



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:57 AM UTC

PDB ID : 5XAF / pdb_00005xaf
Title : Crystal structure of tubulin-stathmin-TTL-Compound Z1 complex
Authors : Zhang, H.; Luo, C.; Wang, Y.
Deposited on : 2017-03-12
Resolution : 2.55 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

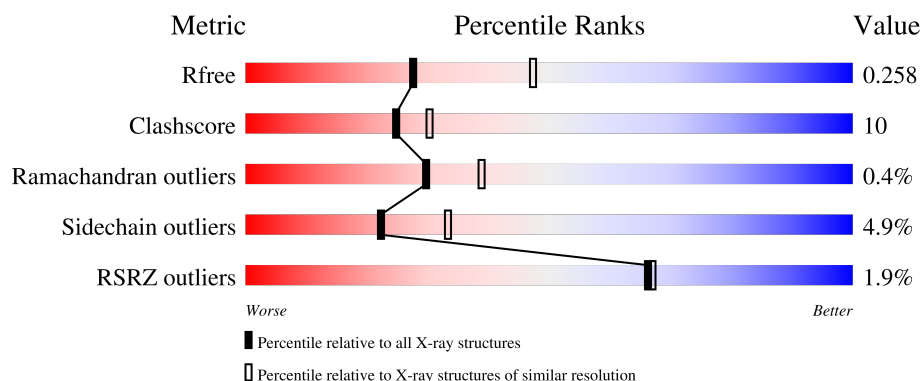
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	73% 23% ..
1	C	451	79% 18% ..
2	B	445	68% 25% • 5%
2	D	445	2% 70% 24% • 5%
3	E	189	% 51% 13% • 36%

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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 18303 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	438	Total	C	N	O	S	0	10	0
			3468	2203	583	657	25			
1	C	440	Total	C	N	O	S	0	11	0
			3489	2209	588	668	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	7	0
			3355	2111	567	650	27			
2	D	421	Total	C	N	O	S	0	3	0
			3323	2092	562	641	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1011	624	183	199	5			

- Molecule 4 is a protein called TTL Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	3	0
			2608	1688	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).

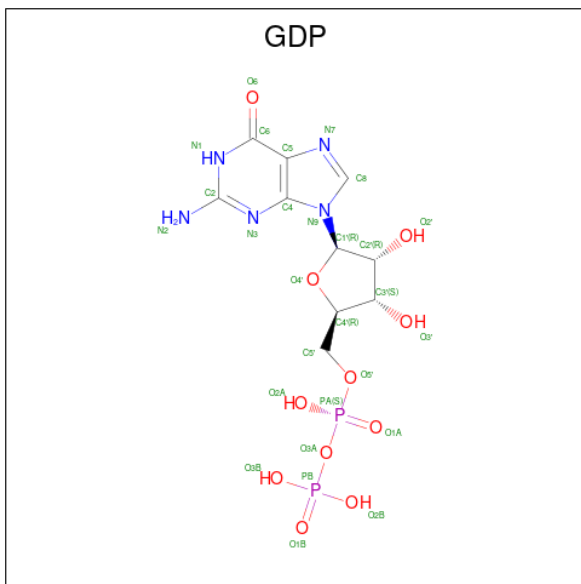


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total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

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



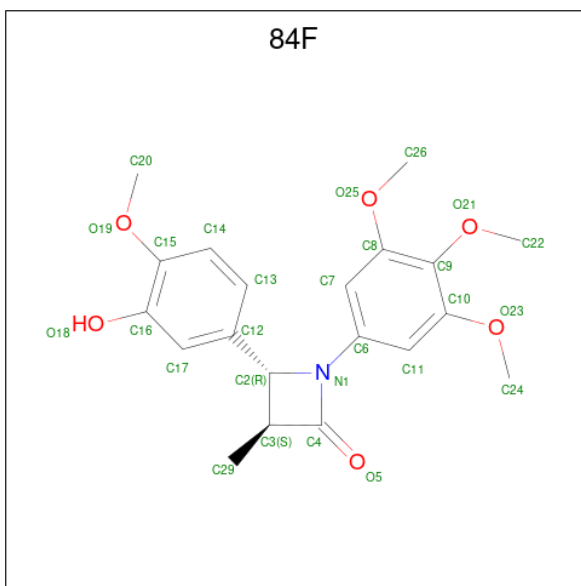
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



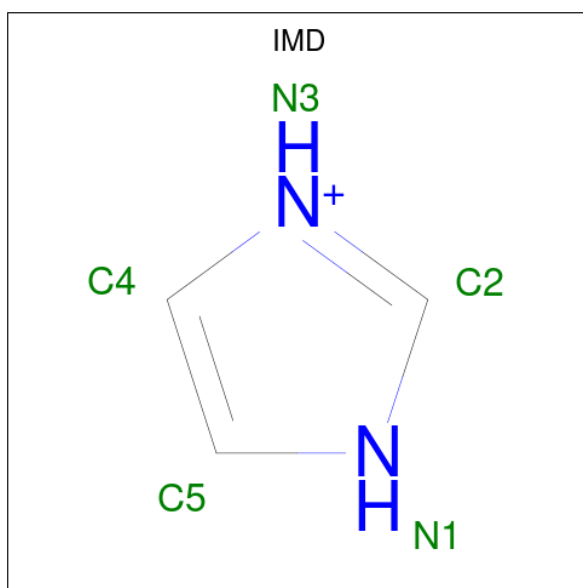
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3S,4R)-4-(3-hydroxy-4-methoxyphenyl)-3-methyl-1-(3,4,5-trimethoxyphenyl)azetidin-2-one (CCD ID: 84F) (formula: $C_{20}H_{23}NO_6$).



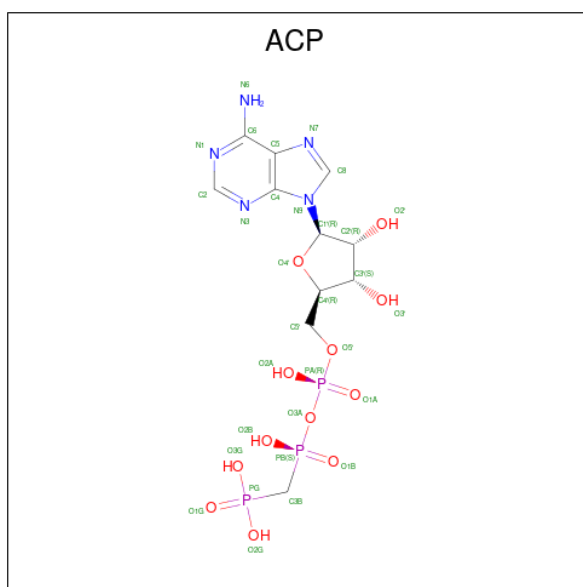
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O		0	0
			27	20	1	6			
11	D	1	Total	C	N	O		0	0
			27	20	1	6			

- 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		

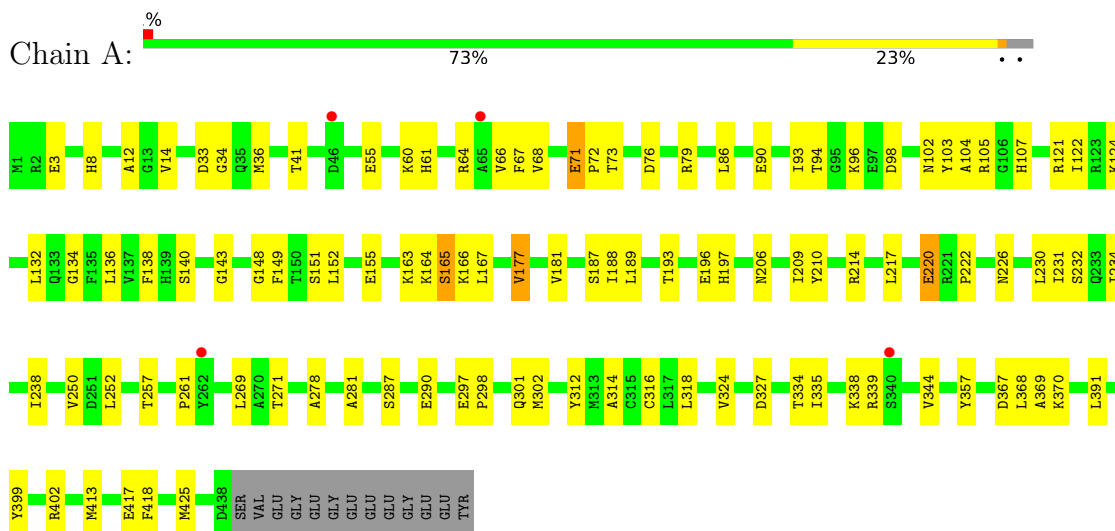
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	131	Total	O	0	0
			131	131		
14	B	136	Total	O	0	0
			136	136		
14	C	211	Total	O	0	0
			211	211		
14	D	99	Total	O	0	0
			99	99		
14	E	59	Total	O	0	0
			59	59		
14	F	101	Total	O	0	0
			101	101		

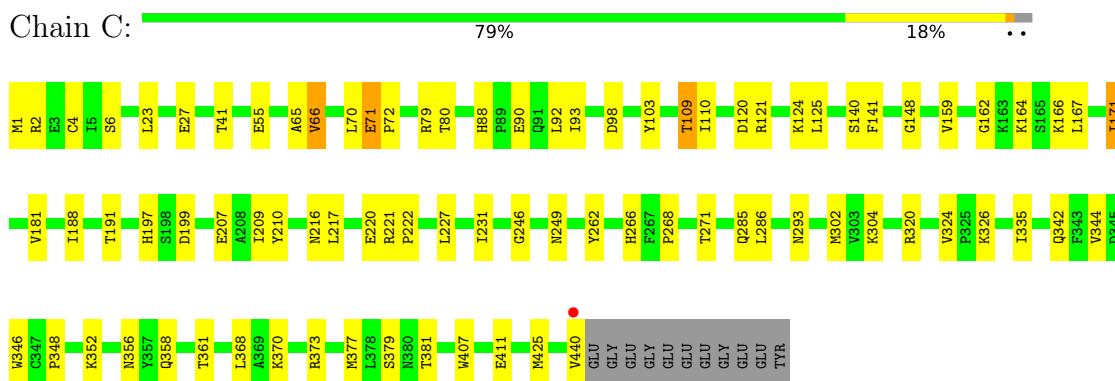
3 Residue-property plots

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.

