



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:46 PM UTC

PDB ID : 5XAG / pdb_00005xag
Title : Crystal structure of tubulin-stathmin-TTL-Compound Z2 complex
Authors : Zhang, H.; Luo, C.; Wang, Y.
Deposited on : 2017-03-12
Resolution : 2.56 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

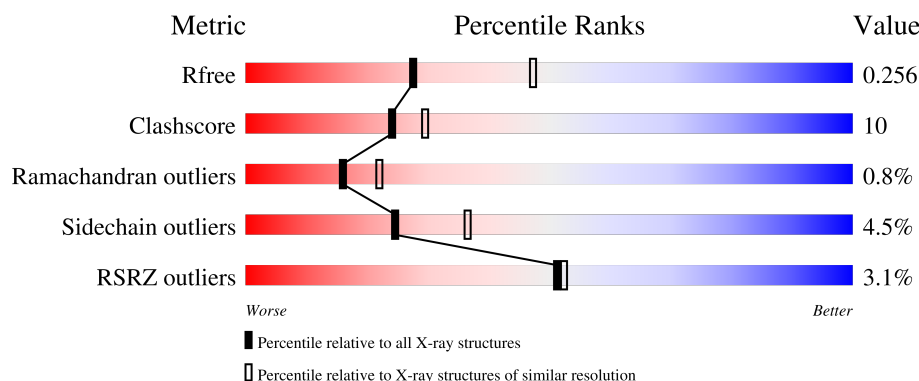
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	2% 76% 20% • •
1	C	451	% 80% 16% • •
2	B	445	2% 71% 23% • 5%
2	D	445	2% 66% 27% • 5%
3	E	189	% 47% 15% • 37%

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Mol	Chain	Length	Quality of chain
4	F	378	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	B	505	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17705 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	439	Total	C	N	O	S	0	10	0
			3476	2206	585	660	25			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2204	588	667	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	9	0
			3376	2125	569	655	27			
2	D	421	Total	C	N	O	S	0	3	0
			3321	2089	562	642	28			

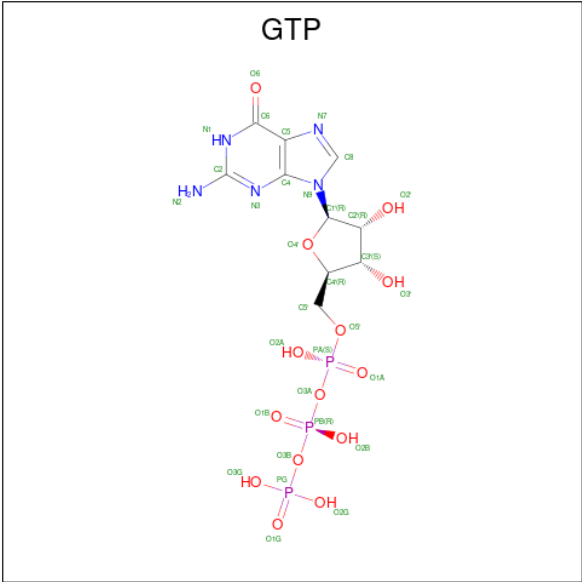
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	1	0
			997	616	181	195	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	3	0
			2609	1689	434	472	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

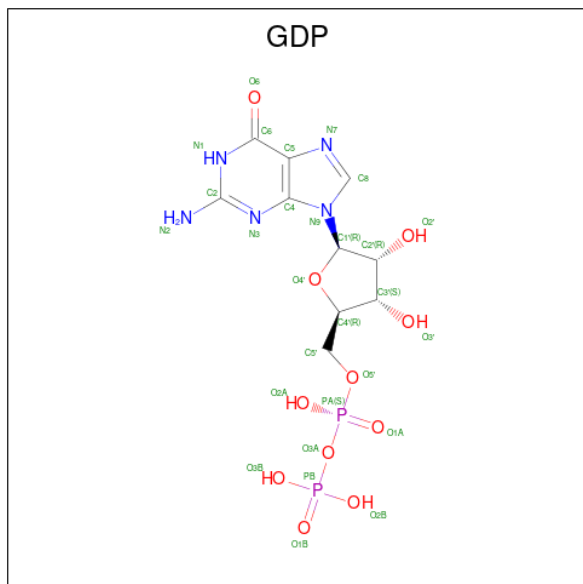


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

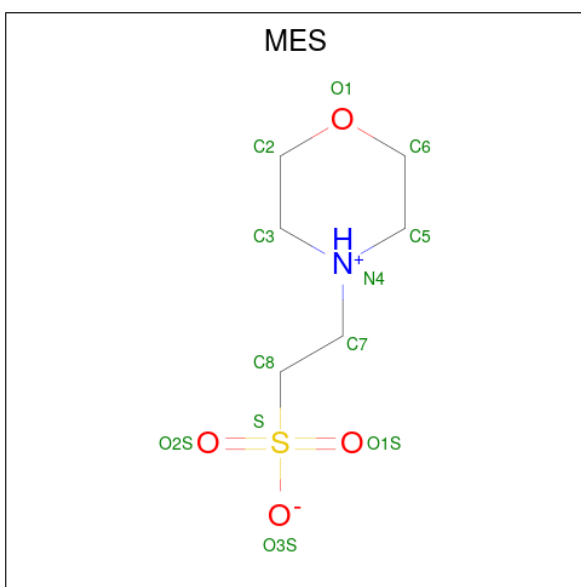
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0
8	B	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

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



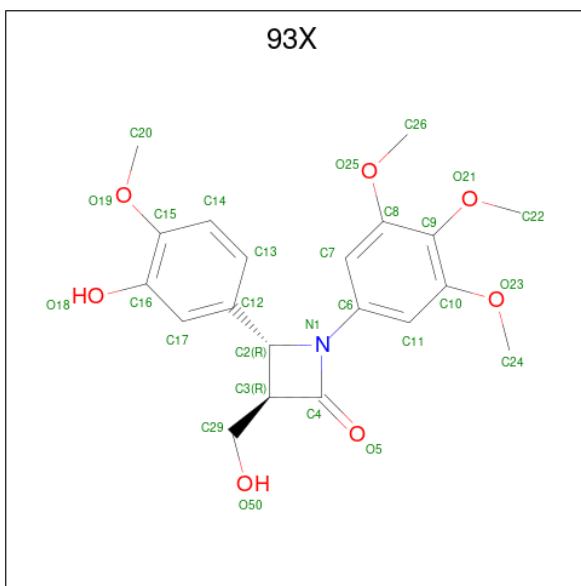
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O P 28 10 5 11 2	0	0
9	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



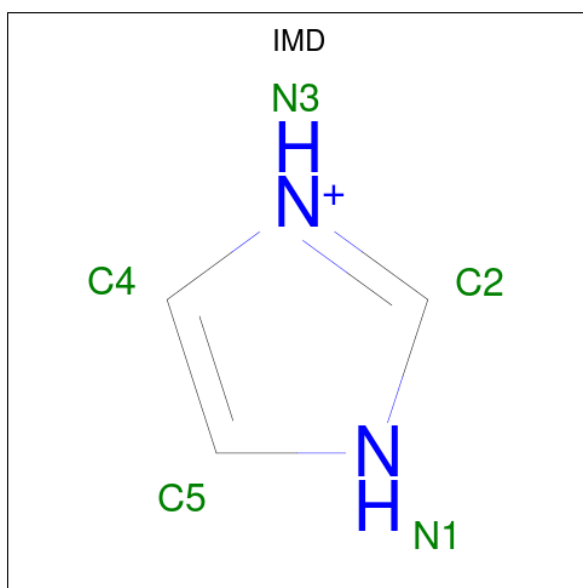
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3 {R},4 {R})-3-(hydroxymethyl)-4-(4-methoxy-3-oxidanyl-phenyl)-1-(3,4,5-trimethoxyphenyl)azetidin-2-one (CCD ID: 93X) (formula: C₂₀H₂₃NO₇).



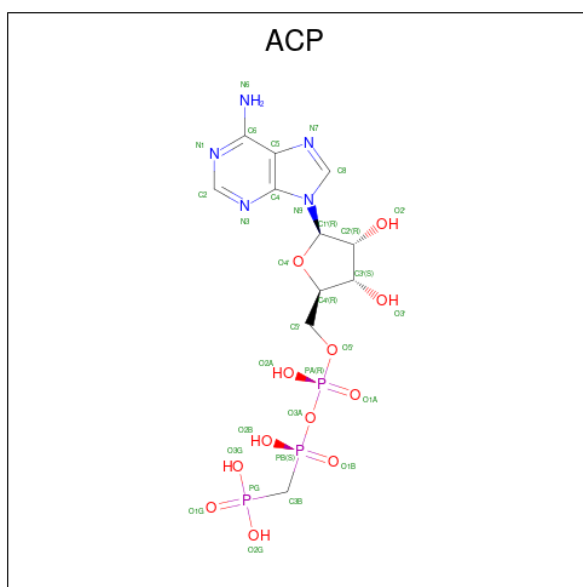
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O		0	0
			28	20	1	7			
11	D	1	Total	C	N	O		0	0
			28	20	1	7			

- Molecule 12 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



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

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



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

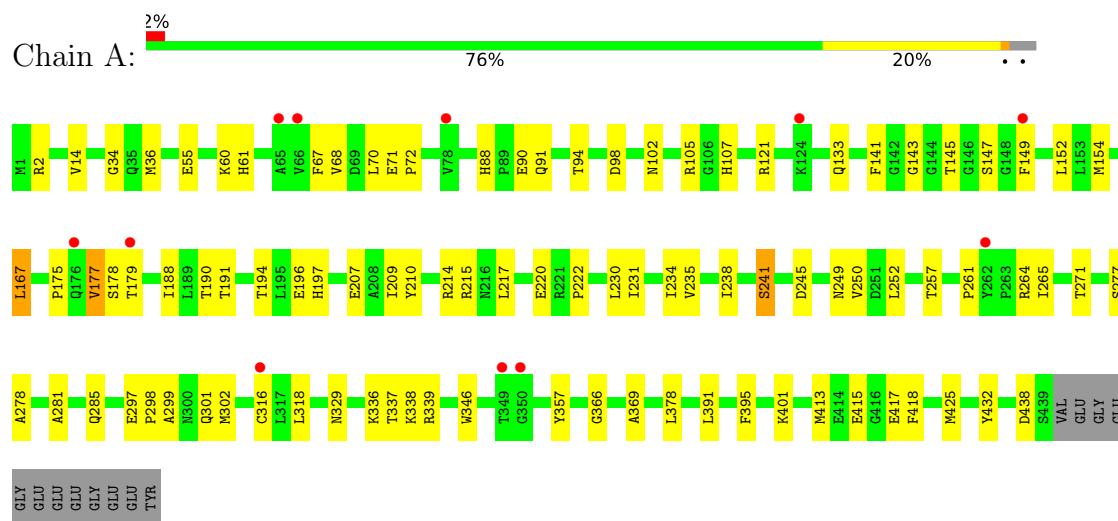
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	20	Total	O	0	0
			20	20		
14	B	20	Total	O	0	0
			20	20		
14	C	48	Total	O	0	0
			48	48		
14	D	9	Total	O	0	0
			9	9		
14	E	15	Total	O	0	0
			15	15		
14	F	18	Total	O	0	0
			18	18		

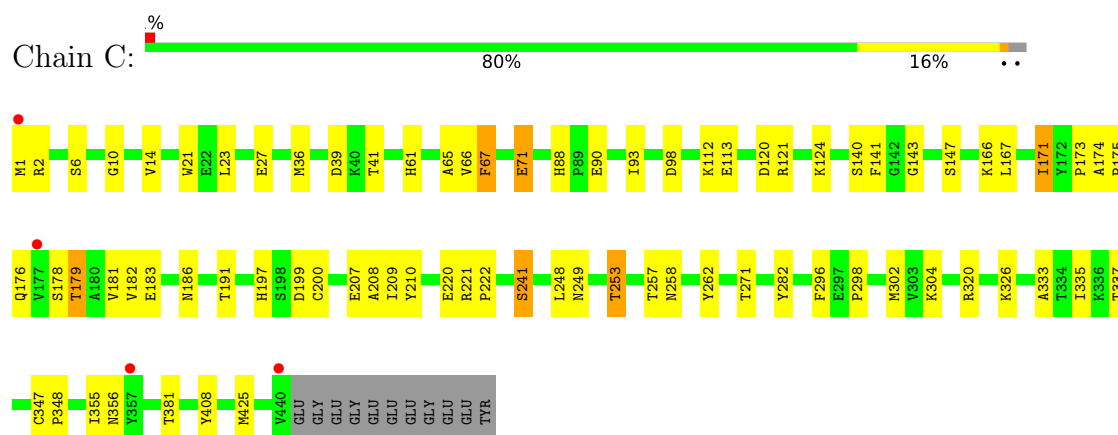
3 Residue-property plots

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.

