



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:06 am BST

PDB ID : 5XAG
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

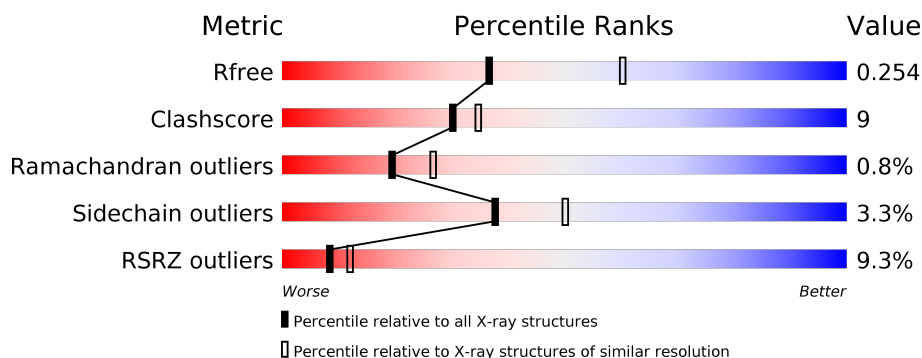
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
2	D	445	<div> <div>9%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div> </div>
3	E	189	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>15%</div> <div>• 37%</div> </div> </div>
4	F	378	<div> <div>29%</div> <div> <div></div> <div>57%</div> <div>24%</div> <div>• 16%</div> </div> </div>

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	A	504	-	-	-	X
7	GOL	B	505	-	-	X	X
7	GOL	C	505	-	-	-	X
7	GOL	D	503	-	-	-	X

2 Entry composition [i](#)

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			

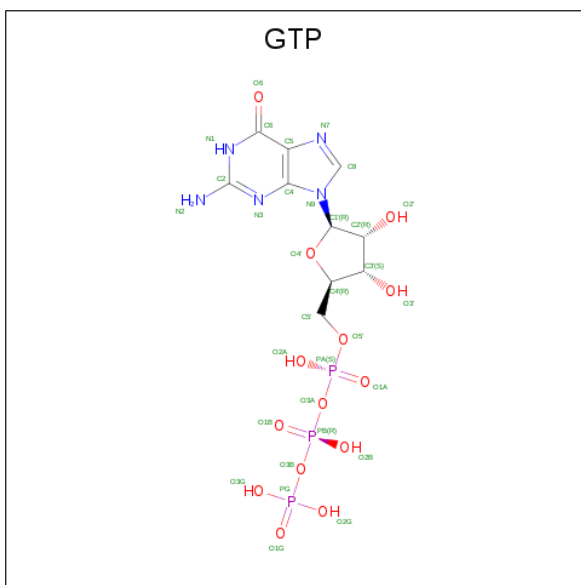
- Molecule 3 is a protein called Stathmin-4.

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 (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

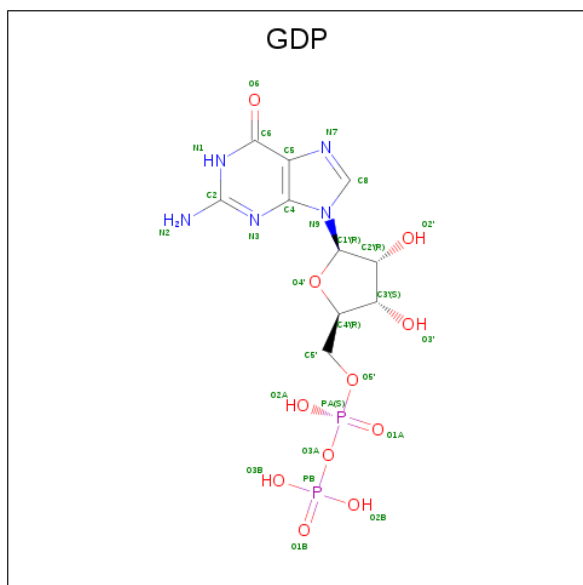


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	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 (three-letter code: CA) (formula: Ca).

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

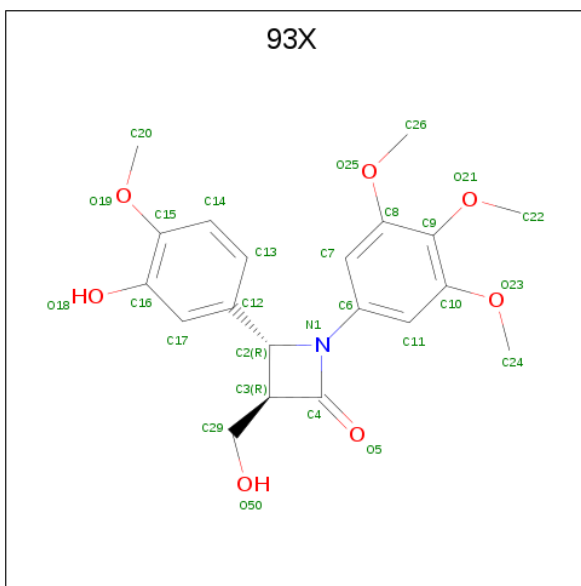
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





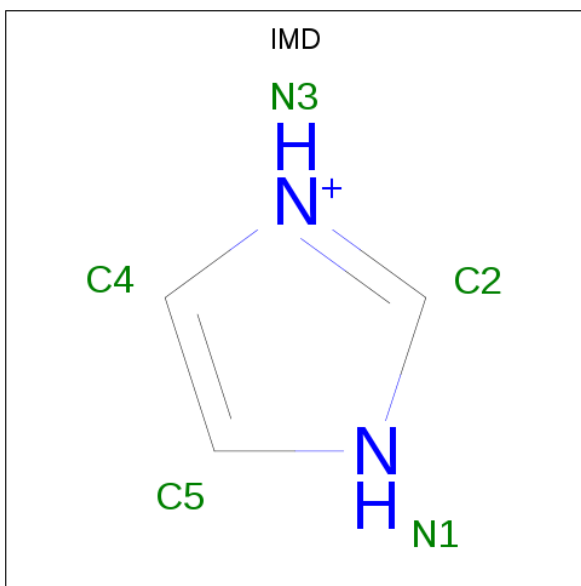
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



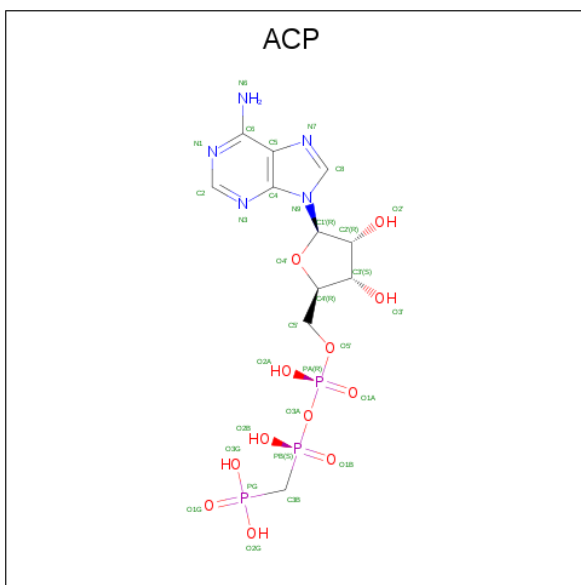
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			28	20	1	7		
11	D	1	Total	C	N	O	0	0
			28	20	1	7		

- Molecule 12 is IMIDAZOLE (three-letter code: 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 (three-letter code: 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		

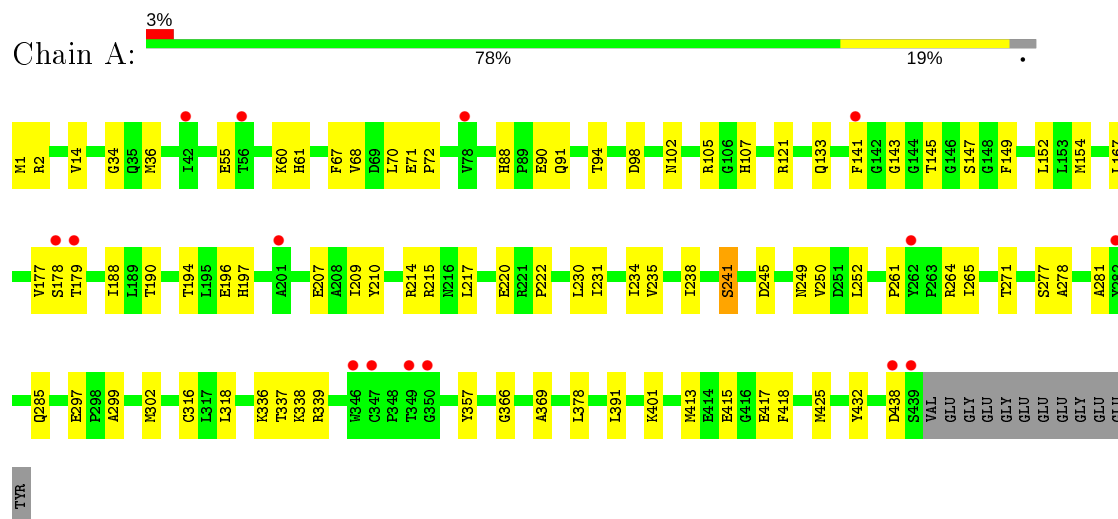
- Molecule 14 is water.