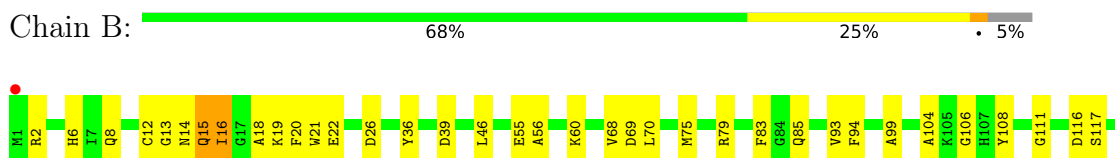
- Molecule 1: Tubulin alpha-1B chain

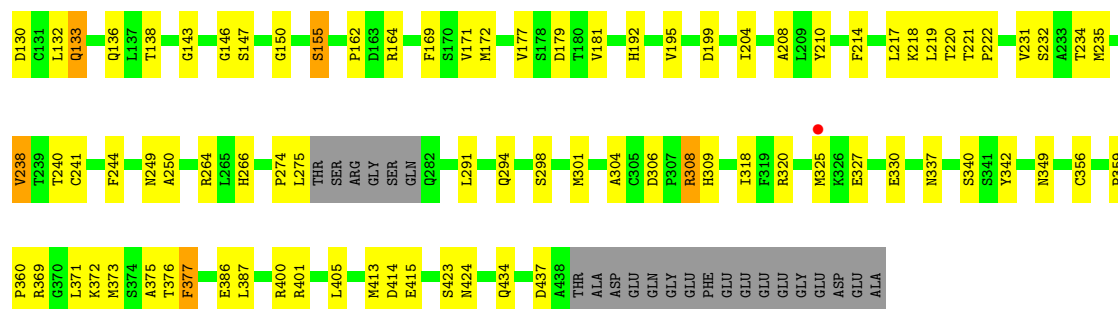


- Molecule 1: Tubulin alpha-1B chain

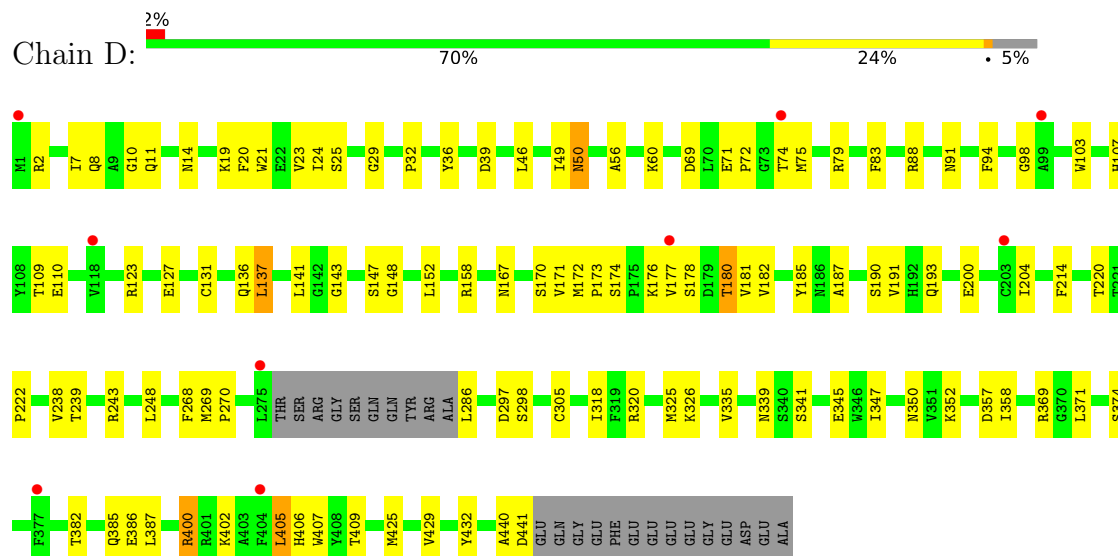


- Molecule 2: Tubulin beta-2B chain

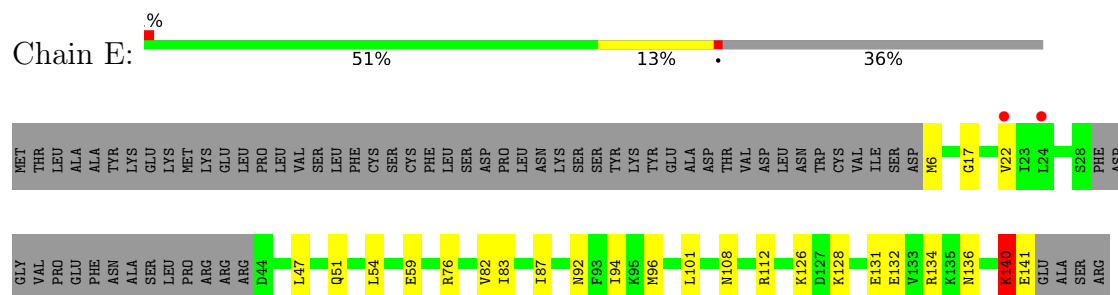




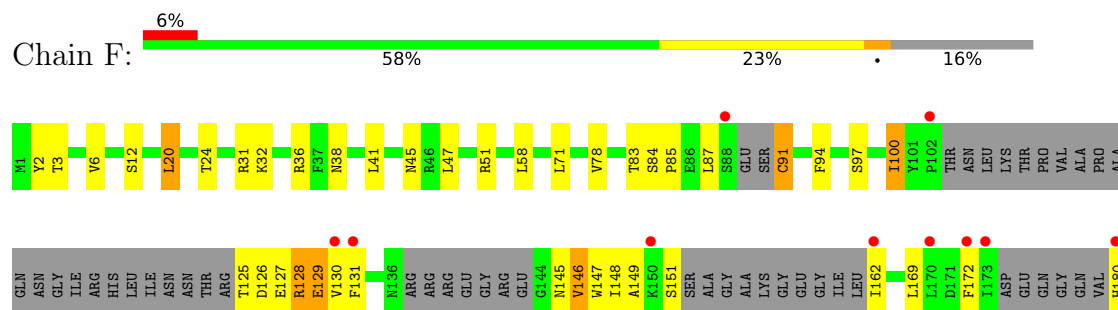
• Molecule 2: Tubulin beta-2B chain

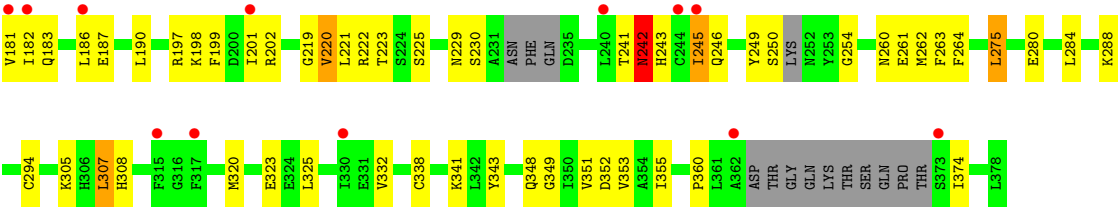


• Molecule 3: Stathmin-4



• Molecule 4: TTL Protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.57Å 156.51Å 182.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.77 – 2.55 49.77 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.77-2.55) 99.9 (49.77-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.206 , 0.257 0.210 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18303	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GTP, MG, 84F, ACP, GOL, GDP, MES, 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	0.36	0/3576	0.56	0/4855
1	C	0.44	0/3597	0.65	2/4885 (0.0%)
2	B	0.39	0/3447	0.59	0/4669
2	D	0.33	0/3405	0.54	0/4614
3	E	0.36	0/1025	0.55	0/1360
4	F	0.34	1/2673 (0.0%)	0.50	0/3608
All	All	0.38	1/17723 (0.0%)	0.57	2/23991 (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	6.58	1.49	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	6.33	129.15	120.67
1	C	171	ILE	C-N-CA	6.33	129.15	120.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3468	0	3413	66	0
1	C	3489	0	3413	56	0
2	B	3355	0	3237	79	0
2	D	3323	0	3216	67	0
3	E	1011	0	1032	21	0
4	F	2608	0	2597	63	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	18	0	24	0	0
7	B	18	0	24	7	0
7	C	24	0	32	1	0
7	D	12	0	15	4	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	1	0
10	B	12	0	12	0	0
11	B	27	0	0	0	0
11	D	27	0	0	0	0
12	C	10	0	10	4	0
12	E	5	0	4	1	0
13	F	31	0	14	1	0
14	A	131	0	0	3	0
14	B	136	0	0	16	1
14	C	211	0	0	3	1
14	D	99	0	0	10	0
14	E	59	0	0	6	0
14	F	101	0	0	10	0
All	All	18303	0	17091	339	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 (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:N	14:B:601:HOH:O	1.93	1.00
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.57	0.86
2:D:10:GLY:O	2:D:14:ASN:ND2	2.12	0.81
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.62	0.81
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.54	0.81
2:B:221:THR:O	14:B:602:HOH:O	1.99	0.79
2:B:401:ARG:HE	7:B:503:GOL:H2	1.49	0.78
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.18	0.77
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.66	0.74
3:E:6:MET:N	14:E:302:HOH:O	2.19	0.74
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.05	0.73
1:A:214:ARG:NH1	1:A:220:GLU:O	2.24	0.71
3:E:140:LYS:O	14:E:301:HOH:O	2.08	0.70
2:D:286:LEU:N	14:D:605:HOH:O	2.23	0.70
4:F:323:GLU:O	14:F:501:HOH:O	2.10	0.69
4:F:151:SER:HB2	4:F:180:HIS:HA	1.75	0.69
2:B:294:GLN:NE2	14:B:610:HOH:O	2.26	0.69
4:F:305:LYS:NZ	14:F:505:HOH:O	2.26	0.69
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.75	0.69
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.74	0.69
2:B:249:ASN:N	14:B:609:HOH:O	2.26	0.68
4:F:31:ARG:HE	4:F:32:LYS:H	1.41	0.66
2:B:162:PRO:O	14:B:603:HOH:O	2.12	0.66
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.30	0.66
4:F:128:ARG:N	14:F:506:HOH:O	2.26	0.66
2:B:337:ASN:HD21	4:F:36:ARG:HH21	1.43	0.66
4:F:201:ILE:HG13	4:F:221:LEU:HD21	1.77	0.66
1:A:90:GLU:OE1	14:A:601:HOH:O	2.14	0.66
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.31	0.65
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.77	0.65
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.79	0.65
2:D:180:THR:O	14:D:602:HOH:O	2.14	0.65
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.79	0.65
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.78	0.64
2:D:75:MET:O	14:D:601:HOH:O	2.14	0.64
2:B:2:ARG:HH21	2:B:133:GLN:HA	1.63	0.64
2:B:309:HIS:ND1	2:B:386:GLU:OE1	2.31	0.63
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.81	0.63
2:D:123:ARG:O	2:D:127:GLU:HG2	1.99	0.63
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.65	0.62
2:D:136:GLN:HA	2:D:167:ASN:O	1.99	0.62
1:A:132:LEU:O	1:A:164:LYS:NZ	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:THR:O	1:C:41:THR:OG1	2.15	0.62
1:A:166:LYS:HE2	1:A:197:HIS:O	1.98	0.62
4:F:145:ASN:HB3	4:F:147:TRP:HE1	1.65	0.61
2:D:325:MET:HG3	14:D:626:HOH:O	2.00	0.61
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.81	0.61
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.66	0.61
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.34	0.61
4:F:261:GLU:O	14:F:503:HOH:O	2.17	0.60
2:D:11:GLN:HB3	9:D:501:GDP:O2A	2.02	0.60
2:D:46:LEU:HA	2:D:49:ILE:HB	1.83	0.60
1:C:166:LYS:HE2	1:C:197:HIS:O	2.02	0.60
2:B:304:ALA:O	14:B:604:HOH:O	2.16	0.59
1:C:286:LEU:O	1:C:373:ARG:NH1	2.35	0.59
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.14	0.59
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.38	0.58
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.85	0.58
1:C:293[A]:ASN:HA	1:C:335:ILE:HD11	1.86	0.58
4:F:197:ARG:HD2	4:F:225:SER:HA	1.84	0.58
2:B:376:THR:OG1	7:B:505:GOL:H32	2.02	0.58
1:C:1:MET:O	14:C:601:HOH:O	2.17	0.58
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.86	0.57
2:D:21:TRP:O	2:D:25:SER:OG	2.14	0.57
2:D:369:ARG:NH1	14:D:612:HOH:O	2.37	0.57
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.39	0.57
2:D:158:ARG:NH1	14:D:611:HOH:O	2.37	0.57
1:C:293[B]:ASN:HA	1:C:335:ILE:HD11	1.87	0.57
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.33	0.57
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.87	0.56
3:E:6:MET:N	14:E:303:HOH:O	2.37	0.56
1:A:413:MET:HE3	1:A:417:GLU:HG2	1.87	0.56
1:C:159:VAL:HA	3:E:94:ILE:HG23	1.86	0.56
2:D:103:TRP:HD1	2:D:147:SER:OG	1.88	0.56
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.89	0.55
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.40	0.55
1:C:324:VAL:HG22	14:C:631:HOH:O	2.06	0.55
1:A:196:GLU:HG3	1:A:197:HIS:CD2	2.42	0.55
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.41	0.55
4:F:246:GLN:HG2	4:F:250:SER:HB3	1.87	0.55
2:D:222:PRO:O	7:D:503:GOL:O2	2.25	0.55
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.43	0.54
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:O	1:A:238:ILE:HG13	2.06	0.54
2:B:308:ARG:HG2	2:B:342:TYR:CE2	2.42	0.54
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.90	0.54
4:F:201:ILE:HG13	4:F:221:LEU:CD2	2.37	0.54
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.88	0.54
2:D:400:ARG:HG3	14:D:628:HOH:O	2.07	0.54
2:B:16:ILE:C	14:B:601:HOH:O	2.50	0.54
2:D:71:GLU:HB3	2:D:98:GLY:HA2	1.90	0.54
4:F:186:LEU:HD23	4:F:320:MET:HE3	1.89	0.54
2:D:19:LYS:O	2:D:23:VAL:HG23	2.08	0.54
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.88	0.53
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.90	0.53
2:B:320:ARG:HD3	7:B:505:GOL:H2	1.90	0.53
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.91	0.53
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.53
2:B:218:LYS:N	14:B:613:HOH:O	2.34	0.52
2:B:15:GLN:O	14:B:601:HOH:O	2.19	0.52
2:B:155[B]:SER:OG	3:E:76:ARG:NH2	2.41	0.52
2:B:400:ARG:NH2	14:B:620:HOH:O	2.41	0.52
2:D:180:THR:HG22	2:D:181:VAL:H	1.75	0.52
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.91	0.52
4:F:131:PHE:HE2	4:F:182:ILE:HG21	1.74	0.52
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.44	0.52
1:C:377:MET:HE3	1:C:379:SER:HB3	1.91	0.52
4:F:2:TYR:OH	4:F:360:PRO:O	2.25	0.52
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.92	0.52
2:D:385:GLN:OE1	14:D:603:HOH:O	2.19	0.52
4:F:351:VAL:HA	4:F:355:ILE:HB	1.92	0.52
2:B:291:LEU:HD13	2:B:375:ALA:HB2	1.92	0.51
1:A:338:LYS:HE2	1:A:339:ARG:HG2	1.92	0.51
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.45	0.51
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.29	0.51
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.44	0.51
1:C:27:GLU:HG2	1:C:361:THR:HG22	1.93	0.51
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.51
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.27	0.51
2:D:177:VAL:HG13	7:D:503:GOL:H2	1.93	0.51
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.46	0.51
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.92	0.51
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.94	0.50
4:F:100:ILE:HD12	4:F:128:ARG:HG3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ILE:O	2:D:137:LEU:HA	2.11	0.50
2:D:320:ARG:NH1	14:D:617:HOH:O	2.44	0.50
1:A:96:LYS:NZ	2:B:130:ASP:O	2.45	0.50
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.47	0.50
1:C:79:ARG:HG2	1:C:92:LEU:HD12	1.94	0.49
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.46	0.49
1:A:68[A]:VAL:HG11	1:A:149:PHE:CE2	2.47	0.49
2:B:401:ARG:HE	7:B:503:GOL:C2	2.24	0.49
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.94	0.49
4:F:146:VAL:HG13	4:F:187:GLU:OE2	2.10	0.49
4:F:186:LEU:HB3	13:F:402:ACP:H2	1.94	0.49
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.53	0.49
