



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:31 am BST

PDB ID : 5BMV
Title : CRYSTAL STRUCTURE OF TUBULIN-STATHMIN-TTL-Vinblastine
COMPLEX
Authors : Wang, Y.; Chen, Q.; Zhang, R.
Deposited on : 2015-05-23
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

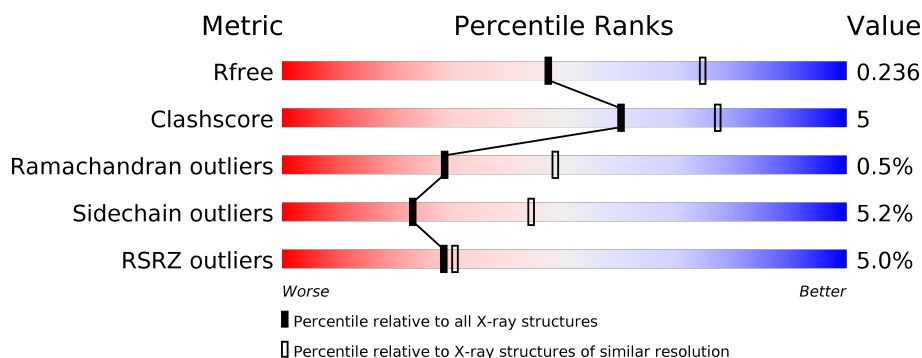
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
1	C	451	<div> <div></div> <div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>•</div> <div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
2	D	445	<div> <div>7%</div> <div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
3	E	143	<div> <div>10%</div> <div> <div>73%</div> <div>10%</div> <div>• 14%</div> </div> </div>
4	F	384	<div> <div>13%</div> <div> <div>74%</div> <div>14%</div> <div>• 10%</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
8	GOL	C	504	-	-	X	-
8	GOL	C	505	-	-	X	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17912 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	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3360	2111	576	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

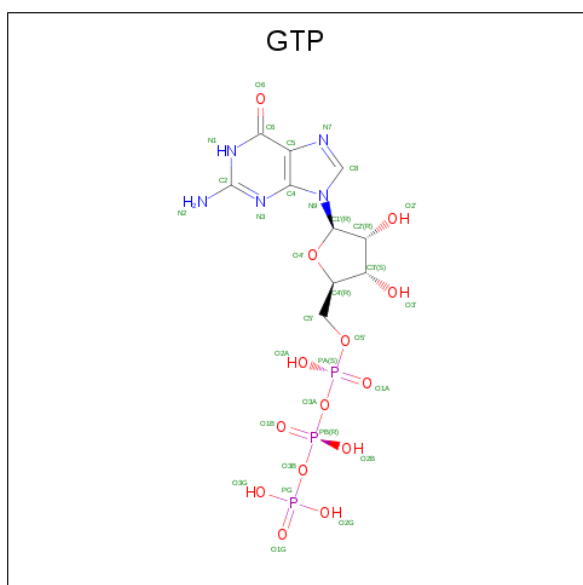
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

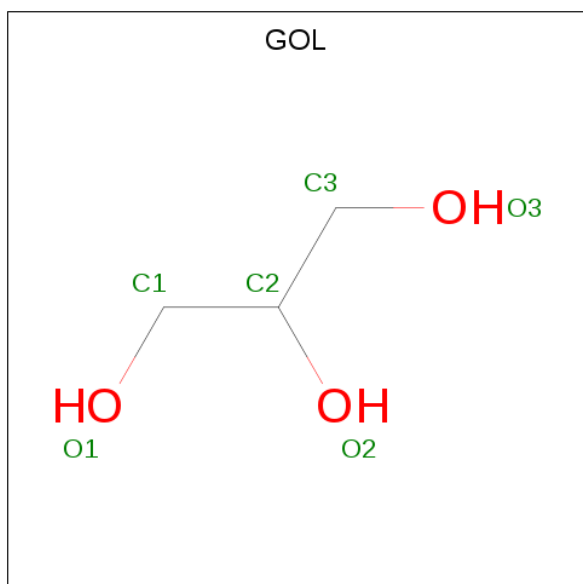
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

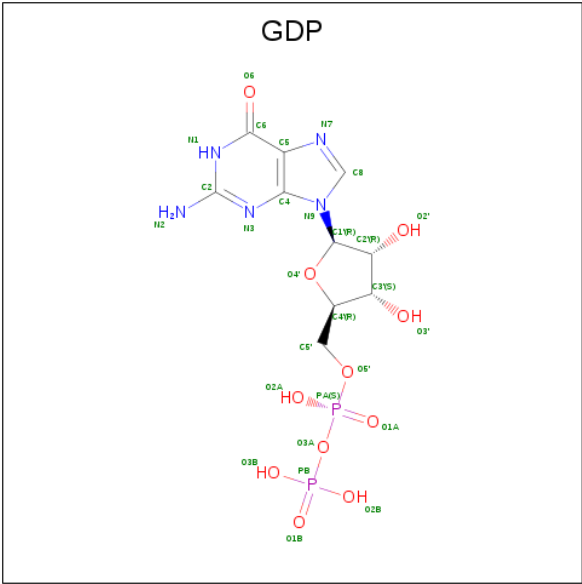
- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

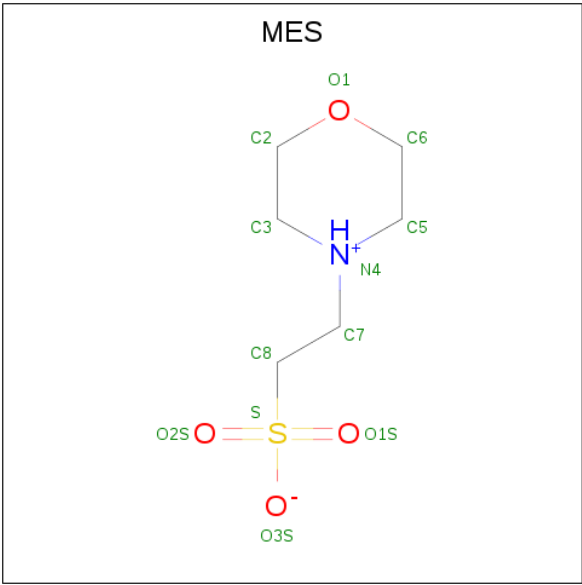
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

C₁₀H₁₅N₅O₁₁P₂).



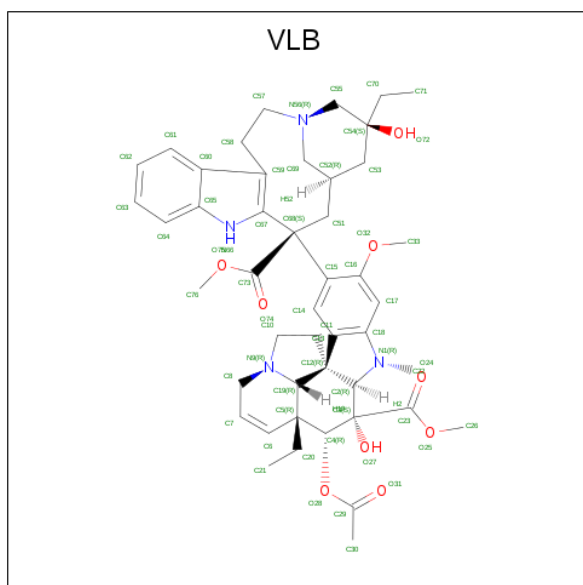
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



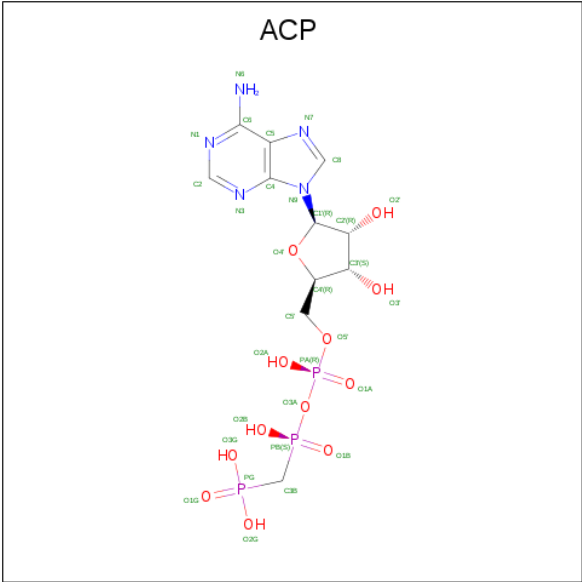
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula: C₄₆H₅₈N₄O₉).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O		0	0
			59	46	4	9			