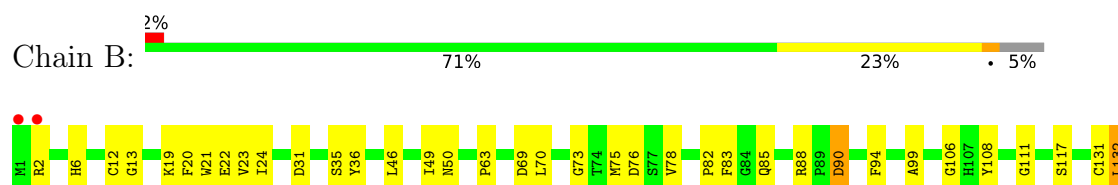
• Molecule 1: Tubulin alpha-1B chain

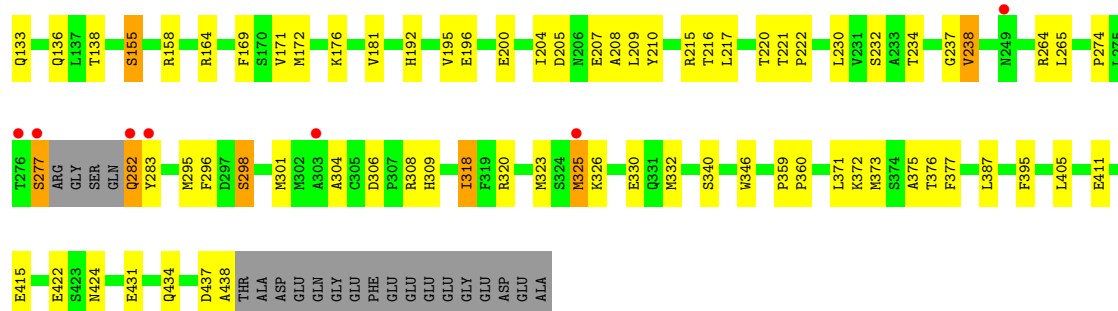


• Molecule 1: Tubulin alpha-1B chain

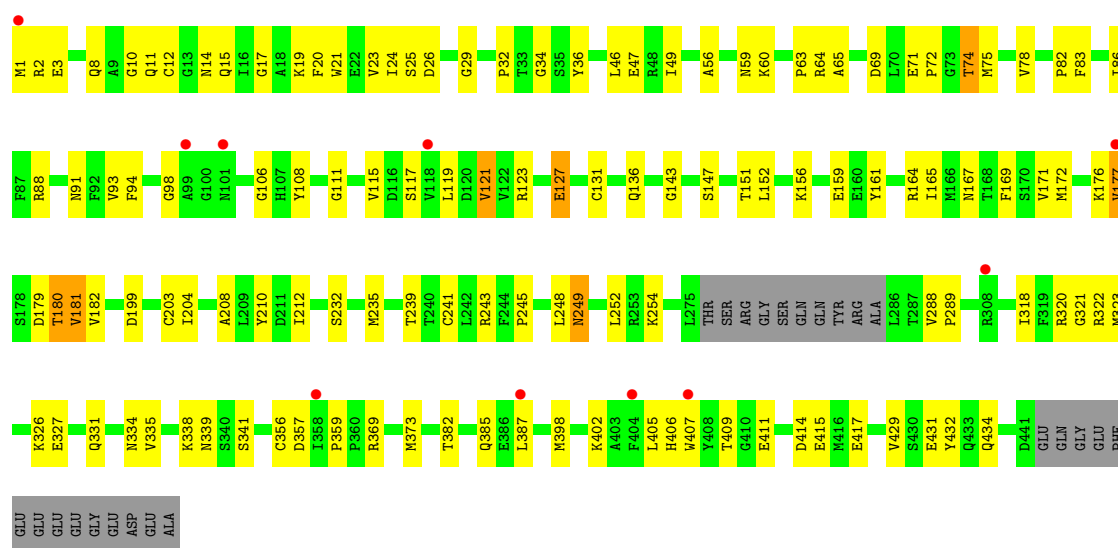


• Molecule 2: Tubulin beta-2B chain

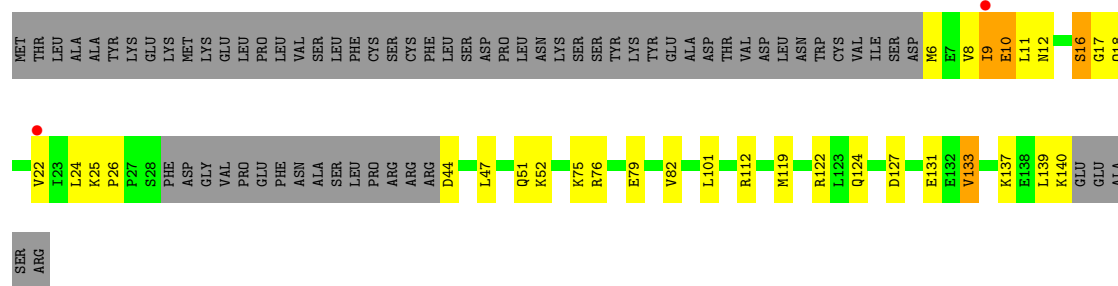




• Molecule 2: Tubulin beta-2B chain



• 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	104.27Å 156.12Å 182.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.56 47.92 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.56) 99.9 (47.92-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.255 0.212 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17705	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: GOL, ACP, GTP, MES, GDP, 93X, MG, CA, IMD

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	0.38	0/3584	0.60	0/4865
1	C	0.45	0/3584	0.66	2/4867 (0.0%)
2	B	0.41	0/3474	0.61	0/4706
2	D	0.35	0/3403	0.55	0/4611
3	E	0.43	0/1008	0.59	0/1337
4	F	0.34	1/2674 (0.0%)	0.52	0/3609
All	All	0.39	1/17727 (0.0%)	0.59	2/23995 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	47	LEU	C-N	6.33	1.48	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ILE	CA-C-N	5.41	131.21	120.94
1	C	171	ILE	C-N-CA	5.41	131.21	120.94

