



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:21 AM UTC

PDB ID : 7ZX2 / pdb_00007zx2
Title : Tubulin-Pelophen B complex
Authors : Estevez-Gallego, J.; Diaz, J.F.; Van der Eycken, J.; Oliva, M.A.
Deposited on : 2022-05-20
Resolution : 2.50 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

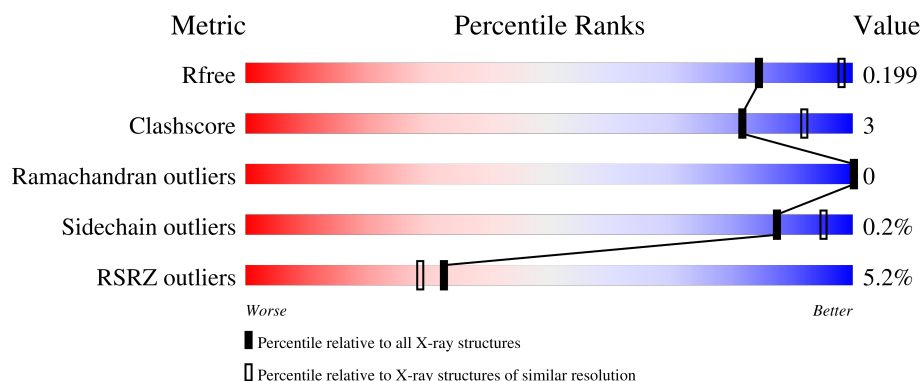
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

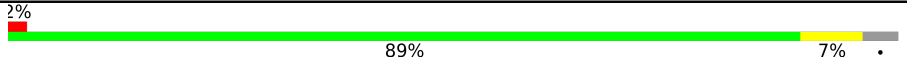
The reported resolution of this entry is 2.50 Å.

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.



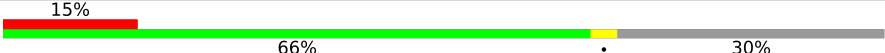
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	189	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment on the left labeled '15%', a green segment in the middle labeled '66%', and a grey segment on the right labeled '30%'. A small yellow segment is visible at the boundary between the green and grey segments.

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 17266 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	434	Total	C	N	O	S	0	7	0
			3439	2174	585	656	24			
1	C	439	Total	C	N	O	S	0	10	0
			3499	2211	593	670	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	6	0
			3375	2119	574	655	27			
2	D	421	Total	C	N	O	S	0	2	0
			3322	2088	564	642	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	3	0
			1019	628	185	201	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	268	Total	C	N	O	S	0	0	0
			2216	1445	373	386	12			

There are 6 discrepancies between the modelled and reference sequences:

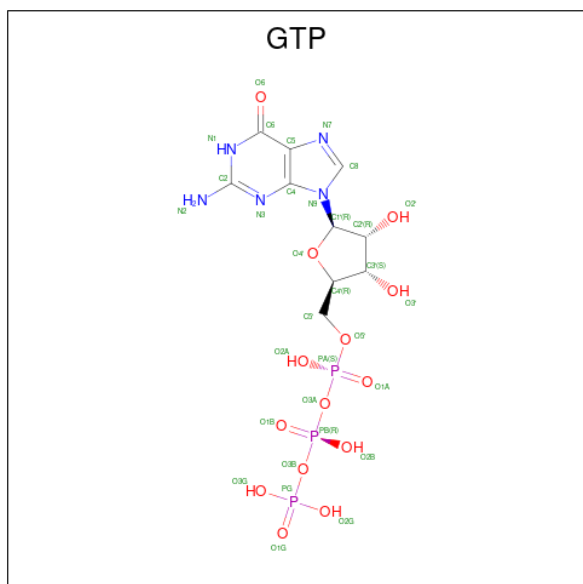
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

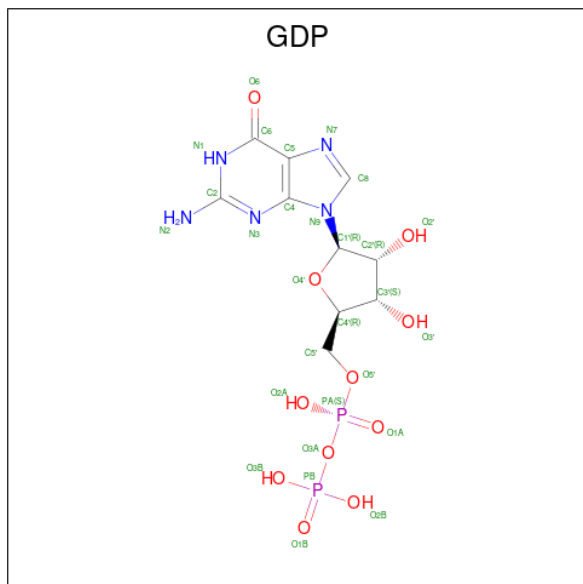
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

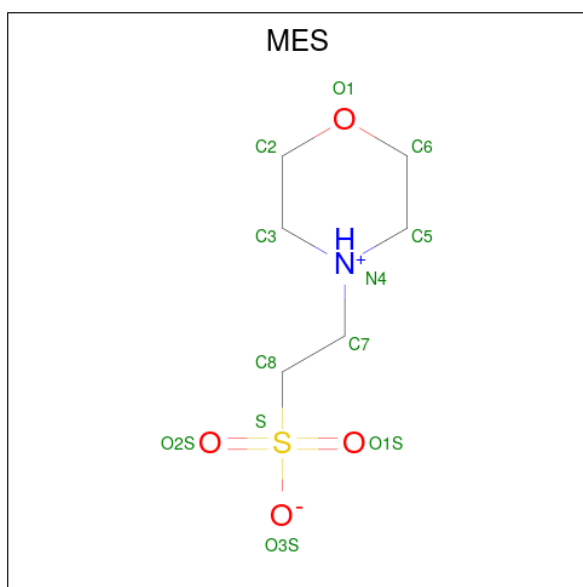
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	B	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



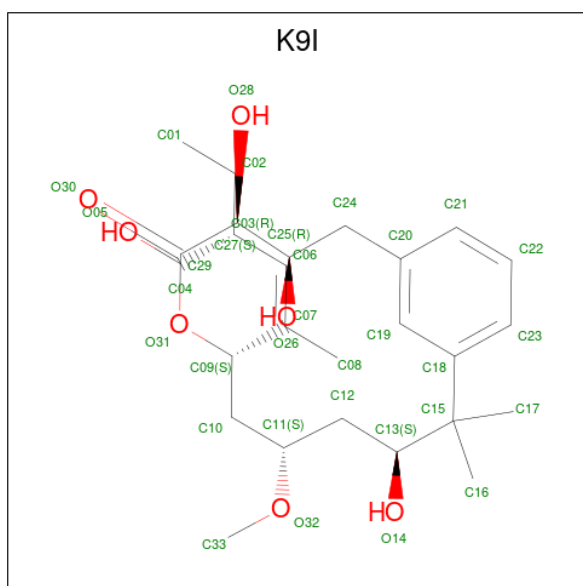
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
10	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



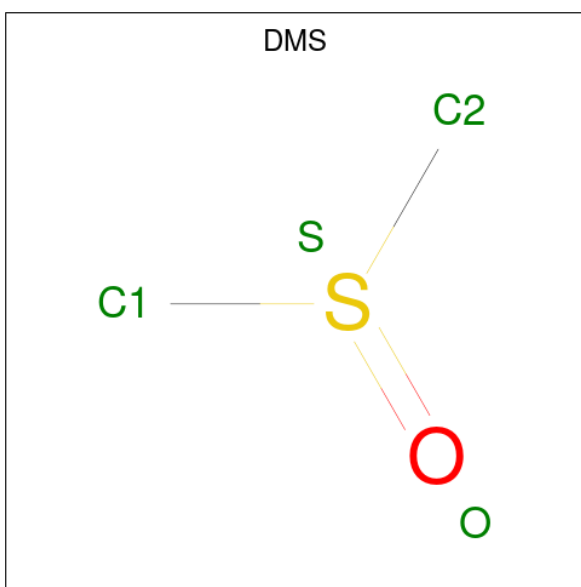
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 12 is (3R,4S,7S,9S,11S)-3,4,11-trihydroxy-7-((R,Z)-4-(hydroxymethyl)hex-2-en-2-yl)-9-methoxy-12,12-dimethyl-6-oxa-1(1,3)-benzenacyclododecaphan-5-one (CCD ID: K9I) (formula: C₂₆H₄₀O₇).