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

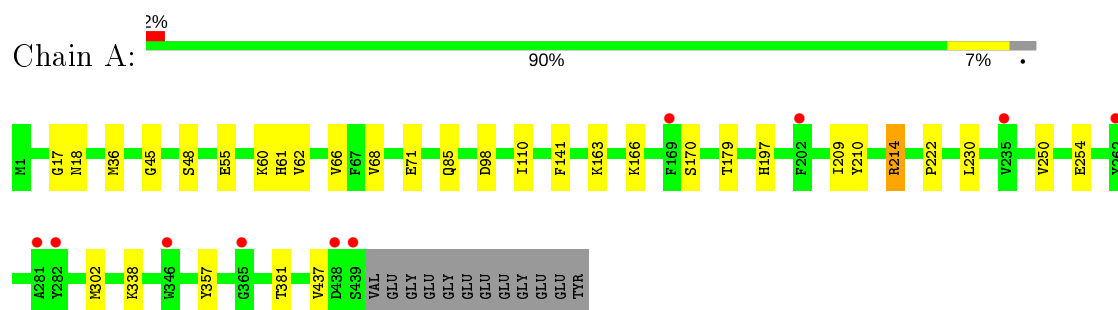
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	47	Total	O	0	0
			47	47		
13	B	56	Total	O	0	0
			56	56		
13	C	83	Total	O	0	0
			83	83		
13	D	8	Total	O	0	0
			8	8		
13	E	1	Total	O	0	0
			1	1		
13	F	24	Total	O	0	0
			24	24		

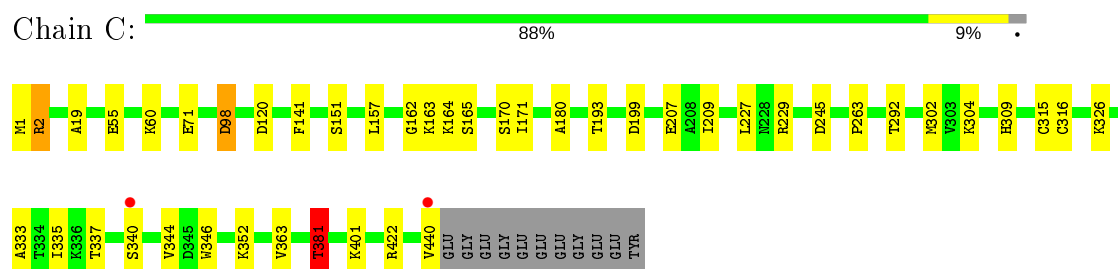
3 Residue-property plots [i](#)

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.

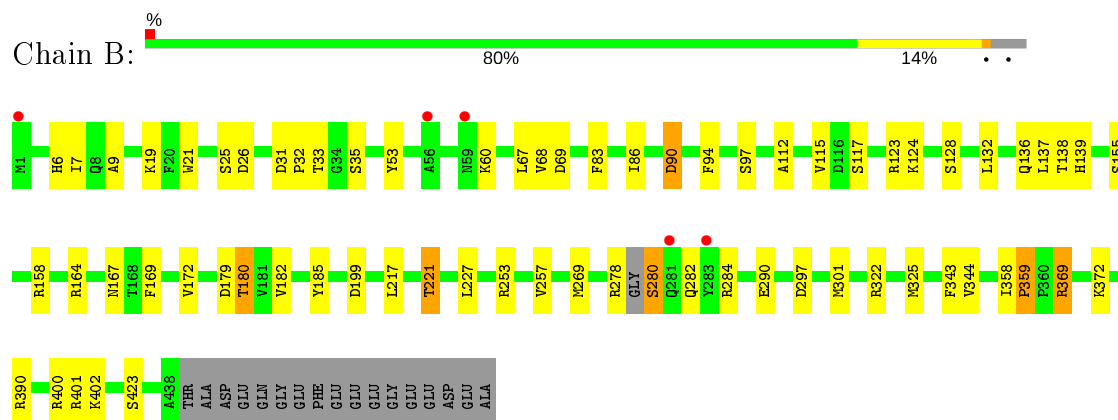
- Molecule 1: Tubulin alpha-1B chain



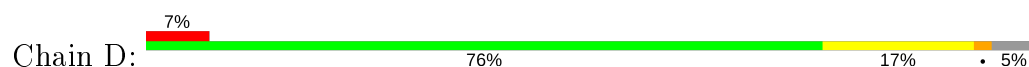
- Molecule 1: Tubulin alpha-1B chain

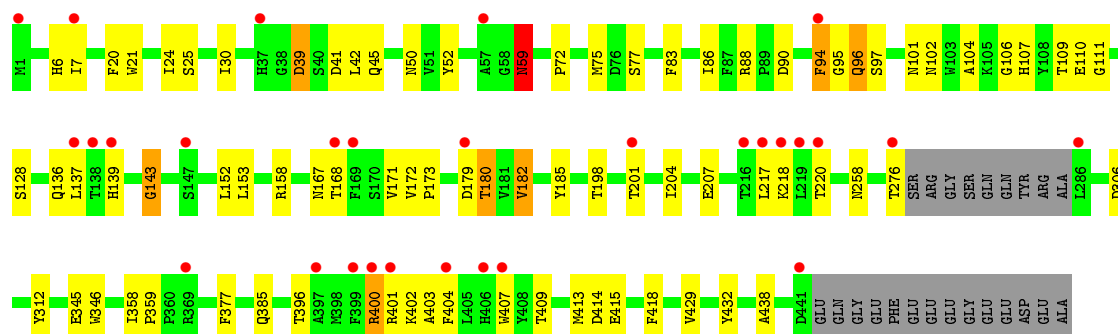


- Molecule 2: Tubulin beta chain

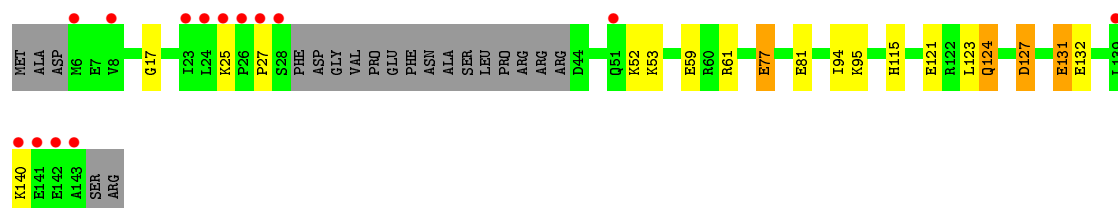
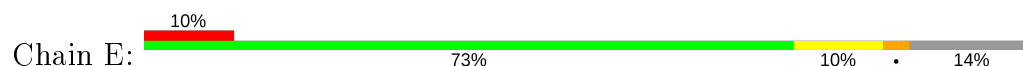


