5	VAL	2.6
4	F	351	VAL	2.6
4	F	253	TYR	2.6
4	F	243	HIS	2.6
4	F	4	PHE	2.6
4	F	87	LEU	2.6
4	F	314	LEU	2.6
4	F	349	GLY	2.6
4	F	72	CYS	2.5
4	F	347	CYS	2.5
4	F	275	LEU	2.5
1	A	346	TRP	2.5
4	F	167[A]	SER	2.5
1	A	283	HIS	2.5
4	F	375	PHE	2.5
2	D	405	LEU	2.5
4	F	21	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	23	ILE	2.5
4	F	204	TRP	2.5
4	F	23	ALA	2.5
4	F	91	CYS	2.4
2	B	272	PHE	2.4
4	F	264	PHE	2.4
4	F	237	THR	2.4
4	F	147	TRP	2.4
4	F	222	ARG	2.4
4	F	219	GLY	2.4
4	F	259	GLY	2.4
4	F	98	TYR	2.4
4	F	228	TYR	2.4
4	F	339	ALA	2.4
1	C	128	GLN	2.4
4	F	95	PRO	2.4
4	F	176	GLN	2.4
4	F	313	GLN	2.4
1	C	365	GLY	2.4
4	F	134	ALA	2.3
4	F	74	LYS	2.3
4	F	302	ILE	2.3
1	C	2	ARG	2.3
4	F	44	ARG	2.3
4	F	153	ALA	2.3
4	F	333	ASN	2.3
4	F	296	MET	2.3
4	F	97	SER	2.2
4	F	146	VAL	2.2
2	D	37	HIS	2.2
2	B	2	ARG	2.2
4	F	128	ARG	2.2
4	F	334	GLY	2.2
2	D	248	LEU	2.2
4	F	41	LEU	2.2
4	F	85	PRO	2.2
4	F	102	PRO	2.2
4	F	231	ALA	2.2
4	F	311	SER	2.2
2	D	371	LEU	2.2
4	F	263	PHE	2.1
4	F	65	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	281	GLN	2.1
4	F	322	ASP	2.1
2	D	178	SER	2.1
4	F	279	LEU	2.1
3	E	25	LYS	2.1
1	C	283	HIS	2.1
1	A	18	ASN	2.1
4	F	232	ASN	2.1
2	B	276	THR	2.1
4	F	32	LYS	2.1
4	F	63	ASN	2.1
1	C	364	PRO	2.1
4	F	301	ALA	2.1
2	B	284	ARG	2.1
4	F	163	SER	2.0
4	F	7	ARG	2.0
4	F	251	LYS	2.0
2	B	83	PHE	2.0
4	F	239	HIS	2.0
1	C	108	TYR	2.0
4	F	101	TYR	2.0
4	F	260	ASN	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	ACP	F	401	31/31	0.77	0.14	92,113,142,145	0

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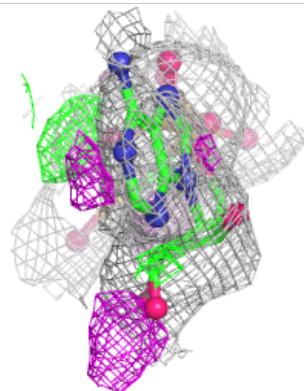
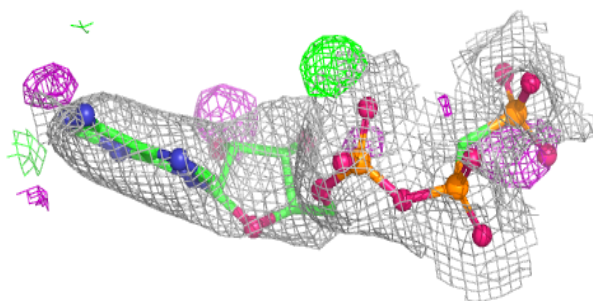
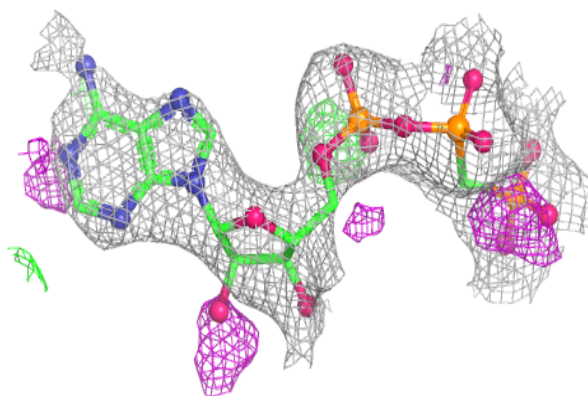
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	A	505	6/6	0.83	0.18	79,80,87,92	0
7	CA	B	503	1/1	0.89	0.09	95,95,95,95	0
10	MES	B	504	12/12	0.90	0.14	64,74,90,98	0
8	GOL	A	506	6/6	0.90	0.12	58,67,78,86	0
11	KLC	B	505	32/32	0.93	0.10	48,62,70,73	0
9	GDP	D	501	28/28	0.93	0.10	49,58,67,73	0
7	CA	A	504	1/1	0.94	0.09	99,99,99,99	0
6	MG	D	502	1/1	0.94	0.07	55,55,55,55	0
7	CA	A	503	1/1	0.98	0.04	70,70,70,70	0
9	GDP	B	501	28/28	0.98	0.05	28,35,39,40	0
5	GTP	A	501	32/32	0.98	0.04	32,37,42,46	0
7	CA	C	503	1/1	0.99	0.04	55,55,55,55	0
6	MG	A	502	1/1	0.99	0.03	38,38,38,38	0
6	MG	B	502	1/1	0.99	0.06	32,32,32,32	0
5	GTP	C	501	32/32	0.99	0.04	27,34,38,40	0
6	MG	C	502	1/1	1.00	0.02	34,34,34,34	0