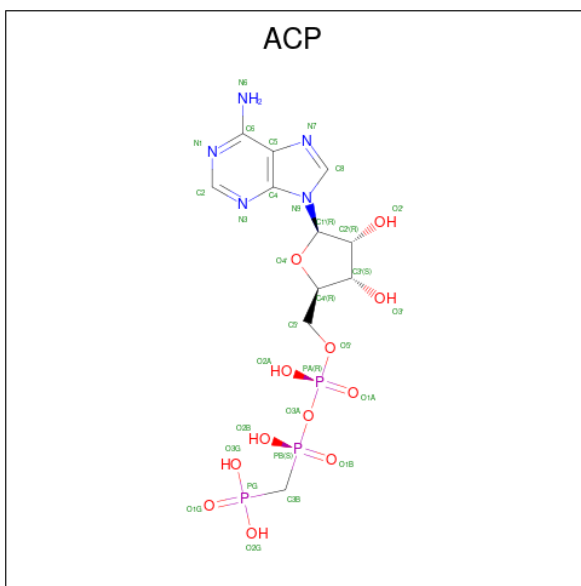
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			33	26	7		

- Molecule 13 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

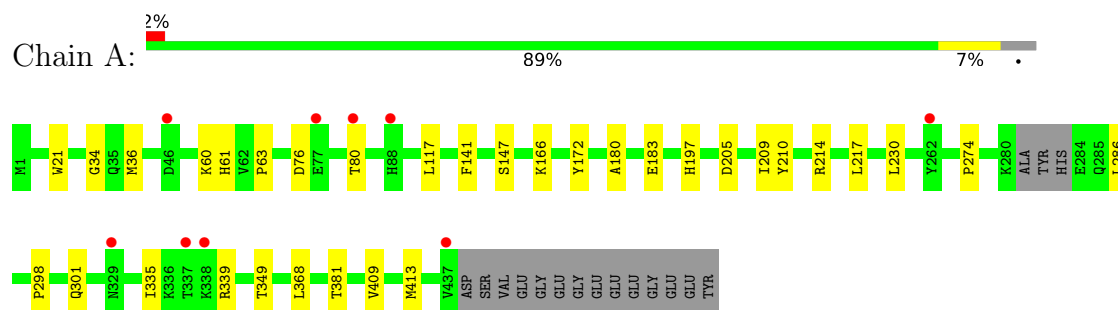


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	18	Total 18	O 18	0	0
15	B	24	Total 24	O 24	0	0
15	C	86	Total 86	O 86	0	0
15	D	10	Total 10	O 10	0	0
15	F	2	Total 2	O 2	0	0

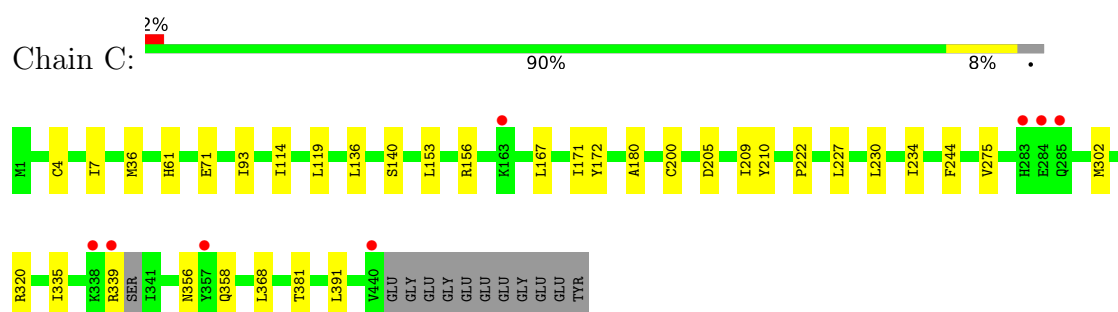
3 Residue-property plots

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.

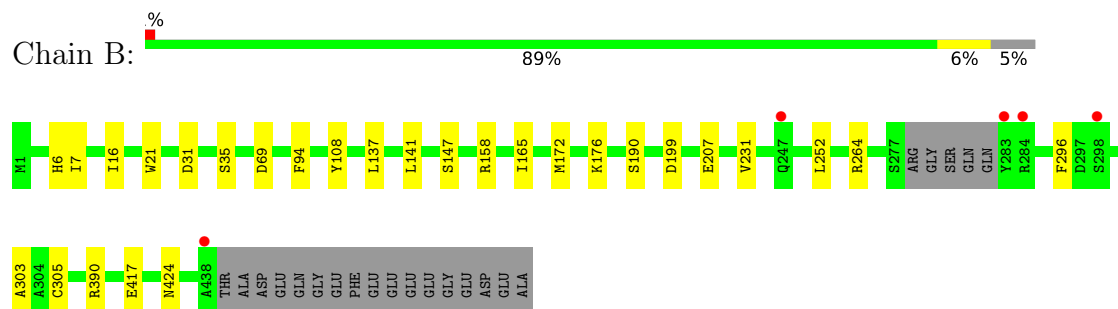
- Molecule 1: Tubulin alpha-1B chain



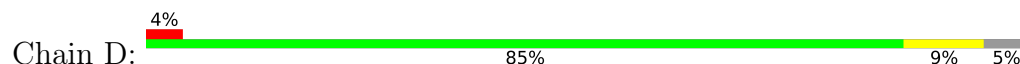
- Molecule 1: Tubulin alpha-1B chain

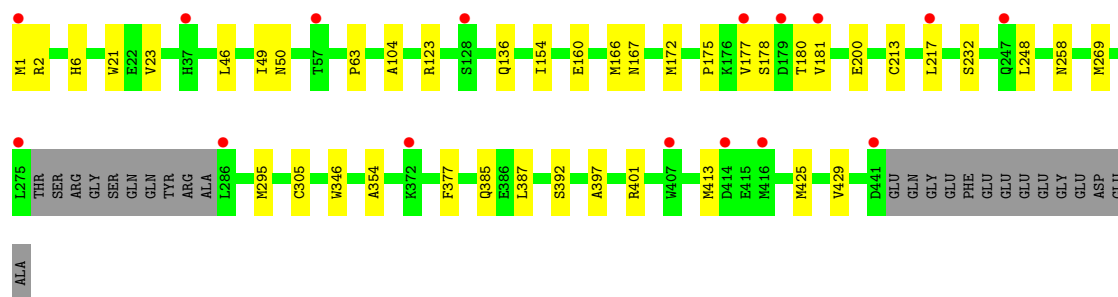


- Molecule 2: Tubulin beta-2B chain

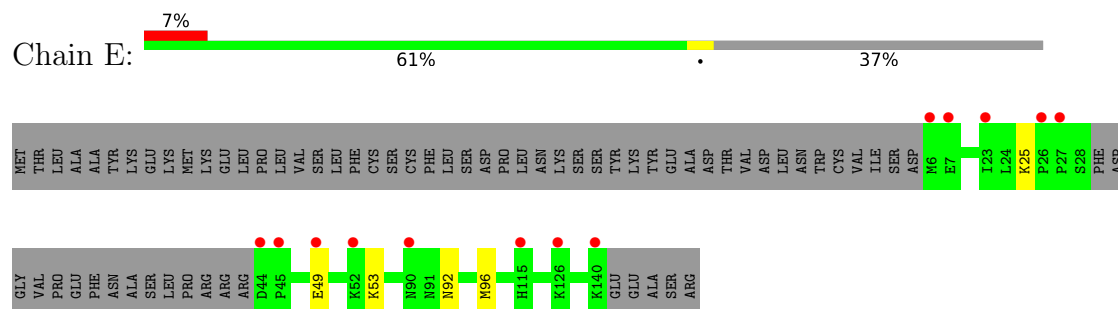


- Molecule 2: Tubulin beta-2B chain

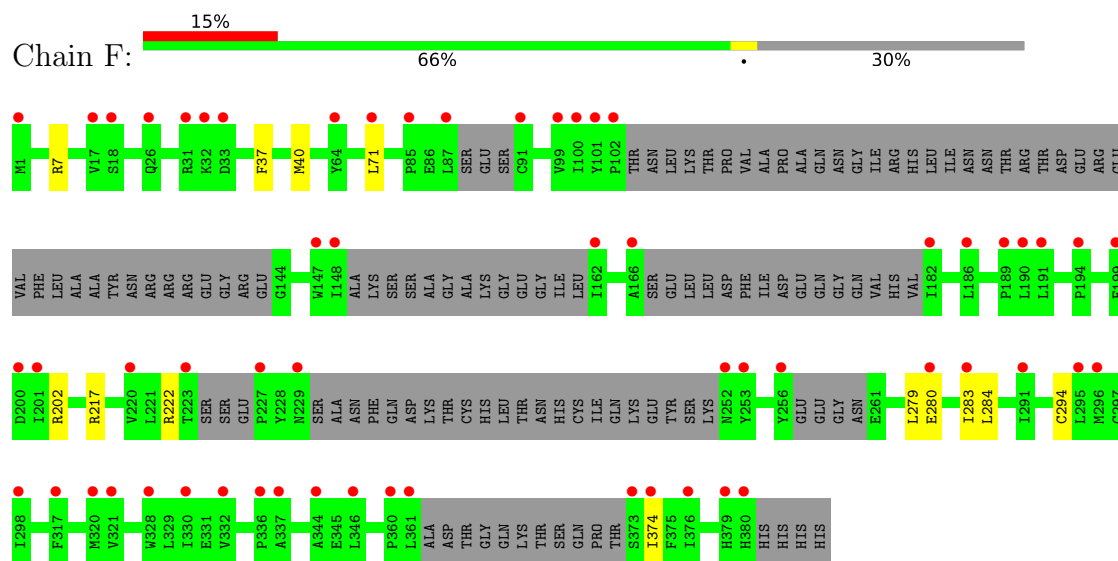




- Molecule 3: Stathmin-4



- Molecule 4: Tubulin 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	104.71Å 156.97Å 181.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.50 49.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.66-2.50) 100.0 (49.66-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.197 , 0.235 0.197 , 0.199	Depositor DCC
R_{free} test set	5239 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17266	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: MES, K9I, DMS, GTP, ACP, MG, GDP, CA, GOL, CL