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	3476	0	3417	60	0
1	C	3482	0	3401	51	1
2	B	3376	0	3265	68	1
2	D	3321	0	3210	82	0
3	E	997	0	1020	23	0
4	F	2609	0	2599	76	0
5	A	32	0	12	2	0
5	C	32	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	18	0	24	1	0
7	B	18	0	24	6	0
7	C	24	0	32	3	0
7	D	12	0	15	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	12	0	12	0	0
11	B	28	0	0	0	0
11	D	28	0	0	1	0
12	C	10	0	10	3	0
12	E	5	0	4	2	0
13	F	31	0	14	1	0
14	A	20	0	0	3	0
14	B	20	0	0	2	0
14	C	48	0	0	0	0
14	D	9	0	0	4	0
14	E	15	0	0	1	0
14	F	18	0	0	9	0
All	All	17705	0	17095	345	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (345) 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:D:411:GLU:HA	3:E:137:LYS:HD2	1.61	0.82
4:F:145:ASN:HB3	4:F:147:TRP:HE1	1.45	0.82
4:F:186:LEU:HD23	4:F:320:MET:HE3	1.61	0.81
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.13	0.81
4:F:31:ARG:HE	4:F:32:LYS:H	1.28	0.81
2:B:217:LEU:HD22	2:B:277:SER:HB3	1.63	0.81
2:D:180:THR:OG1	2:D:181:VAL:N	2.08	0.79
2:B:320:ARG:HH11	7:B:505:GOL:H11	1.49	0.77
2:D:17:GLY:O	14:D:601:HOH:O	2.02	0.77
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.19	0.75
4:F:373:SER:N	14:F:505:HOH:O	2.19	0.75
5:A:501:GTP:O3G	14:A:601:HOH:O	2.05	0.74
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.22	0.73
1:C:199:ASP:OD1	7:C:506:GOL:H31	1.90	0.72
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.23	0.71
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.73	0.71
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.26	0.71
4:F:150:LYS:O	14:F:501:HOH:O	2.08	0.70
4:F:135:TYR:OH	14:F:502:HOH:O	2.09	0.70
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.73	0.69
2:D:334:ASN:HD21	2:D:338:LYS:HE2	1.57	0.69
2:D:10:GLY:O	2:D:14:ASN:ND2	2.21	0.67
2:D:75:MET:HE2	2:D:94:PHE:HD1	1.60	0.67
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.78	0.66
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.29	0.66
1:A:241:SER:HB2	1:A:249:ASN:O	1.95	0.66
2:D:321:GLY:HA2	2:D:359:PRO:HG3	1.78	0.65
2:B:2:ARG:HA	2:B:131:CYS:O	1.96	0.65
2:D:11:GLN:HB3	9:D:501:GDP:O2A	1.95	0.65
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.29	0.65
2:D:21:TRP:O	2:D:25:SER:OG	2.09	0.65
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.62	0.65
3:E:112:ARG:HE	12:E:201:IMD:H5	1.61	0.65
2:D:1:MET:HE2	2:D:2:ARG:HG2	1.79	0.65
2:D:123:ARG:O	2:D:127:GLU:HG2	1.97	0.65
4:F:187:GLU:OE2	14:F:503:HOH:O	2.16	0.63
4:F:373:SER:OG	4:F:374:ILE:N	2.30	0.63
4:F:162:ILE:HD11	4:F:240:LEU:HD13	1.80	0.63
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.72	0.62
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.81	0.62
2:B:376:THR:OG1	7:B:505:GOL:H31	1.99	0.62
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:HIS:HA	2:D:409:THR:HG22	1.81	0.62
4:F:184:LYS:NZ	4:F:187:GLU:OE2	2.33	0.62
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.82	0.61
2:B:106:GLY:O	2:B:111:GLY:HA3	2.00	0.61
3:E:44:ASP:N	14:E:301:HOH:O	2.33	0.61
2:B:155[B]:SER:OG	3:E:76:ARG:NH2	2.32	0.61
2:B:76:ASP:N	14:B:604:HOH:O	2.34	0.61
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.82	0.61
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.81	0.61
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.18	0.60
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.84	0.60
7:A:506:GOL:O2	3:E:44:ASP:OD2	2.20	0.60
1:C:39:ASP:OD2	1:C:41:THR:OG1	2.18	0.60
4:F:166:ALA:N	14:F:502:HOH:O	2.34	0.60
3:E:9:ILE:HG22	3:E:10:GLU:H	1.67	0.59
1:C:179:THR:HG23	5:C:502:GTP:H3'	1.85	0.59
1:C:241:SER:HA	1:C:249:ASN:HD21	1.67	0.59
4:F:2:TYR:OH	4:F:360:PRO:O	2.19	0.59
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.85	0.58
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.85	0.58
2:D:171:VAL:HA	2:D:204:ILE:O	2.04	0.58
4:F:40:MET:HE2	4:F:47:LEU:HG	1.86	0.58
2:B:320:ARG:NH1	7:B:505:GOL:H11	2.18	0.57
4:F:7:ARG:NH2	4:F:43:GLU:OE2	2.30	0.57
4:F:163:SER:OG	4:F:168:GLU:OE1	2.20	0.57
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.86	0.57
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.19	0.57
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.85	0.57
2:D:19:LYS:O	2:D:23:VAL:HG23	2.05	0.57
1:C:253:THR:HB	7:C:501:GOL:H11	1.87	0.57
2:D:93:VAL:HG21	2:D:121:VAL:HG21	1.86	0.57
2:D:75:MET:HE2	2:D:94:PHE:CD1	2.40	0.57
2:D:369:ARG:NH1	14:D:603:HOH:O	2.38	0.56
4:F:136:ASN:O	4:F:145:ASN:ND2	2.38	0.56
2:D:46:LEU:HA	2:D:49:ILE:HB	1.86	0.56
2:B:217:LEU:HD11	2:B:230:LEU:HD21	1.88	0.56
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.88	0.56
2:D:249:ASN:HB3	2:D:254:LYS:NZ	2.20	0.56
4:F:36:ARG:NH1	4:F:55:GLU:OE1	2.36	0.56
3:E:112:ARG:HH21	12:E:201:IMD:C5	2.19	0.55
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:GLN:HA	2:D:167:ASN:O	2.06	0.55
2:D:177:VAL:HG13	7:D:503:GOL:H2	1.87	0.55
1:A:214:ARG:NH1	1:A:220:GLU:O	2.40	0.55
4:F:31:ARG:HE	4:F:32:LYS:HG3	1.72	0.54
2:B:237:GLY:CA	7:B:505:GOL:H12	2.38	0.54
2:D:179:ASP:OD1	2:D:179:ASP:N	2.40	0.54
1:A:245:ASP:HB3	3:E:16:SER:HB2	1.90	0.54
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.43	0.53
2:B:265:LEU:HD11	2:B:431[B]:GLU:HG2	1.91	0.53
2:D:382:THR:HA	2:D:432:TYR:CD1	2.43	0.53
1:A:70:LEU:HG	1:A:145:THR:HG23	1.90	0.53
1:C:210:TYR:OH	1:C:221:ARG:NH2	2.41	0.53
4:F:186:LEU:HB3	13:F:402:ACP:H2	1.91	0.53
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.44	0.53
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.43	0.52
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.44	0.52
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.44	0.52
4:F:101:TYR:CD2	4:F:126:ASP:HB3	2.45	0.52
2:B:221:THR:HG21	1:C:326:LYS:HA	1.91	0.52
4:F:39:LEU:HD13	4:F:61:LEU:HD23	1.90	0.52
2:D:176:LYS:HD2	2:D:210:TYR:CD2	2.44	0.52
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.90	0.52
2:B:19:LYS:HB3	2:B:232:SER:OG	2.10	0.51
2:B:69:ASP:O	2:B:94:PHE:HA	2.10	0.51
2:D:71:GLU:HB3	2:D:98:GLY:HA2	1.90	0.51
4:F:263:PHE:CG	4:F:341:LYS:HE2	2.45	0.51
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.51
1:A:329:ASN:O	3:E:6:MET:HE1	2.10	0.51
1:A:339:ARG:O	14:A:602:HOH:O	2.19	0.51
4:F:181:VAL:O	14:F:501:HOH:O	2.19	0.51
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.92	0.51
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.92	0.51
2:B:132:LEU:O	2:B:164:ARG:NH1	2.43	0.51
2:B:320:ARG:HD3	7:B:505:GOL:H2	1.93	0.51
2:B:181:VAL:HG22	1:C:258:ASN:OD1	2.10	0.50
2:B:326:LYS:NZ	2:B:330:GLU:OE2	2.40	0.50
4:F:100:ILE:HG23	4:F:128:ARG:HG3	1.93	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.46	0.50
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.25	0.50
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.47	0.50
2:D:431:GLU:OE2	14:D:602:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.46	0.50
4:F:128:ARG:HH21	4:F:170:LEU:HD21	1.76	0.50
4:F:12:SER:OG	14:F:504:HOH:O	2.18	0.50
4:F:5:VAL:HG13	4:F:37:PHE:HB3	1.94	0.50
1:A:102:ASN:HB3	1:A:105:ARG:HB3	1.94	0.49
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.47	0.49
4:F:43:GLU:OE1	4:F:43:GLU:N	2.36	0.49
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.48	0.49
2:D:72:PRO:HB3	2:D:94:PHE:CD2	2.47	0.49
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.77	0.49
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.95	0.49
1:C:220:GLU:CD	2:D:326:LYS:HD3	2.38	0.49
1:A:68[A]:VAL:HG11	1:A:149:PHE:CE2	2.47	0.49
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.94	0.49
2:D:208:ALA:O	2:D:212:ILE:HG13	2.12	0.49
4:F:99:VAL:O	4:F:126:ASP:HB2	2.13	0.49
4:F:247:LYS:HG3	4:F:253:TYR:CE2	2.48	0.49
2:B:360:PRO:HG3	7:B:505:GOL:O2	2.13	0.49
2:D:3:GLU:OE2	2:D:3:GLU:N	2.45	0.49
2:D:152:LEU:O	2:D:156:LYS:HG2	2.13	0.49
2:D:357:ASP:O	2:D:359:PRO:HD3	2.13	0.49
4:F:71:LEU:HD13	4:F:298:ILE:HD13	1.94	0.49
4:F:100:ILE:HG13	4:F:182:ILE:HD12	1.94	0.49
4:F:145:ASN:HB3	4:F:147:TRP:NE1	2.19	0.49
1:A:338:LYS:HE2	1:A:339:ARG:HG3	1.95	0.49
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.13	0.48
1:A:230:LEU:O	1:A:234:ILE:HD12	2.14	0.48
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.45	0.48
2:D:182:VAL:HG12	2:D:398:MET:HE1	1.94	0.48
4:F:224:SER:HA	4:F:246:GLN:HE22	1.78	0.48
2:B:195:VAL:HG13	2:B:264:ARG:HG2	1.95	0.48
4:F:189:PRO:HA	4:F:322:ASP:HA	1.95	0.48
4:F:86:GLU:O	4:F:87:LEU:HD23	2.14	0.48
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.78	0.48
4:F:91:CYS:N	14:F:507:HOH:O	2.46	0.48
2:D:327:GLU:O	2:D:331:GLN:HG2	2.14	0.48
4:F:102:PRO:HA	4:F:173:ILE:HG12	1.95	0.48
2:B:415:GLU:HG3	14:B:616:HOH:O	2.14	0.48
4:F:358:VAL:O	4:F:360:PRO:HD3	2.14	0.48
4:F:198:LYS:HD2	4:F:320:MET:HE1	1.94	0.47
1:A:297:GLU:OE2	1:A:339:ARG:NH1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:LYS:HB3	2:D:405:LEU:HD13	1.96	0.47
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.47
3:E:8:VAL:HG22	3:E:22:VAL:HG22	1.96	0.47
3:E:47:LEU:O	3:E:51:GLN:HG2	2.14	0.47
2:B:210:TYR:CE1	2:B:222:PRO:HD2	2.49	0.47
2:B:318:ILE:HD11	2:B:376:THR:HB	1.97	0.47
2:D:161:TYR:HB3	2:D:164:ARG:HG2	1.96	0.47
4:F:128:ARG:O	4:F:131:PHE:HB3	2.15	0.47
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.47
4:F:263:PHE:CD2	4:F:341:LYS:HE2	2.49	0.47
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.97	0.47
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.97	0.47
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:C:166:LYS:HE2	1:C:197:HIS:O	2.15	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
3:E:127:ASP:O	3:E:131:GLU:HG2	2.15	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.47
1:C:21:TRP:CZ2	1:C:65:ALA:HB2	2.50	0.47
1:C:1:MET:O	1:C:2:ARG:HG2	2.14	0.47
2:D:172:MET:HE3	2:D:203:CYS:HA	1.97	0.46
1:C:333:ALA:O	1:C:337:THR:HG23	2.15	0.46
2:B:282:GLN:N	2:B:282:GLN:HE21	2.12	0.46
2:D:63:PRO:O	2:D:65:ALA:N	2.48	0.46
4:F:146:VAL:HG13	14:F:503:HOH:O	2.15	0.46
2:D:323:MET:HE2	2:D:373:MET:HG2	1.96	0.46
4:F:131:PHE:HD1	4:F:132:LEU:HG	1.80	0.46
1:C:141:PHE:O	1:C:147:SER:HB3	2.15	0.46
1:C:174:ALA:HB2	1:C:207:GLU:N	2.31	0.46
1:C:175:PRO:HD2	1:C:207:GLU:OE2	2.16	0.46
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.33	0.46
4:F:241:THR:O	4:F:241:THR:OG1	2.34	0.46
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.98	0.46
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.46
2:D:414:ASP:OD1	2:D:415:GLU:N	2.47	0.46
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.16	0.46
2:B:19:LYS:HA	2:B:19:LYS:HD3	1.77	0.46
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.51	0.46
1:A:415:GLU:O	1:A:418:PHE:HB2	2.16	0.46
1:C:174:ALA:O	1:C:178:SER:HB3	2.15	0.46
2:D:239:THR:O	2:D:243:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HA	1:A:277:SER:HB2	1.98	0.45
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.51	0.45
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.45
2:D:59:ASN:N	14:D:606:HOH:O	2.48	0.45
2:B:298:SER:H	2:B:308:ARG:HH12	1.65	0.45
4:F:3:THR:CG2	4:F:37:PHE:HA	2.46	0.45
2:D:335:VAL:O	2:D:339:ASN:HB2	2.16	0.45
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.99	0.45
4:F:3:THR:HG23	4:F:30:LEU:CD1	2.47	0.45
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.56	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.45
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.80	0.45
2:D:147:SER:O	2:D:151:THR:HG23	2.16	0.45
2:D:322:ARG:O	2:D:373:MET:HE2	2.17	0.45
4:F:284[A]:LEU:HD12	4:F:287:ILE:HB	1.98	0.45
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.50	0.45
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.98	0.45
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.51	0.45
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.98	0.45
2:D:177:VAL:HA	7:D:503:GOL:H32	1.98	0.45
4:F:31:ARG:NE	4:F:32:LYS:H	2.04	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.45
1:A:196:GLU:HG3	1:A:197:HIS:CD2	2.52	0.45
4:F:245:ILE:HG23	4:F:249:TYR:HD2	1.80	0.45
1:A:401:LYS:HE3	2:B:438:ALA:HB1	1.99	0.44
1:C:262:TYR:CB	12:C:508:IMD:H5	2.47	0.44
2:B:296:PHE:CE2	2:B:332:MET:HE1	2.52	0.44
4:F:201:ILE:HG12	4:F:221:LEU:CD2	2.47	0.44
1:A:337:THR:OG1	1:A:338:LYS:N	2.50	0.44
1:C:296:PHE:O	1:C:298:PRO:HD3	2.18	0.44
1:C:262:TYR:CG	12:C:508:IMD:H5	2.52	0.44
4:F:3:THR:HG23	4:F:30:LEU:HD11	1.99	0.44
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.18	0.44
2:B:295:MET:SD	2:B:375:ALA:HB1	2.58	0.44
2:B:372:LYS:O	2:B:373:MET:HE2	2.18	0.44
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.57	0.44
4:F:189:PRO:HG3	4:F:198:LYS:HD3	1.99	0.44
1:C:6:SER:O	1:C:65:ALA:HA	2.18	0.44
1:A:154:MET:HG3	1:A:194:THR:HG23	1.99	0.44
1:C:248:LEU:HB3	1:C:355:ILE:HB	2.00	0.44
1:C:209:ILE:HD11	1:C:302:MET:SD	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:MET:SD	2:D:94:PHE:HB3	2.58	0.43
2:D:82:PRO:O	2:D:83:PHE:HB2	2.19	0.43
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.01	0.43
2:D:108:TYR:CG	3:E:133:VAL:HG11	2.54	0.43
2:B:136:GLN:HG3	2:B:169:PHE:HE1	1.83	0.43
3:E:119:MET:HA	3:E:122:ARG:NH2	2.33	0.43
3:E:139:LEU:HD23	3:E:139:LEU:N	2.33	0.43
2:B:323:MET:HE2	2:B:323:MET:HB3	1.92	0.43
1:C:141:PHE:HE1	1:C:191:THR:OG1	2.02	0.43
2:B:359:PRO:HB2	2:B:371:LEU:O	2.19	0.43
1:C:425:MET:HE3	1:C:425:MET:HB3	1.86	0.43
1:C:257:THR:HG1	7:C:501:GOL:HO1	1.64	0.43
3:E:101:LEU:HD12	3:E:101:LEU:HA	1.86	0.43
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.54	0.43
1:A:346:TRP:CD1	1:A:346:TRP:H	2.35	0.43
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.54	0.43
2:B:274:PRO:HD2	2:B:371:LEU:HD13	2.00	0.43
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.43
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.43
4:F:198:LYS:HG3	4:F:228:TYR:CD1	2.54	0.43
2:B:158:ARG:NH1	2:B:196:GLU:O	2.52	0.43
2:B:176:LYS:HD2	2:B:207:GLU:HG3	2.01	0.43
2:D:248:LEU:HB3	11:D:505:93X:O50	2.19	0.43
1:A:2:ARG:HB3	1:A:133:GLN:HG3	2.00	0.42
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.84	0.42
1:A:285:GLN:HA	1:A:285:GLN:NE2	2.34	0.42
1:A:395:PHE:CD1	1:A:395:PHE:C	2.97	0.42
1:A:72:PRO:HA	1:A:94:THR:HG21	2.02	0.42
1:A:401:LYS:HE2	2:B:346:TRP:CD2	2.55	0.42
1:A:175:PRO:C	1:A:177:VAL:H	2.27	0.42
2:B:431[B]:GLU:O	2:B:434:GLN:HG2	2.19	0.42
4:F:209:HIS:HA	4:F:311:SER:O	2.20	0.42
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.55	0.42
2:B:2:ARG:HB3	2:B:133:GLN:HG2	2.00	0.42
2:D:176:LYS:O	2:D:177:VAL:HB	2.20	0.42
2:D:334:ASN:ND2	2:D:338:LYS:HE2	2.30	0.42
1:C:182:VAL:HB	1:C:408:TYR:OH	2.19	0.42
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.41	0.42
2:B:325:MET:HB3	2:B:325:MET:HE2	1.58	0.42
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.55	0.42
4:F:247:LYS:HG3	4:F:253:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:ND1	1:A:152:LEU:HB2	2.35	0.42
4:F:244:CYS:O	4:F:245:ILE:HG12	2.20	0.42
1:A:167:LEU:HD13	1:A:252:LEU:HD22	2.02	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.85	0.41
2:B:234:THR:O	2:B:238:VAL:HB	2.20	0.41
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.54	0.41
2:D:47:GLU:HG2	2:D:245:PRO:HG3	2.01	0.41
2:D:34:GLY:O	2:D:60:LYS:HD3	2.20	0.41
3:E:75:LYS:O	3:E:79:GLU:HG3	2.20	0.41
4:F:97:SER:HA	4:F:182:ILE:O	2.21	0.41
2:B:298:SER:OG	2:B:308:ARG:NH1	2.53	0.41
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.36	0.41
2:B:301:MET:HE1	2:B:377:PHE:CD2	2.56	0.41
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	0.41
2:D:115:VAL:O	2:D:119:LEU:HG	2.20	0.41
2:B:431[A]:GLU:O	2:B:434:GLN:HG2	2.20	0.41
2:D:29:GLY:O	2:D:36:TYR:HA	2.21	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.46	0.41
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.56	0.41
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.56	0.41
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.85	0.41
1:A:231:ILE:O	1:A:235:VAL:HG23	2.21	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.61	0.41
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.56	0.41
2:B:205:ASP:O	2:B:209:LEU:HG	2.21	0.41
2:D:320:ARG:HG2	2:D:356:CYS:HB3	2.03	0.41
2:D:406:HIS:NE2	2:D:407:TRP:HD1	2.19	0.41
4:F:3:THR:HG22	4:F:37:PHE:HA	2.03	0.41
1:A:2:ARG:O	1:A:133:GLN:NE2	2.53	0.41
1:A:264:ARG:HB2	14:A:612:HOH:O	2.21	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.56	0.41
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.21	0.41
1:C:10:GLY:O	1:C:14:VAL:HG23	2.21	0.40
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	0.40
1:A:90:GLU:O	1:A:121:ARG:HD2	2.21	0.40
1:A:238:ILE:HG12	1:A:378:LEU:HD21	2.02	0.40
2:B:46:LEU:HD23	2:B:49:ILE:HD12	2.04	0.40
1:C:143:GLY:HA3	5:C:502:GTP:O3A	2.21	0.40
1:C:253:THR:HG23	12:C:509:IMD:H4	2.04	0.40
4:F:17:VAL:HG13	4:F:351:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:165:GLU:HB2	4:F:168:GLU:OE2	2.21	0.40
1:A:141:PHE:O	1:A:147:SER:HB3	2.22	0.40
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.56	0.40
1:C:147:SER:OG	1:C:186:ASN:HB3	2.21	0.40
2:D:249:ASN:HB3	2:D:254:LYS:HZ2	1.85	0.40
4:F:31:ARG:NE	4:F:32:LYS:HG3	2.36	0.40
1:C:1:MET:HG3	1:C:2:ARG:N	2.36	0.40
2:D:20:PHE:O	2:D:24:ILE:HG23	2.22	0.40
4:F:242:ASN:O	4:F:246:GLN:HB2	2.21	0.40
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.03	0.40
2:D:320:ARG:HB3	2:D:359:PRO:HA	2.03	0.40
3:E:25:LYS:HA	3:E:26:PRO:HD3	1.86	0.40
4:F:284[A]:LEU:HD12	4:F:284[A]:LEU:HA	1.78	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:GLU:OE1	1:C:282:TYR:OH[4_545]	2.17	0.03