2:B:69:ASP:O	2:B:94:PHE:HA	2.13	0.49
2:B:132:LEU:HB3	2:B:164:ARG:NH1	2.27	0.49
1:C:167:LEU:HD13	12:C:509:IMD:H2	1.94	0.49
1:C:262:TYR:CB	12:C:508:IMD:H5	2.43	0.49
2:B:195:VAL:HG13	2:B:264:ARG:HG2	1.95	0.49
1:C:220:GLU:CD	2:D:326:LYS:HD3	2.38	0.49
3:E:83:ILE:O	3:E:87:ILE:HG13	2.12	0.49
4:F:3:THR:HB	4:F:38:ASN:H	1.77	0.49
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.36	0.48
1:A:151:SER:HB2	1:A:193:THR:HG22	1.94	0.48
2:B:221:THR:HG21	1:C:326:LYS:HA	1.95	0.48
2:D:345:GLU:OE2	2:D:440:ALA:N	2.46	0.48
4:F:6:VAL:HG22	4:F:41:LEU:HD12	1.96	0.48
4:F:31:ARG:HE	4:F:32:LYS:HG3	1.77	0.48
4:F:263:PHE:CG	4:F:341:LYS:HE2	2.48	0.48
1:A:104:ALA:HB2	1:A:413:MET:SD	2.53	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.48
4:F:219:GLY:N	14:F:504:HOH:O	2.45	0.48
1:A:163:LYS:NZ	14:A:606:HOH:O	2.39	0.48
2:B:371:LEU:HD23	2:B:371:LEU:HA	1.72	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.48
3:E:141:GLU:HB3	14:E:332:HOH:O	2.12	0.48
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.94	0.48
2:D:109:THR:HG22	2:D:110:GLU:HG2	1.96	0.48
2:D:405:LEU:O	2:D:409:THR:HG22	2.13	0.48
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.48
2:D:79:ARG:HB2	14:D:601:HOH:O	2.13	0.47
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.32	0.47
2:B:415:GLU:HG3	14:B:685:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:71:LEU:HD23	4:F:332:VAL:HG11	1.97	0.47
4:F:242:ASN:O	4:F:246:GLN:HB2	2.14	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.54	0.47
2:D:335:VAL:O	2:D:339:ASN:HB2	2.14	0.47
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.97	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.47
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.96	0.47
1:C:262:TYR:CG	12:C:508:IMD:H5	2.49	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.47
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.96	0.47
2:D:305:CYS:HA	2:D:386:GLU:OE2	2.15	0.46
4:F:126:ASP:HB2	14:F:506:HOH:O	2.14	0.46
4:F:202:ARG:HB3	4:F:220:VAL:HG12	1.96	0.46
4:F:275:LEU:HD13	4:F:275:LEU:HA	1.80	0.46
2:D:358:ILE:HD12	2:D:358:ILE:H	1.80	0.46
2:B:275:LEU:O	14:B:605:HOH:O	2.20	0.46
1:C:1:MET:N	14:C:612:HOH:O	2.44	0.46
2:D:352:LYS:HD2	2:D:352:LYS:HA	1.78	0.46
4:F:198:LYS:HD2	4:F:320:MET:HE1	1.98	0.46
1:A:3:GLU:HG2	1:A:64:ARG:NH1	2.30	0.46
1:A:196:GLU:HG3	1:A:197:HIS:HD2	1.80	0.46
2:B:199:ASP:O	2:B:266:HIS:HB2	2.16	0.46
1:A:55:GLU:HA	1:A:60:LYS:O	2.16	0.46
1:A:68[A]:VAL:HG11	1:A:149:PHE:HE2	1.81	0.46
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.40	0.46
2:B:234:THR:O	2:B:238:VAL:HB	2.15	0.46
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.96	0.46
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.80	0.46
2:D:72:PRO:HB3	2:D:94:PHE:CD1	2.50	0.46
3:E:140:LYS:HD2	3:E:140:LYS:HA	1.61	0.46
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.16	0.46
2:B:8:GLN:NE2	2:B:14:ASN:HA	2.31	0.46
1:C:207:GLU:HG2	1:C:304:LYS:HD2	1.97	0.46
2:D:50:ASN:OD1	2:D:50:ASN:N	2.43	0.46
2:B:210:TYR:CE1	2:B:222:PRO:HD2	2.51	0.46
4:F:97:SER:OG	4:F:183:GLN:HG2	2.15	0.46
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.51	0.45
2:B:360:PRO:HG3	7:B:505:GOL:O2	2.16	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45
1:C:407:TRP:HZ3	7:D:504:GOL:H11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:129:GLU:H	4:F:129:GLU:HG3	1.46	0.45
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.51	0.45
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.97	0.45
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.82	0.45
2:B:214:PHE:C	14:B:613:HOH:O	2.60	0.45
2:D:239:THR:O	2:D:243:ARG:HG3	2.17	0.45
1:C:266:HIS:O	1:C:268:PRO:HD3	2.16	0.45
2:B:18:ALA:N	14:B:601:HOH:O	2.49	0.45
4:F:223:THR:O	4:F:260:ASN:ND2	2.44	0.45
3:E:92:ASN:O	3:E:96:MET:HG2	2.16	0.45
1:A:324:VAL:HG22	1:A:327:ASP:OD2	2.17	0.45
2:B:274:PRO:HA	14:B:610:HOH:O	2.16	0.45
4:F:229:ASN:CG	4:F:230:SER:H	2.25	0.45
1:A:76:ASP:HA	1:A:79:ARG:HD2	1.99	0.44
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.44
4:F:325:LEU:HA	4:F:325:LEU:HD23	1.74	0.44
1:A:102:ASN:HB3	1:A:105:ARG:HB3	1.98	0.44
2:B:20:PHE:CD1	2:B:235:MET:HE2	2.52	0.44
1:C:41:THR:OG1	1:C:55:GLU:OE2	2.36	0.44
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.52	0.44
2:D:173:PRO:HG3	2:D:187:ALA:HB2	1.98	0.44
2:B:56:ALA:HB3	2:B:60:LYS:H	1.82	0.44
4:F:78:VAL:HG22	4:F:94:PHE:HE2	1.81	0.44
4:F:126:ASP:OD1	4:F:128:ARG:NH2	2.50	0.44
1:C:4:CYS:SG	12:C:509:IMD:H5	2.58	0.44
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.59	0.44
4:F:85:PRO:C	4:F:87:LEU:H	2.25	0.44
4:F:221:LEU:HD23	4:F:221:LEU:HA	1.63	0.44
1:A:370:LYS:HB3	1:A:370:LYS:HE2	1.74	0.44
2:D:191:VAL:HG11	2:D:425:MET:HG3	2.00	0.44
4:F:128:ARG:O	4:F:131:PHE:HB3	2.18	0.44
4:F:349:GLY:O	4:F:353[B]:VAL:HG23	2.17	0.44
4:F:127:GLU:N	14:F:506:HOH:O	2.50	0.44
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.83	0.44
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.52	0.44
4:F:149:ALA:HB3	4:F:169:LEU:HD13	1.99	0.44
1:A:66[B]:VAL:HG11	1:A:122:ILE:HG12	2.00	0.43
1:A:312:TYR:O	1:A:344:VAL:HG13	2.18	0.43
2:B:146:GLY:O	2:B:150:GLY:HA3	2.16	0.43
2:B:325:MET:HE2	2:B:325:MET:HB3	1.80	0.43
4:F:221:LEU:HB2	4:F:262:MET:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:MET:HE1	2:B:377:PHE:HE2	1.83	0.43
1:C:1:MET:O	1:C:2:ARG:HG2	2.18	0.43
1:C:6:SER:O	1:C:65:ALA:HA	2.18	0.43
1:C:199:ASP:OD1	7:C:506:GOL:H32	2.17	0.43
2:D:176:LYS:H	2:D:176:LYS:HG2	1.60	0.43
4:F:288:LYS:HB2	4:F:288:LYS:HE2	1.79	0.43
4:F:51:ARG:HD3	14:F:544:HOH:O	2.18	0.43
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.59	0.43
1:A:413:MET:HE2	1:A:418:PHE:CE1	2.53	0.43
2:B:13:GLY:CA	2:B:138[B]:THR:HG22	2.47	0.43
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.43
1:A:287:SER:OG	1:A:290:GLU:HG3	2.19	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.59	0.43
2:B:320:ARG:HD3	7:B:505:GOL:C3	2.48	0.43
2:B:327:GLU:HA	2:B:330:GLU:HB2	2.00	0.43
2:D:268:PHE:O	2:D:270:PRO:HD3	2.18	0.43
4:F:91:CYS:SG	14:F:512:HOH:O	2.61	0.43
1:A:93:ILE:HD11	1:A:121:ARG:HG3	2.01	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.43
2:B:179:ASP:O	1:C:352:LYS:NZ	2.43	0.43
4:F:245:ILE:HG23	4:F:249:TYR:HD2	1.84	0.43
2:D:297:ASP:OD1	2:D:298:SER:N	2.52	0.42
4:F:222:ARG:HA	4:F:260:ASN:O	2.18	0.42
2:B:241:CYS:O	2:B:250:ALA:HB3	2.19	0.42
1:C:71:GLU:HG2	1:C:72:PRO:N	2.33	0.42
2:D:174:SER:O	2:D:178:SER:HB2	2.19	0.42
2:D:182:VAL:O	2:D:185:TYR:HB2	2.19	0.42
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.88	0.42
2:D:214:PHE:CD1	2:D:220:THR:HA	2.54	0.42
2:D:269[A]:MET:HE2	2:D:305:CYS:HB2	2.01	0.42
2:B:136:GLN:HG3	2:B:169:PHE:HE1	1.83	0.42
1:C:246:GLY:H	1:C:249:ASN:HB2	1.84	0.42
2:D:29:GLY:O	2:D:36:TYR:HA	2.20	0.42
4:F:254:GLY:HA2	14:F:552:HOH:O	2.19	0.42
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.55	0.42
3:E:47:LEU:O	3:E:51:GLN:HG2	2.20	0.42
3:E:51:GLN:HA	14:E:318:HOH:O	2.20	0.42
2:B:26:ASP:HA	14:B:623:HOH:O	2.20	0.42
3:E:132:GLU:O	3:E:136:ASN:HB2	2.20	0.42
4:F:242:ASN:HB3	4:F:243:HIS:H	1.48	0.42
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:O	1:A:402:ARG:NH1	2.53	0.42
2:B:240:THR:HG23	2:B:244:PHE:HD2	1.85	0.42
2:B:320:ARG:HG2	2:B:356:CYS:HB3	2.02	0.42
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.42
4:F:131:PHE:CE2	4:F:182:ILE:HG21	2.54	0.42
4:F:263:PHE:CD2	4:F:341:LYS:HE2	2.54	0.42
1:A:214:ARG:NH2	14:A:615:HOH:O	2.51	0.41
1:C:141:PHE:HE1	1:C:191:THR:OG1	2.03	0.41
3:E:128:LYS:HB2	3:E:128:LYS:HE2	1.84	0.41
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.54	0.41
2:B:359:PRO:HB2	2:B:371:LEU:O	2.20	0.41
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.02	0.41
2:B:16:ILE:HD12	2:B:231:VAL:HG11	2.03	0.41
2:B:218:LYS:O	2:B:219:LEU:HD23	2.19	0.41
4:F:190:LEU:HD23	4:F:199:PHE:HZ	1.86	0.41
2:D:103:TRP:CD1	2:D:148:GLY:HA2	2.55	0.41
1:C:411:GLU:O	3:E:108[A]:ASN:ND2	2.52	0.41
2:D:326:LYS:HB3	2:D:326:LYS:HE2	1.78	0.41
1:A:8:HIS:HD1	1:A:138:PHE:HB2	1.85	0.41
1:A:72:PRO:HA	1:A:94:THR:HG21	2.03	0.41
2:B:132:LEU:HB3	2:B:164:ARG:HH11	1.85	0.41
2:B:320:ARG:HD3	7:B:505:GOL:C2	2.51	0.41
1:C:27:GLU:HG2	1:C:361:THR:CG2	2.50	0.41
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.56	0.41
2:D:107:HIS:ND1	2:D:152:LEU:HB2	2.35	0.41
1:A:71:GLU:HB3	1:A:98:ASP:HB3	2.02	0.41
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.20	0.41
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.56	0.41
2:B:372:LYS:O	2:B:373:MET:HE2	2.20	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.03	0.41
2:B:68:VAL:HA	2:B:93:VAL:O	2.21	0.41
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.56	0.41
2:B:349:ASN:HD22	2:B:349:ASN:HA	1.73	0.41
1:C:216:ASN:O	1:C:217:LEU:HD23	2.21	0.41
2:D:371:LEU:HD23	2:D:371:LEU:HA	1.87	0.41
1:C:70:LEU:HD23	1:C:70:LEU:HA	1.77	0.40
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.95	0.40
2:B:360:PRO:O	2:B:369:ARG:C	2.64	0.40
2:D:382:THR:HA	2:D:432:TYR:CD1	2.56	0.40
3:E:112:ARG:NH1	14:E:305:HOH:O	2.44	0.40
3:E:131:GLU:OE2	3:E:134:ARG:NH2	2.53	0.40