- Molecule 2: Tubulin beta chain

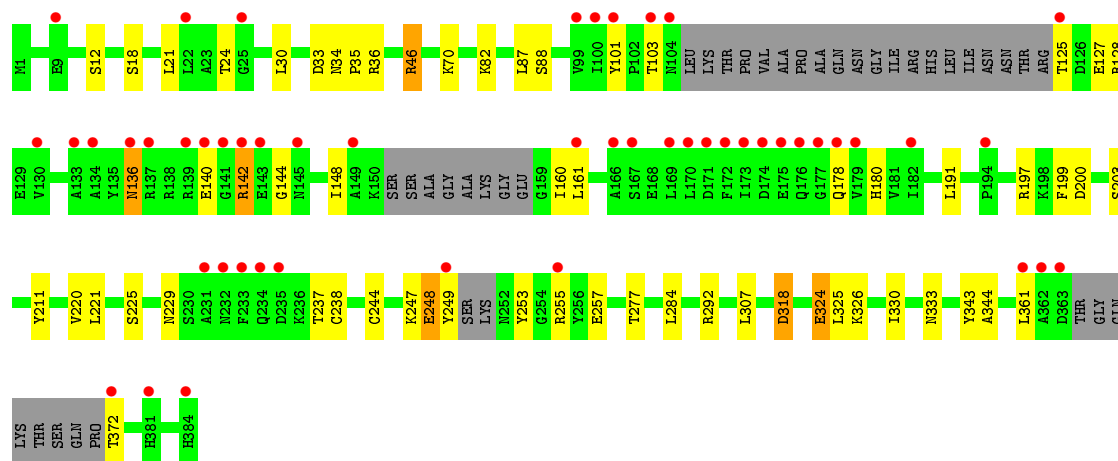




• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.47Å 157.42Å 183.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 39.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.50) 99.5 (39.91-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.184 , 0.235 0.192 , 0.236	Depositor DCC
R_{free} test set	4906 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17912	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GDP, GOL, MG, CA, VLB, GTP, ACP, MES

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	0.71	0/3508	0.82	1/4762 (0.0%)
1	C	0.78	0/3524	0.85	4/4785 (0.1%)
2	B	0.80	1/3434 (0.0%)	0.87	7/4651 (0.2%)
2	D	0.68	2/3384 (0.1%)	0.81	4/4586 (0.1%)
3	E	0.71	0/1022	0.81	1/1356 (0.1%)
4	F	0.59	0/2916	0.78	3/3940 (0.1%)
All	All	0.72	3/17788 (0.0%)	0.83	20/24080 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
4	F	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	179	ASP	CB-CG	-6.36	1.38	1.51
2	D	173	PRO	N-CD	5.23	1.55	1.47
2	D	359	PRO	N-CD	5.20	1.55	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	61	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	C	98	ASP	CB-CG-OD2	-6.31	112.62	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	306	ASP	CB-CG-OD1	6.28	123.95	118.30
2	D	359	PRO	C-N-CD	6.27	141.58	128.40
2	B	179	ASP	CB-CG-OD1	-6.21	112.71	118.30
2	B	390	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	358	ILE	C-N-CD	6.00	141.01	128.40
1	C	381	THR	CB-CA-C	-5.92	95.63	111.60
2	B	359	PRO	C-N-CD	5.87	140.72	128.40
2	B	297	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	98	ASP	CB-CG-OD1	5.73	123.45	118.30
2	D	358	ILE	C-N-CD	5.66	140.28	128.40
4	F	36	ARG	NE-CZ-NH2	-5.51	117.54	120.30
4	F	36	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	422	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	B	179	ASP	CB-CA-C	-5.41	99.58	110.40
2	D	172	VAL	C-N-CD	5.22	139.36	128.40
2	B	172	VAL	C-N-CD	5.16	139.24	128.40
4	F	318	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	214	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	163	LYS	Peptide
4	F	136	ASN	Peptide