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	447/451 (99%)	421 (94%)	22 (5%)	4 (1%)	14	20
1	C	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	43	54
2	B	429/445 (96%)	402 (94%)	24 (6%)	3 (1%)	18	25
2	D	420/445 (94%)	400 (95%)	16 (4%)	4 (1%)	12	17
3	E	117/189 (62%)	105 (90%)	10 (8%)	2 (2%)	7	8
4	F	302/378 (80%)	263 (87%)	37 (12%)	2 (1%)	18	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2162/2359 (92%)	2022 (94%)	124 (6%)	16 (1%)	16 25

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
2	D	177	VAL
3	E	10	GLU
4	F	230	SER
2	D	64	ARG
1	A	366	GLY
2	B	73	GLY
2	B	82	PRO
2	B	216	THR
1	C	176	GLN
1	A	261	PRO
3	E	52	LYS
4	F	242	ASN
1	A	281	ALA
2	D	143	GLY
2	D	181	VAL

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	380/379 (100%)	370 (97%)	10 (3%)	40 57
1	C	380/379 (100%)	370 (97%)	10 (3%)	40 57
2	B	375/383 (98%)	352 (94%)	23 (6%)	17 25
2	D	367/383 (96%)	354 (96%)	13 (4%)	32 46
3	E	109/171 (64%)	103 (94%)	6 (6%)	19 29
4	F	289/336 (86%)	265 (92%)	24 (8%)	10 15
All	All	1900/2031 (94%)	1814 (96%)	86 (4%)	24 36

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LEU
1	A	178	SER
1	A	179	THR
1	A	191	THR
1	A	207	GLU
1	A	241	SER
1	A	250	VAL
1	A	257	THR
1	A	271	THR
1	A	438	ASP
2	B	50[A]	ASN
2	B	50[B]	ASN
2	B	75	MET
2	B	78	VAL
2	B	85	GLN
2	B	90	ASP
2	B	117	SER
2	B	132	LEU
2	B	155[A]	SER
2	B	155[B]	SER
2	B	200	GLU
2	B	215	ARG
2	B	220	THR
2	B	238	VAL
2	B	277	SER
2	B	282	GLN
2	B	283	TYR
2	B	298	SER
2	B	318	ILE
2	B	325	MET
2	B	340	SER
2	B	405	LEU
2	B	437	ASP
1	C	66	VAL
1	C	67	PHE
1	C	71	GLU
1	C	179	THR
1	C	181	VAL
1	C	241	SER
1	C	253	THR
1	C	335	ILE
1	C	347	CYS

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Mol	Chain	Res	Type
1	C	381	THR
2	D	8	GLN
2	D	15	GLN
2	D	26	ASP
2	D	74	THR
2	D	78	VAL
2	D	117	SER
2	D	121	VAL
2	D	127	GLU
2	D	159	GLU
2	D	180	THR
2	D	249	ASN
2	D	341	SER
2	D	434	GLN
3	E	9	ILE
3	E	12	ASN
3	E	16	SER
3	E	124	GLN
3	E	133	VAL
3	E	140	LYS
4	F	13	VAL
4	F	69	ASP
4	F	71	LEU
4	F	127	GLU
4	F	129	GLU
4	F	146	VAL
4	F	150	LYS
4	F	170	LEU
4	F	181	VAL
4	F	191	LEU
4	F	217	ARG
4	F	223	THR
4	F	240	LEU
4	F	245	ILE
4	F	246	GLN
4	F	264	PHE
4	F	275[A]	LEU
4	F	275[B]	LEU
4	F	314	LEU
4	F	331	GLU
4	F	332	VAL
4	F	355	ILE

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Mol	Chain	Res	Type
4	F	361	LEU
4	F	374	ILE

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	309	HIS
1	A	358	GLN
2	B	11	GLN
2	B	59	ASN
2	B	101	ASN
2	B	136	GLN
2	B	336	GLN
2	B	434	GLN
2	B	436	GLN
1	C	128	GLN
1	C	393	HIS
2	D	426	ASN
2	D	436	GLN
3	E	115	HIS
4	F	260	ASN
4	F	306	HIS
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GTP	C	502	6	33,34,34	0.97	2 (6%)	50,54,54	1.73	11 (22%)
7	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.36	0
7	GOL	C	504	-	5,5,5	0.32	0	5,5,5	0.53	0
10	MES	B	507	-	12,12,12	2.21	1 (8%)	15,16,16	2.06	4 (26%)
12	IMD	C	508	-	5,5,5	0.76	0	5,5,5	0.77	0
12	IMD	E	201	7	5,5,5	0.67	0	5,5,5	0.35	0
9	GDP	D	501	-	29,30,30	1.26	4 (13%)	45,47,47	1.89	9 (20%)
7	GOL	D	503	-	5,5,5	0.34	0	5,5,5	0.42	0
7	GOL	B	505	-	5,5,5	0.39	0	5,5,5	0.60	0
7	GOL	C	505	-	5,5,5	0.43	0	5,5,5	0.10	0
7	GOL	B	504	-	5,5,5	0.47	0	5,5,5	0.44	0
9	GDP	B	501	6	29,30,30	1.15	2 (6%)	45,47,47	1.93	11 (24%)
7	GOL	D	504	12	5,5,5	0.37	0	5,5,5	0.33	0
12	IMD	C	509	-	5,5,5	0.64	0	5,5,5	0.36	0
7	GOL	C	506	-	5,5,5	0.55	0	5,5,5	0.59	0
7	GOL	B	503	-	5,5,5	0.37	0	5,5,5	0.25	0
7	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.45	0
5	GTP	A	501	6	33,34,34	0.96	1 (3%)	50,54,54	1.73	13 (26%)
13	ACP	F	402	-	31,33,33	2.69	8 (25%)	47,52,52	2.34	11 (23%)
11	93X	D	505	-	30,30,30	6.51	11 (36%)	41,43,43	4.32	12 (29%)
7	GOL	C	501	-	5,5,5	0.36	0	5,5,5	0.35	0
7	GOL	A	504	-	5,5,5	0.43	0	5,5,5	0.73	0
11	93X	B	508	-	30,30,30	6.42	8 (26%)	41,43,43	4.50	16 (39%)

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	502	6	-	5/22/38/38	0/3/3/3
7	GOL	A	503	-	-	4/4/4/4	-
7	GOL	C	504	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
12	IMD	C	508	-	-	-	0/1/1/1
12	IMD	E	201	7	-	-	0/1/1/1
9	GDP	D	501	-	-	6/16/32/32	0/3/3/3
7	GOL	D	503	-	-	0/4/4/4	-
7	GOL	B	505	-	-	4/4/4/4	-
7	GOL	C	505	-	-	4/4/4/4	-
7	GOL	B	504	-	-	2/4/4/4	-
9	GDP	B	501	6	-	4/16/32/32	0/3/3/3
7	GOL	D	504	12	-	2/4/4/4	-
12	IMD	C	509	-	-	-	0/1/1/1
7	GOL	C	506	-	-	3/4/4/4	-
7	GOL	B	503	-	-	4/4/4/4	-
7	GOL	A	506	-	-	4/4/4/4	-
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
13	ACP	F	402	-	-	3/19/38/38	0/3/3/3
11	93X	D	505	-	-	2/18/34/34	0/3/3/3
7	GOL	C	501	-	-	1/4/4/4	-
7	GOL	A	504	-	-	4/4/4/4	-
11	93X	B	508	-	-	3/18/34/34	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	505	93X	C4-N1	26.07	1.75	1.37
11	B	508	93X	C4-N1	25.66	1.74	1.37
11	B	508	93X	C3-C2	-22.18	1.34	1.57
11	D	505	93X	C3-C2	-21.58	1.35	1.57
13	F	402	ACP	PB-O3A	7.65	1.66	1.58
10	B	507	MES	C8-S	-7.37	1.67	1.77
13	F	402	ACP	PA-O3A	7.08	1.67	1.59
11	D	505	93X	C29-C3	5.79	1.61	1.53
11	D	505	93X	C12-C2	5.17	1.59	1.51
11	B	508	93X	C29-C3	4.99	1.60	1.53
13	F	402	ACP	C6-N6	4.95	1.46	1.34
13	F	402	ACP	C5-N7	4.93	1.48	1.39
11	D	505	93X	O19-C15	3.54	1.42	1.37
11	B	508	93X	C12-C2	3.45	1.56	1.51
11	B	508	93X	O18-C16	3.13	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	C5-C4	3.11	1.47	1.38
11	D	505	93X	C2-N1	3.07	1.51	1.48
11	D	505	93X	O23-C10	2.94	1.41	1.37
13	F	402	ACP	O4'-C1'	2.85	1.48	1.42
11	B	508	93X	O21-C9	2.77	1.43	1.38
11	D	505	93X	O25-C8	2.74	1.41	1.37
5	C	502	GTP	C2-N3	2.68	1.39	1.33
11	D	505	93X	C6-N1	2.67	1.47	1.43
5	A	501	GTP	PA-O3A	2.67	1.62	1.59
13	F	402	ACP	C2'-C3'	-2.66	1.46	1.53
9	B	501	GDP	C5-C4	2.64	1.46	1.38
11	B	508	93X	O19-C15	2.54	1.41	1.37
13	F	402	ACP	C8-N7	2.48	1.36	1.31
13	F	402	ACP	PB-O2B	-2.43	1.50	1.56
11	D	505	93X	O18-C16	2.39	1.41	1.36
5	C	502	GTP	PB-O3B	2.38	1.62	1.59
9	D	501	GDP	C6-N1	-2.38	1.34	1.38
9	D	501	GDP	PA-O3A	2.33	1.62	1.59
11	D	505	93X	O21-C9	2.17	1.42	1.38
9	B	501	GDP	C6-N1	-2.11	1.34	1.38
11	B	508	93X	O25-C8	2.09	1.40	1.37
9	D	501	GDP	C4-N9	-2.08	1.32	1.38