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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	0.40
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.40	0.40
2:D:103:TRP:NE1	2:D:148:GLY:HA2	2.36	0.40
2:D:147:SER:HB2	2:D:190:SER:OG	2.20	0.40
1:A:177:VAL:HG11	1:A:206:ASN:HB3	2.04	0.40
1:C:209:ILE:HD12	1:C:209:ILE:HG23	1.79	0.40
1:C:221:ARG:HD2	1:C:221:ARG:HA	1.88	0.40
7:D:504:GOL:H2	12:E:201:IMD:C2	2.52	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)
14:B:621:HOH:O	14:C:605:HOH:O[4_545]	2.08	0.12

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	446/451 (99%)	419 (94%)	23 (5%)	4 (1%)	14	20
1	C	449/451 (100%)	432 (96%)	16 (4%)	1 (0%)	43	54
2	B	425/445 (96%)	400 (94%)	25 (6%)	0	100	100
2	D	420/445 (94%)	392 (93%)	27 (6%)	1 (0%)	43	54
3	E	119/189 (63%)	114 (96%)	4 (3%)	1 (1%)	16	22
4	F	302/378 (80%)	270 (89%)	31 (10%)	1 (0%)	36	44
All	All	2161/2359 (92%)	2027 (94%)	126 (6%)	8 (0%)	30	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
3	E	140	LYS
4	F	242	ASN
1	A	314	ALA
2	D	143	GLY
1	A	281	ALA
1	C	109	THR
1	A	261	PRO

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	379/379 (100%)	368 (97%)	11 (3%)	37	53
1	C	382/379 (101%)	370 (97%)	12 (3%)	35	50
2	B	371/383 (97%)	345 (93%)	26 (7%)	14	19
2	D	367/383 (96%)	352 (96%)	15 (4%)	27	39
3	E	111/171 (65%)	106 (96%)	5 (4%)	24	36
4	F	289/336 (86%)	265 (92%)	24 (8%)	10	15
All	All	1899/2031 (94%)	1806 (95%)	93 (5%)	22	33

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	41	THR
1	A	71	GLU
1	A	165	SER
1	A	181	VAL
1	A	220	GLU
1	A	232	SER
1	A	250	VAL
1	A	257	THR
1	A	271	THR
1	A	334	THR

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Mol	Chain	Res	Type
2	B	15	GLN
2	B	16	ILE
2	B	39	ASP
2	B	55	GLU
2	B	79	ARG
2	B	85	GLN
2	B	116	ASP
2	B	117	SER
2	B	133	GLN
2	B	155[A]	SER
2	B	155[B]	SER
2	B	177	VAL
2	B	217	LEU
2	B	220	THR
2	B	232	SER
2	B	238	VAL
2	B	298	SER
2	B	308	ARG
2	B	318	ILE
2	B	340	SER
2	B	377	PHE
2	B	405	LEU
2	B	414	ASP
2	B	423	SER
2	B	434	GLN
2	B	437	ASP
1	C	66	VAL
1	C	71	GLU
1	C	80	THR
1	C	181	VAL
1	C	285	GLN
1	C	342	GLN
1	C	358[A]	GLN
1	C	358[B]	GLN
1	C	368	LEU
1	C	370	LYS
1	C	381	THR
1	C	440	VAL
2	D	8	GLN
2	D	39	ASP
2	D	50	ASN
2	D	137	LEU

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Mol	Chain	Res	Type
2	D	180	THR
2	D	200	GLU
2	D	238	VAL
2	D	248	LEU
2	D	318	ILE
2	D	341	SER
2	D	357	ASP
2	D	374	SER
2	D	400	ARG
2	D	405	LEU
2	D	441	ASP
3	E	22	VAL
3	E	54	LEU
3	E	59	GLU
3	E	101	LEU
3	E	140	LYS
4	F	12	SER
4	F	20	LEU
4	F	45	ASN
4	F	83	THR
4	F	84	SER
4	F	91	CYS
4	F	100	ILE
4	F	125	THR
4	F	128	ARG
4	F	129	GLU
4	F	130	VAL
4	F	146	VAL
4	F	148	ILE
4	F	162	ILE
4	F	172	PHE
4	F	181	VAL
4	F	220	VAL
4	F	241	THR
4	F	242	ASN
4	F	245	ILE
4	F	264	PHE
4	F	275	LEU
4	F	307	LEU
4	F	374	ILE

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

Mol	Chain	Res	Type
1	A	285	GLN
1	A	301	GLN
1	A	393	HIS
2	B	15	GLN
2	B	249	ASN
2	B	349	ASN
2	B	385	GLN
2	B	436	GLN
1	C	35	GLN
1	C	61	HIS
1	C	301	GLN
2	D	331	GLN
3	E	90	ASN
3	E	92	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	$\# Z > 2$
7	GOL	A	503	-	5,5,5	0.33	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	IMD	E	201	7	5,5,5	0.67	0	5,5,5	0.36	0
7	GOL	D	503	-	5,5,5	0.37	0	5,5,5	0.34	0
7	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.50	0
9	GDP	B	501	6	29,30,30	1.23	3 (10%)	45,47,47	1.97	12 (26%)
7	GOL	C	501	-	5,5,5	0.41	0	5,5,5	0.25	0
7	GOL	C	506	-	5,5,5	0.51	0	5,5,5	0.58	0
5	GTP	C	502	6	33,34,34	1.02	2 (6%)	50,54,54	1.83	13 (26%)
7	GOL	C	504	-	5,5,5	0.36	0	5,5,5	0.28	0
7	GOL	B	503	-	5,5,5	0.24	0	5,5,5	0.75	0
7	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.75	0
7	GOL	D	504	12	5,5,5	0.42	0	5,5,5	0.36	0
7	GOL	B	505	-	5,5,5	0.43	0	5,5,5	0.49	0
13	ACP	F	402	-	31,33,33	2.72	10 (32%)	47,52,52	2.35	10 (21%)
12	IMD	C	509	-	5,5,5	0.66	0	5,5,5	0.35	0
5	GTP	A	501	6	33,34,34	1.06	2 (6%)	50,54,54	1.76	12 (24%)
10	MES	B	507	-	12,12,12	2.10	1 (8%)	15,16,16	1.95	6 (40%)
11	84F	B	508	-	28,29,29	6.31	11 (39%)	38,42,42	4.31	13 (34%)
11	84F	D	505	-	28,29,29	6.44	11 (39%)	38,42,42	4.46	14 (36%)
12	IMD	C	508	-	5,5,5	0.72	0	5,5,5	0.58	0
7	GOL	C	505	-	5,5,5	0.38	0	5,5,5	0.30	0
7	GOL	B	504	-	5,5,5	0.46	0	5,5,5	0.51	0
9	GDP	D	501	6	29,30,30	1.29	4 (13%)	45,47,47	1.74	8 (17%)

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	A	503	-	-	2/4/4/4	-
12	IMD	E	201	7	-	-	0/1/1/1
7	GOL	D	503	-	-	2/4/4/4	-
7	GOL	A	506	-	-	3/4/4/4	-
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
7	GOL	C	501	-	-	2/4/4/4	-
7	GOL	C	506	-	-	4/4/4/4	-
5	GTP	C	502	6	-	7/22/38/38	0/3/3/3
7	GOL	C	504	-	-	2/4/4/4	-
7	GOL	B	503	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	504	-	-	3/4/4/4	-
7	GOL	D	504	12	-	4/4/4/4	-
7	GOL	B	505	-	-	2/4/4/4	-
13	ACP	F	402	-	-	6/19/38/38	0/3/3/3
12	IMD	C	509	-	-	-	0/1/1/1
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
11	84F	B	508	-	-	2/16/32/32	0/3/3/3
11	84F	D	505	-	-	6/16/32/32	0/3/3/3
12	IMD	C	508	-	-	-	0/1/1/1
7	GOL	C	505	-	-	0/4/4/4	-
7	GOL	B	504	-	-	2/4/4/4	-
9	GDP	D	501	6	-	5/16/32/32	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	505	84F	C4-N1	26.34	1.75	1.37
11	B	508	84F	C4-N1	26.00	1.75	1.37
11	D	505	84F	C3-C2	-19.19	1.35	1.57
11	B	508	84F	C3-C2	-18.93	1.35	1.57
13	F	402	ACP	PB-O3A	7.45	1.66	1.58
13	F	402	ACP	PA-O3A	7.16	1.67	1.59
10	B	507	MES	C8-S	-6.95	1.67	1.77
13	F	402	ACP	C6-N6	5.02	1.47	1.34
13	F	402	ACP	C5-N7	4.97	1.48	1.39
11	D	505	84F	C12-C2	4.77	1.58	1.51
11	D	505	84F	C29-C3	4.20	1.62	1.53
11	B	508	84F	C12-C2	4.07	1.57	1.51
11	B	508	84F	C29-C3	3.70	1.61	1.53
9	B	501	GDP	PA-O3A	3.47	1.63	1.59
11	B	508	84F	O23-C10	3.42	1.42	1.37
11	D	505	84F	O19-C15	3.42	1.42	1.37
11	D	505	84F	C2-N1	3.41	1.51	1.48
13	F	402	ACP	O4'-C1'	3.19	1.49	1.42
9	D	501	GDP	C5-C4	3.05	1.47	1.38
13	F	402	ACP	C2'-C3'	-3.03	1.45	1.53
9	D	501	GDP	C6-N1	-2.80	1.33	1.38
9	B	501	GDP	C5-C4	2.63	1.45	1.38
9	D	501	GDP	C5-N7	-2.63	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	508	84F	C2-N1	2.57	1.50	1.48
11	D	505	84F	O25-C8	2.56	1.41	1.37
13	F	402	ACP	C8-N7	2.51	1.36	1.31
5	A	501	GTP	C2-N3	2.51	1.39	1.33
13	F	402	ACP	PB-O2B	-2.47	1.50	1.56
9	B	501	GDP	C6-N1	-2.46	1.34	1.38
11	D	505	84F	O21-C9	2.44	1.42	1.38
11	D	505	84F	O23-C10	2.43	1.41	1.37
11	B	508	84F	O19-C15	2.35	1.41	1.37
5	C	502	GTP	PB-O3B	2.26	1.61	1.59
11	B	508	84F	O18-C16	2.24	1.40	1.36
11	B	508	84F	O25-C8	2.24	1.40	1.37
11	D	505	84F	C6-N1	2.18	1.46	1.43
5	C	502	GTP	C2-N3	2.17	1.38	1.33
9	D	501	GDP	PA-O3A	2.17	1.61	1.59
13	F	402	ACP	O3'-C3'	-2.14	1.37	1.43
13	F	402	ACP	PA-O5'	2.09	1.67	1.59
5	A	501	GTP	C5-N7	-2.08	1.34	1.39
11	B	508	84F	O21-C9	2.06	1.42	1.38
11	D	505	84F	O18-C16	2.03	1.40	1.36
11	B	508	84F	O5-C4	-2.02	1.18	1.22