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		

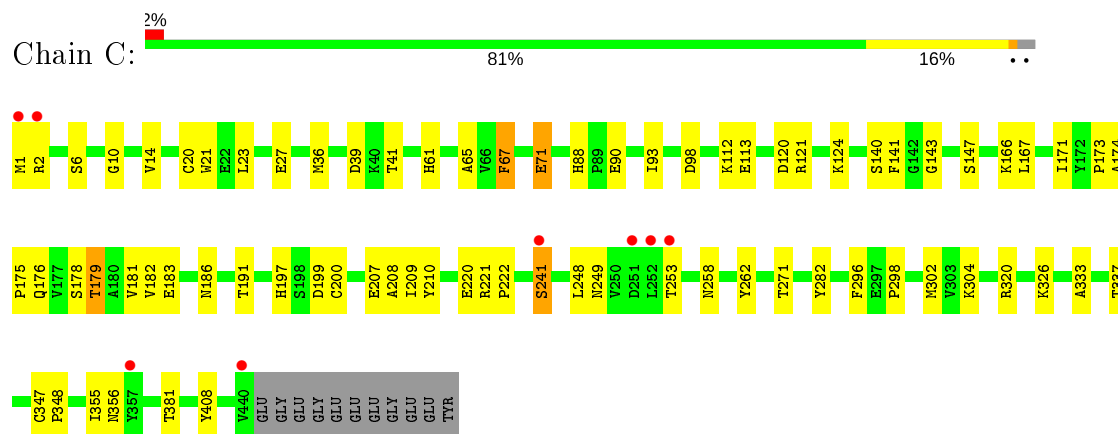
3 Residue-property plots [i](#)

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

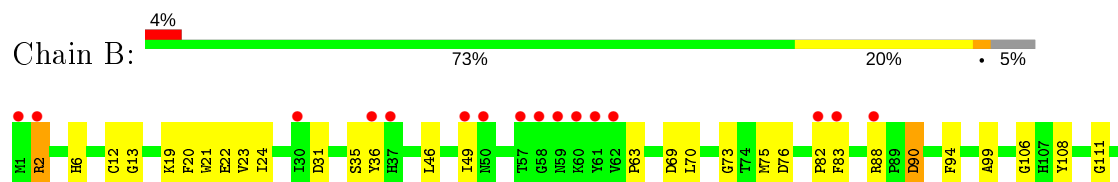
- Molecule 1: Tubulin alpha-1B chain

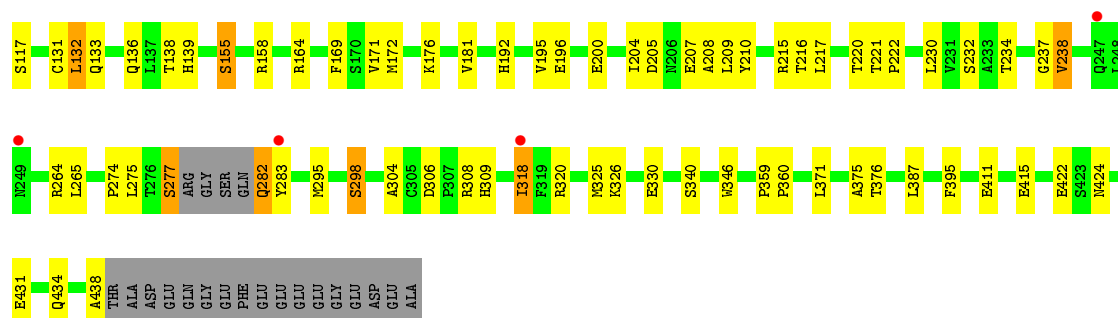


- Molecule 1: Tubulin alpha-1B chain

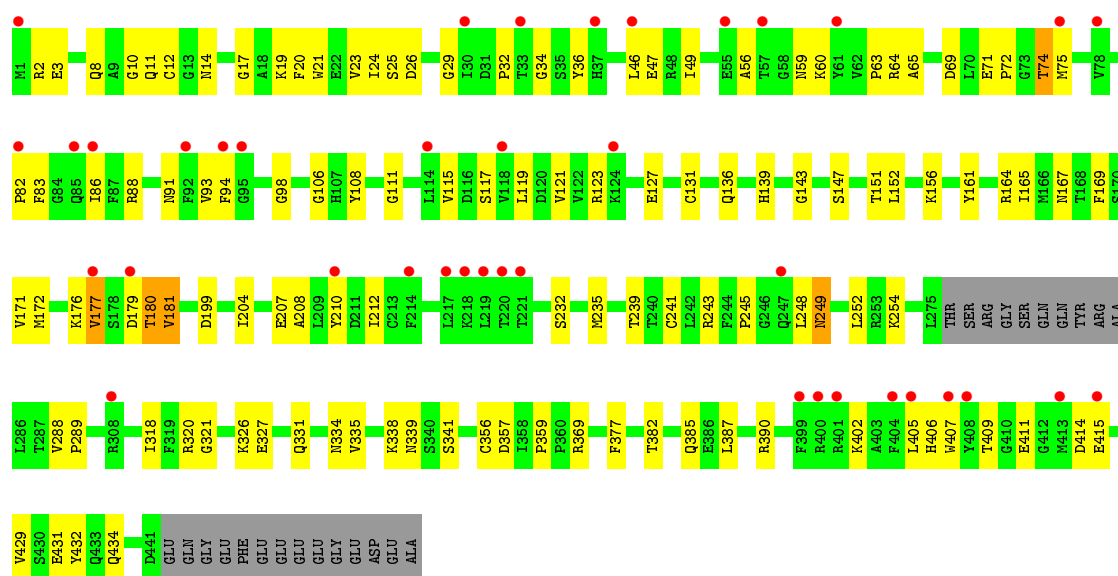


- Molecule 2: Tubulin beta-2B chain

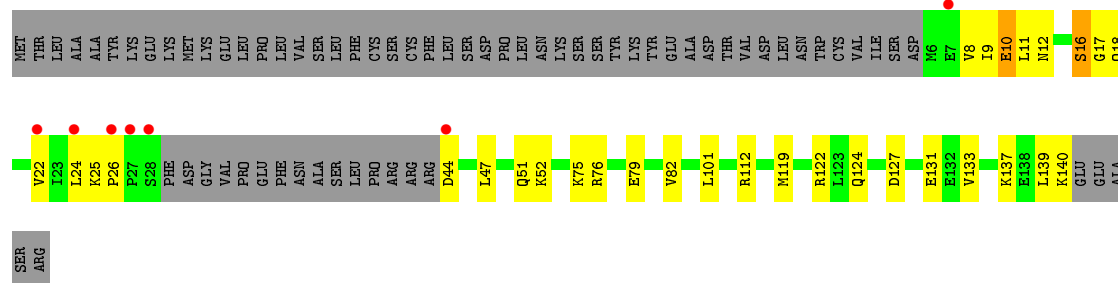




• Molecule 2: Tubulin beta-2B chain

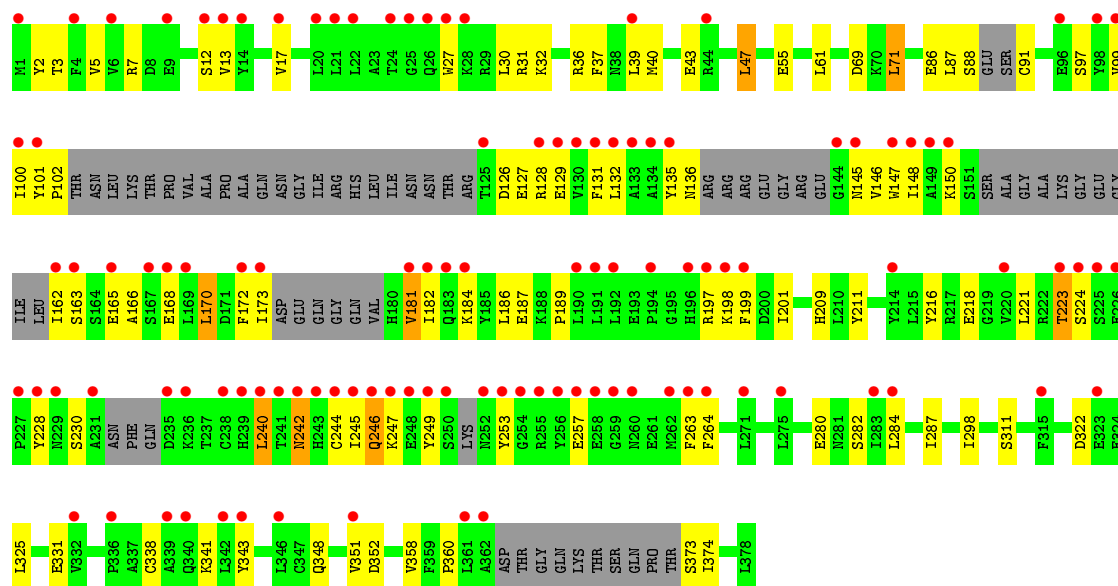


• Molecule 3: Stathmin-4



• 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 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.56) 99.9 (47.92-2.55)	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 0.211 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (2.07%)	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 , 52.7	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: GDP, GOL, MG, IMD, CA, GTP, 93X, MES, ACP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/3584	0.60	0/4865
1	C	0.52	1/3584 (0.0%)	0.66	0/4867
2	B	0.46	0/3474	0.62	1/4706 (0.0%)
2	D	0.42	0/3403	0.57	0/4611
3	E	0.50	0/1008	0.56	0/1337
4	F	0.41	1/2674 (0.0%)	0.57	0/3609
All	All	0.46	2/17727 (0.0%)	0.60	1/23995 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	47	LEU	C-N	7.58	1.48	1.34
1	C	20	CYS	CB-SG	-5.15	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	LEU	CA-CB-CG	-5.21	103.31	115.30

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	55	0
1	C	3482	0	3401	49	1
2	B	3376	0	3265	63	1
2	D	3321	0	3210	74	0
3	E	997	0	1020	22	0
4	F	2609	0	2599	72	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	2	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	321	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 9.

All (321) 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
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
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:320:ARG:NH1	7:B:505:GOL:H11	2.18	0.57
4:F:163:SER:OG	4:F:168:GLU:OE1	2.20	0.57
4:F:7:ARG:NH2	4:F:43:GLU:OE2	2.30	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
4:F:40:MET:HE2	4:F:47:LEU:HG	1.86	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: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:N	2:D:179:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.44	0.52
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.43	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
4:F:88:SER:HG	4:F:91:CYS:N	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:D:3:GLU:N	2:D:3:GLU:OE2	2.45	0.49
4:F:145:ASN:HB3	4:F:147:TRP:NE1	2.19	0.49
4:F:100:ILE:HG13	4:F:182:ILE:HD12	1.94	0.49
4:F:71:LEU:HD13	4:F:298:ILE:HD13	1.94	0.49
1:A:338:LYS:HE2	1:A:339:ARG:HG3	1.95	0.49
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.93	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
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
1:A:297:GLU:OE2	1:A:339:ARG:NH1	2.44	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:A:88:HIS:HB3	1:A:91:GLN:HG3	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
4:F:2:TYR:OH	4:F:360:PRO:O	2.19	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
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
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:175:PRO:HD2	1:C:207:GLU:OE2	2.16	0.46
1:C:174:ALA:HB2	1:C:207:GLU:N	2.31	0.46
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.33	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
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:336:LYS:HD2	1:A:336:LYS:HA	1.80	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:SER:O	2:D:151:THR:HG23	2.16	0.45
4:F:284[A]:LEU:HD12	4:F:287:ILE:HB	1.98	0.45
2:B:325:MET:HB3	2:B:325:MET:HE2	1.86	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:D:177:VAL:HA	7:D:503:GOL:H32	1.98	0.45
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.98	0.45
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.51	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
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:220:GLU:CD	2:D:326:LYS:HD3	2.38	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
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
2:D:75:MET:SD	2:D:94:PHE:HB3	2.58	0.43
2:D:249:ASN:HB3	2:D:254:LYS:HZ2	1.82	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:N	3:E:139:LEU:HD23	2.33	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
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
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:285:GLN:HE21	1:A:285:GLN:HA	1.84	0.42
1:A:2:ARG:HB3	1:A:133:GLN:HG3	2.00	0.42
1:A:285:GLN:NE2	1:A:285:GLN:HA	2.34	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
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
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
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:D:115:VAL:O	2:D:119:LEU:HG	2.20	0.41
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:264:ARG:HB2	14:A:612:HOH:O	2.21	0.41
1:A:2:ARG:O	1:A:133:GLN:NE2	2.53	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:165:GLU:HB2	4:F:168:GLU:OE2	2.21	0.40
4:F:17:VAL:HG13	4:F:351:VAL:HG22	2.03	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
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