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	3430	0	3340	16	0
1	C	3446	0	3354	33	0
2	B	3360	0	3242	40	0
2	D	3311	0	3192	40	0
3	E	1014	0	1029	9	0
4	F	2849	0	2796	22	0
5	A	32	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	0	0
8	B	6	0	8	1	0
8	C	18	0	24	12	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	C	59	0	58	5	0
12	F	31	0	14	2	0
13	A	47	0	0	1	0
13	B	56	0	0	1	0
13	C	83	0	0	6	0
13	D	8	0	0	2	0
13	E	1	0	0	0	0
13	F	24	0	0	1	0
All	All	17912	0	17155	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (159) 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:35:SER:OG	2:B:60:LYS:NZ	1.65	1.30
2:D:432:TYR:OH	13:D:601:HOH:O	1.71	1.09
11:C:507:VLB:H511	11:C:507:VLB:H582	1.43	1.01
2:B:33:THR:HG22	2:B:60:LYS:HE3	1.58	0.85
2:B:83:PHE:O	2:B:86:ILE:HG22	1.79	0.82
2:B:33:THR:CG2	2:B:60:LYS:HE3	2.14	0.77
2:D:96:GLN:HG2	2:D:97:SER:N	1.99	0.77
1:C:381:THR:HG23	13:C:667:HOH:O	1.87	0.73
8:C:506:GOL:O1	8:C:506:GOL:O3	2.11	0.69
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.75	0.68
11:C:507:VLB:C51	11:C:507:VLB:H582	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:TYR:CD1	2:D:418:PHE:HE2	2.12	0.67
13:C:663:HOH:O	3:E:115:HIS:HE1	1.76	0.67
2:B:278:ARG:C	2:B:280:SER:N	2.49	0.66
2:B:33:THR:HG22	2:B:60:LYS:CE	2.26	0.64
2:D:7:ILE:O	2:D:137:LEU:HD12	1.96	0.63
3:E:131:GLU:HA	3:E:131:GLU:OE2	1.96	0.63
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.79	0.63
2:B:35:SER:HG	2:B:60:LYS:NZ	1.95	0.63
1:A:60:LYS:NZ	1:A:85:GLN:O	2.18	0.62
2:B:199:ASP:OD1	10:B:504:MES:H32	1.99	0.62
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.36	0.61
11:C:507:VLB:O32	11:C:507:VLB:C73	2.47	0.61
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.35	0.61
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.33	0.61
2:B:132:LEU:O	2:B:164:ARG:NH1	2.30	0.61
2:D:414:ASP:OD1	2:D:415:GLU:N	2.34	0.60
2:B:401:ARG:HH21	8:B:506:GOL:H11	1.66	0.60
2:D:136:GLN:HA	2:D:167:ASN:O	2.01	0.60
1:C:309:HIS:CE1	13:C:612:HOH:O	2.55	0.59
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.38	0.59
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.85	0.58
1:C:229:ARG:HG2	8:C:505:GOL:O2	2.04	0.57
2:D:21:TRP:O	2:D:25:SER:OG	2.09	0.57
2:B:221:THR:CG2	2:B:221:THR:O	2.53	0.56
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.05	0.56
2:D:217:LEU:C	2:D:218:LYS:HG2	2.27	0.55
4:F:324:GLU:O	4:F:325:LEU:HB2	2.05	0.55
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.42	0.55
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.26	0.54
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.89	0.54
2:B:31:ASP:OD1	2:B:33:THR:HB	2.07	0.54
3:E:124:GLN:O	3:E:127:ASP:N	2.40	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.53
2:D:401:ARG:O	2:D:403:ALA:N	2.41	0.53
2:D:59:ASN:OD1	2:D:59:ASN:N	2.40	0.53
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.12	0.53
2:B:284:ARG:NH2	2:B:290:GLU:OE1	2.43	0.52
1:C:229:ARG:CG	8:C:505:GOL:O2	2.57	0.52
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.44	0.52
3:E:124:GLN:HA	3:E:124:GLN:OE1	2.10	0.52
1:C:207:GLU:OE2	8:C:504:GOL:H11	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:THR:HB	13:C:608:HOH:O	2.09	0.51
2:B:90:ASP:OD1	2:B:90:ASP:N	2.44	0.51
1:C:363:VAL:HG21	8:C:505:GOL:H11	1.93	0.51
2:D:39:ASP:N	2:D:39:ASP:OD1	2.41	0.51
1:C:304:LYS:HG3	8:C:504:GOL:H12	1.93	0.51
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.29	0.50
2:B:253:ARG:O	2:B:257:VAL:HG23	2.12	0.50
4:F:191:LEU:HA	4:F:197:ARG:O	2.10	0.50
2:B:269:MET:HE1	2:B:301:MET:HG3	1.93	0.50
1:C:171:ILE:HD13	1:C:171:ILE:N	2.25	0.50
1:C:1:MET:O	1:C:2:ARG:HB2	2.11	0.50
2:D:182:VAL:HG22	2:D:185:TYR:HD2	1.76	0.50
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.94	0.50
4:F:200:ASP:OD2	12:F:401:ACP:O3'	2.30	0.49
1:C:229:ARG:HG2	8:C:505:GOL:C2	2.41	0.49
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.42	0.49
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.12	0.49
1:C:209:ILE:HD11	1:C:302:MET:HG2	1.93	0.49
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.12	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.27	0.48
4:F:248:GLU:O	4:F:249:TYR:CD2	2.66	0.48
1:C:19:ALA:HA	8:C:505:GOL:H12	1.95	0.48
3:E:121:GLU:O	3:E:124:GLN:HB2	2.13	0.48
2:D:96:GLN:HG2	2:D:97:SER:H	1.76	0.48
2:B:164:ARG:HD2	13:B:614:HOH:O	2.13	0.48
11:C:507:VLB:H19	11:C:507:VLB:H213	1.72	0.48
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.96	0.47
2:D:400:ARG:HG3	2:D:401:ARG:N	2.30	0.47
1:C:304:LYS:HE3	8:C:504:GOL:H31	1.95	0.47
1:A:110:ILE:O	1:A:110:ILE:HG22	2.15	0.47
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.15	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.47
2:B:7:ILE:O	2:B:137:LEU:HA	2.15	0.46
1:C:55:GLU:HA	1:C:60:LYS:O	2.14	0.46
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.98	0.46
2:D:102:ASN:ND2	2:D:407:TRP:O	2.47	0.46
2:B:227:LEU:HD22	11:C:507:VLB:H711	1.97	0.46
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.46
2:B:158:ARG:NE	10:B:504:MES:O1	2.49	0.46
1:C:381:THR:CG2	13:C:667:HOH:O	2.53	0.46
2:B:199:ASP:OD2	10:B:504:MES:H52	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:O	2:B:280:SER:N	2.50	0.45
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.99	0.45
2:D:83:PHE:O	2:D:86:ILE:HG22	2.16	0.45
4:F:247:LYS:HE3	4:F:253:TYR:CZ	2.52	0.45
4:F:343:TYR:O	4:F:344:ALA:C	2.55	0.45
2:B:25:SER:HA	2:B:53:TYR:OH	2.17	0.44
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.17	0.44
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
2:D:107:HIS:O	2:D:152:LEU:HD22	2.18	0.44
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.52	0.44
2:B:343:PHE:O	2:B:344:VAL:C	2.53	0.44
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.53	0.44
8:C:506:GOL:HO1	8:C:506:GOL:HO3	1.61	0.44
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.44
4:F:46:ARG:NH2	4:F:46:ARG:HB3	2.33	0.43
2:B:158:ARG:HG3	10:B:504:MES:H62	2.00	0.43
1:A:166:LYS:HE2	1:A:197:HIS:O	2.18	0.43
1:A:55:GLU:HA	1:A:60:LYS:O	2.18	0.43
1:A:17:GLY:O	1:A:18:ASN:C	2.56	0.43
4:F:330:ILE:HD13	4:F:330:ILE:HA	1.77	0.43
2:B:269:MET:HE2	2:B:301:MET:SD	2.58	0.43
4:F:333:ASN:HB3	13:F:518:HOH:O	2.18	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.43
1:C:304:LYS:HB3	8:C:504:GOL:H31	2.01	0.42
2:D:101:ASN:ND2	2:D:180:THR:HG21	2.34	0.42
1:A:209:ILE:HD11	1:A:302:MET:SD	2.59	0.42
2:B:112:ALA:O	2:B:115:VAL:HG12	2.19	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.42
2:D:438:ALA:O	13:D:602:HOH:O	2.21	0.42
2:B:269:MET:CE	2:B:301:MET:HG3	2.49	0.42
3:E:77:GLU:O	3:E:81:GLU:HG3	2.19	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
4:F:101:TYR:O	4:F:128:ARG:NH2	2.52	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.54	0.42
2:B:9:ALA:HA	2:B:68:VAL:O	2.20	0.42
1:C:304:LYS:CB	8:C:504:GOL:H31	2.50	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.20	0.41
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.02	0.41
1:C:157:LEU:HA	1:C:157:LEU:HD23	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:PRO:HD2	13:C:641:HOH:O	2.20	0.41
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.51	0.41
2:D:102:ASN:OD1	2:D:102:ASN:C	2.59	0.41
2:B:97:SER:O	1:C:2:ARG:NH2	2.53	0.41
1:C:316:CYS:HA	1:C:352:LYS:O	2.20	0.41
2:D:168:THR:HG23	2:D:198:THR:HG21	2.02	0.41
2:D:52:TYR:OH	2:D:136:GLN:OE1	2.32	0.41
4:F:136:ASN:O	4:F:140:GLU:HG2	2.21	0.41
4:F:178:GLN:OE1	4:F:178:GLN:N	2.54	0.41
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.41
1:A:45:GLY:HA3	13:A:624:HOH:O	2.21	0.41
2:D:41:ASP:C	2:D:45:GLN:N	2.73	0.41
2:D:171:VAL:HA	2:D:204:ILE:O	2.21	0.41
2:D:168:THR:OG1	2:D:201:THR:HG23	2.21	0.40
2:D:41:ASP:C	2:D:45:GLN:H	2.24	0.40
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.40
2:B:182:VAL:O	2:B:185:TYR:HB2	2.20	0.40
2:D:185:TYR:CD1	2:D:418:PHE:CE2	3.02	0.40
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.40
2:B:180:THR:HG22	1:C:352:LYS:NZ	2.37	0.40
2:D:72:PRO:HG3	2:D:95:GLY:O	2.22	0.40
2:B:69:ASP:O	2:B:94:PHE:HA	2.21	0.40
1:C:151:SER:HB2	1:C:193:THR:HG22	2.03	0.40
4:F:244:CYS:O	4:F:247:LYS:N	2.55	0.40
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/451 (97%)	417 (95%)	20 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	439/451 (97%)	423 (96%)	14 (3%)	2 (0%)	29	48
2	B	423/445 (95%)	417 (99%)	6 (1%)	0	100	100
2	D	418/445 (94%)	390 (93%)	23 (6%)	5 (1%)	13	24
3	E	119/143 (83%)	111 (93%)	7 (6%)	1 (1%)	19	35
4	F	336/384 (88%)	306 (91%)	27 (8%)	3 (1%)	17	31
All	All	2172/2319 (94%)	2064 (95%)	97 (4%)	11 (0%)	29	48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	402	LYS
3	E	27	PRO
1	C	2	ARG
1	C	164	LYS
2	D	143	GLY
2	D	404	PHE
4	F	142	ARG
2	D	59	ASN
2	D	180	THR
4	F	88	SER
4	F	144	GLY

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	370/379 (98%)	360 (97%)	10 (3%)	44	71
1	C	372/379 (98%)	365 (98%)	7 (2%)	57	80
2	B	368/381 (97%)	347 (94%)	21 (6%)	20	39
2	D	363/381 (95%)	341 (94%)	22 (6%)	18	36
3	E	110/127 (87%)	99 (90%)	11 (10%)	7	15
4	F	312/342 (91%)	284 (91%)	28 (9%)	9	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1895/1989 (95%)	1796 (95%)	99 (5%)	23	44