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	93X	C2-N1-C4	-14.66	82.45	95.30
11	D	505	93X	C2-N1-C4	-14.27	82.79	95.30
11	B	508	93X	C3-C2-N1	12.43	98.01	86.56
11	D	505	93X	C3-C2-N1	11.63	97.28	86.56
11	D	505	93X	C3-C4-N1	-10.99	81.99	93.08
11	B	508	93X	C3-C4-N1	-10.79	82.19	93.08
11	D	505	93X	C2-C3-C4	9.07	97.91	85.08
13	F	402	ACP	C4-N9-C8	8.95	115.13	105.74
11	B	508	93X	C6-N1-C2	8.91	143.41	130.33
11	B	508	93X	C2-C3-C4	8.56	97.19	85.08
11	D	505	93X	C6-N1-C2	7.91	141.94	130.33
11	D	505	93X	O5-C4-C3	6.21	142.01	135.44
11	B	508	93X	O5-C4-C3	6.05	141.84	135.44
9	B	501	GDP	C5-C4-N3	-6.01	118.83	128.39
9	D	501	GDP	C5-C4-N3	-5.87	119.05	128.39
10	B	507	MES	C5-N4-C3	5.36	120.39	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C2-N3-C4	5.27	121.37	112.30
13	F	402	ACP	N3-C4-N9	5.19	136.00	127.17
13	F	402	ACP	C5-C4-N3	-5.17	119.60	126.72
11	B	508	93X	C26-O25-C8	-5.11	110.02	117.51
9	D	501	GDP	C2-N3-C4	5.07	121.04	112.30
11	D	505	93X	O23-C10-C9	4.96	123.64	115.14
5	A	501	GTP	C5-C4-N3	-4.92	120.56	128.39
11	B	508	93X	O23-C10-C9	4.73	123.25	115.14
5	A	501	GTP	C2-N3-C4	4.57	120.17	112.30
5	C	502	GTP	C2-N3-C4	4.56	120.15	112.30
5	C	502	GTP	C5-C4-N3	-4.53	121.18	128.39
9	B	501	GDP	N9-C4-N3	4.42	134.79	125.95
13	F	402	ACP	N9-C8-N7	-4.41	107.68	113.94
11	D	505	93X	O25-C8-C9	4.32	122.55	115.14
11	D	505	93X	O23-C10-C11	-4.28	116.70	124.08
9	D	501	GDP	N9-C4-N3	4.27	134.49	125.95
13	F	402	ACP	N3-C2-N1	-4.23	122.18	128.58
11	D	505	93X	O25-C8-C7	-4.16	116.91	124.08
9	D	501	GDP	C6-C5-N7	3.99	137.56	130.29
13	F	402	ACP	O3'-C3'-C4'	3.92	122.35	111.08
11	B	508	93X	O23-C10-C11	-3.83	117.48	124.08
11	B	508	93X	O25-C8-C7	-3.69	117.72	124.08
5	C	502	GTP	N9-C8-N7	-3.55	106.82	113.40
9	D	501	GDP	O2A-PA-O3A	3.36	116.37	107.27
10	B	507	MES	O3S-S-C8	3.33	112.52	106.00
13	F	402	ACP	C4-C5-N7	-3.30	106.81	110.58
9	B	501	GDP	C6-C5-N7	3.24	136.19	130.29
11	B	508	93X	C24-O23-C10	-3.22	112.79	117.51
13	F	402	ACP	C2-N3-C4	3.21	119.67	111.83
5	C	502	GTP	C2-N1-C6	-3.19	119.33	125.11
11	D	505	93X	O5-C4-N1	3.13	135.99	131.85
9	B	501	GDP	O6-C6-C5	-3.12	118.30	126.53
11	B	508	93X	O5-C4-N1	3.09	135.93	131.85
11	B	508	93X	O25-C8-C9	2.99	120.26	115.14
5	C	502	GTP	C8-N7-C5	2.98	109.57	104.26
5	A	501	GTP	N9-C4-N3	2.93	131.82	125.95
5	C	502	GTP	N9-C4-N3	2.93	131.81	125.95
9	D	501	GDP	C4-C5-N7	-2.92	106.05	110.67
13	F	402	ACP	C3'-C2'-C1'	2.91	106.98	101.46
5	C	502	GTP	C5-C6-N1	2.90	120.63	113.25
10	B	507	MES	C6-C5-N4	-2.89	105.72	110.12
5	A	501	GTP	C2-N1-C6	-2.83	119.97	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	505	93X	C7-C6-N1	2.79	122.15	119.36
5	A	501	GTP	N9-C8-N7	-2.75	108.31	113.40
9	B	501	GDP	O2B-PB-O3A	2.74	113.82	104.64
13	F	402	ACP	C1'-N9-C8	-2.71	121.09	127.09
11	B	508	93X	O21-C9-C10	2.67	123.95	120.12
9	B	501	GDP	C2'-C1'-N9	2.60	120.48	113.25
9	B	501	GDP	C5-C6-N1	2.57	119.78	113.25
9	B	501	GDP	O4'-C1'-N9	-2.56	102.56	108.36
5	A	501	GTP	C8-N7-C5	2.54	108.79	104.26
5	A	501	GTP	O3B-PB-O1B	-2.54	103.07	110.70
5	A	501	GTP	O2B-PB-O3A	2.53	114.11	107.27
11	B	508	93X	C14-C13-C12	-2.50	118.69	121.18
11	B	508	93X	C7-C6-N1	2.47	121.83	119.36
5	C	502	GTP	O4'-C1'-N9	-2.46	102.78	108.36
5	A	501	GTP	O6-C6-C5	-2.41	120.18	126.53
9	B	501	GDP	C4-C5-N7	-2.38	106.90	110.67
5	C	502	GTP	O6-C6-C5	-2.37	120.28	126.53
5	C	502	GTP	O3G-PG-O3B	2.36	112.57	104.64
5	A	501	GTP	O2B-PB-O3B	2.35	113.63	107.27
13	F	402	ACP	C2'-C3'-C4'	2.34	107.13	102.61
5	C	502	GTP	O2B-PB-O3B	2.32	113.54	107.27
5	A	501	GTP	C5-C6-N1	2.31	119.14	113.25
9	B	501	GDP	C2-N1-C6	-2.26	121.02	125.11
9	D	501	GDP	C2'-C3'-C4'	2.23	106.93	102.61
5	A	501	GTP	O3'-C3'-C2'	-2.19	104.78	111.82
5	A	501	GTP	O2A-PA-O3A	2.16	113.11	107.27
9	D	501	GDP	C5-C6-N1	2.08	118.54	113.25
10	B	507	MES	O1S-S-C8	2.05	109.82	106.73
9	D	501	GDP	O4'-C1'-N9	-2.01	103.79	108.36

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
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	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
7	A	503	GOL	O1-C1-C2-C3
7	A	503	GOL	O2-C2-C3-O3
7	A	504	GOL	O1-C1-C2-C3
7	A	506	GOL	C1-C2-C3-O3
7	A	506	GOL	O2-C2-C3-O3
7	B	503	GOL	O1-C1-C2-C3
7	B	503	GOL	C1-C2-C3-O3
7	B	503	GOL	O2-C2-C3-O3
7	B	505	GOL	O1-C1-C2-O2
7	B	505	GOL	O1-C1-C2-C3
7	C	504	GOL	O1-C1-C2-O2
7	C	504	GOL	O1-C1-C2-C3
7	C	505	GOL	O1-C1-C2-O2
7	C	505	GOL	O1-C1-C2-C3
7	C	506	GOL	O1-C1-C2-C3
7	D	504	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
13	F	402	ACP	C5'-O5'-PA-O1A
13	F	402	ACP	C5'-O5'-PA-O3A
11	D	505	93X	C9-C10-O23-C24
11	D	505	93X	C11-C10-O23-C24
7	A	504	GOL	O1-C1-C2-O2
7	B	504	GOL	O1-C1-C2-O2
7	C	506	GOL	O1-C1-C2-O2
11	B	508	93X	C8-C9-O21-C22
7	A	503	GOL	C1-C2-C3-O3
7	A	506	GOL	O1-C1-C2-C3
7	B	504	GOL	O1-C1-C2-C3
7	B	505	GOL	C1-C2-C3-O3
7	A	503	GOL	O1-C1-C2-O2
7	A	506	GOL	O1-C1-C2-O2
7	B	503	GOL	O1-C1-C2-O2
7	B	505	GOL	O2-C2-C3-O3
7	D	504	GOL	O1-C1-C2-O2
9	D	501	GDP	C3'-C4'-C5'-O5'
9	D	501	GDP	O4'-C4'-C5'-O5'
11	B	508	93X	C10-C9-O21-C22

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Mol	Chain	Res	Type	Atoms
13	F	402	ACP	C3'-C4'-C5'-O5'
7	A	504	GOL	O2-C2-C3-O3
7	A	504	GOL	C1-C2-C3-O3
7	C	501	GOL	C1-C2-C3-O3
7	C	505	GOL	C1-C2-C3-O3
7	C	506	GOL	O2-C2-C3-O3
7	C	505	GOL	O2-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O2G
11	B	508	93X	C9-C10-O23-C24
5	C	502	GTP	PB-O3B-PG-O1G
9	B	501	GDP	PB-O3A-PA-O2A
9	D	501	GDP	PB-O3A-PA-O2A

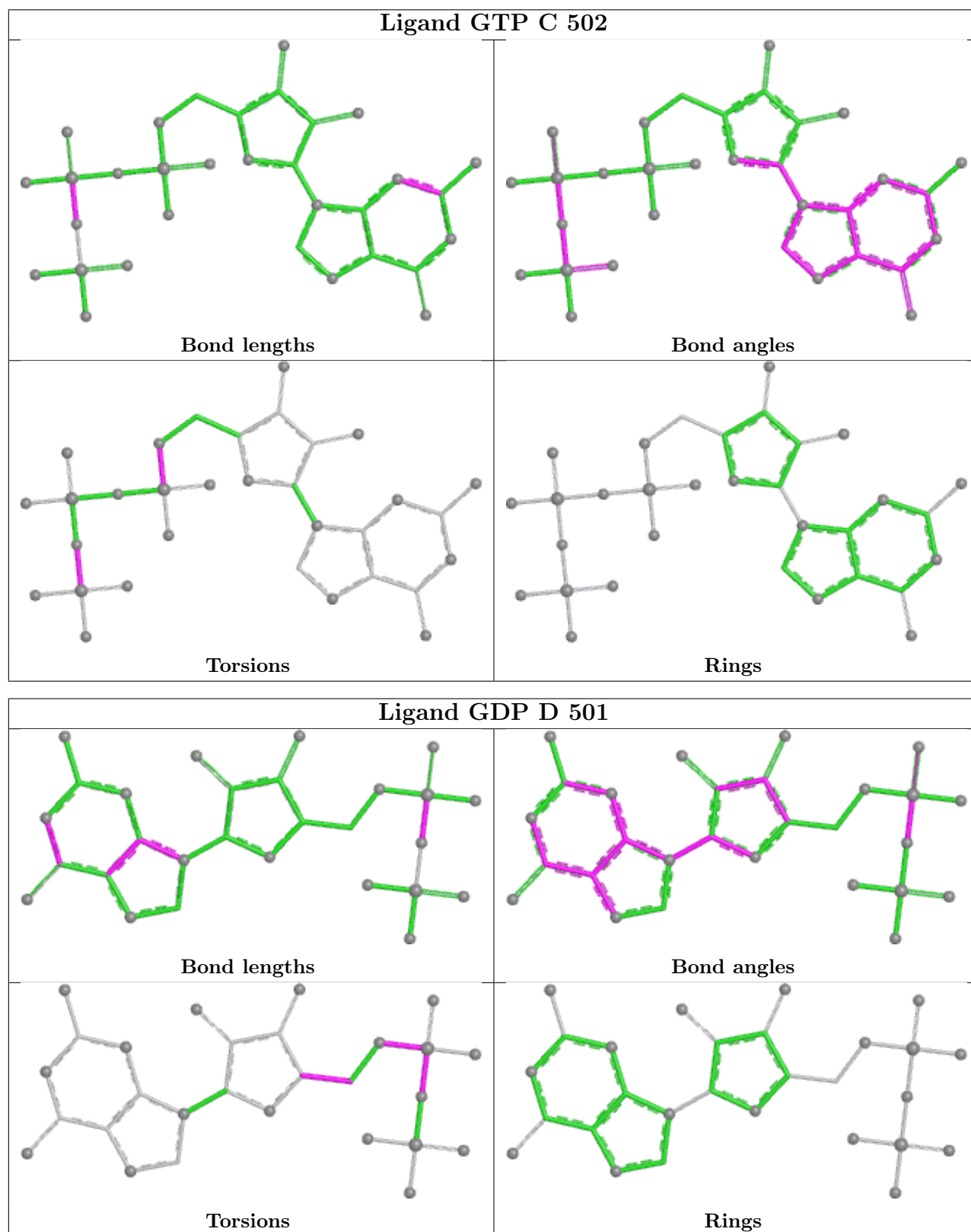
There are no ring outliers.