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	447/451 (99%)	421 (94%)	22 (5%)	4 (1%)	17	24
1	C	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	47	58
2	B	429/445 (96%)	402 (94%)	24 (6%)	3 (1%)	22	29
2	D	420/445 (94%)	400 (95%)	16 (4%)	4 (1%)	15	21
3	E	117/189 (62%)	105 (90%)	10 (8%)	2 (2%)	9	11
4	F	302/378 (80%)	263 (87%)	37 (12%)	2 (1%)	22	29
All	All	2162/2359 (92%)	2022 (94%)	124 (6%)	16 (1%)	19	29

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%)	372 (98%)	8 (2%)	53	67
1	C	380/379 (100%)	373 (98%)	7 (2%)	59	73
2	B	375/383 (98%)	357 (95%)	18 (5%)	25	34
2	D	367/383 (96%)	355 (97%)	12 (3%)	38	50
3	E	109/171 (64%)	105 (96%)	4 (4%)	34	45
4	F	289/336 (86%)	275 (95%)	14 (5%)	25	34
All	All	1900/2031 (94%)	1837 (97%)	63 (3%)	38	50

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	178	SER
1	A	179	THR
1	A	207	GLU
1	A	241	SER
1	A	250	VAL
1	A	271	THR
1	A	438	ASP
2	B	2	ARG
2	B	75	MET
2	B	90	ASP
2	B	117	SER
2	B	132	LEU
2	B	139	HIS
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

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Mol	Chain	Res	Type
2	B	283	TYR
2	B	298	SER
2	B	318	ILE
2	B	340	SER
1	C	67	PHE
1	C	71	GLU
1	C	179	THR
1	C	181	VAL
1	C	241	SER
1	C	347	CYS
1	C	381	THR
2	D	8	GLN
2	D	26	ASP
2	D	74	THR
2	D	117	SER
2	D	139	HIS
2	D	180	THR
2	D	207	GLU
2	D	249	ASN
2	D	341	SER
2	D	377	PHE
2	D	390	ARG
2	D	434	GLN
3	E	12	ASN
3	E	16	SER
3	E	124	GLN
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	170	LEU
4	F	172	PHE
4	F	181	VAL
4	F	211	TYR
4	F	223	THR
4	F	240	LEU
4	F	246	GLN
4	F	264	PHE
4	F	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	249	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 carbohydrates 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	$\# Z > 2$
7	GOL	B	504	-	5,5,5	0.45	0	5,5,5	0.43	0
7	GOL	D	504	12	5,5,5	0.36	0	5,5,5	0.30	0
7	GOL	C	504	-	5,5,5	0.31	0	5,5,5	0.48	0
12	IMD	E	201	7	3,5,5	0.36	0	4,5,5	0.49	0
11	93X	D	505	-	30,30,30	6.24	11 (36%)	40,43,43	3.97	12 (30%)
9	GDP	D	501	-	24,30,30	1.35	3 (12%)	31,47,47	2.00	8 (25%)
7	GOL	D	503	-	5,5,5	0.33	0	5,5,5	0.38	0
7	GOL	B	505	-	5,5,5	0.38	0	5,5,5	0.58	0
7	GOL	C	505	-	5,5,5	0.42	0	5,5,5	0.09	0
13	ACP	F	402	-	27,33,33	2.50	8 (29%)	32,52,52	1.56	5 (15%)
9	GDP	B	501	6	24,30,30	1.13	1 (4%)	31,47,47	1.91	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	504	-	5,5,5	0.41	0	5,5,5	0.70	0
7	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.33	0
12	IMD	C	508	-	3,5,5	0.45	0	4,5,5	0.51	0
10	MES	B	507	-	12,12,12	2.16	1 (8%)	14,16,16	2.22	4 (28%)
5	GTP	C	502	6	26,34,34	1.11	2 (7%)	33,54,54	1.73	7 (21%)
7	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.40	0
11	93X	B	508	-	30,30,30	6.16	8 (26%)	40,43,43	4.17	15 (37%)
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.71	6 (18%)
7	GOL	B	503	-	5,5,5	0.36	0	5,5,5	0.23	0
12	IMD	C	509	-	3,5,5	0.43	0	4,5,5	0.53	0
7	GOL	C	506	-	5,5,5	0.54	0	5,5,5	0.57	0
7	GOL	C	501	-	5,5,5	0.36	0	5,5,5	0.31	0

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
7	GOL	B	504	-	-	2/4/4/4	-
7	GOL	D	504	12	-	2/4/4/4	-
7	GOL	C	504	-	-	2/4/4/4	-
12	IMD	E	201	7	-	-	0/1/1/1
11	93X	D	505	-	-	3/18/34/34	0/3/3/3
9	GDP	D	501	-	-	5/12/32/32	0/3/3/3
7	GOL	D	503	-	-	0/4/4/4	-
12	IMD	C	508	-	-	-	0/1/1/1
7	GOL	C	505	-	-	4/4/4/4	-
13	ACP	F	402	-	-	3/15/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
7	GOL	A	504	-	-	4/4/4/4	-
7	GOL	A	503	-	-	4/4/4/4	-
7	GOL	B	505	-	-	4/4/4/4	-
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
5	GTP	C	502	6	-	5/18/38/38	0/3/3/3
7	GOL	A	506	-	-	4/4/4/4	-
11	93X	B	508	-	-	3/18/34/34	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	503	-	-	4/4/4/4	-
12	IMD	C	509	-	-	-	0/1/1/1
7	GOL	C	506	-	-	4/4/4/4	-
7	GOL	C	501	-	-	1/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	505	93X	C4-N1	24.39	1.75	1.37
11	B	508	93X	C4-N1	24.01	1.74	1.37
11	B	508	93X	C3-C2	-21.86	1.34	1.57
11	D	505	93X	C3-C2	-21.27	1.35	1.57
13	F	402	ACP	PB-O3A	7.66	1.66	1.58
10	B	507	MES	C8-S	-7.21	1.67	1.77
13	F	402	ACP	O4'-C1'	5.38	1.48	1.41
11	D	505	93X	C29-C3	5.37	1.61	1.53
11	D	505	93X	C12-C2	5.15	1.59	1.51
9	D	501	GDP	C6-C5	4.76	1.49	1.41
11	B	508	93X	C29-C3	4.63	1.60	1.53
13	F	402	ACP	C2'-C1'	-3.77	1.48	1.53
11	D	505	93X	O19-C15	3.61	1.42	1.37
13	F	402	ACP	C6-N6	3.51	1.46	1.34
11	B	508	93X	C12-C2	3.43	1.56	1.51
9	B	501	GDP	C6-C5	3.29	1.47	1.41
5	A	501	GTP	C6-N1	3.20	1.38	1.33
13	F	402	ACP	C4-N3	-3.17	1.31	1.35
5	C	502	GTP	C6-N1	3.16	1.38	1.33
11	B	508	93X	O18-C16	3.06	1.42	1.36
11	D	505	93X	O23-C10	3.00	1.41	1.37
11	D	505	93X	C2-N1	2.89	1.51	1.48
11	D	505	93X	O25-C8	2.79	1.41	1.37
11	B	508	93X	O21-C9	2.77	1.43	1.38
13	F	402	ACP	C2'-C3'	-2.63	1.46	1.53
11	D	505	93X	C6-N1	2.61	1.47	1.43
11	B	508	93X	O19-C15	2.59	1.41	1.37
13	F	402	ACP	PB-O2B	-2.53	1.50	1.56
9	D	501	GDP	C5-C4	2.40	1.47	1.40
11	D	505	93X	O18-C16	2.34	1.41	1.36
5	C	502	GTP	C2-N1	2.32	1.39	1.35
13	F	402	ACP	C5-N7	2.31	1.48	1.39
11	D	505	93X	O21-C9	2.17	1.42	1.38
9	D	501	GDP	C2'-C1'	-2.15	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	508	93X	O25-C8	2.13	1.40	1.37