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	0.15	0/3514	0.31	0/4769
1	C	0.18	0/3579	0.36	0/4858
2	B	0.17	0/3449	0.34	0/4671
2	D	0.14	0/3398	0.30	0/4603
3	E	0.15	0/1028	0.24	0/1364
4	F	0.12	0/2267	0.26	0/3058
All	All	0.16	0/17235	0.32	0/23323

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	3439	0	3351	17	0
1	C	3499	0	3396	18	0
2	B	3375	0	3243	17	0
2	D	3322	0	3203	24	0
3	E	1019	0	1028	3	0
4	F	2216	0	2220	8	0
5	A	32	0	12	0	0

Continued on next page...

Continued from previous page...

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	30	0	40	1	0
7	B	6	0	8	0	0
7	C	12	0	16	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	0	0
11	B	12	0	12	3	0
12	B	33	0	0	1	0
13	C	4	0	6	0	0
14	F	31	0	14	0	0
15	A	18	0	0	0	0
15	B	24	0	0	0	0
15	C	86	0	0	0	0
15	D	10	0	0	0	0
15	F	2	0	0	0	0
All	All	17266	0	16585	85	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 (85) 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:264:ARG:HH12	2:B:424[B]:ASN:HD21	1.41	0.68
2:B:199:ASP:OD1	11:B:503:MES:H51	1.99	0.61
4:F:217:ARG:HE	4:F:374:ILE:HA	1.66	0.61
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.83	0.60
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.82	0.60
2:D:1:MET:HE2	2:D:2:ARG:HG2	1.85	0.58
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.41	0.56
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.88	0.55
4:F:202:ARG:HB2	4:F:222:ARG:HH11	1.73	0.54
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:CZ	11:B:503:MES:H61	2.37	0.53
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.49	0.53
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.91	0.53
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.90	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.91	0.52
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.92	0.52
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.91	0.51
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.92	0.51
2:B:199:ASP:OD2	11:B:503:MES:H31	2.12	0.50
2:D:167:ASN:ND2	2:D:200:GLU:HG3	2.27	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.49
2:D:123:ARG:NH2	2:D:160:GLU:OE2	2.42	0.49
2:D:1:MET:N	2:D:50[B]:ASN:OD1	2.45	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.95	0.49
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.95	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.48
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.94	0.48
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.96	0.48
2:D:175:PRO:HA	2:D:178:SER:HB2	1.96	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.47
1:A:117:LEU:HD13	7:A:509:GOL:H32	1.97	0.47
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.96	0.47
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.47
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.46
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.46
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.98	0.46
2:B:141:LEU:HD12	2:B:172:MET:SD	2.56	0.45
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.50	0.45
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.98	0.45
2:D:46:LEU:HA	2:D:49:ILE:HB	1.99	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.97	0.45
2:B:303:ALA:O	2:B:305:CYS:N	2.47	0.45
2:D:269[A]:MET:HE2	2:D:305:CYS:HB2	1.99	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.44
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.44
1:A:166:LYS:HE2	1:A:197:HIS:O	2.17	0.44
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.52	0.44
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.99	0.44
1:A:76:ASP:O	1:A:80:THR:HG22	2.18	0.43
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:397:ALA:O	2:D:401:ARG:NH1	2.51	0.43
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.31	0.43
2:D:392:SER:HB2	2:D:425:MET:HE3	1.99	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.43
2:D:104:ALA:HB2	2:D:413:MET:SD	2.58	0.43
4:F:37:PHE:CE1	4:F:40:MET:HB2	2.54	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.19	0.43
2:B:207:GLU:OE1	2:B:390:ARG:NH1	2.51	0.43
2:D:180:THR:OG1	2:D:181:VAL:N	2.52	0.43
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.00	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.83	0.42
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.22	0.42
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.00	0.42
2:D:346:TRP:CD1	2:D:346:TRP:H	2.36	0.42
3:E:49[B]:GLU:HG2	3:E:53:LYS:HE3	2.01	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.42
2:D:295:MET:CG	2:D:377:PHE:HB2	2.50	0.42
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.54	0.42
1:A:349:THR:HB	3:E:25:LYS:HB3	2.01	0.42
3:E:92:ASN:O	3:E:96:MET:HG2	2.20	0.42
1:C:234:ILE:HG12	1:C:302[A]:MET:HE3	2.01	0.42
4:F:202:ARG:HB2	4:F:222:ARG:NH1	2.34	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.41
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.02	0.41
2:B:31:ASP:OD1	2:B:35:SER:N	2.53	0.40
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.02	0.40
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.03	0.40
1:A:180:ALA:O	1:A:183:GLU:HG3	2.22	0.40
1:A:298:PRO:HA	1:A:301:GLN:CD	2.46	0.40
2:B:7:ILE:O	2:B:137:LEU:HA	2.22	0.40
2:B:296:PHE:O	12:B:506:K9I:O05	2.39	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	437/451 (97%)	425 (97%)	12 (3%)	0	100	100
1	C	445/451 (99%)	437 (98%)	8 (2%)	0	100	100
2	B	425/445 (96%)	417 (98%)	8 (2%)	0	100	100
2	D	419/445 (94%)	410 (98%)	9 (2%)	0	100	100
3	E	119/189 (63%)	118 (99%)	1 (1%)	0	100	100
4	F	250/384 (65%)	241 (96%)	9 (4%)	0	100	100
All	All	2095/2365 (89%)	2048 (98%)	47 (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	94
1	C	380/379 (100%)	378 (100%)	2 (0%)	81	92
2	B	372/383 (97%)	372 (100%)	0	100	100
2	D	366/383 (96%)	365 (100%)	1 (0%)	86	94
3	E	111/171 (65%)	111 (100%)	0	100	100
4	F	243/342 (71%)	243 (100%)	0	100	100
All	All	1845/2037 (91%)	1841 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	THR
1	C	71	GLU
1	C	381	THR
2	D	177	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	300	ASN
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	136	GLN
2	B	334	ASN
1	C	15	GLN
1	C	101	ASN
1	C	107	HIS
1	C	393	HIS
2	D	15	GLN
2	D	167	ASN
3	E	12	ASN
4	F	306	HIS
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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	1.04	4 (12%)	50,54,54	1.53	10 (20%)
7	GOL	A	508	-	5,5,5	0.83	0	5,5,5	1.09	0
7	GOL	B	505	-	5,5,5	1.05	0	5,5,5	0.81	0
13	DMS	C	506	-	3,3,3	0.69	0	3,3,3	0.71	0
7	GOL	A	505	-	5,5,5	0.97	0	5,5,5	1.04	0
7	GOL	C	505	-	5,5,5	0.82	0	5,5,5	1.14	0
7	GOL	A	507	-	5,5,5	0.89	0	5,5,5	1.16	1 (20%)
10	GDP	B	501	6	29,30,30	1.25	3 (10%)	45,47,47	1.78	8 (17%)
7	GOL	A	509	-	5,5,5	1.08	0	5,5,5	0.94	0
11	MES	B	503	-	12,12,12	2.04	1 (8%)	15,16,16	2.04	6 (40%)
7	GOL	C	503	-	5,5,5	0.94	0	5,5,5	1.02	0
14	ACP	F	401	-	31,33,33	0.66	1 (3%)	47,52,52	1.04	1 (2%)
7	GOL	A	503	-	5,5,5	0.86	0	5,5,5	1.19	1 (20%)
12	K9I	B	506	-	34,34,34	1.71	4 (11%)	42,48,48	1.32	5 (11%)
10	GDP	D	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
5	GTP	A	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.62	11 (22%)