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	62	VAL
1	A	66	VAL
1	A	68	VAL
1	A	71	GLU
1	A	163	LYS
1	A	179	THR
1	A	338	LYS
1	A	381	THR
1	A	437	VAL
2	B	19	LYS
2	B	90	ASP
2	B	117	SER
2	B	123	ARG
2	B	124	LYS
2	B	128	SER
2	B	139	HIS
2	B	155	SER
2	B	180	THR
2	B	217	LEU
2	B	221	THR
2	B	280	SER
2	B	282	GLN
2	B	322	ARG
2	B	325	MET
2	B	359	PRO
2	B	369	ARG
2	B	372	LYS
2	B	400	ARG
2	B	402	LYS
2	B	423	SER
1	C	120	ASP
1	C	245	ASP
1	C	315	CYS
1	C	326	LYS
1	C	340	SER
1	C	381	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	440	VAL
2	D	30	ILE
2	D	39	ASP
2	D	42	LEU
2	D	50	ASN
2	D	59	ASN
2	D	77	SER
2	D	88	ARG
2	D	90	ASP
2	D	94	PHE
2	D	96	GLN
2	D	128	SER
2	D	139	HIS
2	D	153	LEU
2	D	179	ASP
2	D	182	VAL
2	D	207	GLU
2	D	220	THR
2	D	276	THR
2	D	345	GLU
2	D	396	THR
2	D	400	ARG
2	D	409	THR
3	E	25	LYS
3	E	52	LYS
3	E	53	LYS
3	E	59	GLU
3	E	77	GLU
3	E	95	LYS
3	E	124	GLN
3	E	127	ASP
3	E	131	GLU
3	E	132	GLU
3	E	140	LYS
4	F	12	SER
4	F	18	SER
4	F	30	LEU
4	F	33	ASP
4	F	46	ARG
4	F	70	LYS
4	F	87	LEU
4	F	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	125	THR
4	F	142	ARG
4	F	161	LEU
4	F	180	HIS
4	F	203	SER
4	F	211	TYR
4	F	220	VAL
4	F	225	SER
4	F	229	ASN
4	F	237	THR
4	F	238	CYS
4	F	248	GLU
4	F	255	ARG
4	F	277	THR
4	F	292	ARG
4	F	307	LEU
4	F	324	GLU
4	F	326	LYS
4	F	361	LEU
4	F	372	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	281	GLN
2	D	96	GLN
2	D	101	ASN
3	E	18	GLN
4	F	229	ASN
4	F	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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
8	GOL	B	506	-	5,5,5	0.41	0	5,5,5	0.32	0
8	GOL	C	504	-	5,5,5	0.62	0	5,5,5	1.02	0
8	GOL	A	504	-	5,5,5	0.48	0	5,5,5	0.52	0
12	ACP	F	401	-	27,33,33	2.13	9 (33%)	32,52,52	1.25	2 (6%)
10	MES	B	505	-	12,12,12	2.35	1 (8%)	14,16,16	1.49	1 (7%)
5	GTP	C	501	6	26,34,34	1.28	4 (15%)	33,54,54	2.02	10 (30%)
9	GDP	B	501	6	24,30,30	1.25	3 (12%)	31,47,47	1.74	6 (19%)
5	GTP	A	501	6	26,34,34	1.16	3 (11%)	33,54,54	1.76	8 (24%)
11	VLB	C	507	-	63,67,67	2.96	17 (26%)	79,108,108	2.28	22 (27%)
8	GOL	A	506	-	5,5,5	0.74	0	5,5,5	0.51	0
9	GDP	D	501	6	24,30,30	1.23	3 (12%)	31,47,47	1.70	8 (25%)
8	GOL	C	506	-	5,5,5	0.37	0	5,5,5	0.62	0
10	MES	B	504	-	12,12,12	2.27	3 (25%)	14,16,16	6.61	7 (50%)
8	GOL	C	505	-	5,5,5	0.66	0	5,5,5	0.74	0
8	GOL	A	505	-	5,5,5	0.45	0	5,5,5	1.09	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
8	GOL	B	506	-	-	2/4/4/4	-
8	GOL	C	504	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	504	-	-	2/4/4/4	-
12	ACP	F	401	-	-	6/15/38/38	0/3/3/3
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
11	VLB	C	507	-	-	6/38/131/131	0/7/9/9
8	GOL	A	506	-	-	2/4/4/4	-
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3
8	GOL	C	506	-	-	2/4/4/4	-
10	MES	B	504	-	-	5/6/14/14	0/1/1/1
8	GOL	C	505	-	-	1/4/4/4	-
8	GOL	A	505	-	-	2/4/4/4	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	507	VLB	C6-C7	11.72	1.54	1.32
11	C	507	VLB	C68-C73	-9.90	1.45	1.53
11	C	507	VLB	C68-C67	-9.42	1.44	1.53
10	B	505	MES	C8-S	-7.78	1.66	1.77
10	B	504	MES	C8-S	-6.58	1.68	1.77
11	C	507	VLB	C12-C13	-6.13	1.41	1.51
12	F	401	ACP	PB-O3A	6.02	1.65	1.58
12	F	401	ACP	PG-O1G	5.78	1.62	1.50
11	C	507	VLB	C58-C59	-4.49	1.44	1.52
11	C	507	VLB	C18-C13	-3.95	1.34	1.39
11	C	507	VLB	C19-N9	3.75	1.53	1.47
9	D	501	GDP	C6-C5	3.69	1.47	1.41
5	A	501	GTP	C6-C5	3.42	1.47	1.41
11	C	507	VLB	C20-C5	-3.40	1.49	1.55
9	B	501	GDP	C6-C5	3.30	1.47	1.41
5	C	501	GTP	C4-N3	-3.30	1.30	1.35
11	C	507	VLB	C60-C65	-3.24	1.33	1.42
11	C	507	VLB	C17-C18	-3.21	1.34	1.39
11	C	507	VLB	C57-C58	3.13	1.61	1.52
12	F	401	ACP	PG-O3G	3.11	1.62	1.54
11	C	507	VLB	C61-C60	-3.07	1.36	1.42
11	C	507	VLB	C14-C13	-3.04	1.34	1.39
11	C	507	VLB	C64-C65	-3.02	1.36	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PG-O2G	-2.94	1.48	1.54
9	B	501	GDP	O4'-C1'	2.85	1.45	1.41
11	C	507	VLB	O75-C73	2.81	1.38	1.33
10	B	504	MES	O2S-S	2.75	1.53	1.45
11	C	507	VLB	C68-C15	-2.56	1.45	1.54
12	F	401	ACP	C5-C4	2.52	1.47	1.40
11	C	507	VLB	C18-N1	-2.38	1.35	1.39
5	C	501	GTP	C2-N2	2.34	1.38	1.33
12	F	401	ACP	PB-O2B	2.33	1.61	1.56
5	C	501	GTP	C2'-C1'	-2.31	1.50	1.53
9	D	501	GDP	C2'-C1'	-2.25	1.50	1.53
9	B	501	GDP	C5-C4	2.23	1.46	1.40
9	D	501	GDP	C5-C4	2.20	1.46	1.40
12	F	401	ACP	C2-N3	2.17	1.35	1.32
12	F	401	ACP	C2'-C1'	-2.17	1.50	1.53
12	F	401	ACP	O4'-C1'	2.10	1.44	1.41
5	A	501	GTP	C5-C4	2.09	1.46	1.40
10	B	504	MES	O1S-S	2.05	1.51	1.45
5	A	501	GTP	C6-N1	2.03	1.36	1.33
5	C	501	GTP	C8-N7	2.00	1.38	1.34