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

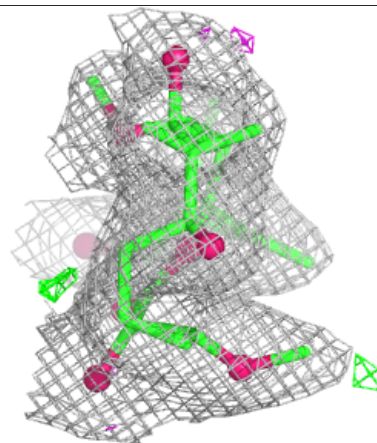
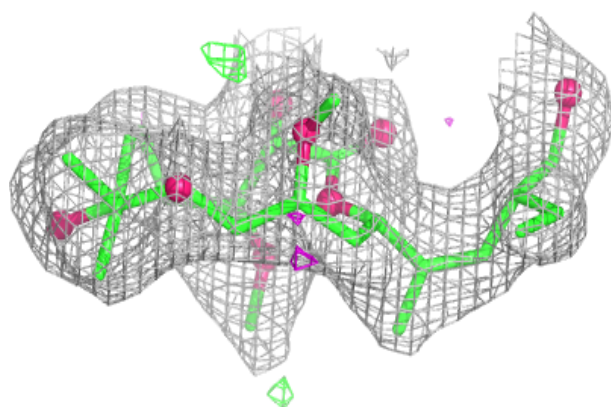
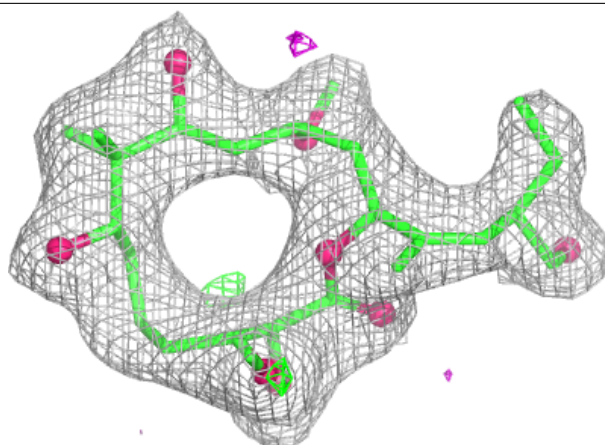
Electron density around ACP F 401:

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



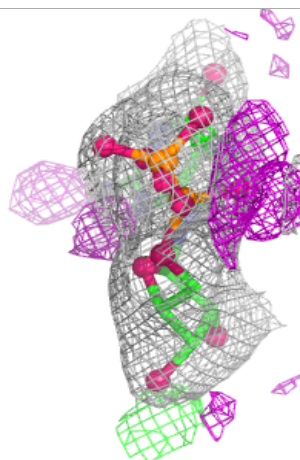
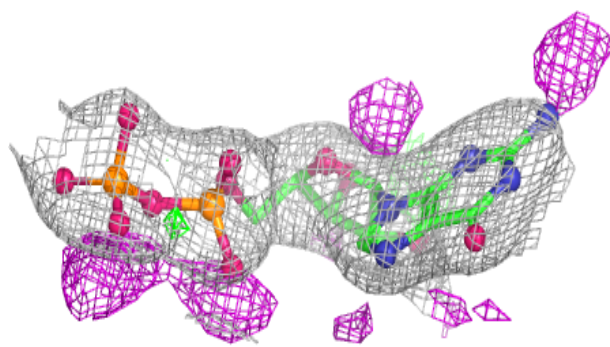
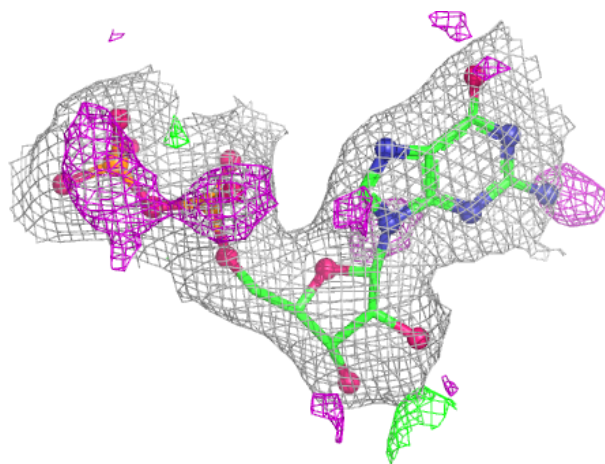
Electron density around KLC B 505:

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



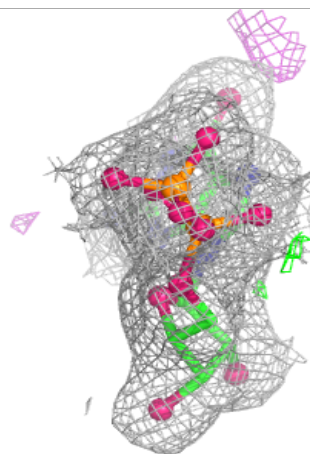
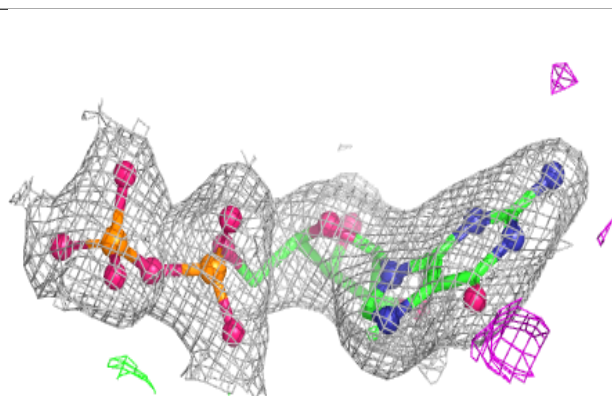
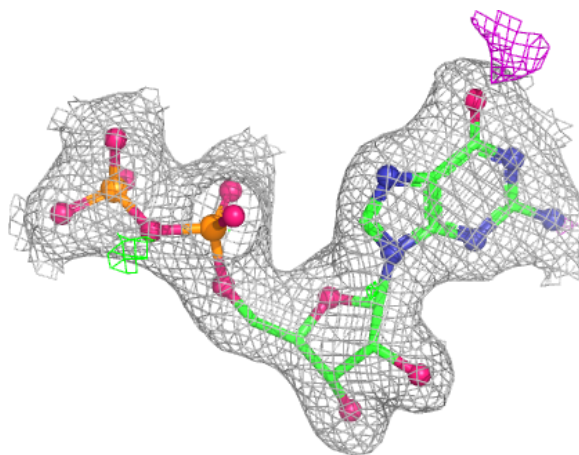
Electron density around GDP D 501:

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



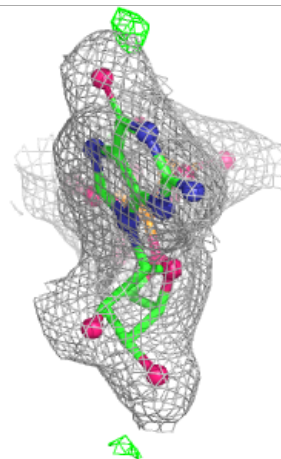
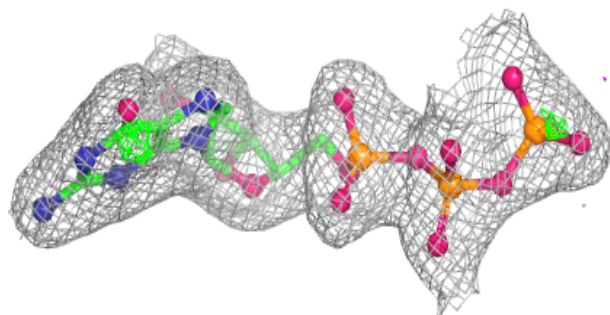
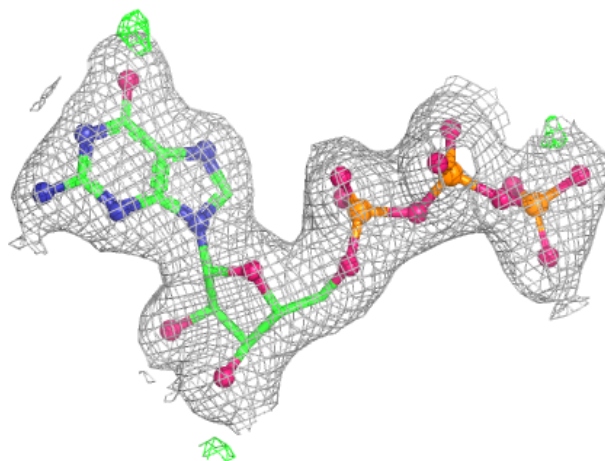
Electron density around GDP B 501:

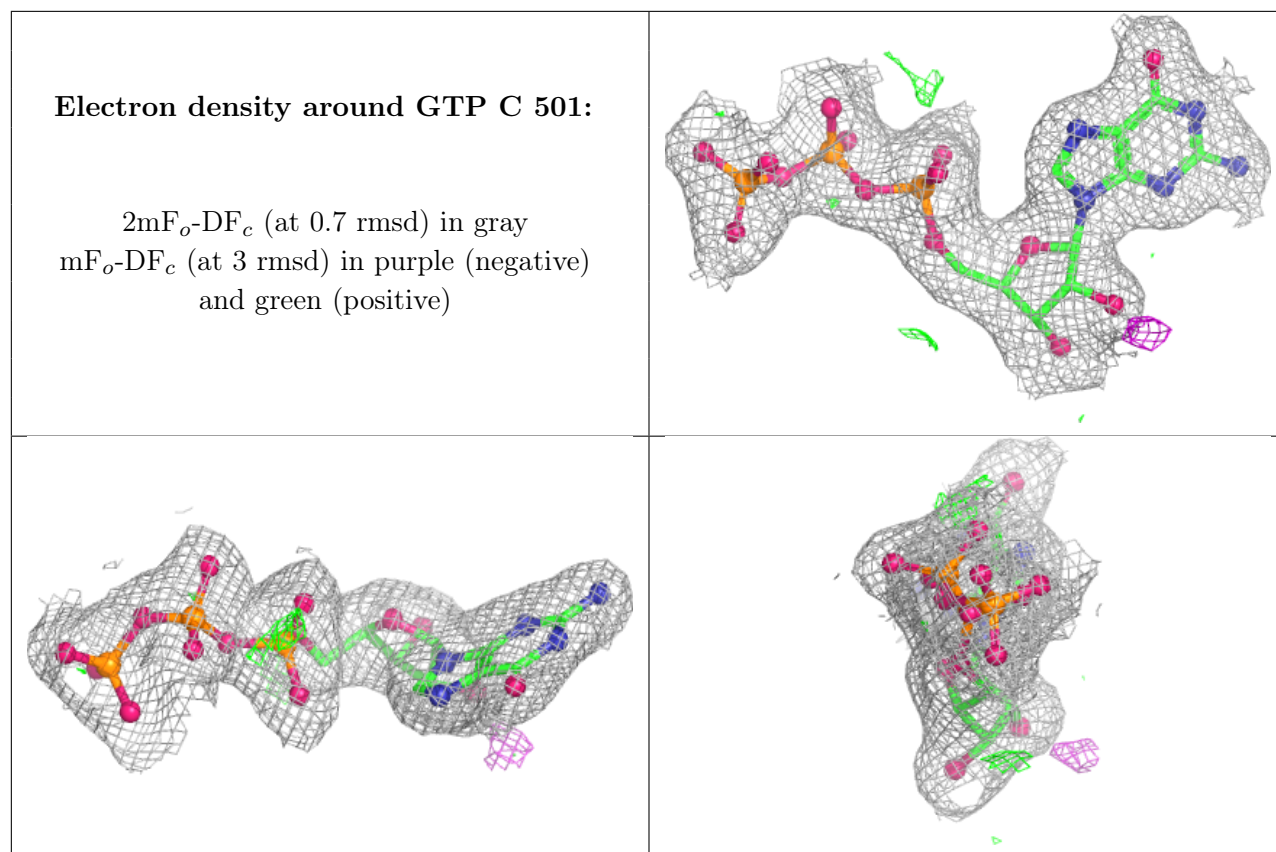
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP A 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.