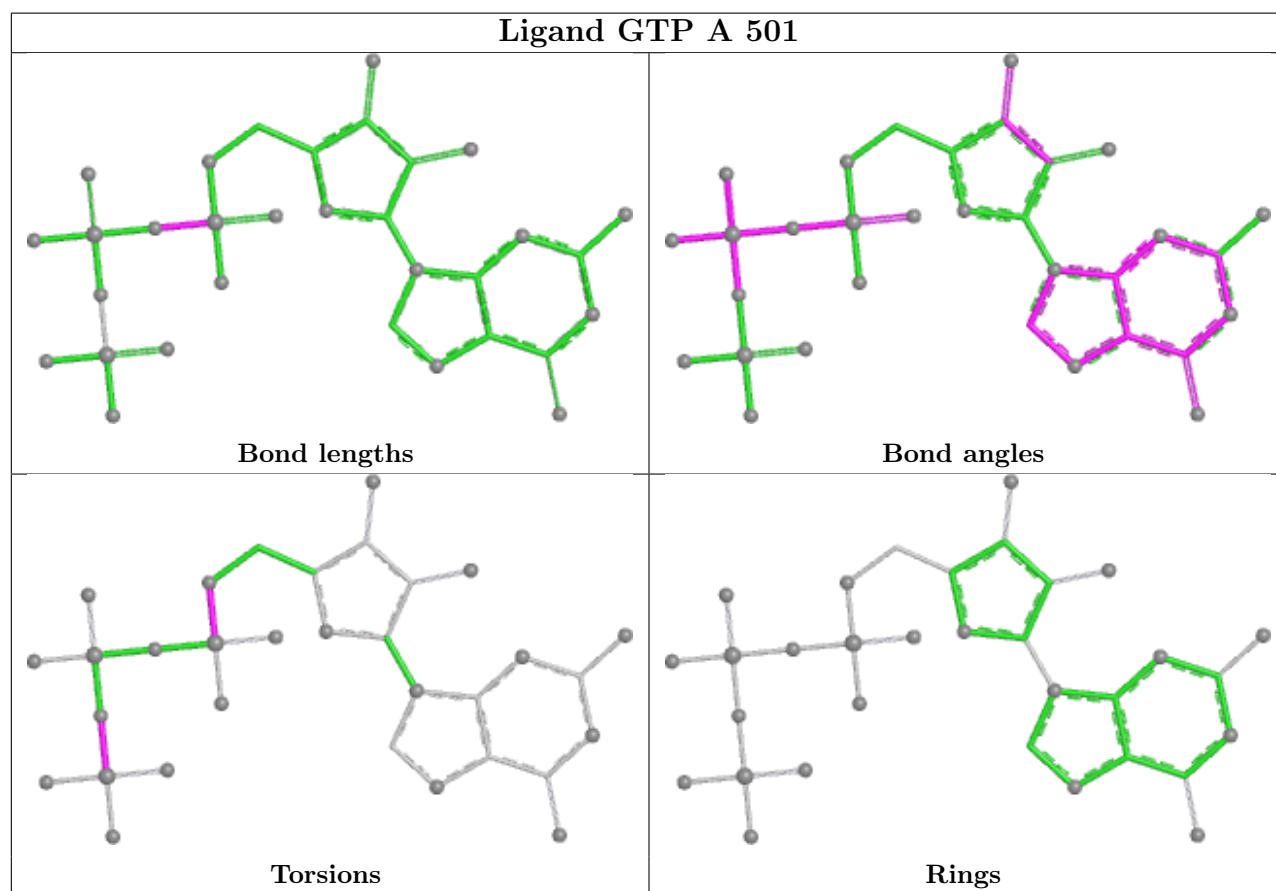
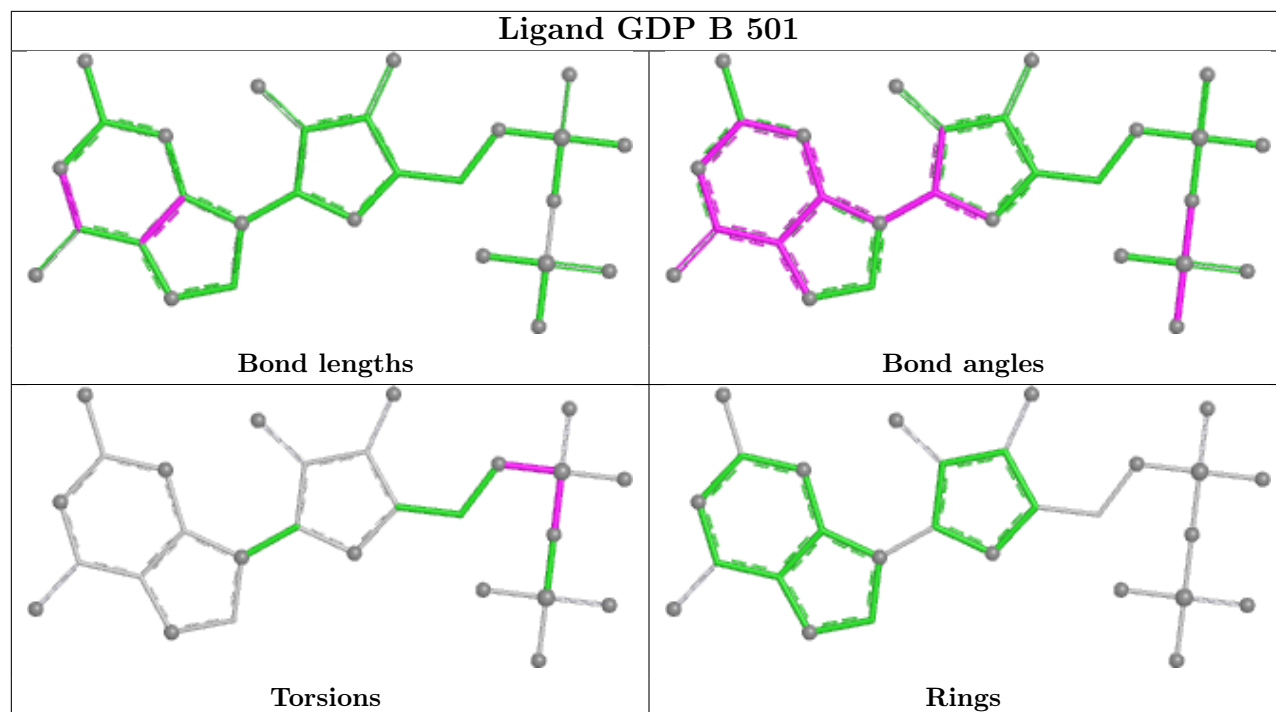
14 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	GTP	2	0
12	C	508	IMD	2	0
12	E	201	IMD	2	0
9	D	501	GDP	2	0
7	D	503	GOL	2	0
7	B	505	GOL	6	0
9	B	501	GDP	1	0
12	C	509	IMD	1	0
7	C	506	GOL	1	0
7	A	506	GOL	1	0
5	A	501	GTP	2	0
13	F	402	ACP	1	0
11	D	505	93X	1	0
7	C	501	GOL	2	0

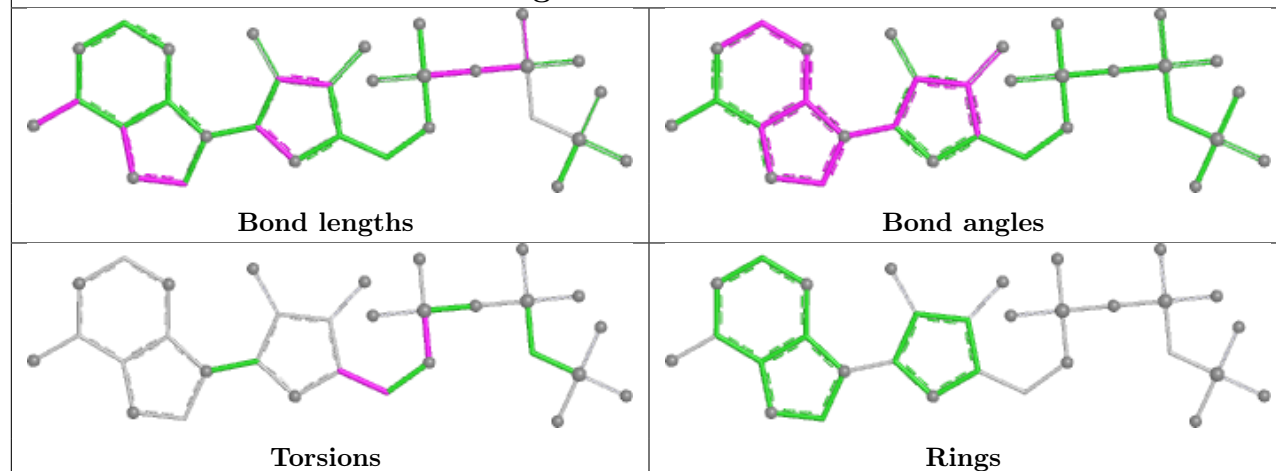
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