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
7	GOL	A	508	-	-	2/4/4/4	-
7	GOL	B	505	-	-	0/4/4/4	-
7	GOL	A	505	-	-	0/4/4/4	-
7	GOL	C	505	-	-	0/4/4/4	-
7	GOL	A	507	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GDP	B	501	6	-	5/16/32/32	0/3/3/3
7	GOL	A	509	-	-	0/4/4/4	-
11	MES	B	503	-	-	2/6/14/14	0/1/1/1
7	GOL	C	503	-	-	0/4/4/4	-
14	ACP	F	401	-	-	3/19/38/38	0/3/3/3
7	GOL	A	503	-	-	1/4/4/4	-
12	K9I	B	506	-	-	15/50/50/50	0/1/2/2
10	GDP	D	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	503	MES	C8-S	-6.71	1.68	1.77
12	B	506	K9I	O31-C29	5.20	1.46	1.34
12	B	506	K9I	C15-C18	4.66	1.62	1.54
14	F	401	ACP	PB-O3A	3.09	1.61	1.58
10	B	501	GDP	C5-C4	3.06	1.47	1.38
10	D	501	GDP	C5-C4	3.06	1.47	1.38
10	B	501	GDP	PA-O3A	2.93	1.62	1.59
10	B	501	GDP	C6-N1	-2.61	1.34	1.38
5	C	501	GTP	PA-O3A	2.53	1.62	1.59
12	B	506	K9I	C03-C06	2.51	1.54	1.49
10	D	501	GDP	C6-N1	-2.38	1.34	1.38
5	C	501	GTP	PB-O3B	2.35	1.62	1.59
10	D	501	GDP	C5-N7	-2.10	1.34	1.39
12	B	506	K9I	O31-C09	-2.09	1.42	1.45
5	C	501	GTP	PB-O3A	2.02	1.61	1.59
5	A	501	GTP	C2-N3	2.01	1.38	1.33
5	C	501	GTP	C2-N3	2.00	1.38	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	401	ACP	PB-O3A-PA	-6.96	109.67	132.37
10	B	501	GDP	C5-C4-N3	-6.01	118.83	128.39
10	D	501	GDP	C5-C4-N3	-6.00	118.83	128.39
10	B	501	GDP	C2-N3-C4	5.08	121.06	112.30
10	D	501	GDP	C2-N3-C4	4.91	120.75	112.30
12	B	506	K9I	O31-C29-C27	4.74	118.64	111.13
11	B	503	MES	C5-N4-C3	4.72	119.02	108.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C4-N3	-4.68	120.94	128.39
5	A	501	GTP	C2-N3-C4	4.54	120.12	112.30
5	C	501	GTP	C5-C4-N3	-4.52	121.19	128.39
10	B	501	GDP	N9-C4-N3	4.49	134.94	125.95
10	D	501	GDP	N9-C4-N3	4.46	134.88	125.95
5	C	501	GTP	C2-N3-C4	4.38	119.85	112.30
10	B	501	GDP	C6-C5-N7	3.49	136.64	130.29
10	D	501	GDP	C6-C5-N7	3.21	136.14	130.29
11	B	503	MES	C7-N4-C3	2.94	119.08	111.24
12	B	506	K9I	C08-C07-C09	-2.88	108.42	114.94
12	B	506	K9I	C10-C09-C07	-2.82	108.71	113.28
5	C	501	GTP	N9-C8-N7	-2.72	108.35	113.40
5	C	501	GTP	N9-C4-N3	2.70	131.35	125.95
5	A	501	GTP	N9-C8-N7	-2.69	108.40	113.40
10	B	501	GDP	C4-C5-N7	-2.61	106.54	110.67
10	D	501	GDP	C4-C5-N7	-2.61	106.54	110.67
5	A	501	GTP	C8-N7-C5	2.59	108.88	104.26
5	A	501	GTP	N9-C4-N3	2.59	131.14	125.95
10	B	501	GDP	O2A-PA-O3A	2.57	114.22	107.27
5	A	501	GTP	O2B-PB-O3B	2.56	114.20	107.27
5	C	501	GTP	C2-N1-C6	-2.54	120.50	125.11
5	A	501	GTP	C2-N1-C6	-2.51	120.55	125.11
5	C	501	GTP	C8-N7-C5	2.49	108.70	104.26
11	B	503	MES	O1S-S-C8	2.44	110.42	106.73
5	C	501	GTP	C5-C6-N1	2.40	119.36	113.25
5	C	501	GTP	O2A-PA-O3A	2.39	113.73	107.27
5	A	501	GTP	C5-C6-N1	2.35	119.24	113.25
5	A	501	GTP	O2G-PG-O3B	2.31	112.40	104.64
5	A	501	GTP	O3B-PB-O1B	-2.25	103.93	110.70
11	B	503	MES	C7-N4-C5	2.19	117.07	111.24
5	C	501	GTP	O3'-C3'-C4'	-2.16	104.87	111.08
5	C	501	GTP	O6-C6-C5	-2.09	121.02	126.53
11	B	503	MES	O2S-S-C8	2.08	109.87	106.73
11	B	503	MES	C2-C3-N4	-2.08	106.97	110.12
12	B	506	K9I	C20-C24-C25	-2.07	109.62	113.39
5	A	501	GTP	C4-C5-N7	-2.06	107.41	110.67
10	D	501	GDP	O6-C6-C5	-2.05	121.12	126.53
12	B	506	K9I	C12-C13-C15	-2.03	113.19	115.49
7	A	503	GOL	C3-C2-C1	-2.03	104.34	111.80
10	B	501	GDP	O6-C6-C5	-2.03	121.18	126.53
10	B	501	GDP	C5-C6-N1	2.01	118.37	113.25
7	A	507	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (44) 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
10	B	501	GDP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O2A
12	B	506	K9I	C09-C10-C11-O32
12	B	506	K9I	O14-C13-C15-C17
12	B	506	K9I	C03-C06-C07-C09
12	B	506	K9I	C09-C10-C11-C12
12	B	506	K9I	C03-C06-C07-C08
11	B	503	MES	C8-C7-N4-C3
11	B	503	MES	C8-C7-N4-C5
5	C	501	GTP	PB-O3B-PG-O1G
12	B	506	K9I	C10-C11-O32-C33
12	B	506	K9I	C12-C11-O32-C33
12	B	506	K9I	C25-C27-C29-O31
5	C	501	GTP	C5'-O5'-PA-O2A
10	B	501	GDP	C5'-O5'-PA-O2A
14	F	401	ACP	C5'-O5'-PA-O1A
14	F	401	ACP	C5'-O5'-PA-O2A
14	F	401	ACP	C5'-O5'-PA-O3A
7	A	508	GOL	O1-C1-C2-C3
10	B	501	GDP	PB-O3A-PA-O2A
12	B	506	K9I	C16-C15-C18-C19
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
12	B	506	K9I	C16-C15-C18-C23
12	B	506	K9I	C12-C13-C15-C17
12	B	506	K9I	O14-C13-C15-C16
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
12	B	506	K9I	C21-C20-C24-C25
12	B	506	K9I	C17-C15-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	503	GOL	O2-C2-C3-O3
7	A	508	GOL	O1-C1-C2-O2
12	B	506	K9I	C19-C20-C24-C25
10	B	501	GDP	PB-O3A-PA-O1A