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O3S-S-O1S	-12.81	79.98	111.27
10	B	504	MES	O1S-S-C8	12.24	121.66	106.92
10	B	504	MES	O3S-S-C8	-11.81	86.66	105.77
10	B	504	MES	O3S-S-O2S	-8.31	90.97	111.27
11	C	507	VLB	C8-C7-C6	-8.13	109.72	123.02
10	B	504	MES	O2S-S-C8	7.57	116.03	106.92
11	C	507	VLB	C19-C5-C6	6.95	115.39	108.28
11	C	507	VLB	C5-C6-C7	-5.25	112.34	124.02
5	C	501	GTP	C5-C6-N1	-4.94	116.67	123.43
11	C	507	VLB	C11-C12-C13	-4.84	103.53	112.35
11	C	507	VLB	O28-C29-C30	4.71	119.75	111.09
11	C	507	VLB	C12-C19-C5	-4.48	114.88	118.20
9	B	501	GDP	C5-C6-N1	-4.48	117.31	123.43
5	C	501	GTP	C6-N1-C2	4.40	122.93	115.93
9	D	501	GDP	C2-N3-C4	4.32	120.30	115.36
11	C	507	VLB	C4-O28-C29	4.20	124.13	117.65
11	C	507	VLB	O28-C4-C3	4.11	112.93	106.30
5	C	501	GTP	C6-C5-C4	-4.09	116.89	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	-4.08	117.86	123.43
5	C	501	GTP	N3-C2-N1	-3.93	121.98	127.22
9	B	501	GDP	C6-N1-C2	3.92	122.16	115.93
11	C	507	VLB	C52-C69-N56	3.81	117.24	111.28
9	B	501	GDP	C6-C5-C4	-3.78	117.19	120.80
10	B	505	MES	O2S-S-C8	3.77	111.45	106.92
5	A	501	GTP	C4-C5-N7	-3.69	105.55	109.40
12	F	401	ACP	N3-C2-N1	-3.59	123.07	128.68
11	C	507	VLB	C5-C19-N9	3.53	119.15	111.72
5	C	501	GTP	C2-N3-C4	3.45	119.29	115.36
11	C	507	VLB	C13-C12-C2	3.37	107.46	102.21
9	D	501	GDP	C5-C6-N1	-3.27	118.96	123.43
9	D	501	GDP	O3B-PB-O1B	3.27	123.47	110.68
9	B	501	GDP	C4-C5-N7	-3.14	106.13	109.40
10	B	504	MES	C5-N4-C3	3.12	115.86	108.83
5	A	501	GTP	C2-N3-C4	3.10	118.89	115.36
5	A	501	GTP	C1'-N9-C4	-2.94	121.47	126.64
5	C	501	GTP	N2-C2-N1	2.92	121.79	117.25
5	A	501	GTP	C6-N1-C2	2.88	120.50	115.93
10	B	504	MES	C6-C5-N4	2.84	114.41	110.10
11	C	507	VLB	O75-C73-C68	2.77	115.48	111.32
5	C	501	GTP	PB-O3B-PG	-2.70	123.58	132.83
11	C	507	VLB	C53-C52-C69	2.65	111.82	108.72
11	C	507	VLB	C2-C12-C19	2.65	118.55	114.07
11	C	507	VLB	C63-C62-C61	-2.60	116.79	120.44
11	C	507	VLB	C13-C18-N1	2.57	113.90	110.98
12	F	401	ACP	C4-C5-N7	-2.56	106.73	109.40
5	A	501	GTP	O3G-PG-O3B	-2.56	96.05	104.64
5	C	501	GTP	O2A-PA-O1A	2.56	124.88	112.24
9	D	501	GDP	C4-C5-N7	-2.55	106.74	109.40
9	D	501	GDP	C6-N1-C2	2.53	119.95	115.93
5	C	501	GTP	C1'-N9-C4	-2.41	122.40	126.64
9	D	501	GDP	C6-C5-C4	-2.41	118.50	120.80
11	C	507	VLB	C17-C18-C13	-2.37	119.18	122.00
5	A	501	GTP	O3G-PG-O1G	2.34	119.85	110.68
9	D	501	GDP	O3A-PB-O1B	-2.29	98.47	111.19
5	A	501	GTP	C6-C5-C4	-2.28	118.62	120.80
11	C	507	VLB	C17-C16-C15	-2.21	120.17	122.20
11	C	507	VLB	C8-N9-C19	2.18	118.20	112.50
11	C	507	VLB	C11-C12-C2	-2.16	108.28	112.34
11	C	507	VLB	C53-C54-C55	2.15	111.92	109.29
11	C	507	VLB	C70-C54-C55	-2.13	106.84	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	O2A-PA-O5'	2.12	117.61	107.75
9	B	501	GDP	C3'-C2'-C1'	-2.10	97.81	100.98
9	B	501	GDP	C1'-N9-C4	-2.06	123.02	126.64
5	C	501	GTP	C4-C5-N7	-2.05	107.26	109.40

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	A	506	GOL	O1-C1-C2-O2
8	A	506	GOL	O1-C1-C2-C3
9	D	501	GDP	C5'-O5'-PA-O1A
8	C	506	GOL	O2-C2-C3-O3
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	N4-C7-C8-S
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
8	B	506	GOL	C1-C2-C3-O3
8	A	505	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
11	C	507	VLB	C30-C29-O28-C4
11	C	507	VLB	O31-C29-O28-C4
8	A	504	GOL	C1-C2-C3-O3
8	C	506	GOL	C1-C2-C3-O3
8	C	504	GOL	O1-C1-C2-C3
8	A	505	GOL	O1-C1-C2-O2
12	F	401	ACP	PB-O3A-PA-O1A
12	F	401	ACP	O4'-C4'-C5'-O5'
8	B	506	GOL	O2-C2-C3-O3
8	C	505	GOL	O1-C1-C2-O2
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O1S
5	C	501	GTP	C4'-C5'-O5'-PA
8	A	504	GOL	O2-C2-C3-O3
11	C	507	VLB	C58-C57-N56-C69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	504	MES	C8-C7-N4-C3
11	C	507	VLB	C67-C68-C73-O75
11	C	507	VLB	C3-C23-O25-C26
11	C	507	VLB	C67-C68-C73-O74
8	C	504	GOL	O1-C1-C2-O2
12	F	401	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
10	B	504	MES	C7-C8-S-O2S

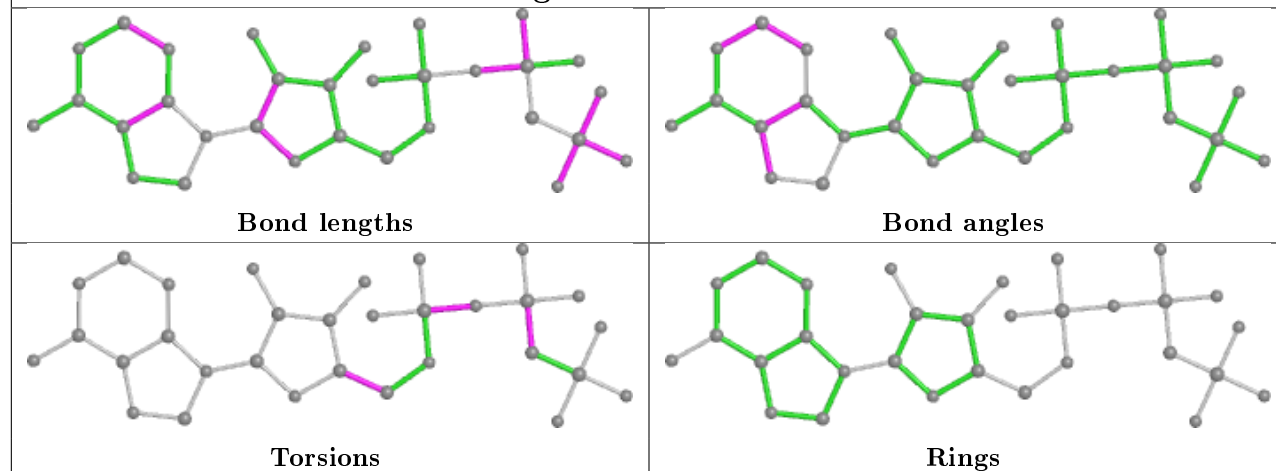
There are no ring outliers.

9 monomers are involved in 26 short contacts:

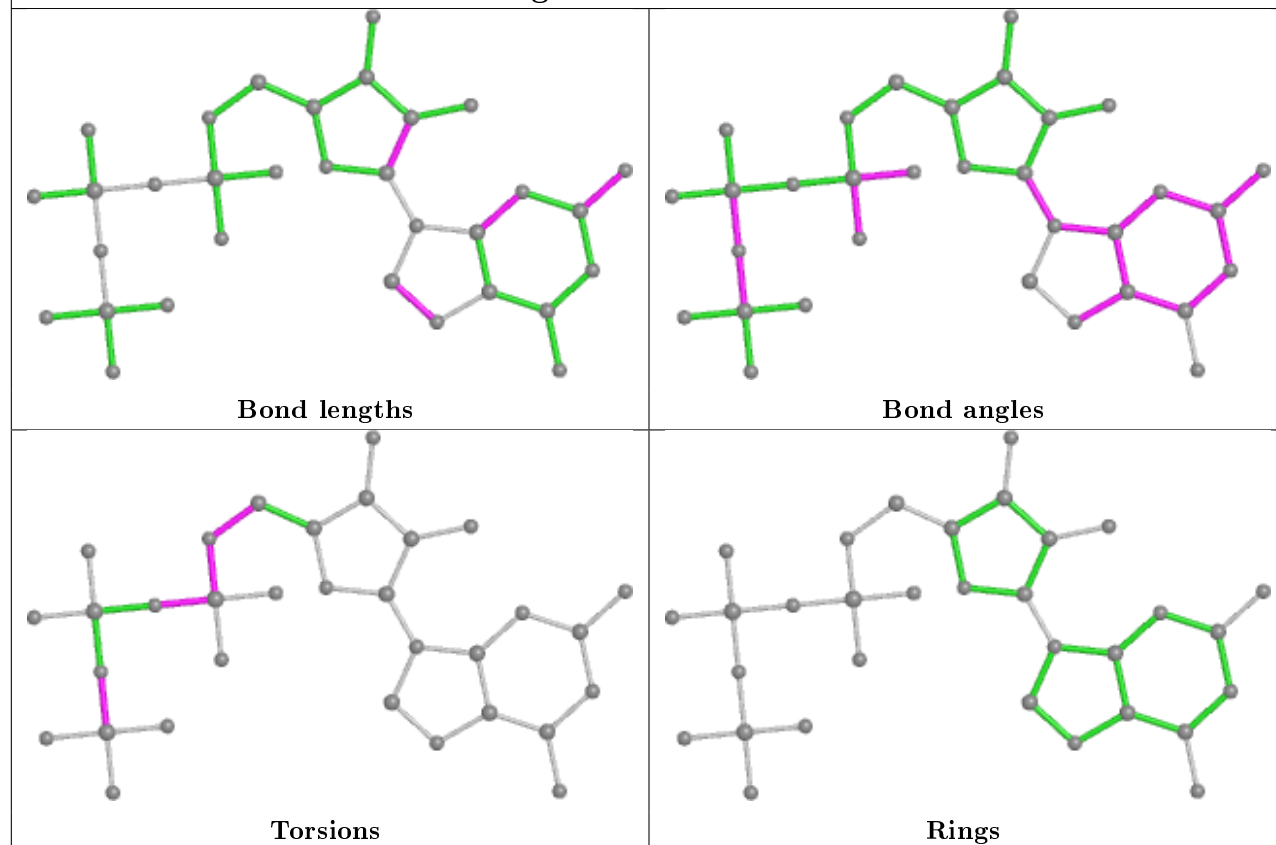
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	506	GOL	1	0
8	C	504	GOL	5	0
12	F	401	ACP	2	0
5	A	501	GTP	1	0
11	C	507	VLB	5	0
9	D	501	GDP	1	0
8	C	506	GOL	2	0
10	B	504	MES	4	0
8	C	505	GOL	5	0

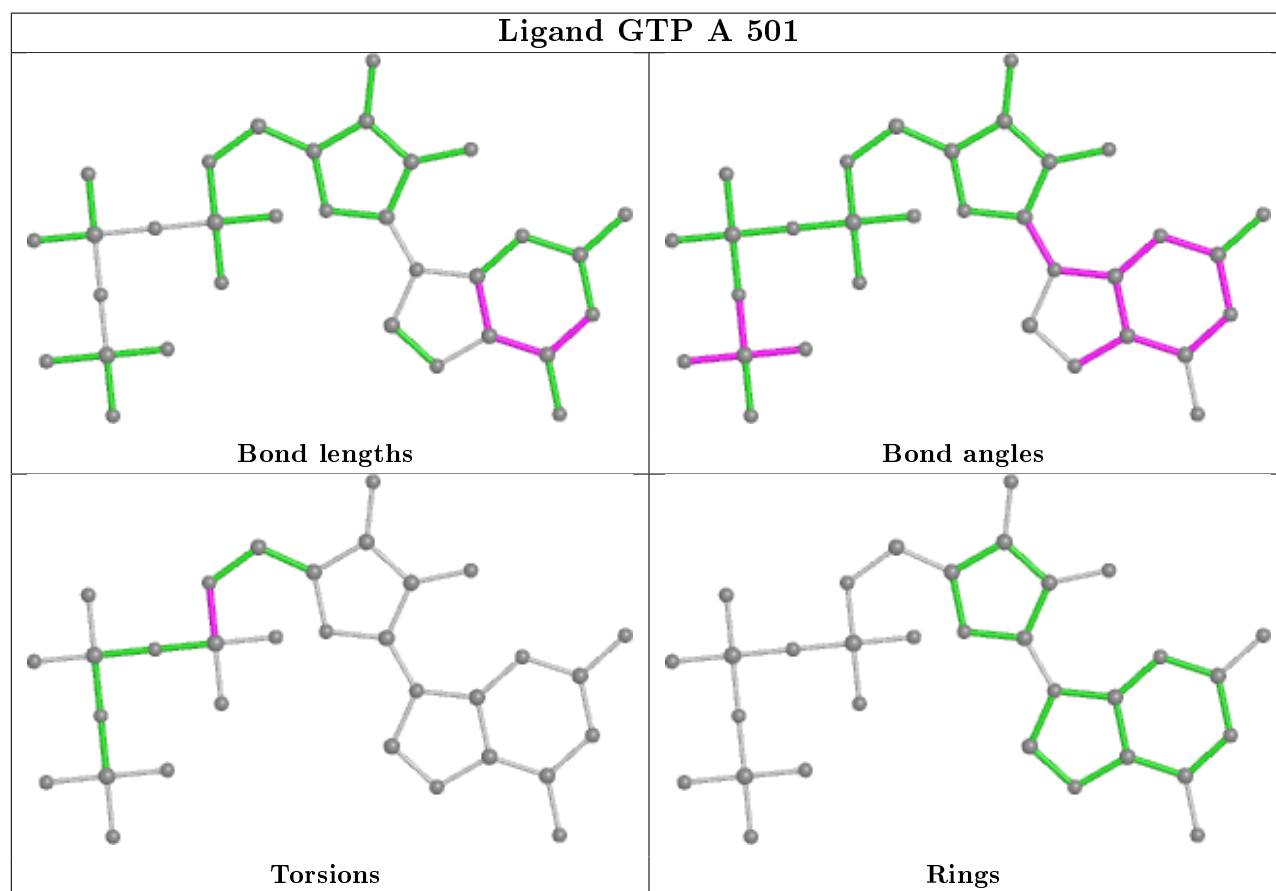
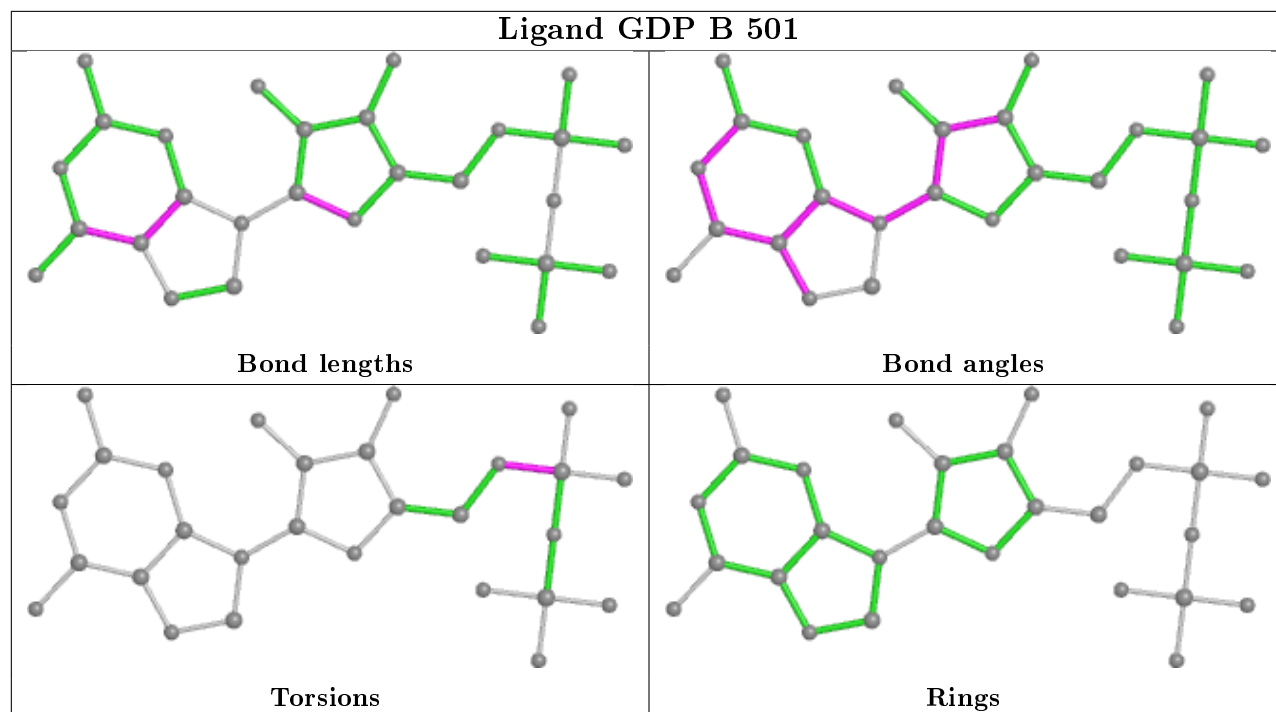
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 401