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	93X	C2-N1-C4	-13.19	82.45	95.27
11	D	505	93X	C2-N1-C4	-12.84	82.79	95.27
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	B	508	93X	C6-N1-C2	8.18	143.41	130.29
11	D	505	93X	C6-N1-C2	7.26	141.94	130.29
11	D	505	93X	O5-C4-C3	6.15	142.01	135.43
11	B	508	93X	O5-C4-C3	5.99	141.84	135.43
5	C	502	GTP	N3-C2-N1	-5.56	119.80	127.22
9	B	501	GDP	C2-N3-C4	5.27	121.37	115.36
10	B	507	MES	C5-N4-C3	5.14	120.39	108.83
11	B	508	93X	C26-O25-C8	-4.98	110.02	117.53
9	D	501	GDP	C2-N3-C4	4.98	121.04	115.36
5	A	501	GTP	N3-C2-N1	-4.83	120.77	127.22
11	D	505	93X	O23-C10-C9	4.82	123.64	115.16
9	D	501	GDP	C6-C5-C4	-4.61	116.40	120.80
11	B	508	93X	O23-C10-C9	4.60	123.25	115.16
11	D	505	93X	O23-C10-C11	-4.31	116.70	124.12
5	A	501	GTP	C2-N3-C4	4.22	120.17	115.36
11	D	505	93X	O25-C8-C9	4.20	122.55	115.16
5	C	502	GTP	C2-N3-C4	4.20	120.15	115.36
11	D	505	93X	O25-C8-C7	-4.19	116.91	124.12
10	B	507	MES	O3S-S-C8	4.18	112.52	105.77
13	F	402	ACP	N3-C2-N1	-4.16	122.18	128.68
9	B	501	GDP	C6-C5-C4	-4.08	116.90	120.80
13	F	402	ACP	C3'-C2'-C1'	3.98	106.98	100.98
9	D	501	GDP	C6-N1-C2	3.94	122.19	115.93
13	F	402	ACP	O3'-C3'-C4'	3.91	122.35	111.05
11	B	508	93X	O23-C10-C11	-3.86	117.48	124.12
9	B	501	GDP	N3-C2-N1	-3.85	122.09	127.22
11	B	508	93X	O25-C8-C7	-3.72	117.72	124.12
9	D	501	GDP	C5-C6-N1	-3.58	118.54	123.43
9	D	501	GDP	N3-C2-N1	-3.32	122.79	127.22
9	D	501	GDP	C4-C5-N7	-3.22	106.05	109.40
9	B	501	GDP	C6-N1-C2	3.20	121.02	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	-3.14	119.14	123.43
11	B	508	93X	C24-O23-C10	-3.14	112.79	117.53
11	D	505	93X	O5-C4-N1	2.97	135.99	131.80
11	B	508	93X	O5-C4-N1	2.93	135.93	131.80
11	B	508	93X	O25-C8-C9	2.90	120.26	115.16
10	B	507	MES	C6-C5-N4	-2.89	105.72	110.10
9	B	501	GDP	O2B-PB-O3A	2.74	113.82	104.64
9	B	501	GDP	C5-C6-N1	-2.67	119.78	123.43
11	B	508	93X	O21-C9-C10	2.65	123.95	120.12
9	D	501	GDP	PA-O3A-PB	-2.56	124.03	132.83
5	A	501	GTP	C6-N1-C2	2.55	119.97	115.93
5	C	502	GTP	PB-O3B-PG	-2.52	124.19	132.83
11	D	505	93X	C7-C6-N1	2.50	122.15	119.47
11	B	508	93X	C14-C13-C12	-2.49	118.69	121.20
13	F	402	ACP	C4-C5-N7	-2.49	106.81	109.40
9	B	501	GDP	PA-O3A-PB	-2.48	124.31	132.83
10	B	507	MES	O1S-S-C8	2.41	109.82	106.92
9	B	501	GDP	C4-C5-N7	-2.40	106.90	109.40
5	C	502	GTP	O3G-PG-O3B	2.36	112.57	104.64
13	F	402	ACP	C2'-C3'-C4'	2.31	107.13	102.64
5	C	502	GTP	N2-C2-N1	2.28	120.79	117.25
9	D	501	GDP	C2'-C3'-C4'	2.21	106.93	102.64
11	B	508	93X	C7-C6-N1	2.20	121.83	119.47
5	A	501	GTP	O3'-C3'-C2'	-2.18	104.78	111.82
5	C	502	GTP	C6-N1-C2	2.14	119.33	115.93
5	A	501	GTP	N2-C2-N1	2.06	120.45	117.25
5	C	502	GTP	C5-C6-N1	-2.05	120.63	123.43
11	D	505	93X	O19-C15-C16	2.02	117.50	114.57

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	504	GOL	O1-C1-C2-C3
7	C	504	GOL	O1-C1-C2-O2
7	C	504	GOL	O1-C1-C2-C3
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
7	B	505	GOL	O1-C1-C2-O2
7	B	505	GOL	O1-C1-C2-C3
7	C	505	GOL	O1-C1-C2-O2
7	C	505	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	F	402	ACP	C5'-O5'-PA-O1A
13	F	402	ACP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
7	A	504	GOL	O1-C1-C2-C3
7	A	503	GOL	O1-C1-C2-C3
7	A	503	GOL	O2-C2-C3-O3
5	C	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
7	A	506	GOL	C1-C2-C3-O3
7	A	506	GOL	O2-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
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	C	506	GOL	O1-C1-C2-C3
11	D	505	93X	C9-C10-O23-C24
11	D	505	93X	C11-C10-O23-C24
7	B	504	GOL	O1-C1-C2-O2
7	A	504	GOL	O1-C1-C2-O2
7	C	506	GOL	O1-C1-C2-O2
11	B	508	93X	C8-C9-O21-C22
7	B	504	GOL	O1-C1-C2-C3
7	B	505	GOL	C1-C2-C3-O3
7	A	503	GOL	C1-C2-C3-O3
7	A	506	GOL	O1-C1-C2-C3
7	D	504	GOL	O1-C1-C2-O2
7	B	505	GOL	O2-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
9	D	501	GDP	O4'-C4'-C5'-O5'
9	D	501	GDP	C3'-C4'-C5'-O5'
11	B	508	93X	C10-C9-O21-C22
9	B	501	GDP	C5'-O5'-PA-O3A
7	C	505	GOL	C1-C2-C3-O3
13	F	402	ACP	C3'-C4'-C5'-O5'
7	A	504	GOL	C1-C2-C3-O3
7	A	504	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	C	501	GOL	C1-C2-C3-O3
7	C	505	GOL	O2-C2-C3-O3
7	C	506	GOL	O2-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O2G
9	D	501	GDP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
11	B	508	93X	C9-C10-O23-C24
7	C	506	GOL	C1-C2-C3-O3
5	C	502	GTP	PB-O3B-PG-O1G
11	D	505	93X	C8-C9-O21-C22

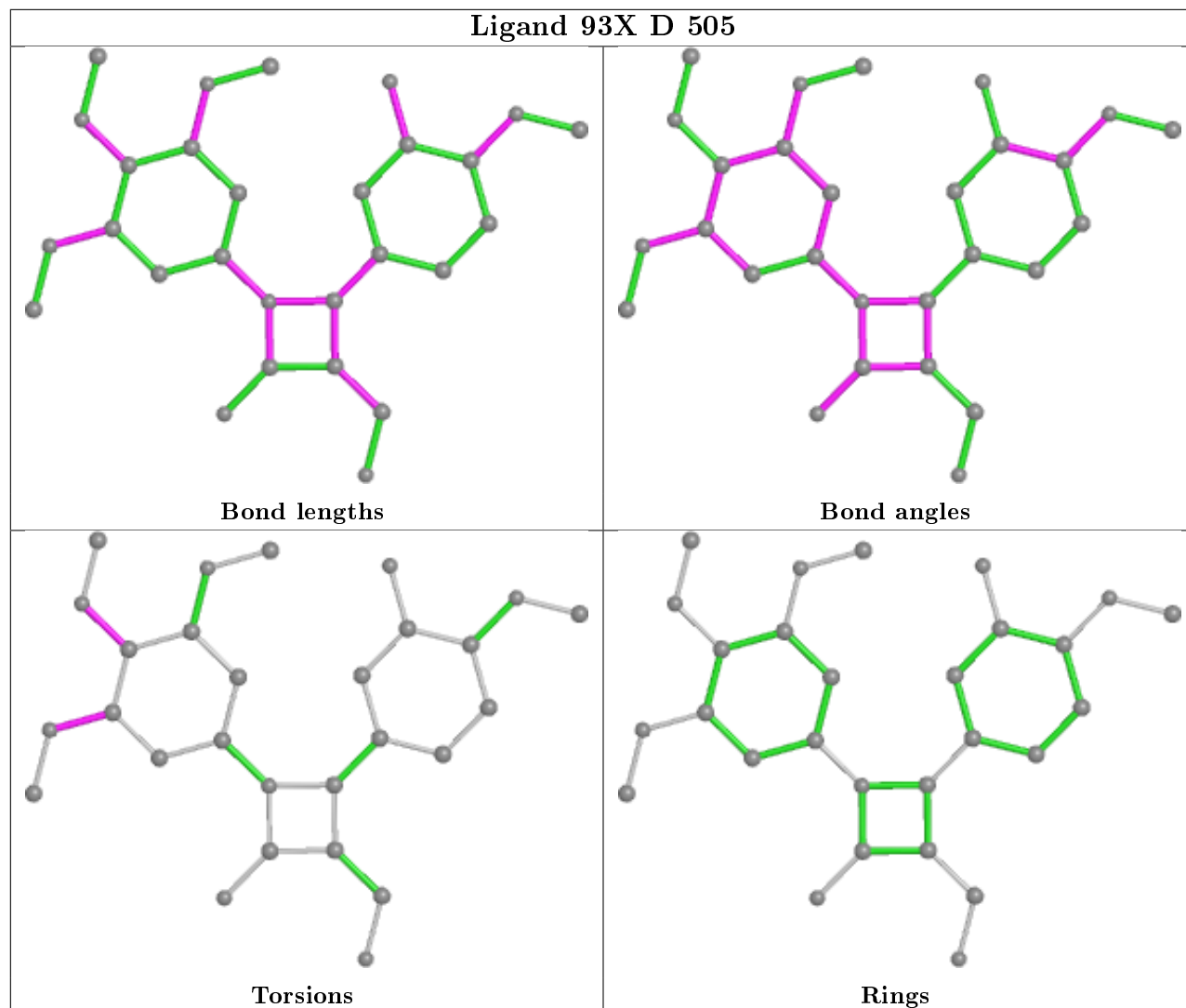
There are no ring outliers.