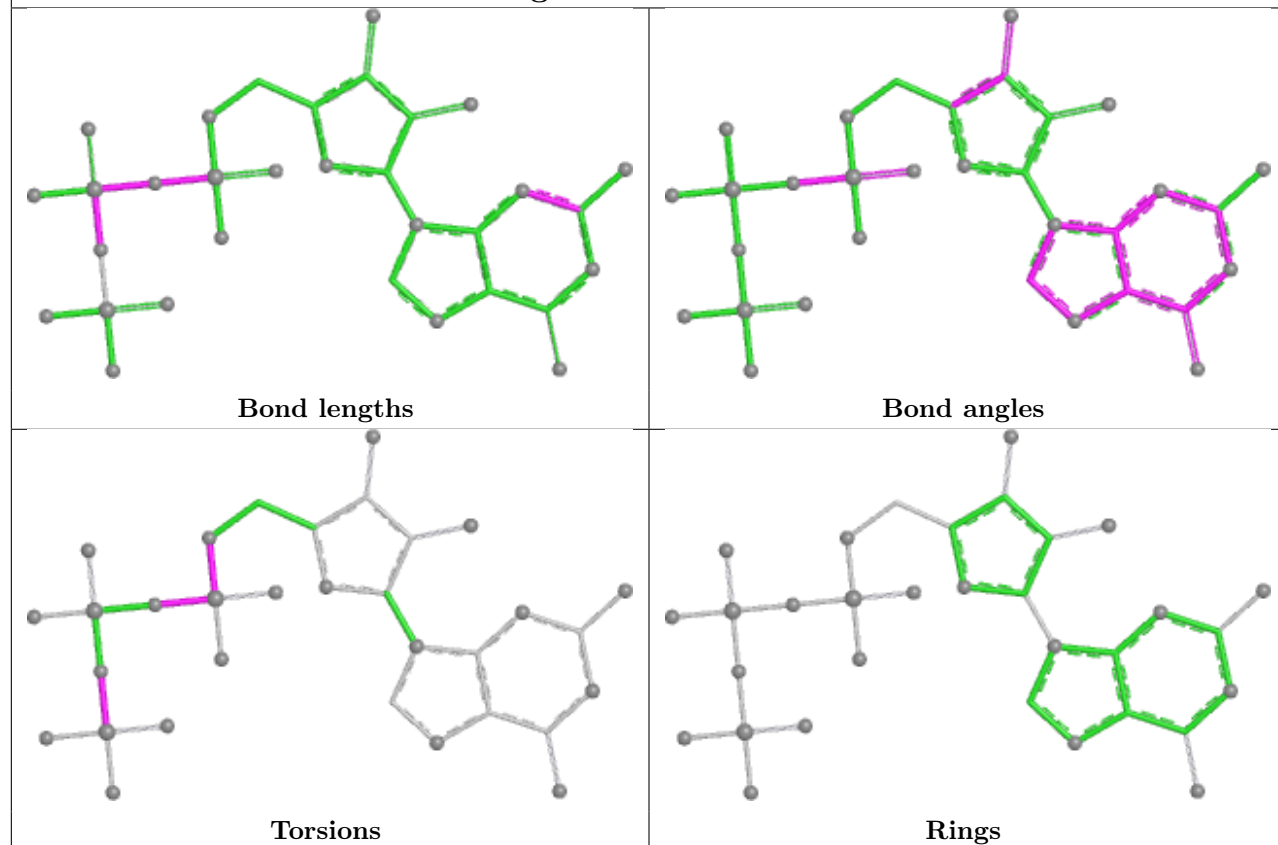
There are no ring outliers.

3 monomers are involved in 5 short contacts:

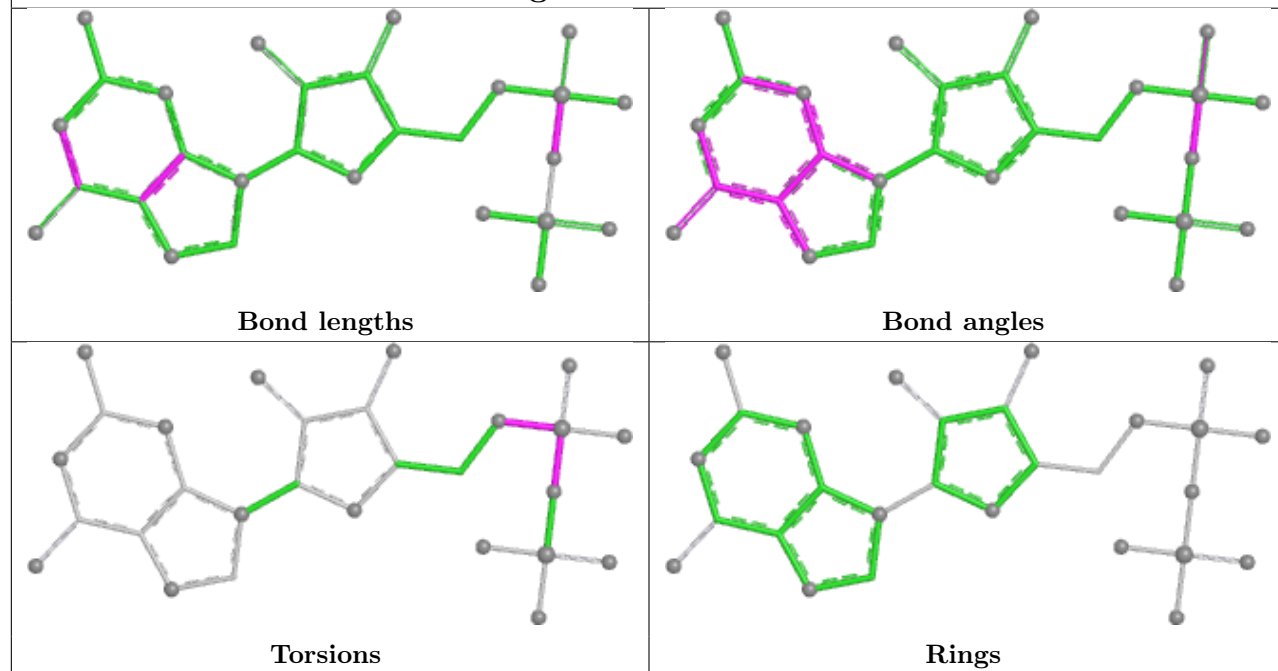
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	509	GOL	1	0
11	B	503	MES	3	0
12	B	506	K9I	1	0

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.