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	84F	C2-N1-C4	-14.02	83.01	95.30
11	D	505	84F	C2-N1-C4	-13.65	83.33	95.30
11	D	505	84F	C2-C3-C4	13.52	98.49	85.82
11	B	508	84F	C2-C3-C4	13.04	98.04	85.82
11	D	505	84F	C3-C4-N1	-11.25	81.43	92.76
11	B	508	84F	C3-C4-N1	-10.78	81.90	92.76
11	B	508	84F	C6-N1-C2	8.59	142.94	130.33
13	F	402	ACP	C4-N9-C8	8.44	114.60	105.74
11	D	505	84F	C6-N1-C2	8.18	142.34	130.33
13	F	402	ACP	O3'-C3'-C4'	5.92	128.09	111.08
9	D	501	GDP	C5-C4-N3	-5.88	119.04	128.39
11	D	505	84F	O23-C10-C9	5.75	124.99	115.14
9	B	501	GDP	C5-C4-N3	-5.73	119.27	128.39
11	D	505	84F	O23-C10-C11	-5.54	114.53	124.08
11	B	508	84F	O23-C10-C9	5.49	124.55	115.14
9	B	501	GDP	C2-N3-C4	5.38	121.57	112.30
13	F	402	ACP	N3-C4-N9	5.27	136.13	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	402	ACP	C5-C4-N3	-5.27	119.46	126.72
5	C	502	GTP	C2-N3-C4	5.20	121.26	112.30
11	D	505	84F	O25-C8-C9	5.17	124.00	115.14
5	A	501	GTP	C5-C4-N3	-5.10	120.27	128.39
5	C	502	GTP	C5-C4-N3	-5.06	120.34	128.39
11	D	505	84F	O25-C8-C7	-5.01	115.45	124.08
9	D	501	GDP	N9-C4-N3	4.72	135.39	125.95
11	B	508	84F	O25-C8-C7	-4.61	116.13	124.08
5	A	501	GTP	C2-N3-C4	4.50	120.05	112.30
9	D	501	GDP	C2-N3-C4	4.42	119.92	112.30
11	B	508	84F	O25-C8-C9	4.24	122.41	115.14
11	B	508	84F	O23-C10-C11	-4.22	116.81	124.08
9	B	501	GDP	N9-C4-N3	4.18	134.31	125.95
13	F	402	ACP	N3-C2-N1	-4.11	122.36	128.58
11	D	505	84F	C24-O23-C10	-4.04	111.59	117.51
5	C	502	GTP	N9-C8-N7	-3.99	106.00	113.40
13	F	402	ACP	N9-C8-N7	-3.94	108.34	113.94
11	B	508	84F	O5-C4-N1	3.85	136.94	131.85
5	C	502	GTP	C8-N7-C5	3.84	111.11	104.26
10	B	507	MES	C5-N4-C3	3.74	116.91	108.84
11	D	505	84F	C26-O25-C8	-3.63	112.19	117.51
9	B	501	GDP	O4'-C1'-N9	-3.57	100.26	108.36
11	D	505	84F	O5-C4-N1	3.48	136.46	131.85
5	C	502	GTP	C2-N1-C6	-3.38	118.99	125.11
9	B	501	GDP	C6-C5-N7	3.30	136.30	130.29
10	B	507	MES	O1S-S-C8	3.29	111.70	106.73
13	F	402	ACP	C2-N3-C4	3.24	119.74	111.83
9	B	501	GDP	O6-C6-C5	-3.21	118.05	126.53
5	A	501	GTP	N9-C4-N3	3.17	132.30	125.95
13	F	402	ACP	C4-C5-N7	-3.08	107.06	110.58
5	C	502	GTP	C4-C5-N7	-3.07	105.81	110.67
11	D	505	84F	C7-C6-N1	3.06	122.41	119.36
11	B	508	84F	C12-C2-C3	-2.99	114.72	118.28
13	F	402	ACP	C3'-C2'-C1'	2.97	107.08	101.46
5	A	501	GTP	C2-N1-C6	-2.94	119.79	125.11
5	A	501	GTP	C8-N7-C5	2.84	109.32	104.26
9	D	501	GDP	C6-C5-N7	2.79	135.36	130.29
10	B	507	MES	O3S-S-C8	2.78	111.45	106.00
5	C	502	GTP	C5-C6-N1	2.76	120.29	113.25
11	D	505	84F	C11-C6-N1	-2.75	116.62	119.36
5	C	502	GTP	N9-C4-N3	2.71	131.37	125.95
5	A	501	GTP	O3'-C3'-C4'	-2.67	103.40	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C2'-C1'-N9	2.65	120.64	113.25
13	F	402	ACP	C1'-N9-C8	-2.64	121.24	127.09
11	B	508	84F	O19-C15-C16	2.63	118.50	114.55
5	A	501	GTP	N9-C8-N7	-2.60	108.59	113.40
5	A	501	GTP	O3G-PG-O3B	2.58	113.30	104.64
5	A	501	GTP	O6-C6-C5	-2.50	119.93	126.53
9	D	501	GDP	O2A-PA-O3A	2.45	113.91	107.27
9	B	501	GDP	O5'-PA-O1A	2.43	118.58	108.94
9	D	501	GDP	C2'-C3'-C4'	2.40	107.25	102.61
5	C	502	GTP	C6-C5-N7	2.40	134.66	130.29
5	A	501	GTP	C5-C6-N1	2.36	119.26	113.25
5	C	502	GTP	N2-C2-N1	2.35	121.72	116.76
5	C	502	GTP	O2A-PA-O3A	2.35	113.62	107.27
11	B	508	84F	C26-O25-C8	-2.29	114.16	117.51
9	D	501	GDP	O6-C6-C5	-2.24	120.61	126.53
9	B	501	GDP	C5-C6-N1	2.24	118.95	113.25
10	B	507	MES	C6-C5-N4	-2.21	106.77	110.12
11	D	505	84F	C12-C2-C3	-2.20	115.66	118.28
10	B	507	MES	C7-N4-C5	2.20	117.09	111.24
9	B	501	GDP	O2A-PA-O3A	2.19	113.20	107.27
9	B	501	GDP	C4-C5-N7	-2.17	107.23	110.67
5	A	501	GTP	C4-C5-N7	-2.15	107.26	110.67
11	B	508	84F	O19-C15-C14	-2.15	120.69	124.30
5	C	502	GTP	O6-C6-C5	-2.14	120.88	126.53
5	A	501	GTP	O3B-PB-O1B	-2.13	104.29	110.70
9	D	501	GDP	C4-C5-N7	-2.10	107.34	110.67
9	B	501	GDP	N2-C2-N1	2.05	121.09	116.76
5	C	502	GTP	N1-C2-N3	-2.03	119.60	123.32
10	B	507	MES	O3S-S-O1S	-2.03	106.32	111.40

There are no chirality outliers.

All (63) 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	504	GOL	O1-C1-C2-C3
7	A	506	GOL	C1-C2-C3-O3
7	B	503	GOL	O1-C1-C2-C3
7	B	504	GOL	O1-C1-C2-O2
7	C	504	GOL	O1-C1-C2-C3
7	C	506	GOL	C1-C2-C3-O3
7	D	503	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-O3A
11	D	505	84F	C9-C10-O23-C24
11	D	505	84F	C11-C10-O23-C24
7	C	504	GOL	O1-C1-C2-O2
7	D	504	GOL	O2-C2-C3-O3
13	F	402	ACP	C3'-C4'-C5'-O5'
11	D	505	84F	C9-C8-O25-C26
7	A	504	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	O1-C1-C2-C3
7	C	501	GOL	O1-C1-C2-C3
7	C	506	GOL	O1-C1-C2-C3
7	D	504	GOL	O1-C1-C2-C3
7	D	504	GOL	C1-C2-C3-O3
7	A	506	GOL	O2-C2-C3-O3
7	B	503	GOL	O1-C1-C2-O2
7	C	501	GOL	O1-C1-C2-O2
7	C	506	GOL	O2-C2-C3-O3
7	D	504	GOL	O1-C1-C2-O2
11	D	505	84F	C7-C8-O25-C26
7	A	503	GOL	O1-C1-C2-O2
7	A	504	GOL	O1-C1-C2-O2
7	B	505	GOL	O1-C1-C2-O2
7	D	503	GOL	O1-C1-C2-O2
13	F	402	ACP	O4'-C4'-C5'-O5'
7	C	506	GOL	O1-C1-C2-O2
11	B	508	84F	C8-C9-O21-C22

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O1G
13	F	402	ACP	PG-C3B-PB-O2B
13	F	402	ACP	C5'-O5'-PA-O1A
11	B	508	84F	C10-C9-O21-C22
11	D	505	84F	C8-C9-O21-C22
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	502	GTP	C4'-C5'-O5'-PA
13	F	402	ACP	PG-C3B-PB-O1B
9	D	501	GDP	C4'-C5'-O5'-PA
5	C	502	GTP	PB-O3B-PG-O1G
5	C	502	GTP	PB-O3B-PG-O2G
11	D	505	84F	C10-C9-O21-C22
9	D	501	GDP	PB-O3A-PA-O2A

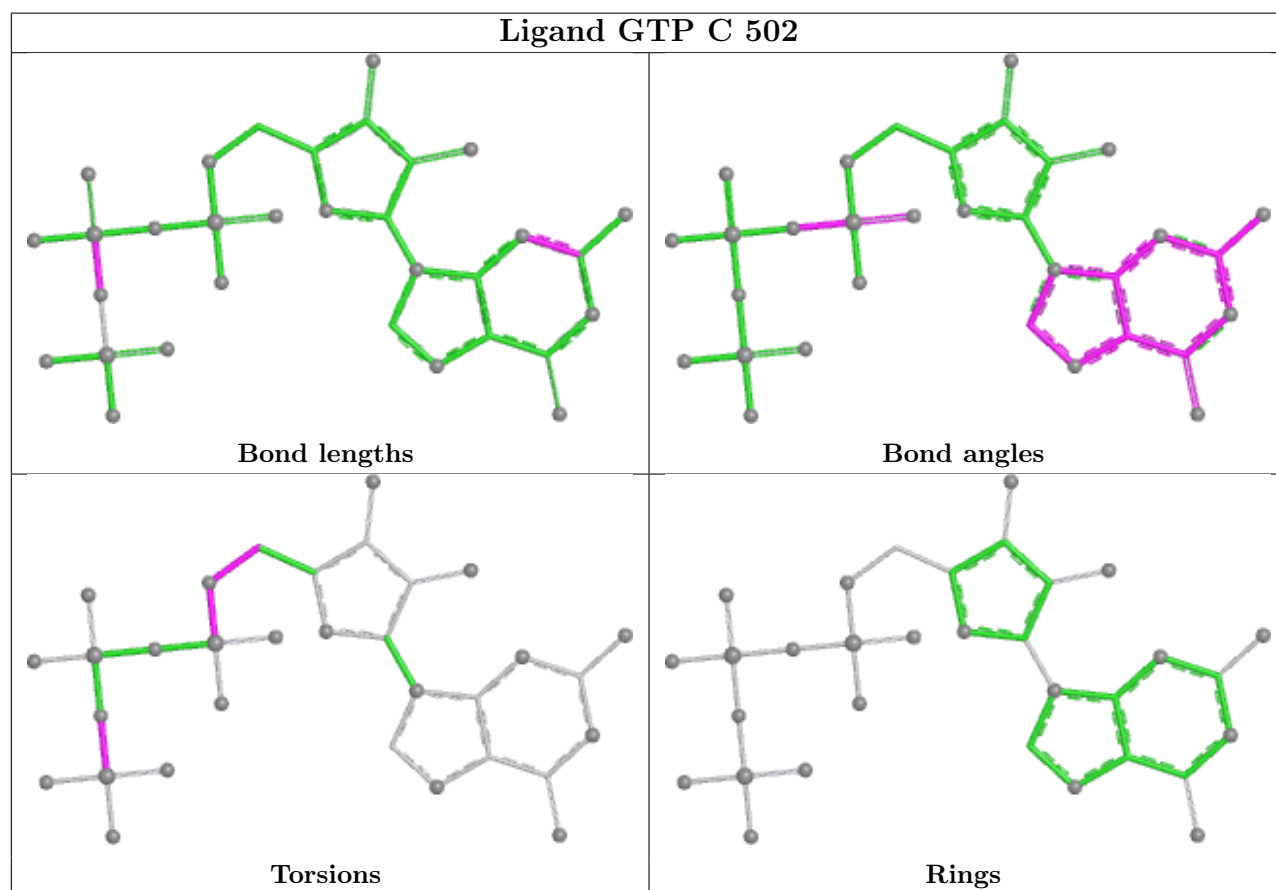
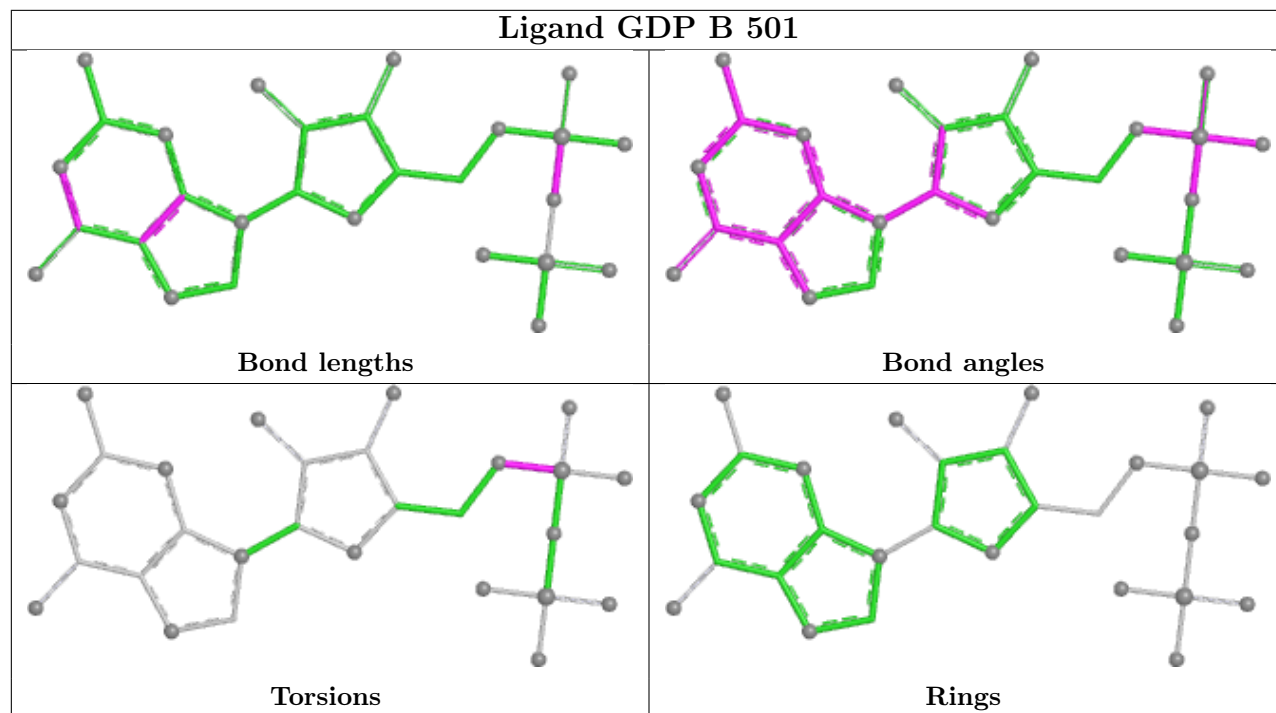
There are no ring outliers.