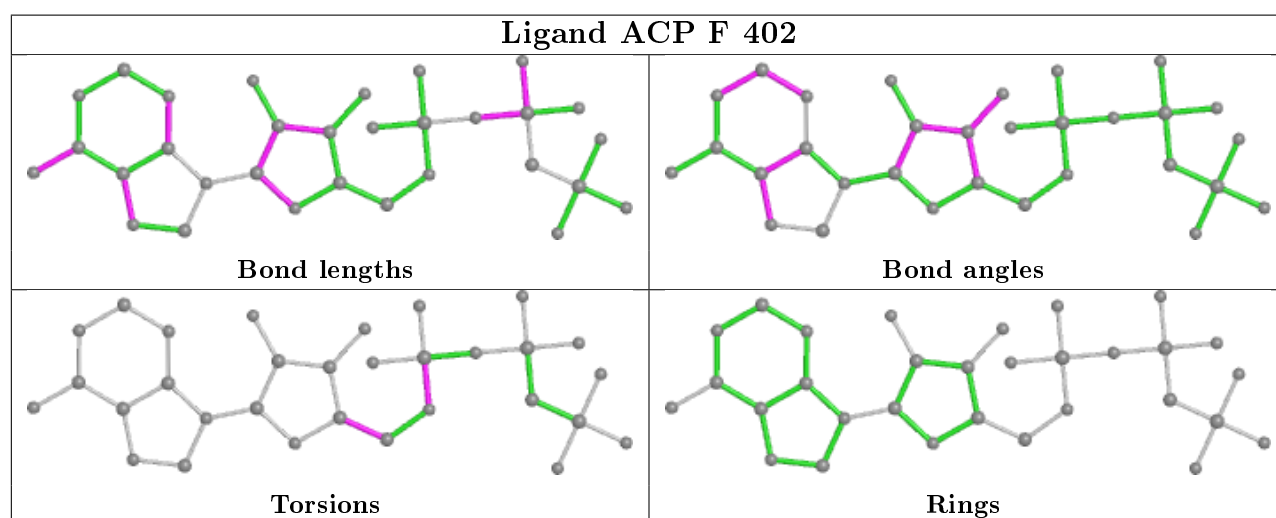
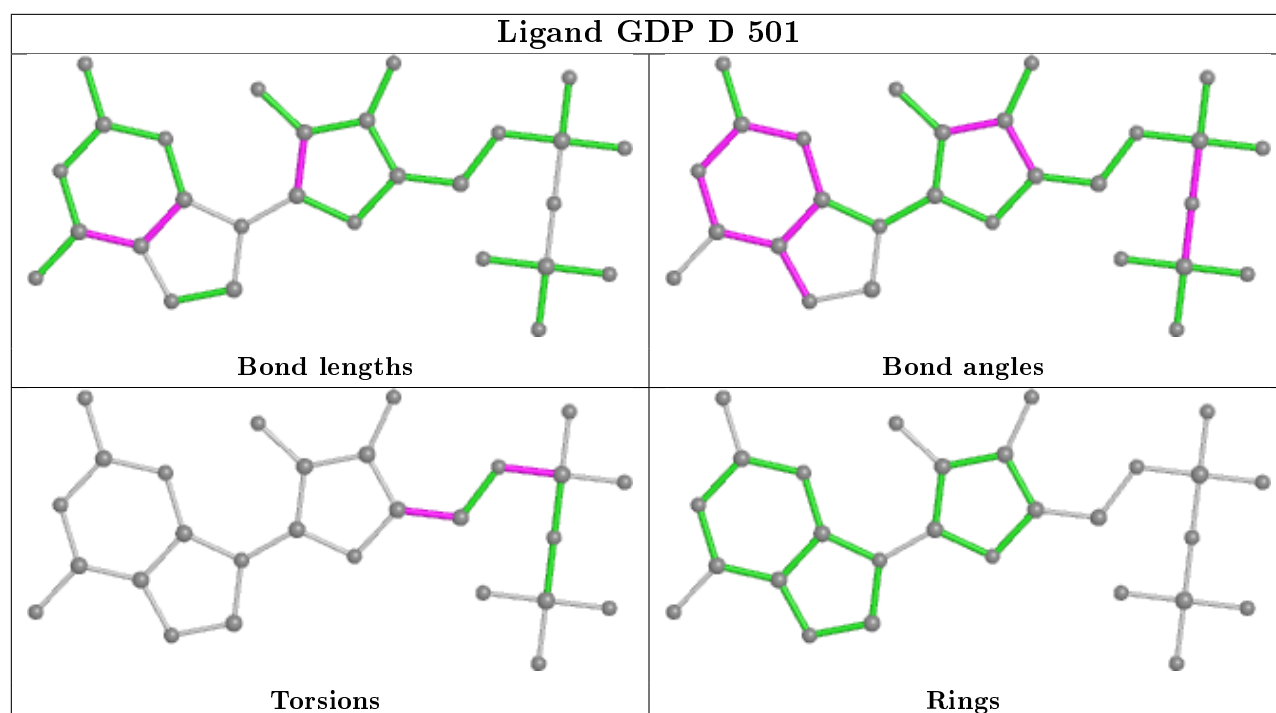
14 monomers are involved in 25 short contacts:

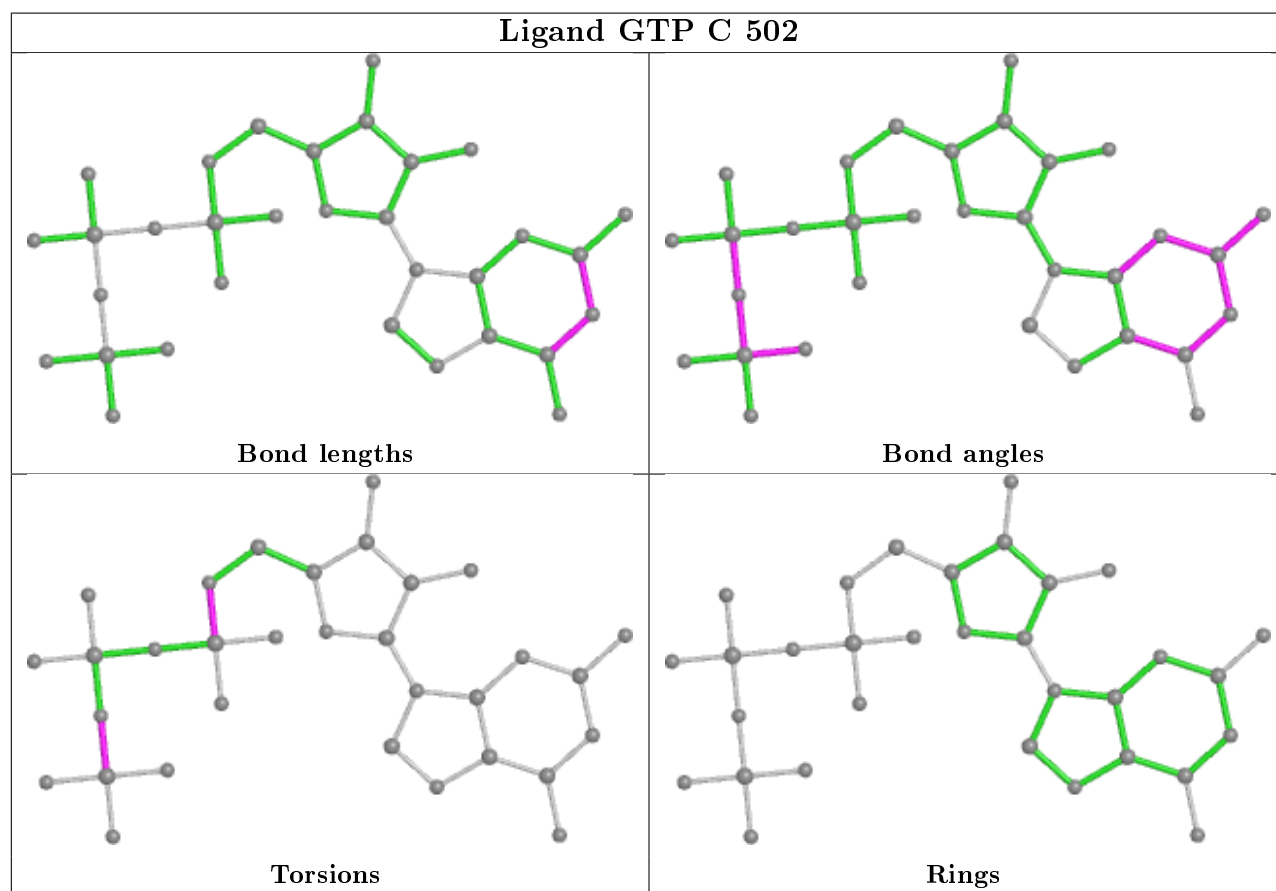
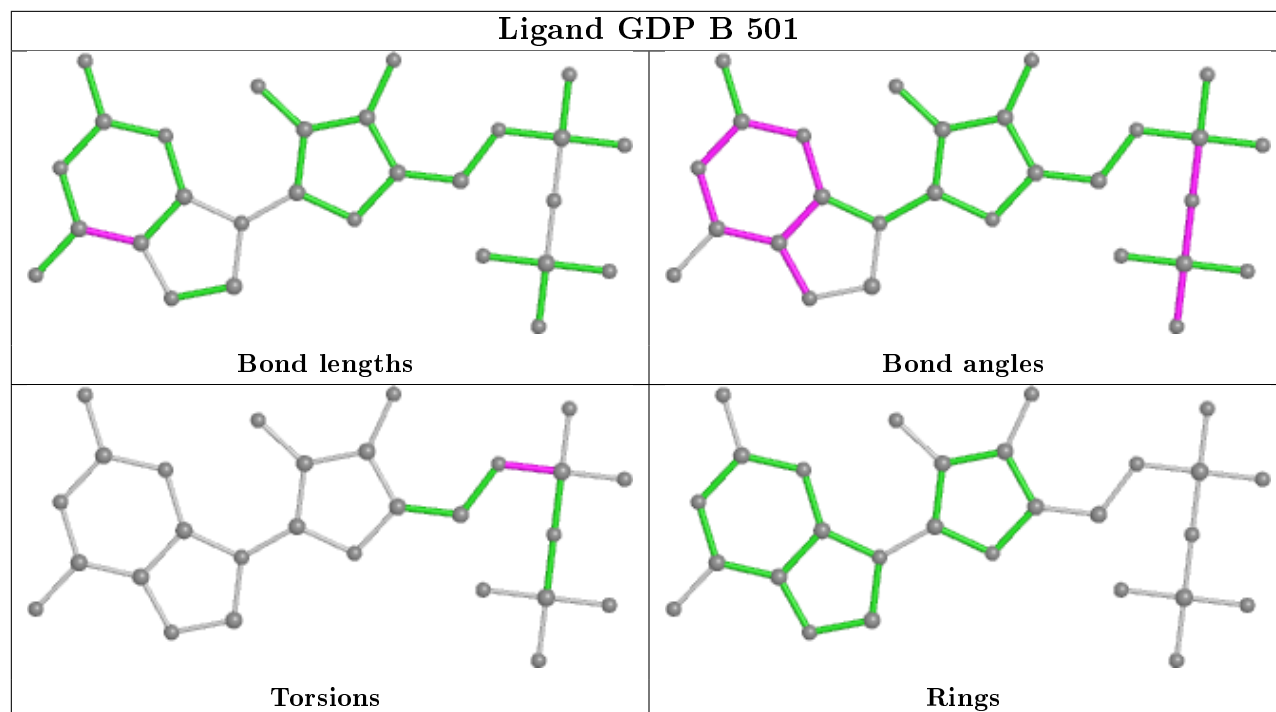
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	201	IMD	2	0
11	D	505	93X	1	0
9	D	501	GDP	2	0
7	D	503	GOL	2	0
7	B	505	GOL	6	0
13	F	402	ACP	1	0
9	B	501	GDP	1	0
12	C	508	IMD	2	0
5	C	502	GTP	2	0
7	A	506	GOL	1	0
5	A	501	GTP	2	0
12	C	509	IMD	1	0
7	C	506	GOL	1	0
7	C	501	GOL	1	0

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

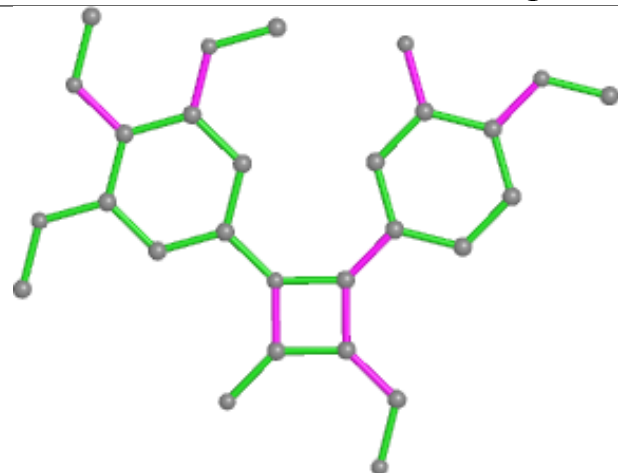
equivalents in the CSD to analyse the geometry.