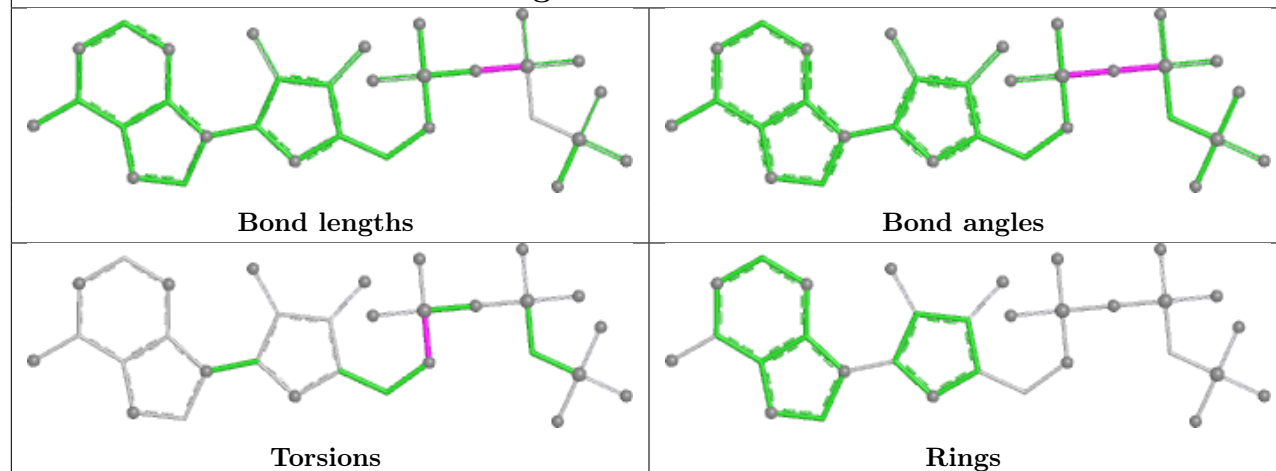
Ligand GTP C 501



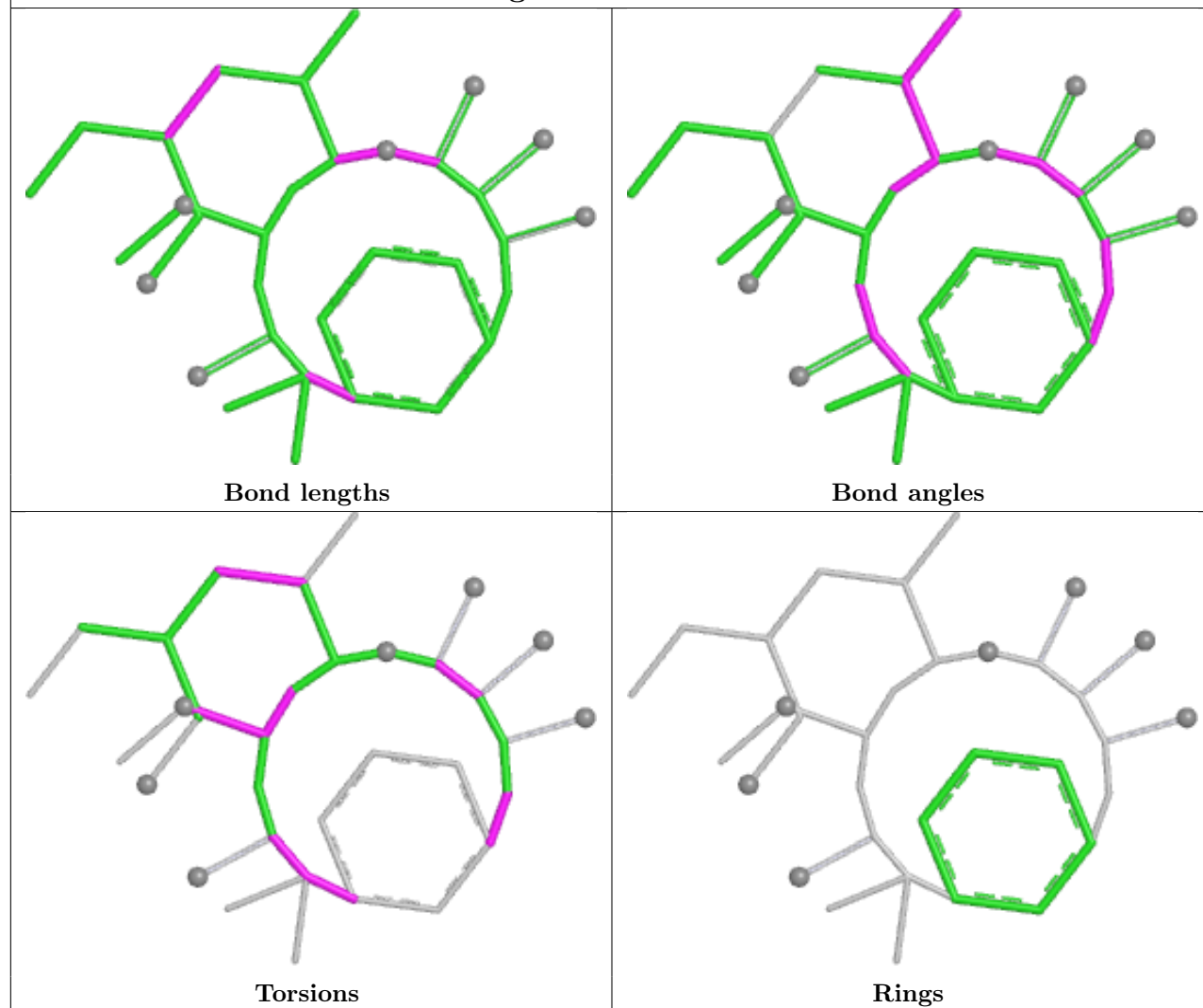
Ligand GDP B 501

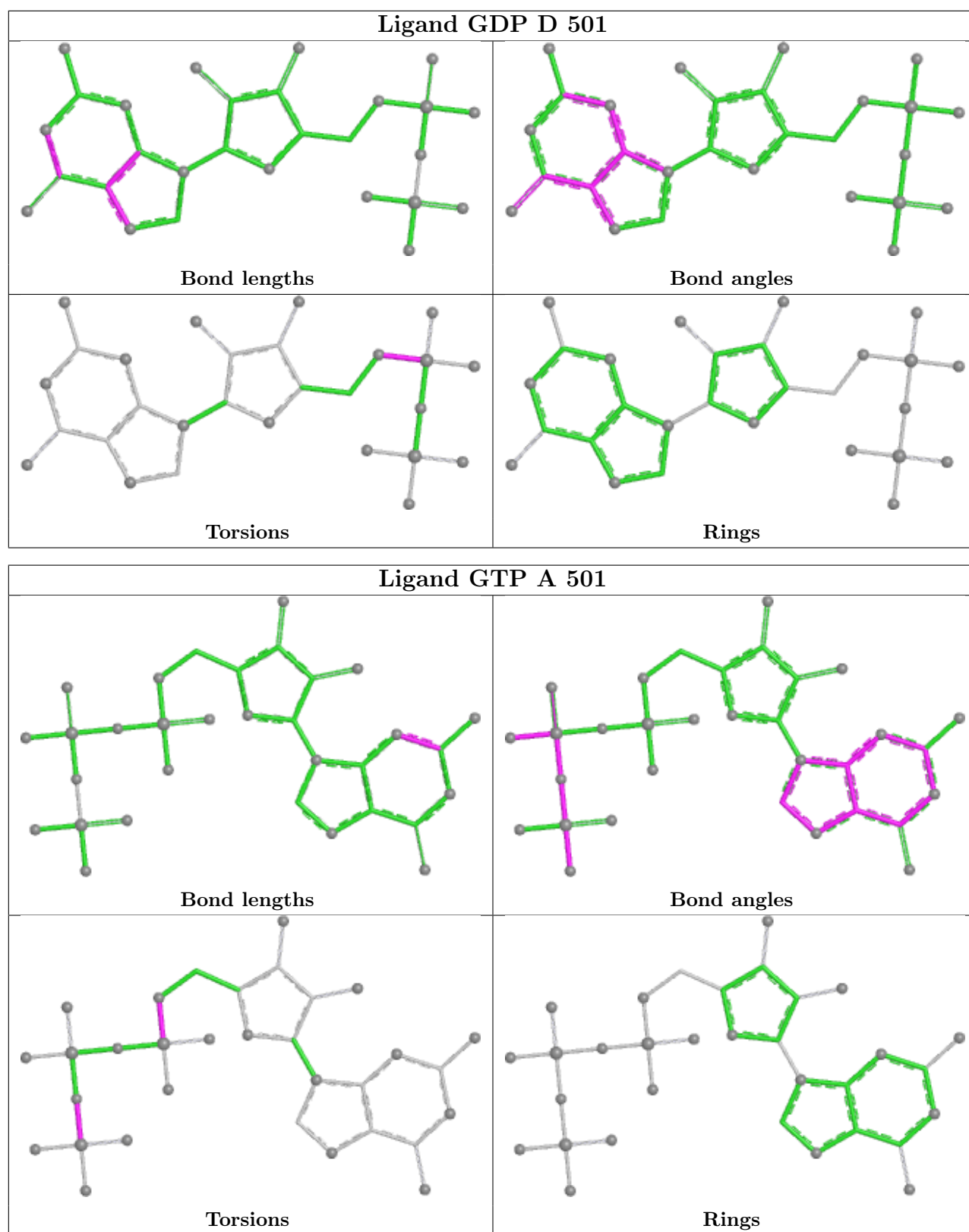


Ligand ACP F 401



Ligand K9I B 506





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	434/451 (96%)	0.14	9 (2%) 63 59	26, 59, 96, 120	7 (1%)
1	C	439/451 (97%)	-0.10	8 (1%) 67 64	19, 47, 74, 104	10 (2%)
2	B	423/445 (95%)	0.01	5 (1%) 76 73	19, 53, 86, 142	8 (1%)
2	D	421/445 (94%)	0.48	16 (3%) 44 39	32, 72, 106, 150	4 (0%)
3	E	120/189 (63%)	0.64	13 (10%) 11 9	29, 72, 112, 124	3 (2%)
4	F	268/384 (69%)	1.32	59 (22%) 2 2	53, 95, 130, 154	5 (1%)
All	All	2105/2365 (89%)	0.31	110 (5%) 33 29	19, 62, 109, 154	37 (1%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	5.3
4	F	182	ILE	4.9
4	F	102	PRO	4.2
1	C	440	VAL	4.1
4	F	166	ALA	3.9
4	F	186	LEU	3.8
2	D	247	GLN	3.5
1	A	437	VAL	3.5
4	F	361	LEU	3.4
4	F	91	CYS	3.4
3	E	27	PRO	3.3
4	F	344	ALA	3.2
4	F	320	MET	3.1
3	E	140	LYS	3.1
4	F	201	ILE	3.1
1	C	357	TYR	3.0
4	F	376	ILE	3.0
1	C	283	HIS	2.9
2	D	407	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	87	LEU	2.9
4	F	199	PHE	2.9
4	F	256	TYR	2.9
4	F	33	ASP	2.8
4	F	99	VAL	2.8
2	D	286	LEU	2.7
4	F	190	LEU	2.7
4	F	229	ASN	2.7
4	F	321	VAL	2.7
4	F	373	SER	2.7
4	F	346	LEU	2.7
3	E	52	LYS	2.7
1	A	88	HIS	2.7
4	F	227	PRO	2.7
2	B	284	ARG	2.7
1	C	284	GLU	2.7
3	E	44	ASP	2.6
3	E	23	ILE	2.6
4	F	148	ILE	2.6
1	C	163	LYS	2.6
4	F	189	PRO	2.6
4	F	283	ILE	2.6
1	A	262	TYR	2.6
4	F	223	THR	2.6
4	F	85	PRO	2.6
4	F	194	PRO	2.6
4	F	295	LEU	2.5
1	C	285	GLN	2.5
2	B	247	GLN	2.5
4	F	17	VAL	2.5
4	F	379	HIS	2.5
4	F	71	LEU	2.5
3	E	115[A]	HIS	2.5
3	E	126	LYS	2.5
4	F	332	VAL	2.5
1	A	80	THR	2.5
4	F	330	ILE	2.5
2	B	438	ALA	2.5
3	E	6	MET	2.5
4	F	298	ILE	2.5
2	D	275	LEU	2.5
4	F	337	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	283	TYR	2.4
4	F	147	TRP	2.4
1	A	329	ASN	2.4
4	F	220	VAL	2.4
1	A	337	THR	2.4
3	E	49[A]	GLU	2.4
2	D	128	SER	2.4
4	F	100	ILE	2.4
2	D	217	LEU	2.4
4	F	200	ASP	2.4
2	D	372	LYS	2.4
2	D	179	ASP	2.3
4	F	101	TYR	2.3
4	F	317	PHE	2.3