12 monomers are involved in 20 short contacts:

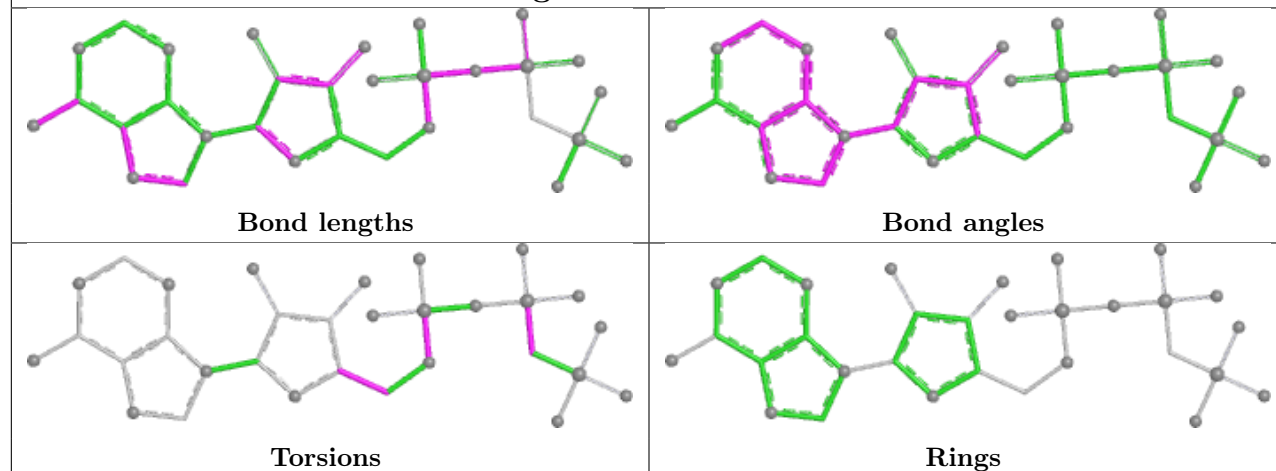
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	201	IMD	1	0
7	D	503	GOL	2	0
9	B	501	GDP	1	0
7	C	506	GOL	1	0
7	B	503	GOL	2	0
7	D	504	GOL	2	0
7	B	505	GOL	5	0
13	F	402	ACP	1	0
12	C	509	IMD	2	0
5	A	501	GTP	1	0
12	C	508	IMD	2	0
9	D	501	GDP	1	0

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

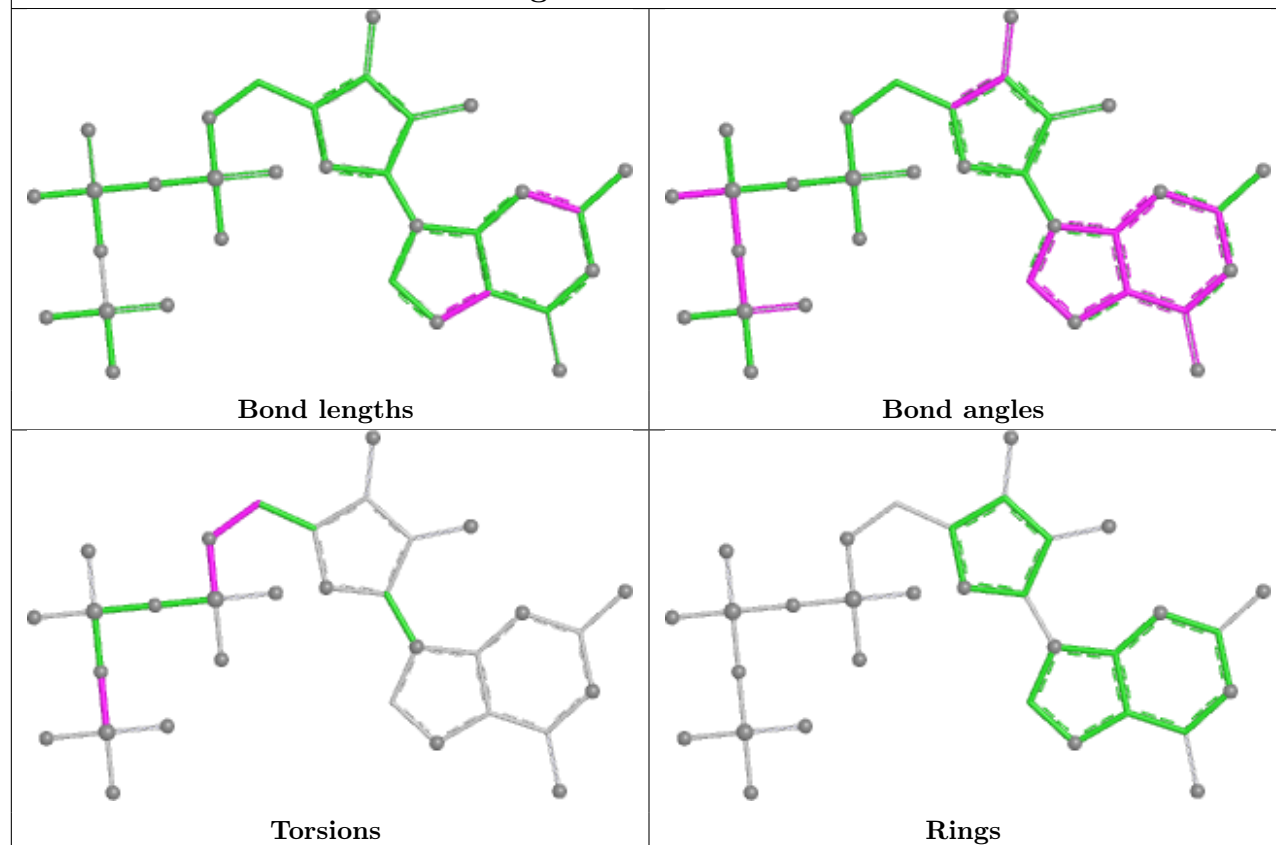
equivalents in the CSD to analyse the geometry.