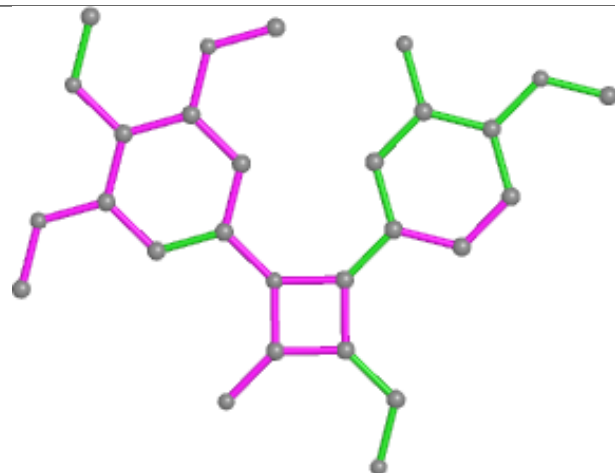




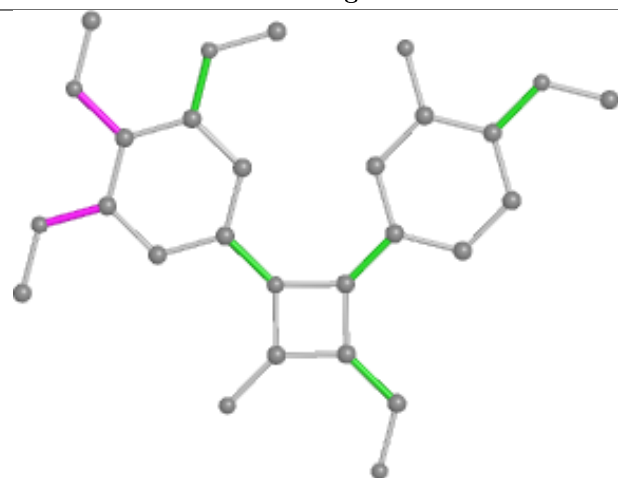
Ligand 93X B 508



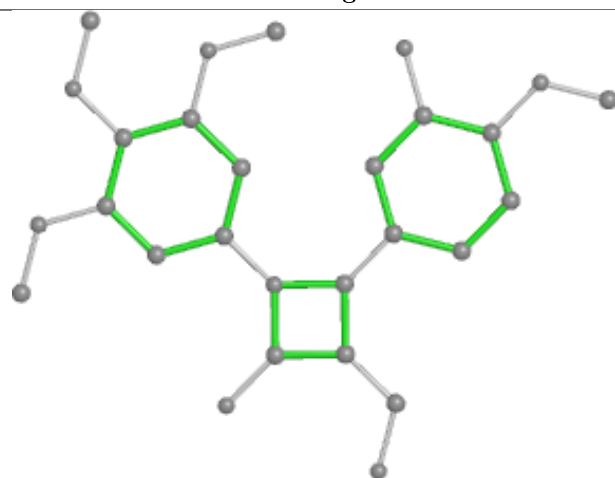
Bond lengths



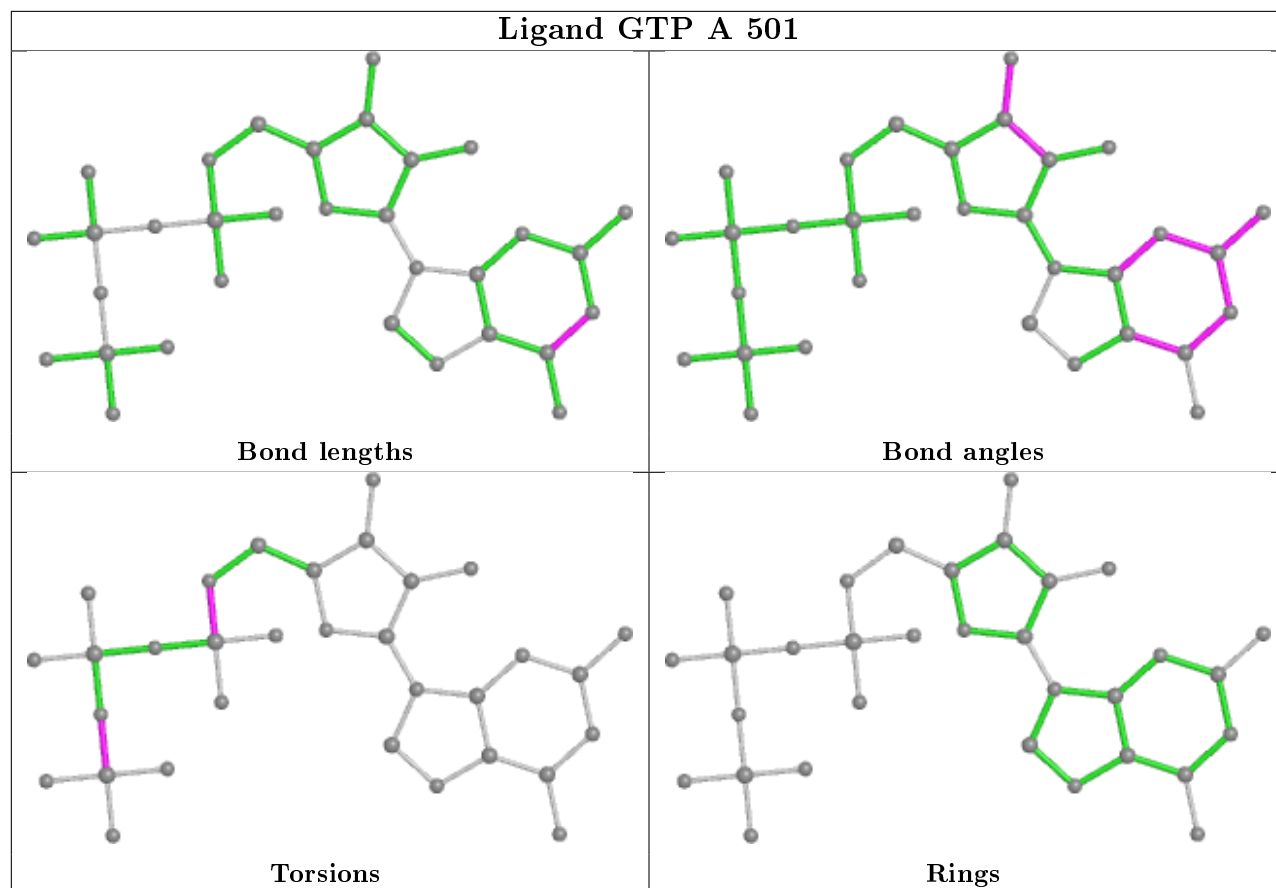
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	0.34	15 (3%) 45 54	48, 71, 104, 153	0
1	C	440/451 (97%)	0.02	8 (1%) 68 75	40, 55, 82, 106	0
2	B	424/445 (95%)	0.28	20 (4%) 31 40	38, 64, 102, 176	0
2	D	421/445 (94%)	0.59	39 (9%) 8 12	48, 85, 122, 181	4 (0%)
3	E	120/189 (63%)	0.35	7 (5%) 23 29	50, 80, 115, 154	0
4	F	317/378 (83%)	1.55	111 (35%) 0 0	55, 100, 170, 220	0
All	All	2161/2359 (91%)	0.49	200 (9%) 8 12	38, 73, 124, 220	4 (0%)