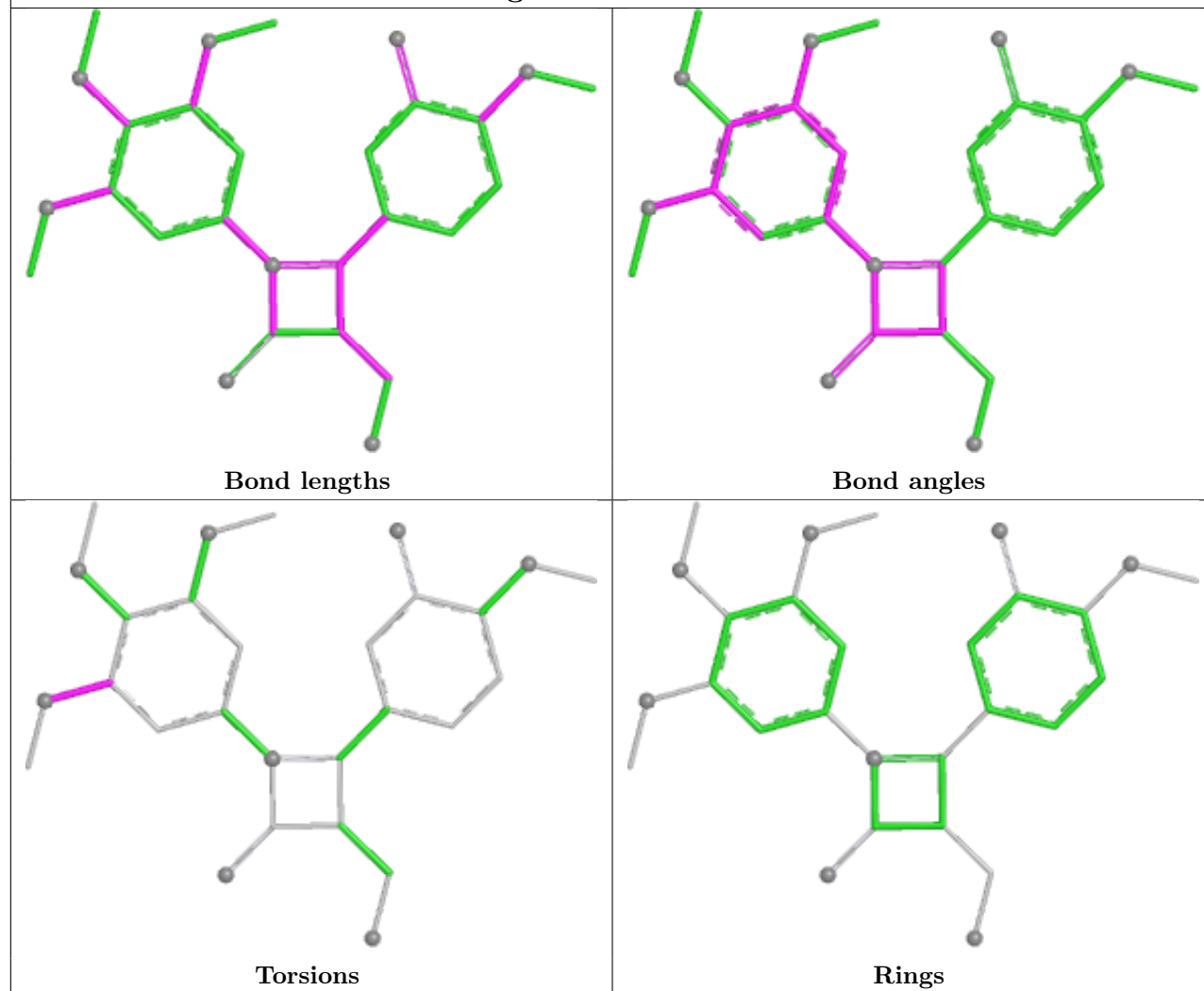


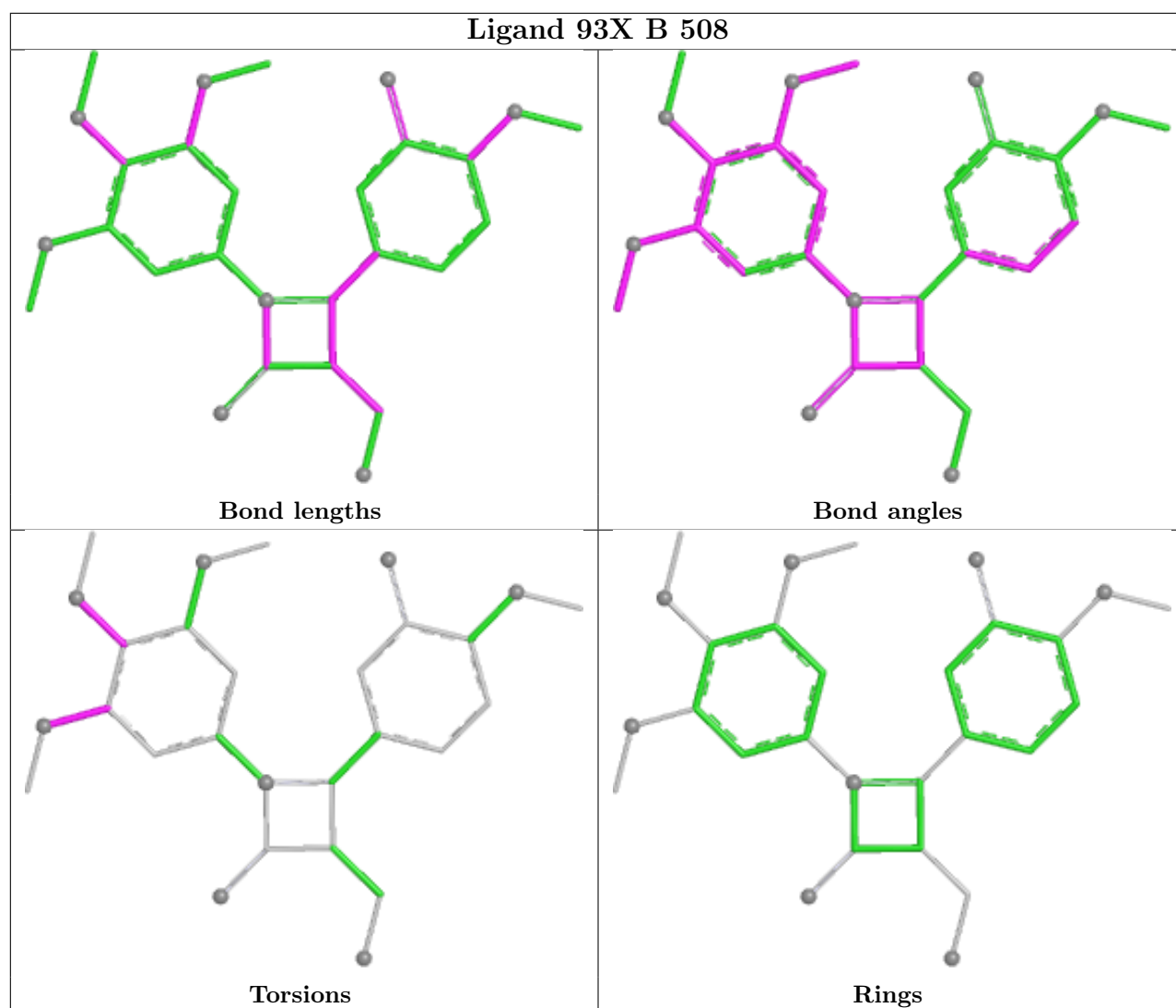


Ligand ACP F 402



Ligand 93X D 505





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	0.28	11 (2%) 58 59	34, 71, 104, 153	10 (2%)
1	C	440/451 (97%)	-0.19	4 (0%) 81 83	27, 55, 82, 106	9 (2%)
2	B	424/445 (95%)	0.07	9 (2%) 63 64	29, 64, 102, 176	9 (2%)
2	D	421/445 (94%)	0.52	10 (2%) 59 61	45, 84, 122, 181	6 (1%)
3	E	120/189 (63%)	0.40	2 (1%) 69 70	32, 80, 115, 154	1 (0%)
4	F	317/378 (83%)	0.76	30 (9%) 14 14	46, 100, 170, 220	3 (0%)
All	All	2161/2359 (91%)	0.27	66 (3%) 51 52	27, 72, 124, 220	38 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	315	PHE	5.0
4	F	150	LYS	4.6
4	F	245	ILE	4.0
4	F	173	ILE	3.8
2	B	2	ARG	3.7
4	F	362	ALA	3.6
4	F	169	LEU	3.3
4	F	172	PHE	3.2
4	F	102	PRO	3.2
4	F	240	LEU	3.0
4	F	88	SER	3.0
4	F	182	ILE	3.0
2	D	1	MET	3.0
3	E	22	VAL	3.0
4	F	131	PHE	3.0
2	B	276	THR	2.9
1	A	350	GLY	2.9
2	D	308	ARG	2.8
2	D	387	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	404	PHE	2.8
4	F	250	SER	2.8
4	F	170	LEU	2.8
2	D	118	VAL	2.7
2	B	325	MET	2.7
4	F	317	PHE	2.7
2	B	249	ASN	2.7
4	F	231	ALA	2.6
2	D	177	VAL	2.6
4	F	334	GLY	2.6
4	F	149	ALA	2.6
4	F	244	CYS	2.6
1	A	262	TYR	2.5
2	B	283	TYR	2.5
1	A	179	THR	2.5
1	A	349	THR	2.5
1	A	65	ALA	2.5
2	B	277	SER	2.5
1	A	316[A]	CYS	2.4
1	C	177	VAL	2.4
2	B	1	MET	2.4
2	B	282	GLN	2.4
1	A	78	VAL	2.4
4	F	332	VAL	2.4
4	F	130	VAL	2.4
2	D	407	TRP	2.4
4	F	180	HIS	2.3
1	A	149	PHE	2.3
1	A	66	VAL	2.3
2	B	303	ALA	2.3
2	D	101	ASN	2.3
2	D	358	ILE	2.3
3	E	9	ILE	2.3
1	A	124	LYS	2.2
4	F	264	PHE	2.2
1	C	1	MET	2.2
4	F	132	LEU	2.1
4	F	151	SER	2.1
4	F	296	MET	2.1
1	A	176	GLN	2.1
4	F	162	ILE	2.1
1	C	440	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	196	HIS	2.1
4	F	330	ILE	2.0
4	F	181	VAL	2.0
2	D	99	ALA	2.0
1	C	357	TYR	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
13	ACP	F	402	31/31	0.67	0.13	86,147,176,178	0
7	GOL	A	506	6/6	0.69	0.16	86,93,98,101	0
7	GOL	D	503	6/6	0.70	0.16	139,142,144,145	0
6	MG	D	502	1/1	0.72	0.16	95,95,95,95	0
7	GOL	A	504	6/6	0.74	0.22	111,113,114,115	0
7	GOL	C	505	6/6	0.74	0.19	108,114,117,119	0
7	GOL	B	504	6/6	0.80	0.16	77,95,99,102	0
7	GOL	B	503	6/6	0.80	0.23	82,96,105,110	0
7	GOL	D	504	6/6	0.82	0.18	101,109,113,118	0
7	GOL	C	501	6/6	0.83	0.17	78,88,91,93	0
7	GOL	B	505	6/6	0.85	0.18	100,107,115,123	0
7	GOL	C	504	6/6	0.85	0.13	91,98,99,101	0
12	IMD	E	201	5/5	0.86	0.21	123,124,128,129	0
7	GOL	C	506	6/6	0.88	0.14	79,86,88,88	0
9	GDP	D	501	28/28	0.88	0.13	79,90,101,102	0
6	MG	F	401	1/1	0.90	0.08	119,119,119,119	0
6	MG	B	502	1/1	0.91	0.18	51,51,51,51	0
12	IMD	C	509	5/5	0.91	0.27	110,112,113,114	0

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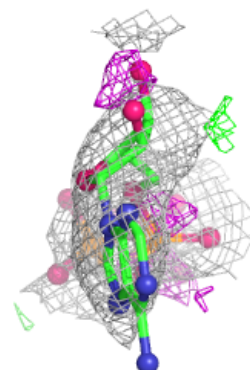
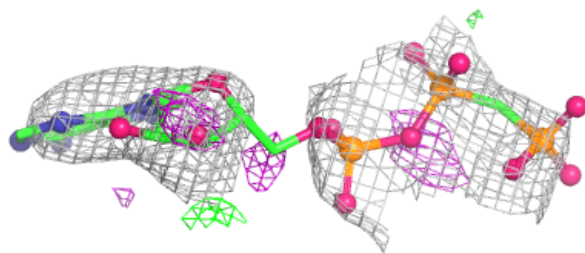
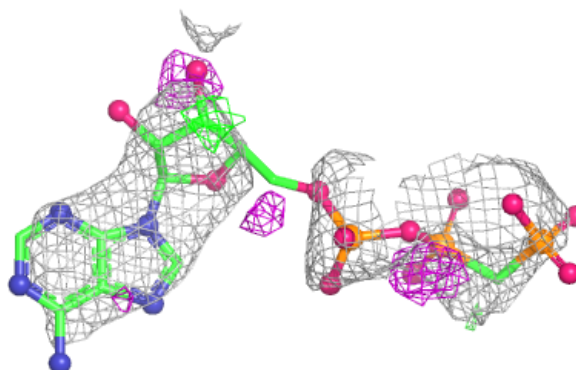
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	A	505	1/1	0.92	0.11	97,97,97,97	0
7	GOL	A	503	6/6	0.93	0.10	89,92,95,99	0
10	MES	B	507	12/12	0.93	0.09	52,69,81,85	0
12	IMD	C	508	5/5	0.93	0.12	66,73,74,78	0
11	93X	B	508	28/28	0.94	0.12	34,62,74,83	0
11	93X	D	505	28/28	0.94	0.10	55,66,75,83	0
6	MG	C	503	1/1	0.95	0.11	52,52,52,52	0
8	CA	B	506	1/1	0.95	0.08	118,118,118,118	0
5	GTP	A	501	32/32	0.96	0.07	49,55,60,62	0
6	MG	A	502	1/1	0.96	0.08	80,80,80,80	0
9	GDP	B	501	28/28	0.97	0.06	36,46,54,66	0
5	GTP	C	502	32/32	0.97	0.07	43,51,57,60	0
8	CA	C	507	1/1	0.97	0.05	112,112,112,112	0