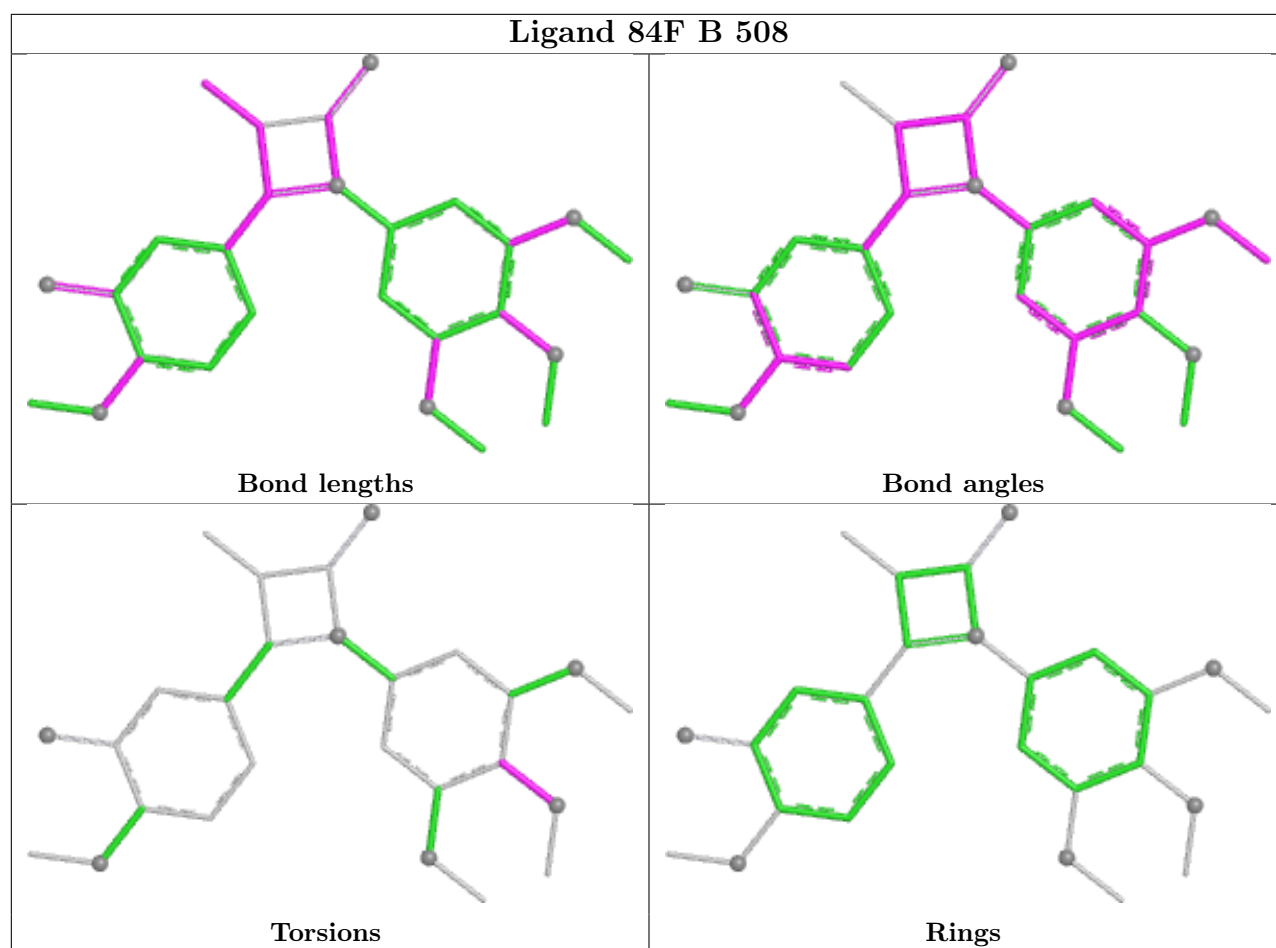


Ligand ACP F 402

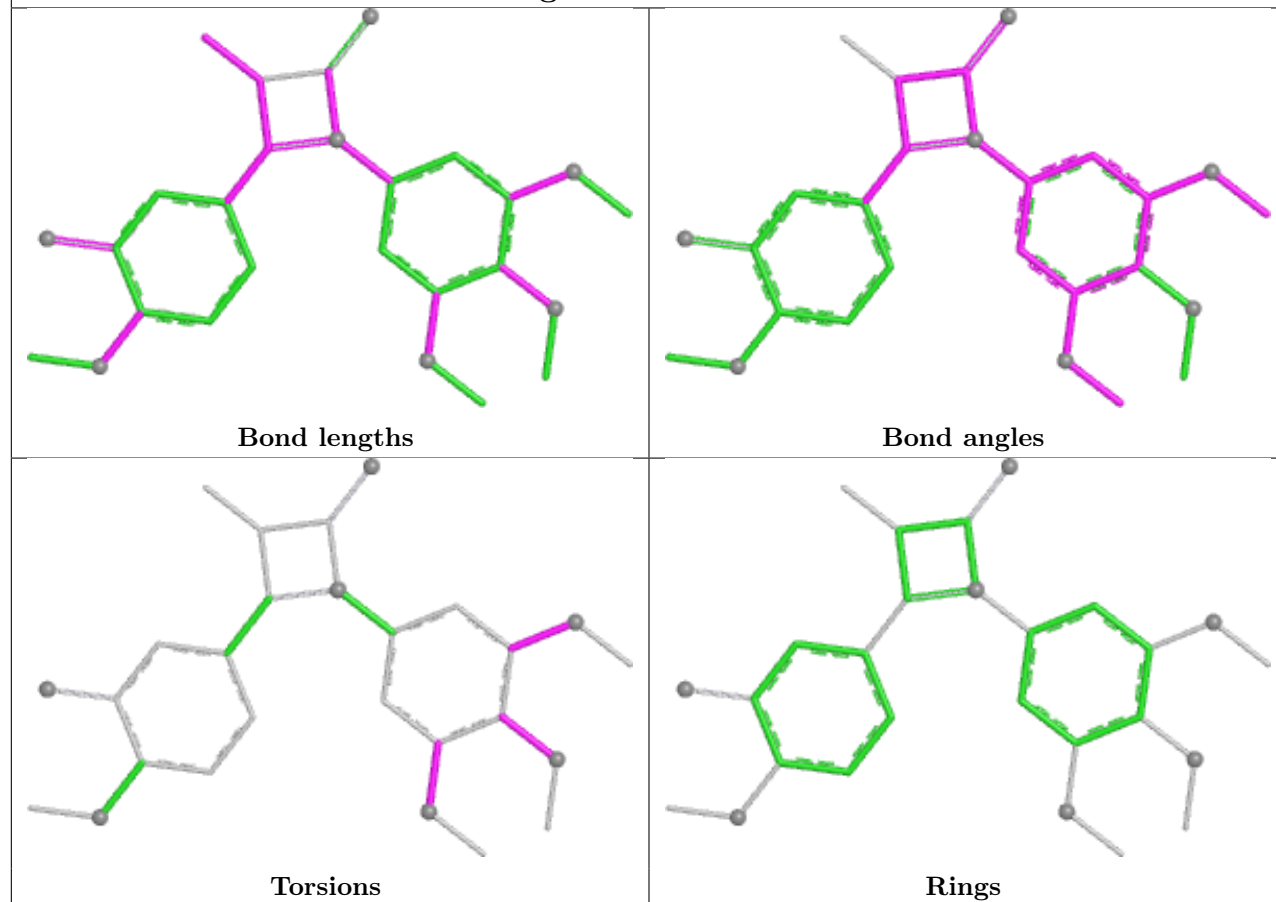


Ligand GTP A 501

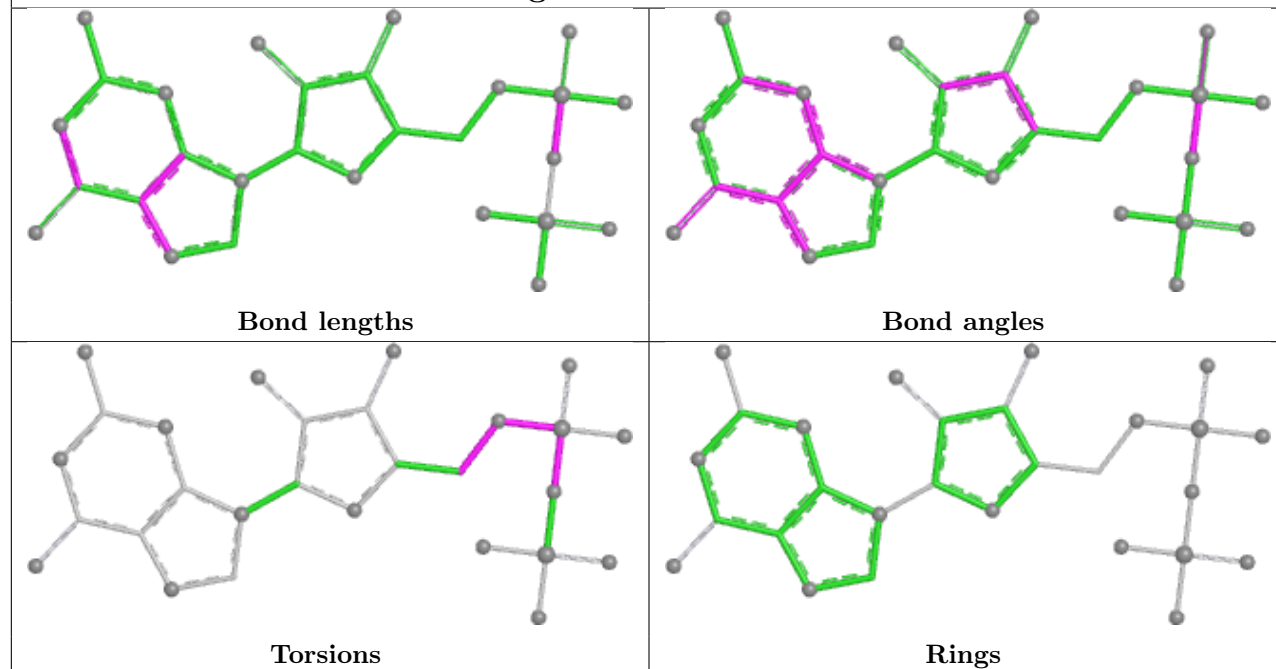




Ligand 84F D 505



Ligand GDP D 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.16	4 (0%) 81 83	33, 71, 107, 149	10 (2%)
1	C	440/451 (97%)	-0.33	1 (0%) 91 92	28, 54, 87, 106	11 (2%)
2	B	422/445 (94%)	-0.11	2 (0%) 87 89	32, 63, 105, 186	7 (1%)
2	D	421/445 (94%)	0.38	9 (2%) 63 64	41, 85, 126, 180	5 (1%)
3	E	121/189 (64%)	0.32	2 (1%) 69 70	32, 83, 120, 171	2 (1%)
4	F	317/378 (83%)	0.59	22 (6%) 23 22	47, 105, 194, 234	3 (0%)
All	All	2159/2359 (91%)	0.12	40 (1%) 66 67	28, 74, 129, 234	38 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	22	VAL	4.6
2	D	177	VAL	4.4
4	F	173	ILE	3.5
4	F	172	PHE	3.4
4	F	245	ILE	3.2
1	C	440	VAL	3.1
4	F	240	LEU	3.1
4	F	88	SER	3.0
3	E	24	LEU	2.9
4	F	150	LYS	2.8
4	F	373	SER	2.7
4	F	131	PHE	2.6
4	F	102	PRO	2.6
4	F	330	ILE	2.6
4	F	130	VAL	2.6
1	A	340	SER	2.6
1	A	46	ASP	2.6
2	D	118	VAL	2.6
2	B	325	MET	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	180	HIS	2.5
4	F	315	PHE	2.4
4	F	362	ALA	2.4
1	A	65	ALA	2.4
2	D	99	ALA	2.4
4	F	181	VAL	2.3
4	F	244	CYS	2.3
1	A	262	TYR	2.3
4	F	186	LEU	2.3
2	D	404	PHE	2.3
4	F	162	ILE	2.2
2	D	74	THR	2.2
4	F	182	ILE	2.2
2	D	203	CYS	2.2
4	F	317	PHE	2.2
2	B	1	MET	2.1
2	D	1	MET	2.1
2	D	275	LEU	2.1
2	D	377	PHE	2.1
4	F	170	LEU	2.1
4	F	201	ILE	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($\text{\AA}^2$)	Q<0.9
13	ACP	F	402	31/31	0.64	0.12	83,201,241,243	0
6	MG	D	502	1/1	0.72	0.12	97,97,97,97	0

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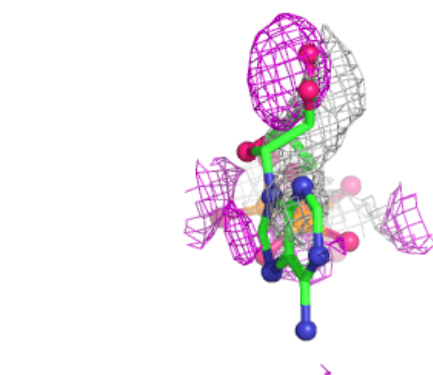
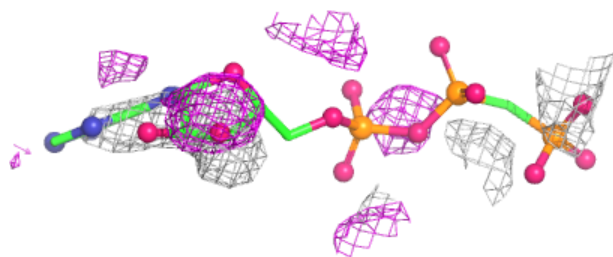
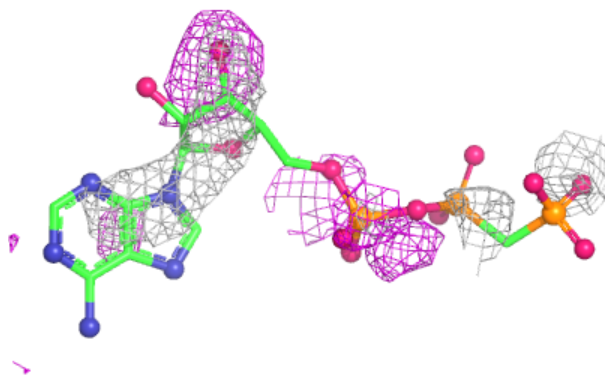
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	506	6/6	0.73	0.15	90,98,107,109	0
7	GOL	D	503	6/6	0.76	0.14	150,152,158,158	0
6	MG	F	401	1/1	0.78	0.15	162,162,162,162	0
7	GOL	B	504	6/6	0.79	0.17	74,115,118,121	0
7	GOL	A	504	6/6	0.82	0.21	106,113,114,117	0
7	GOL	B	505	6/6	0.82	0.21	102,115,129,143	0
7	GOL	C	505	6/6	0.83	0.17	99,113,123,127	0
7	GOL	C	504	6/6	0.85	0.14	105,110,112,112	0
6	MG	A	502	1/1	0.86	0.31	67,67,67,67	0
12	IMD	E	201	5/5	0.87	0.21	130,130,138,138	0
7	GOL	B	503	6/6	0.87	0.15	88,95,100,115	0
7	GOL	C	501	6/6	0.89	0.18	82,100,104,107	0
7	GOL	D	504	6/6	0.89	0.15	89,105,114,118	0
7	GOL	A	503	6/6	0.90	0.13	88,100,107,109	0
9	GDP	D	501	28/28	0.90	0.11	65,94,108,113	0
12	IMD	C	508	5/5	0.91	0.15	77,78,85,85	0
6	MG	B	502	1/1	0.92	0.24	58,58,58,58	0
7	GOL	C	506	6/6	0.92	0.14	79,94,98,99	0
10	MES	B	507	12/12	0.93	0.09	46,75,86,99	0
12	IMD	C	509	5/5	0.93	0.23	113,117,121,122	0
8	CA	A	505	1/1	0.95	0.09	106,106,106,106	0
8	CA	B	506	1/1	0.95	0.07	121,121,121,121	0
11	84F	B	508	27/27	0.95	0.09	44,59,72,86	0
11	84F	D	505	27/27	0.95	0.09	49,60,77,91	0
5	GTP	A	501	32/32	0.96	0.07	43,51,65,70	0
8	CA	C	507	1/1	0.96	0.06	135,135,135,135	0
9	GDP	B	501	28/28	0.98	0.06	35,48,58,60	0
6	MG	C	503	1/1	0.98	0.05	48,48,48,48	0
5	GTP	C	502	32/32	0.98	0.05	42,50,56,58	0