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	15.4
4	F	245	ILE	10.9
4	F	133	ALA	9.2
4	F	249	TYR	8.4
4	F	248	GLU	7.6
4	F	256	TYR	7.2
4	F	225	SER	7.1
4	F	239	HIS	6.6
4	F	17	VAL	6.5
4	F	253	TYR	6.3
4	F	240	LEU	6.0
4	F	224	SER	5.9
2	B	59	ASN	5.9
1	A	439	SER	5.8
2	D	219	LEU	5.7
4	F	132	LEU	5.6
4	F	231	ALA	5.6
4	F	134	ALA	5.5
4	F	100	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
4	F	255	ARG	5.3
2	B	62	VAL	5.3
4	F	21	LEU	5.1
3	E	27	PRO	5.0
4	F	257	GLU	5.0
2	B	1	MET	5.0
4	F	130	VAL	4.9
4	F	147	TRP	4.8
4	F	131	PHE	4.6
4	F	236	LYS	4.5
4	F	9	GLU	4.5
2	D	1	MET	4.5
2	D	94	PHE	4.4
2	D	177	VAL	4.4
4	F	252	ASN	4.3
4	F	14	TYR	4.3
4	F	235	ASP	4.3
4	F	346	LEU	4.3
4	F	199	PHE	4.3
4	F	144	GLY	4.2
2	B	50[A]	ASN	4.1
4	F	182	ILE	4.0
4	F	241	THR	3.9
2	D	401	ARG	3.9
4	F	190	LEU	3.9
4	F	27	TRP	3.8
4	F	250	SER	3.8
4	F	259	GLY	3.8
2	D	218	LYS	3.7
2	B	60	LYS	3.7
4	F	227	PRO	3.7
4	F	238	CYS	3.7
4	F	13	VAL	3.7
4	F	361	LEU	3.7
2	B	37	HIS	3.6
4	F	339	ALA	3.5
4	F	242	ASN	3.5
2	B	249	ASN	3.5
4	F	315	PHE	3.5
4	F	150	LYS	3.4
2	B	36	TYR	3.4
2	D	400	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	254	GLY	3.4
2	D	57	THR	3.3
4	F	228	TYR	3.3
4	F	24	THR	3.3
4	F	99	VAL	3.3
2	D	404	PHE	3.3
4	F	243	HIS	3.3
4	F	264	PHE	3.3
2	D	95	GLY	3.3
4	F	135	TYR	3.3
4	F	169	LEU	3.3
4	F	263	PHE	3.3
1	A	262	TYR	3.2
4	F	283	ILE	3.2
2	D	37	HIS	3.2
4	F	128	ARG	3.2
2	D	220	THR	3.2
4	F	198	LYS	3.2
2	B	61	TYR	3.2
1	C	1	MET	3.1
2	D	179	ASP	3.1
3	E	28	SER	3.1
4	F	163	SER	3.1
4	F	148	ILE	3.1
2	D	407	TRP	3.1
1	A	349	THR	3.1
4	F	129	GLU	3.0
4	F	172	PHE	3.0
4	F	197	ARG	3.0
4	F	20	LEU	3.0
3	E	7	GLU	3.0
2	D	75	MET	3.0
4	F	168	GLU	3.0
1	C	241	SER	3.0
4	F	101	TYR	3.0
1	A	179	THR	3.0
4	F	125	THR	3.0
4	F	247	LYS	2.9
2	D	210	TYR	2.9
2	D	408	TYR	2.9
4	F	1	MET	2.9
4	F	96	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	399	PHE	2.9
2	B	57	THR	2.9
2	D	92	PHE	2.9
3	E	22	VAL	2.8
4	F	323	GLU	2.8
2	D	308	ARG	2.8
4	F	167	SER	2.7
4	F	22	LEU	2.7
2	D	124	LYS	2.7
4	F	220	VAL	2.7
4	F	258	GLU	2.7
4	F	271	LEU	2.7
4	F	149	ALA	2.7
2	D	405	LEU	2.7
1	A	438	ASP	2.7
4	F	260	ASN	2.7
4	F	165	GLU	2.6
1	A	141	PHE	2.6
2	B	283	TYR	2.6
1	A	350	GLY	2.6
1	A	347	CYS	2.6
4	F	28	LYS	2.6
3	E	24	LEU	2.6
2	D	61	TYR	2.6
2	B	247	GLN	2.6
4	F	262	MET	2.6
4	F	362	ALA	2.5
2	D	118	VAL	2.5
4	F	192	LEU	2.5
3	E	26	PRO	2.5
4	F	145	ASN	2.5
2	D	30	ILE	2.5
4	F	4	PHE	2.5
2	D	82	PRO	2.5
4	F	25	GLY	2.5
4	F	214	TYR	2.4
2	B	30	ILE	2.4
2	D	78	VAL	2.4
4	F	226	GLU	2.4
4	F	183	GLN	2.4
2	B	49	ILE	2.4
2	D	33	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	85	GLN	2.4
4	F	336	PRO	2.4
1	C	251	ASP	2.4
2	D	413	MET	2.3
2	B	83	PHE	2.3
1	A	346	TRP	2.3
2	D	247	GLN	2.3
4	F	223	THR	2.3
4	F	229	ASN	2.3
4	F	194	PRO	2.3
4	F	26	GLN	2.3
1	C	253	THR	2.3
4	F	162	ILE	2.2
4	F	184	LYS	2.2
1	A	42	ILE	2.2
1	A	282	TYR	2.2
4	F	181	VAL	2.2
4	F	342	LEU	2.2
4	F	196	HIS	2.2
2	D	86	ILE	2.2
2	D	114	LEU	2.2
2	D	415	GLU	2.2
4	F	39	LEU	2.2
2	D	46	LEU	2.2
4	F	44	ARG	2.1
1	A	78	VAL	2.1
4	F	351	VAL	2.1
4	F	173	ILE	2.1
2	B	88	ARG	2.1
4	F	98	TYR	2.1
4	F	332	VAL	2.1
2	D	214	PHE	2.1
1	A	178	SER	2.1
4	F	12	SER	2.1
3	E	44	ASP	2.1
2	B	318	ILE	2.1
1	C	252	LEU	2.1
4	F	340	GLN	2.1
1	C	440	VAL	2.1
2	D	217	LEU	2.1
4	F	284[A]	LEU	2.1
2	B	58	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	2	ARG	2.1
2	B	82	PRO	2.1
1	C	357	TYR	2.1
4	F	275[A]	LEU	2.1
1	A	201	ALA	2.0
2	D	221[A]	THR	2.0
4	F	246	GLN	2.0
2	D	55	GLU	2.0
1	A	56	THR	2.0
4	F	6	VAL	2.0
1	C	2	ARG	2.0
4	F	191	LEU	2.0
4	F	343	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 carbohydrates 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(\AA^2)	Q<0.9
7	GOL	A	504	6/6	0.50	0.45	111,113,114,115	0
7	GOL	B	505	6/6	0.58	0.77	100,107,115,123	0
7	GOL	D	503	6/6	0.66	0.57	139,142,144,145	0
6	MG	D	502	1/1	0.68	0.13	95,95,95,95	0
7	GOL	B	504	6/6	0.70	0.38	77,95,99,102	0
13	ACP	F	402	31/31	0.70	0.33	86,147,176,178	0
7	GOL	B	503	6/6	0.71	0.37	82,96,105,110	0
7	GOL	C	505	6/6	0.74	0.74	108,114,117,119	0
7	GOL	A	506	6/6	0.74	0.26	86,93,98,101	0
7	GOL	C	501	6/6	0.80	0.36	78,88,91,93	0

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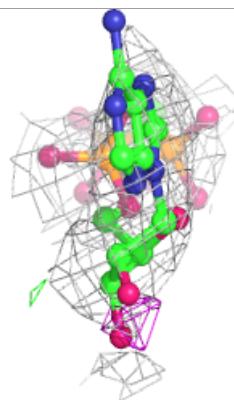
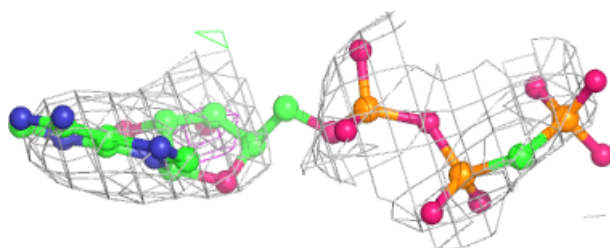
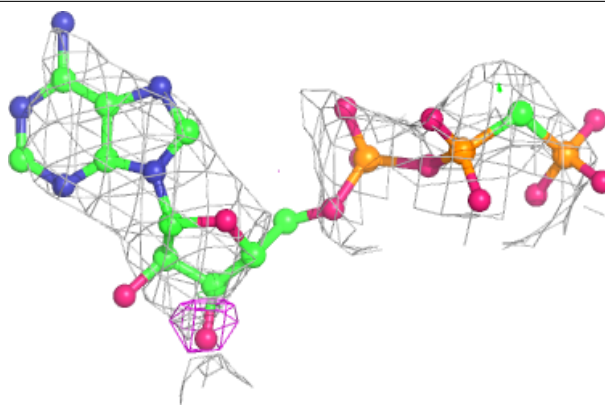
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	IMD	C	509	5/5	0.82	0.36	110,112,113,114	0
7	GOL	D	504	6/6	0.83	0.31	101,109,113,118	0
7	GOL	C	504	6/6	0.85	0.23	91,98,99,101	0
7	GOL	C	506	6/6	0.86	0.23	79,86,88,88	0
12	IMD	E	201	5/5	0.86	0.33	123,124,128,129	0
7	GOL	A	503	6/6	0.89	0.21	89,92,95,99	0
9	GDP	D	501	28/28	0.90	0.17	79,90,101,102	0
12	IMD	C	508	5/5	0.91	0.18	66,73,74,78	0
8	CA	A	505	1/1	0.92	0.08	97,97,97,97	0
6	MG	F	401	1/1	0.92	0.23	119,119,119,119	0
6	MG	B	502	1/1	0.95	0.40	51,51,51,51	0
11	93X	B	508	28/28	0.95	0.24	34,62,74,83	0
11	93X	D	505	28/28	0.96	0.19	55,66,75,83	0
6	MG	C	503	1/1	0.96	0.28	52,52,52,52	0
10	MES	B	507	12/12	0.96	0.15	52,69,81,85	0
8	CA	C	507	1/1	0.96	0.07	112,112,112,112	0
9	GDP	B	501	28/28	0.97	0.21	36,46,54,66	0
6	MG	A	502	1/1	0.98	0.26	80,80,80,80	0
5	GTP	A	501	32/32	0.98	0.23	49,55,60,62	0
8	CA	B	506	1/1	0.98	0.08	118,118,118,118	0
5	GTP	C	502	32/32	0.98	0.20	43,51,57,60	0

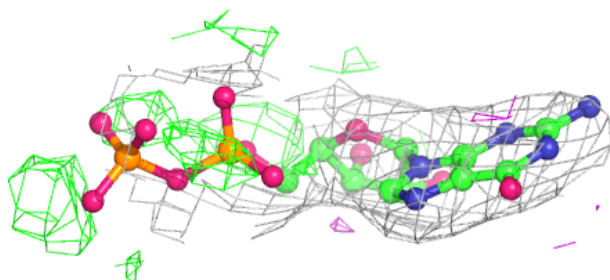
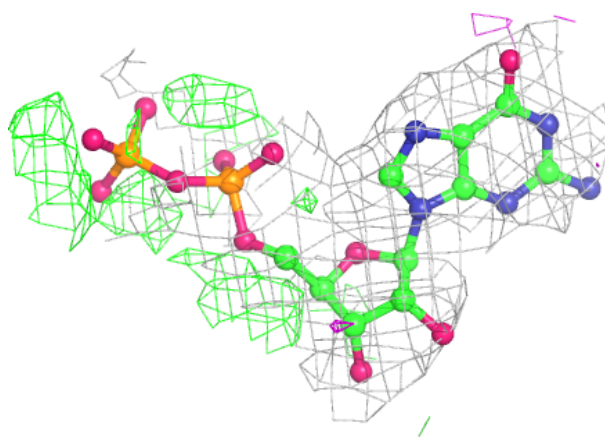
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