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

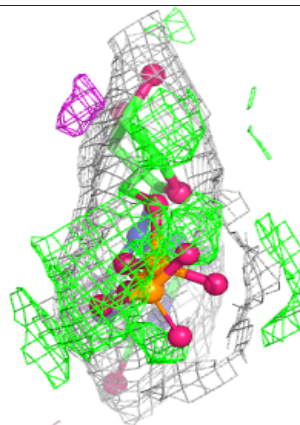
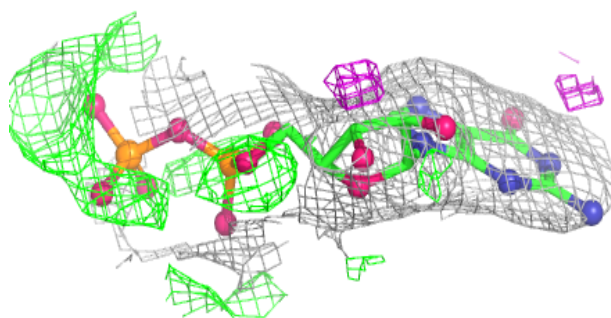
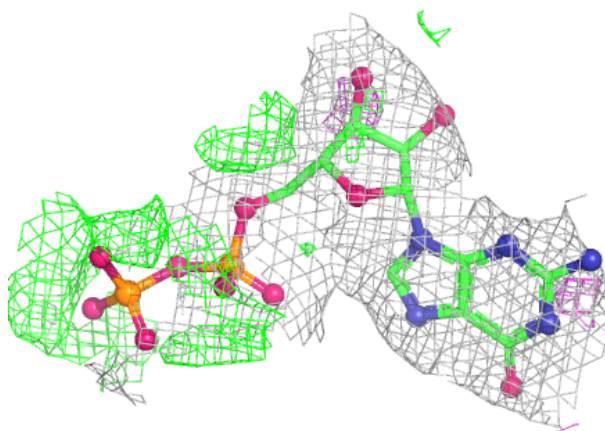
Electron density around ACP F 402:

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

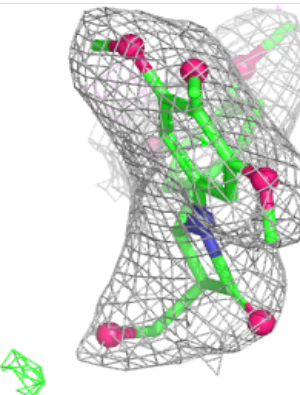
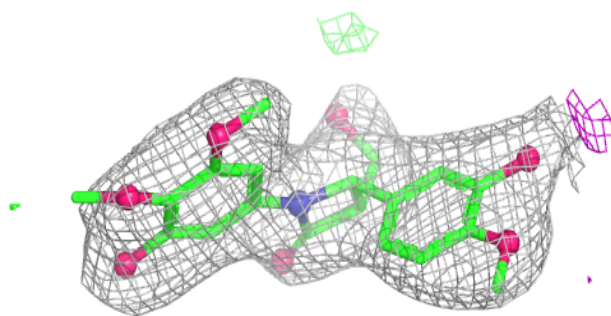
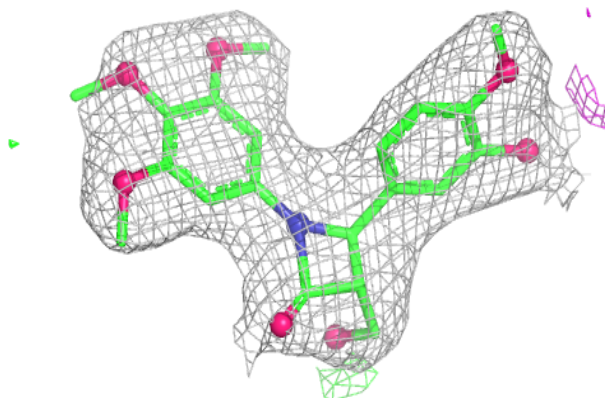


Electron density around GDP D 501:

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

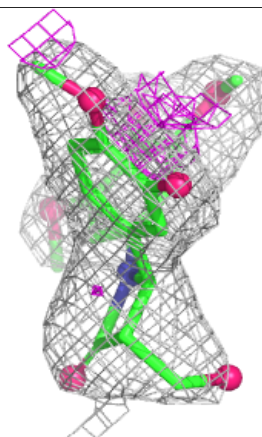
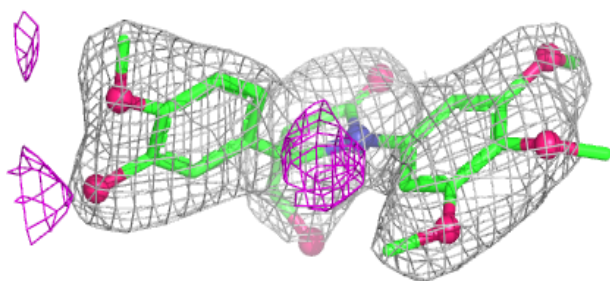
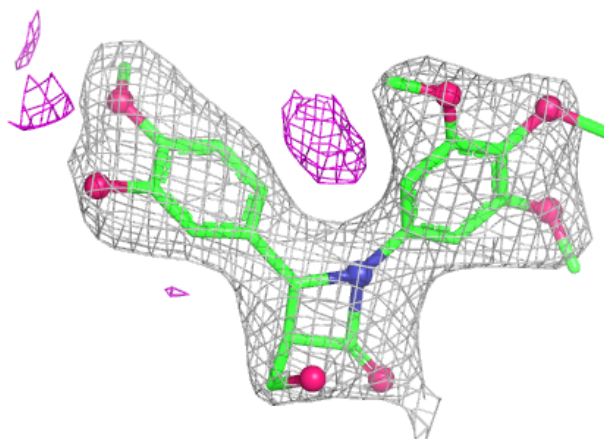
**Electron density around 93X B 508:**

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

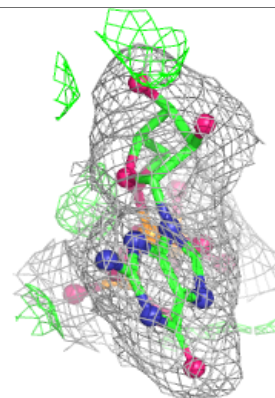
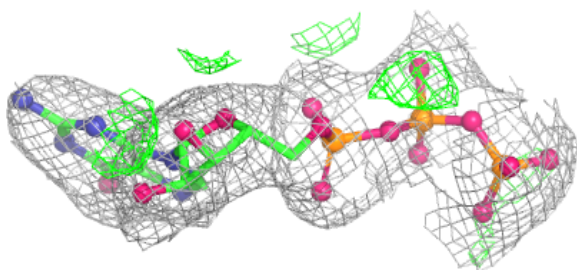
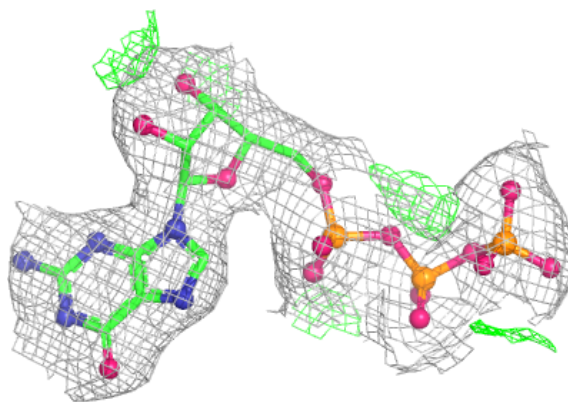


Electron density around 93X D 505:

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

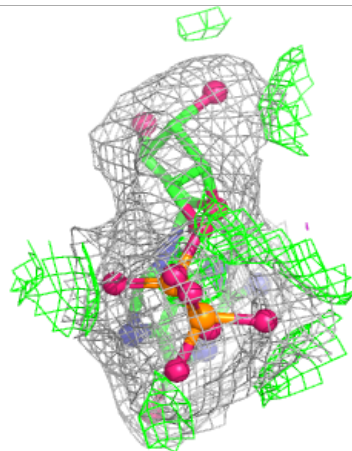
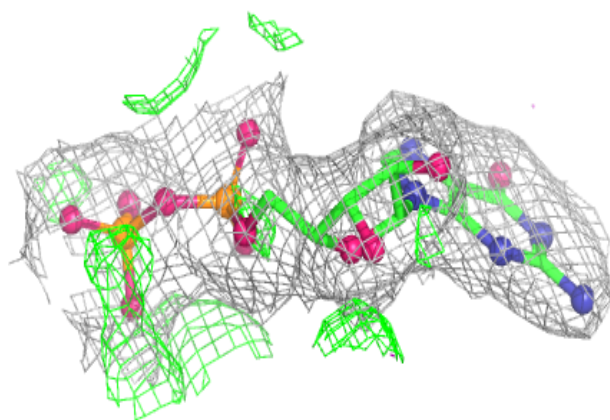
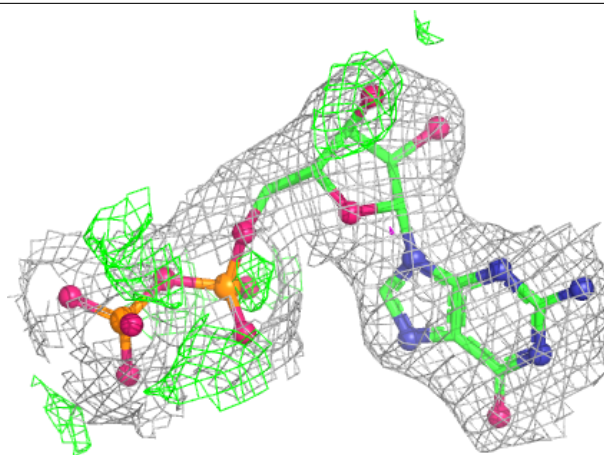
**Electron density around GTP A 501:**

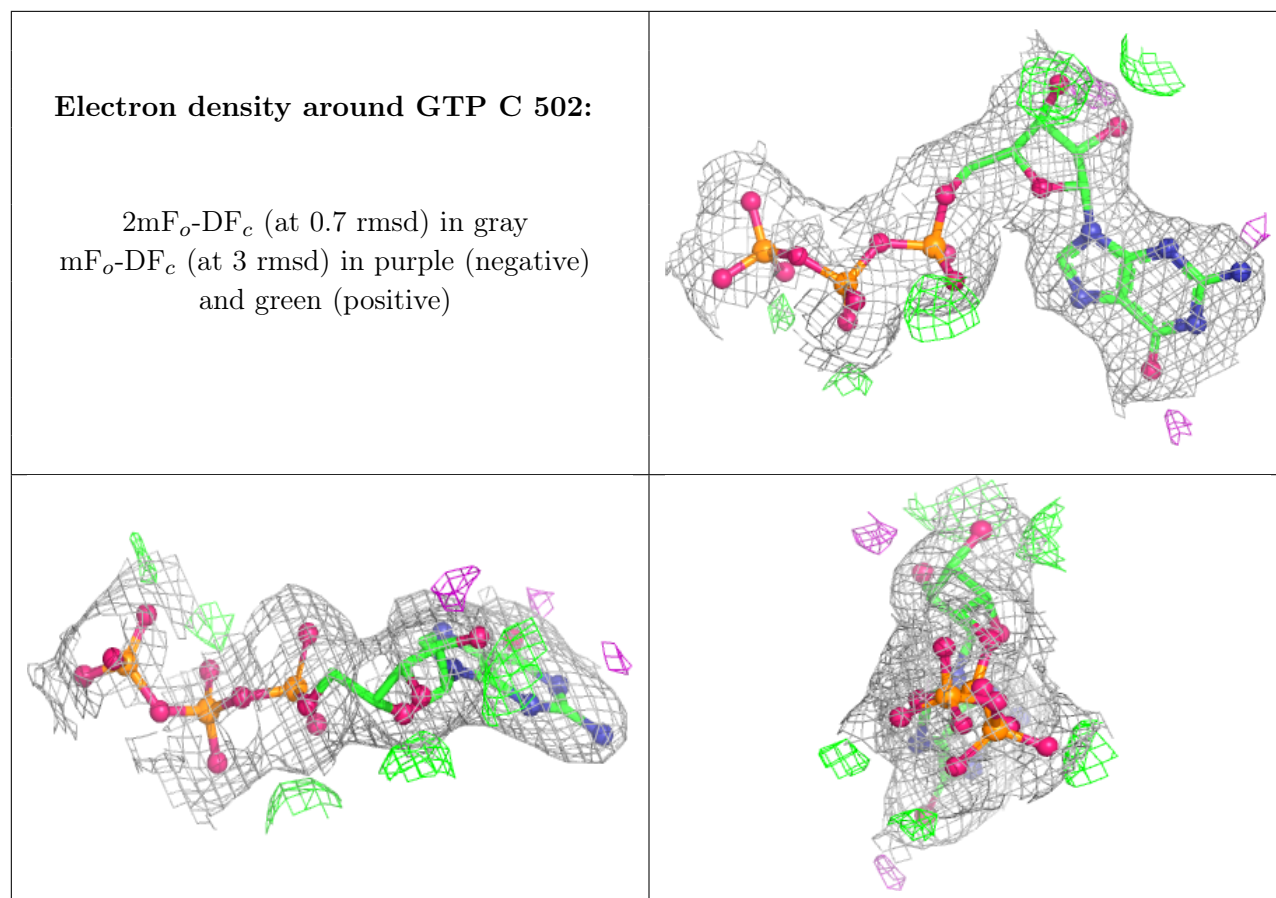
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.