3	E	7	GLU	2.3
4	F	26	GLN	2.3
1	C	338	LYS	2.3
2	D	57	THR	2.2
4	F	291	ILE	2.2
1	C	339	ARG	2.2
2	D	181	VAL	2.2
4	F	162	ILE	2.2
4	F	280	GLU	2.2
3	E	26	PRO	2.2
1	A	338	LYS	2.2
4	F	253	TYR	2.2
3	E	45	PRO	2.2
4	F	360	PRO	2.2
3	E	90	ASN	2.2
4	F	191	LEU	2.1
4	F	31	ARG	2.1
4	F	380	HIS	2.1
4	F	374	ILE	2.1
2	B	298	SER	2.1
2	D	414	ASP	2.1
1	A	77	GLU	2.1
4	F	64	TYR	2.1
4	F	336	PRO	2.1
4	F	252	ASN	2.1
4	F	296	MET	2.1
2	D	177	VAL	2.0
1	A	46	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	441	ASP	2.0
4	F	18	SER	2.0
4	F	32	LYS	2.0
4	F	328	TRP	2.0
2	D	416	MET	2.0
4	F	1	MET	2.0
2	D	37	HIS	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
7	GOL	C	503	6/6	0.62	0.17	65,72,76,79	0
7	GOL	A	509	6/6	0.64	0.20	72,75,83,93	0
7	GOL	A	505	6/6	0.74	0.21	65,69,73,74	6
14	ACP	F	401	31/31	0.75	0.15	96,102,108,113	31
13	DMS	C	506	4/4	0.80	0.29	48,63,65,76	4
7	GOL	A	503	6/6	0.80	0.20	60,64,65,67	6
7	GOL	A	507	6/6	0.84	0.17	60,60,67,75	0
7	GOL	A	508	6/6	0.86	0.15	58,63,65,68	0
7	GOL	B	505	6/6	0.87	0.14	61,64,65,68	0
6	MG	D	502	1/1	0.88	0.10	68,68,68,68	0
7	GOL	C	505	6/6	0.89	0.19	55,57,65,75	0
12	K9I	B	506	33/33	0.89	0.12	54,62,69,71	0
8	CL	A	504	1/1	0.92	0.09	71,71,71,71	0
10	GDP	D	501	28/28	0.93	0.10	60,67,74,84	0
11	MES	B	503	12/12	0.94	0.12	43,47,58,60	12
10	GDP	B	501	28/28	0.98	0.05	30,40,43,49	0

Continued on next page...

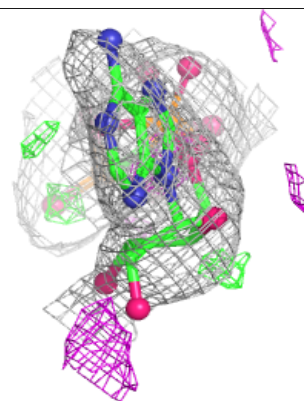
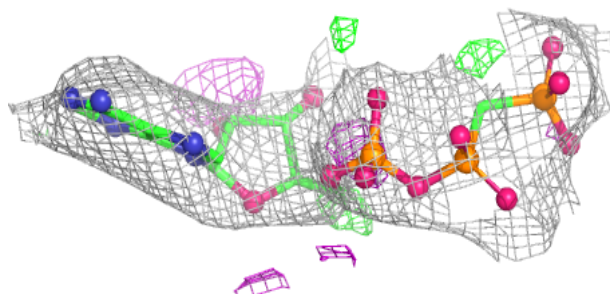
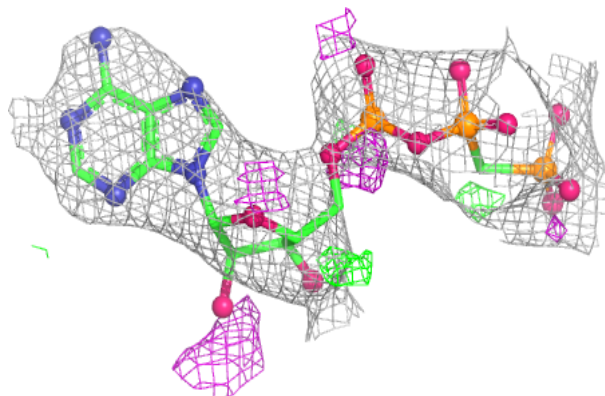
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	0.98	0.05	37,42,47,49	0
9	CA	B	504	1/1	0.98	0.14	79,79,79,79	0
6	MG	C	502	1/1	0.99	0.02	38,38,38,38	0
5	GTP	C	501	32/32	0.99	0.04	29,37,42,45	0
6	MG	A	502	1/1	0.99	0.03	40,40,40,40	0
9	CA	A	506	1/1	0.99	0.05	79,79,79,79	0
6	MG	B	502	1/1	0.99	0.02	35,35,35,35	0
9	CA	C	504	1/1	0.99	0.05	58,58,58,58	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.

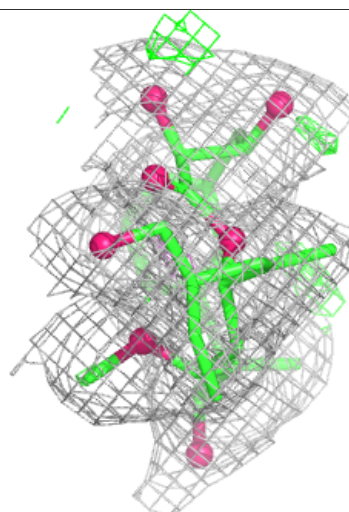
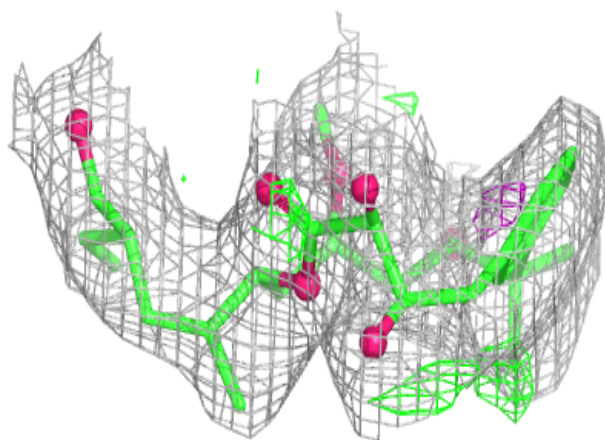
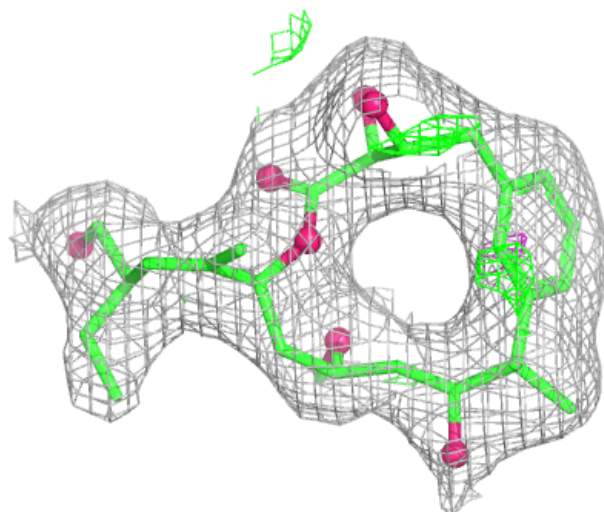
Electron density around ACP F 401:

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



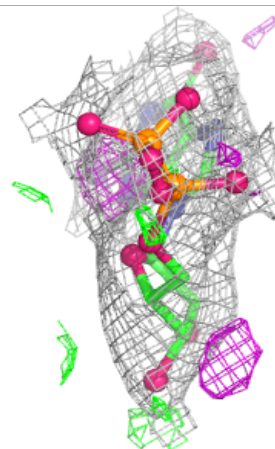
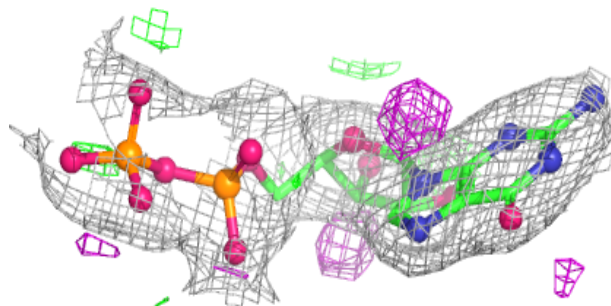
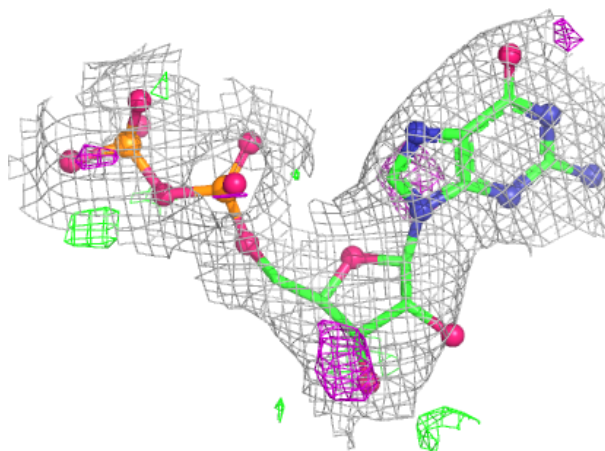
Electron density around K9I B 506:

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



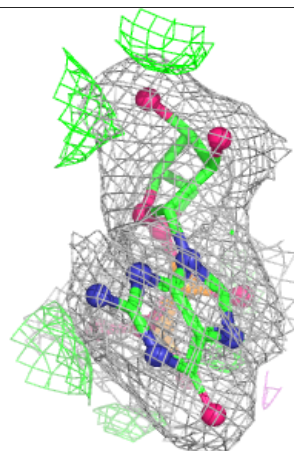
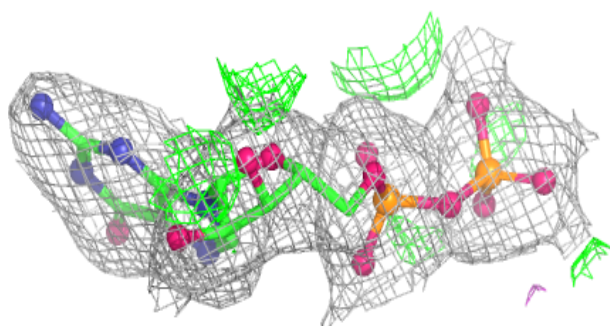
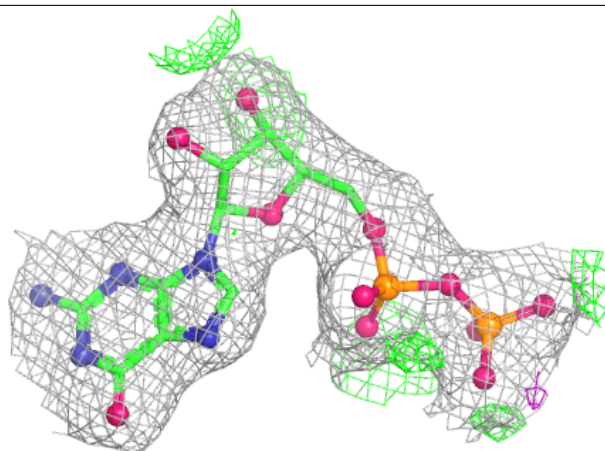
Electron density around GDP D 501:

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

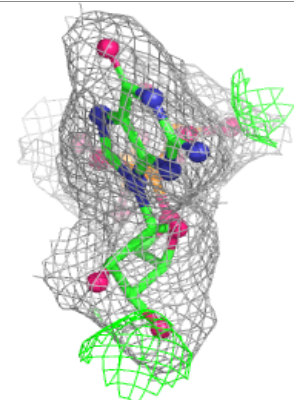
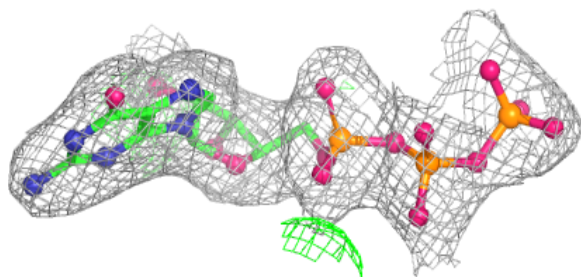
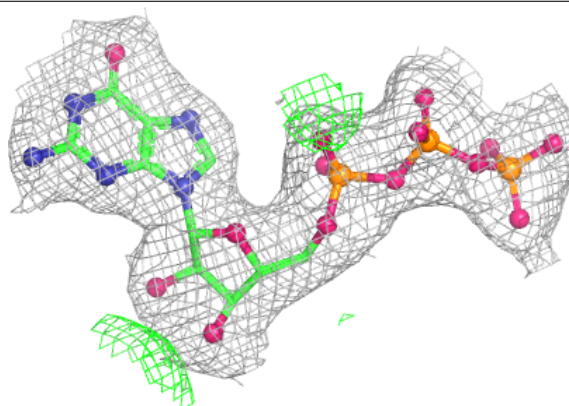


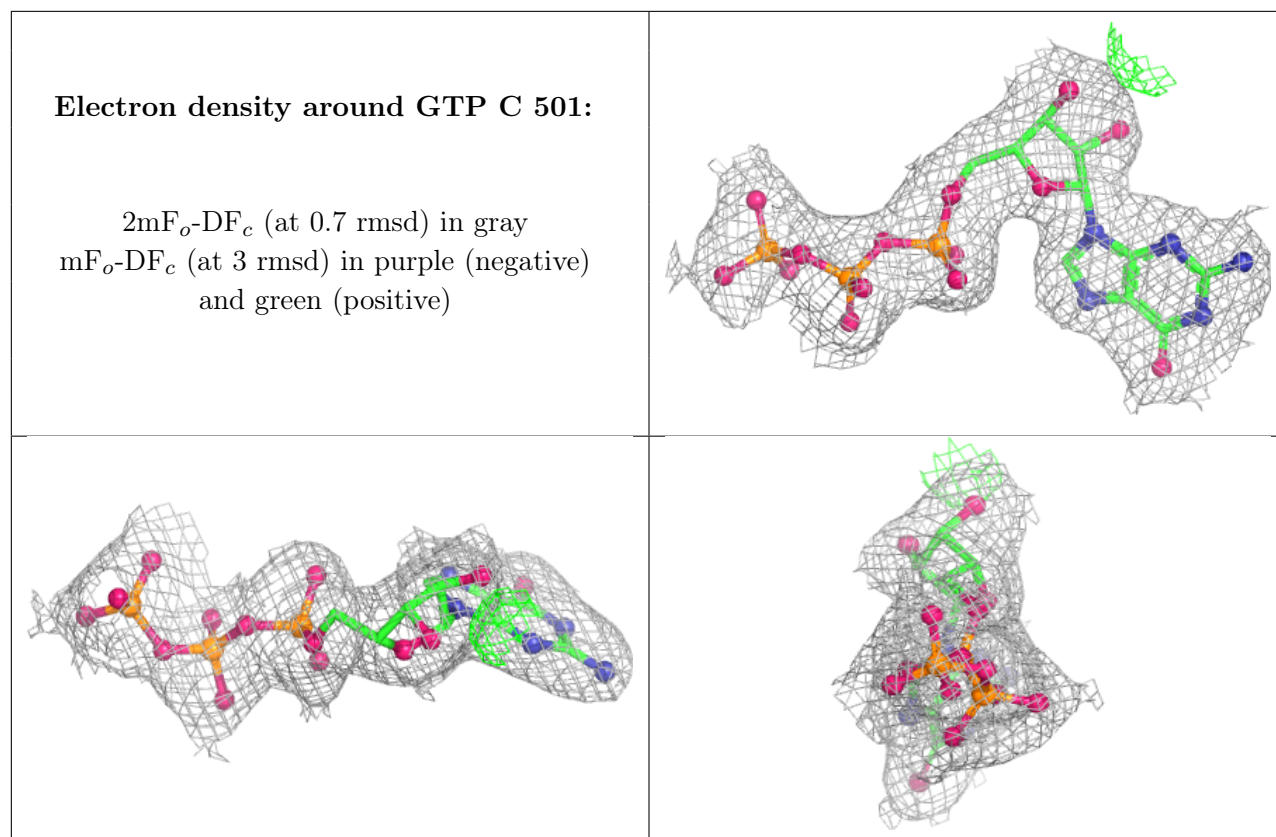
Electron density around GDP B 501:

$2mF_o-DF_c$ (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.