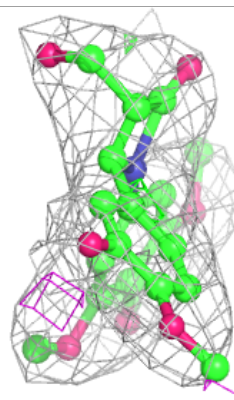
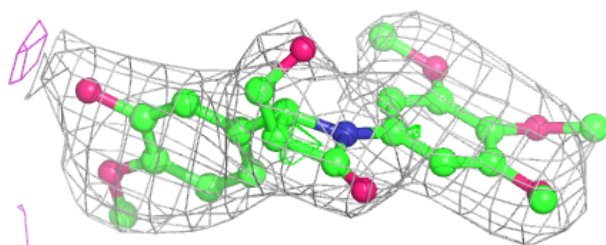
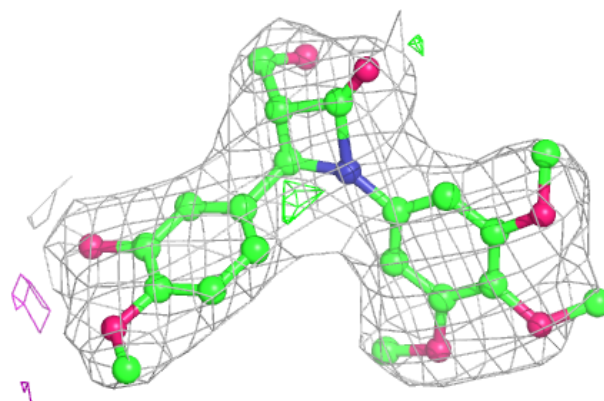
**Electron density around GDP D 501:**

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

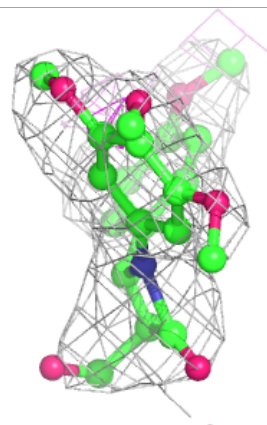
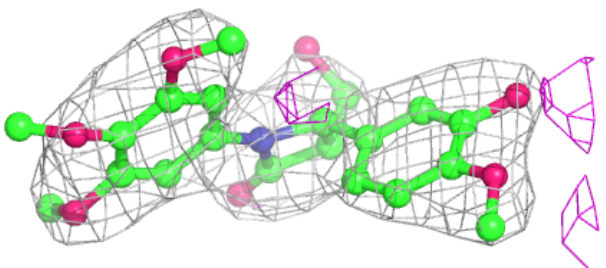
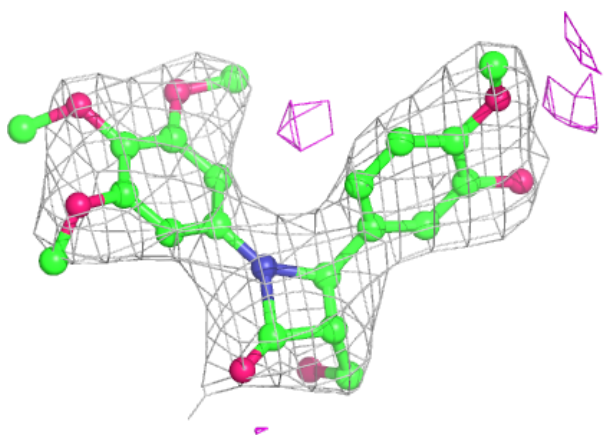


Electron density around 93X B 508:

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

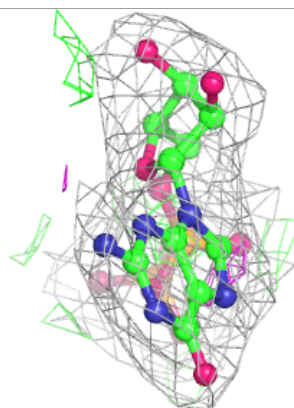
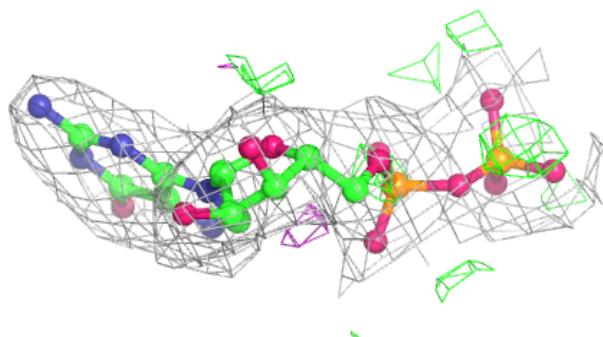
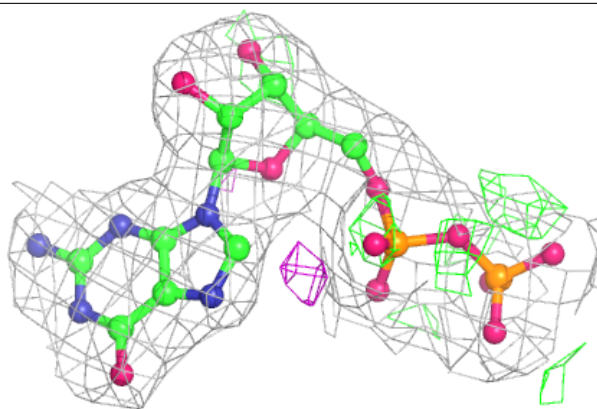
**Electron density around 93X D 505:**

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

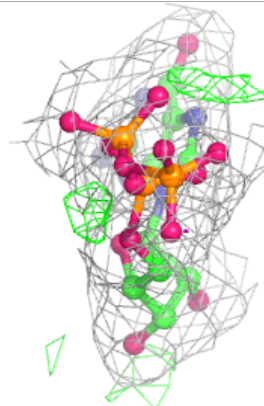
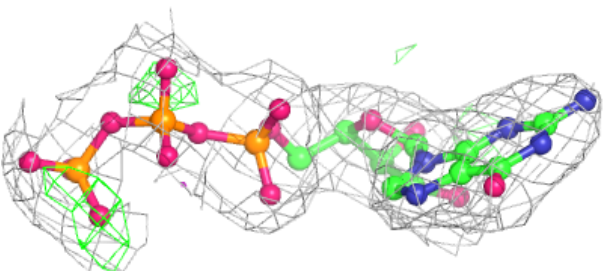
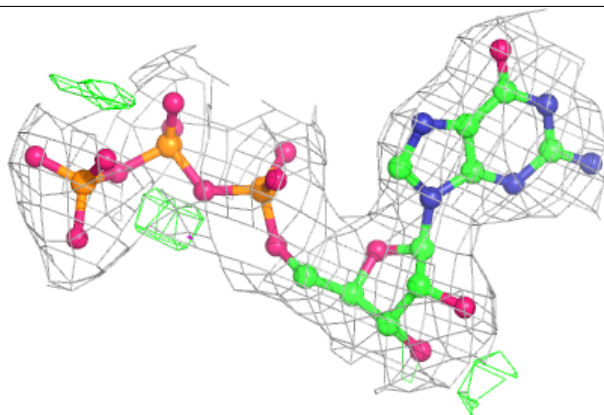


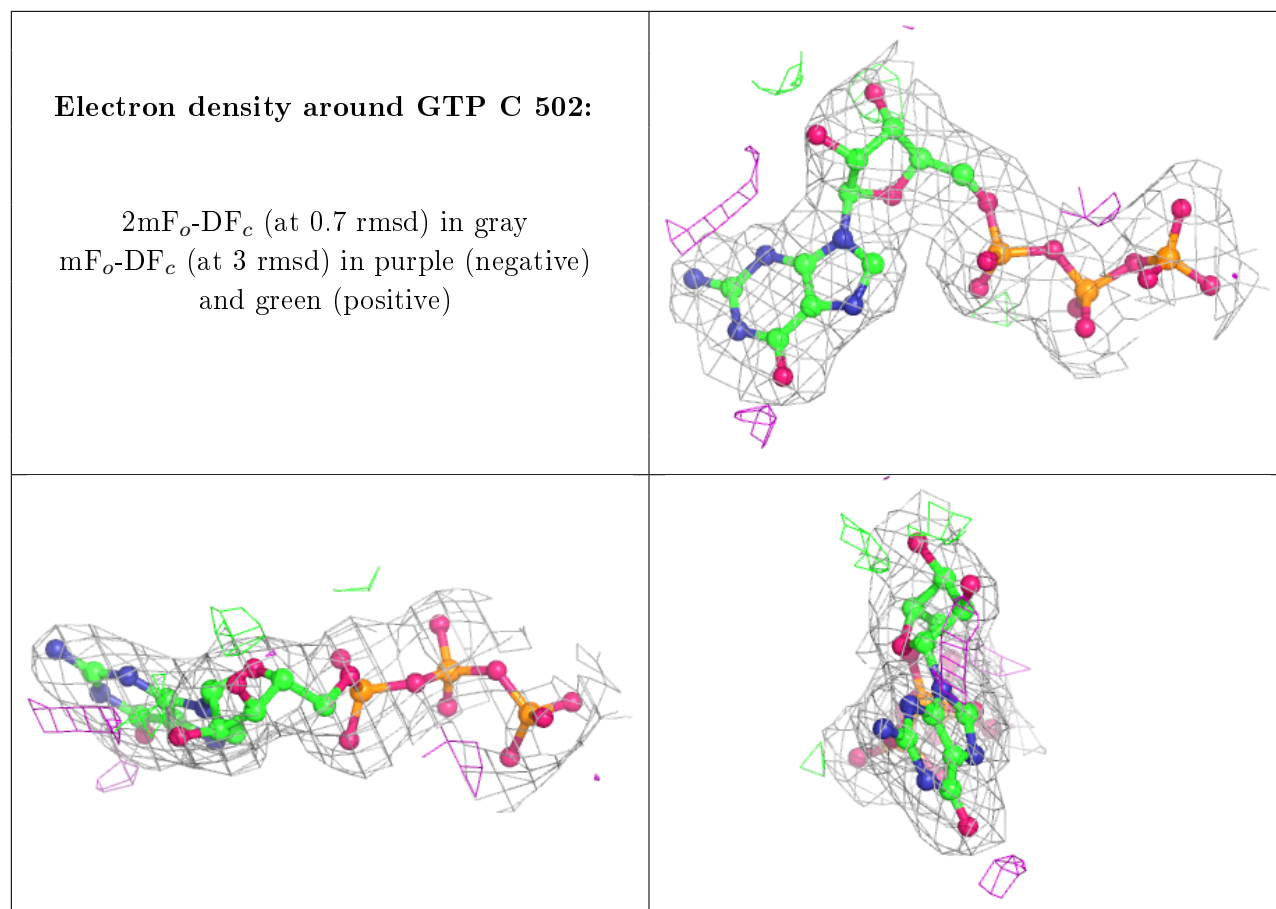
Electron density around GDP B 501:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.