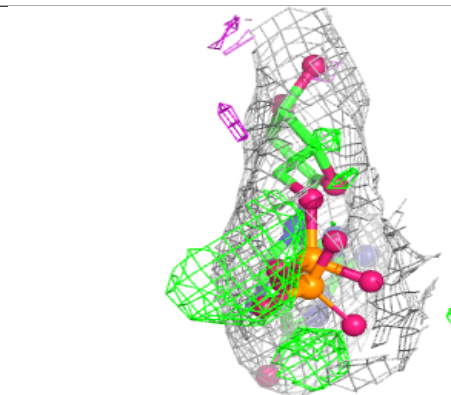
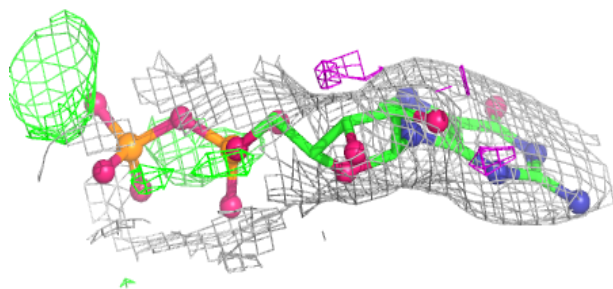
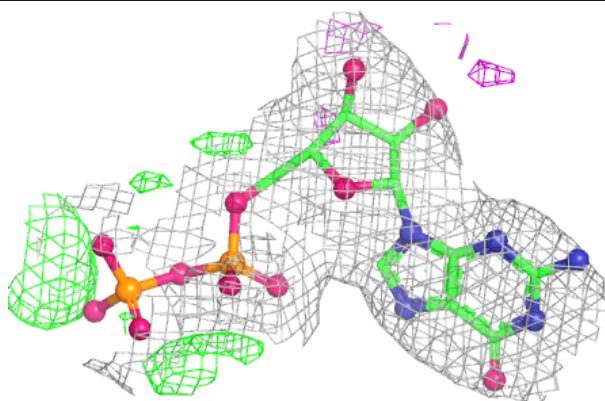
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

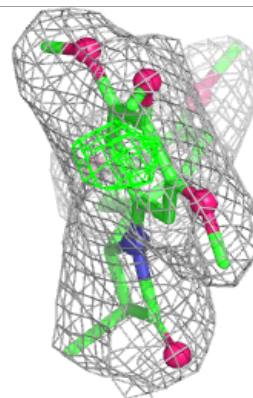
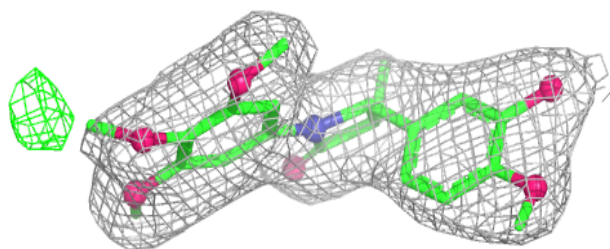
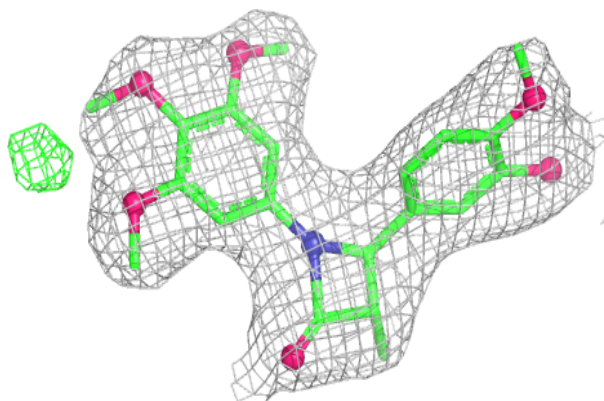
**Electron density around GDP D 501:**

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

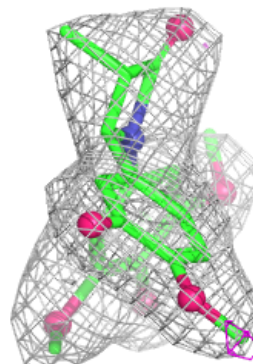
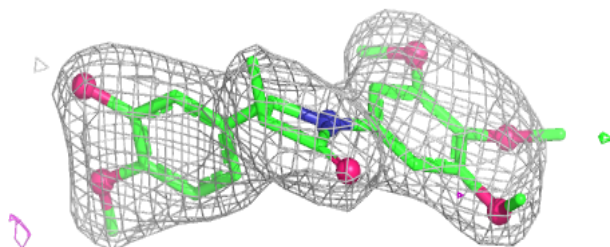
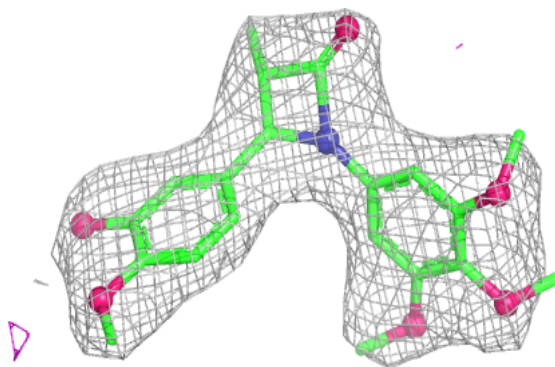


Electron density around 84F B 508:

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

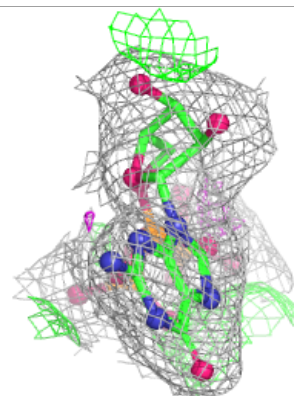
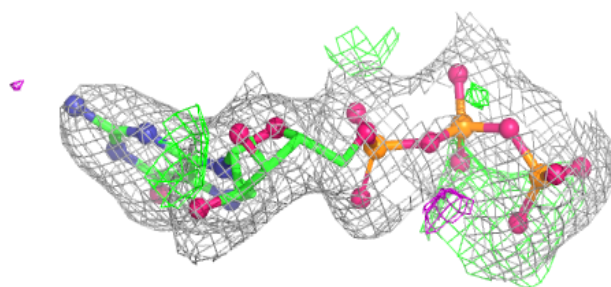
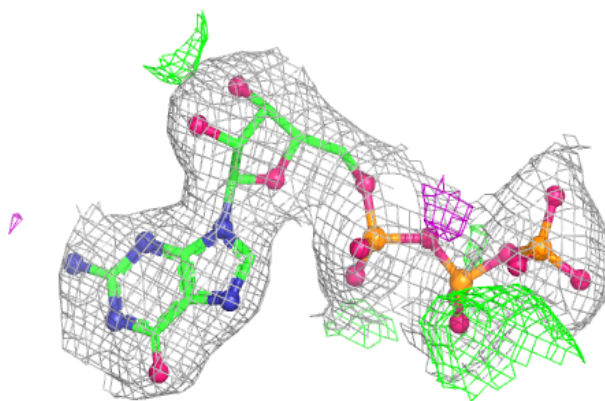
**Electron density around 84F D 505:**

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

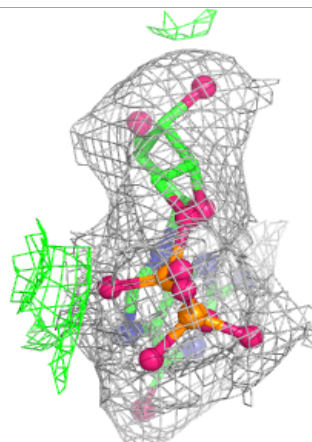
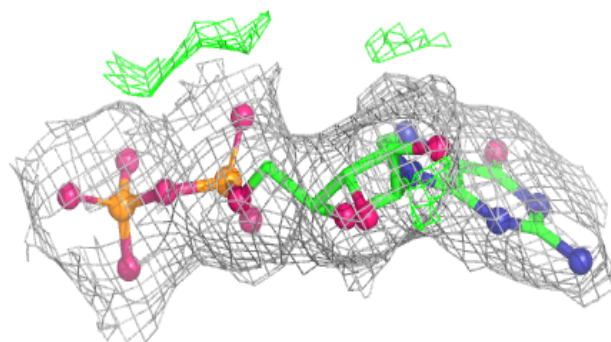
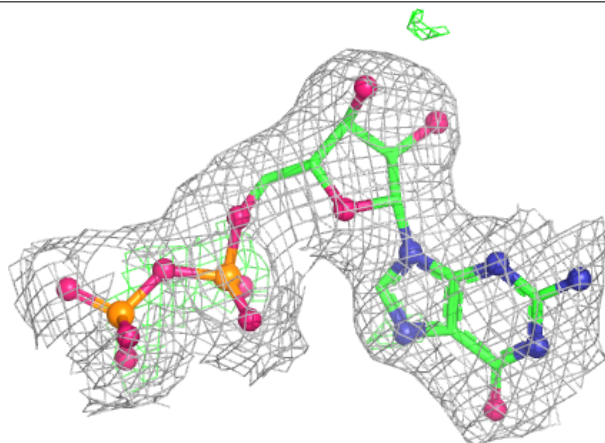


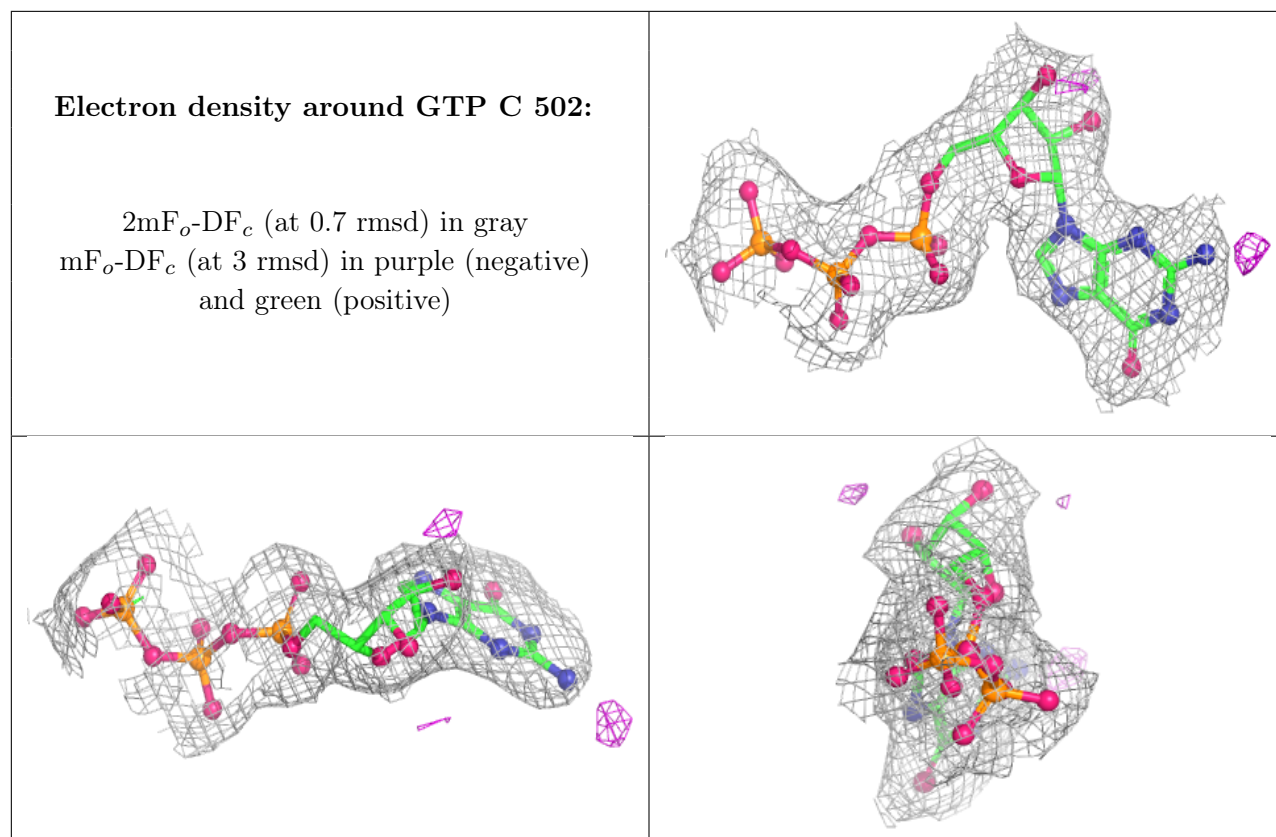
Electron density around GTP A 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.