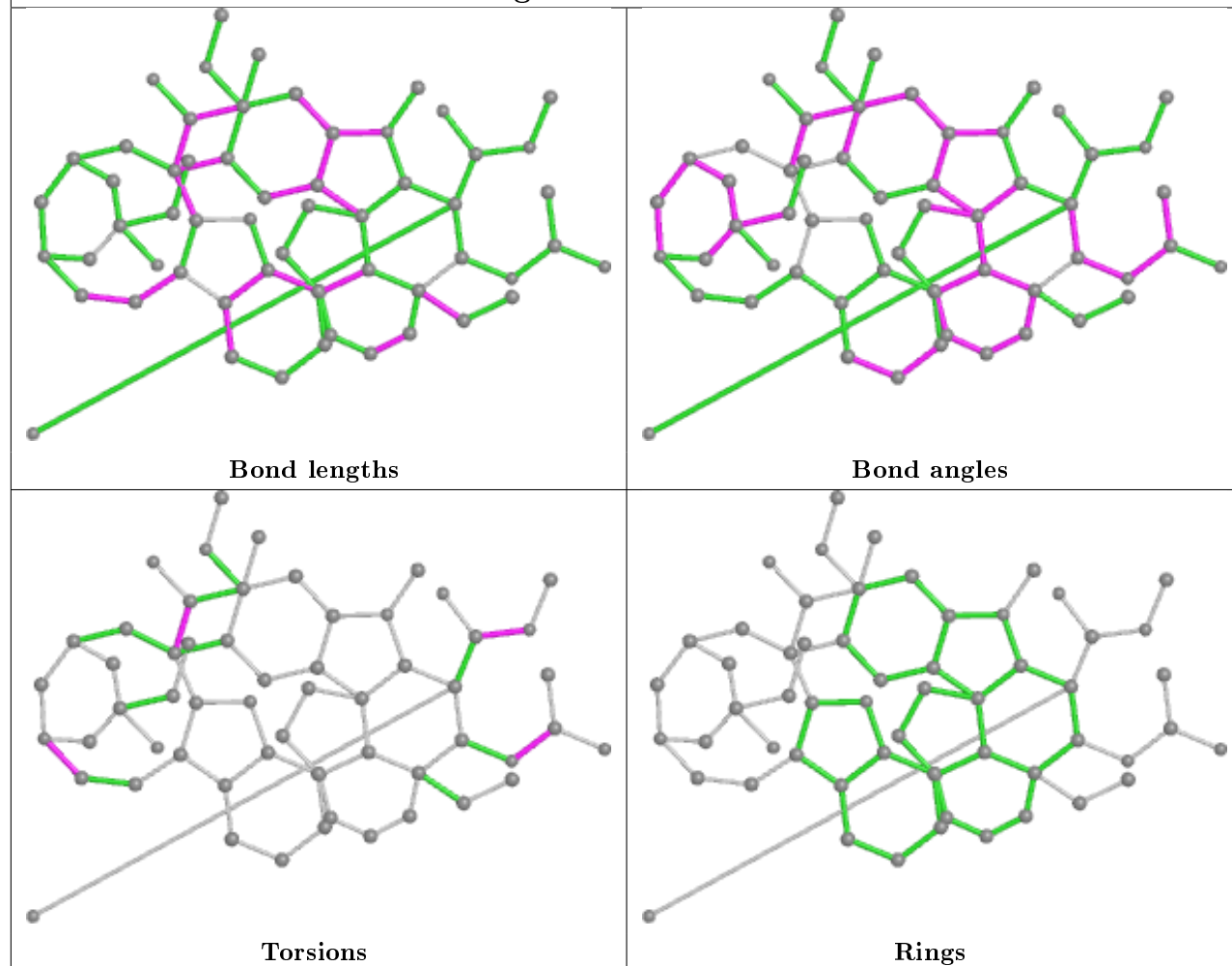


Ligand GTP C 501

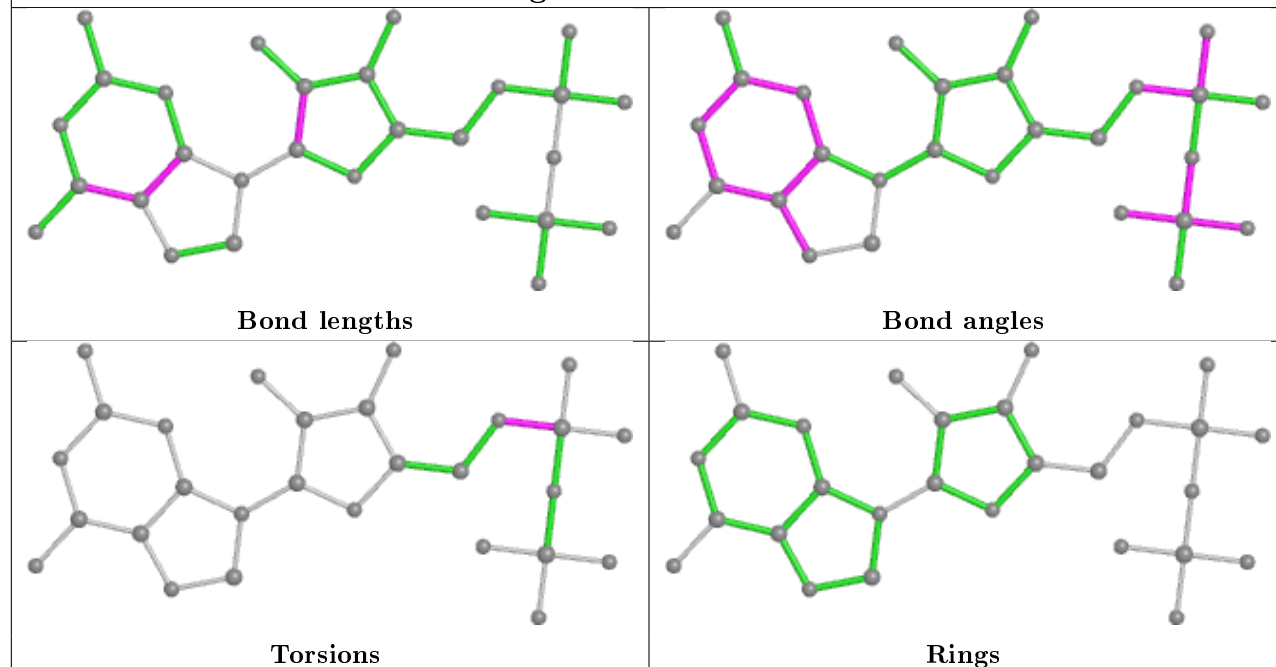




Ligand VLB C 507



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	439/451 (97%)	0.03	10 (2%) 60 63	26, 45, 74, 106	0
1	C	440/451 (97%)	-0.25	2 (0%) 91 91	24, 38, 66, 97	0
2	B	427/445 (95%)	-0.14	5 (1%) 79 80	24, 38, 75, 109	0
2	D	422/445 (94%)	0.23	29 (6%) 16 17	33, 58, 89, 111	0
3	E	123/143 (86%)	0.50	14 (11%) 5 4	35, 62, 101, 125	0
4	F	346/384 (90%)	0.49	50 (14%) 2 2	33, 68, 121, 136	0
All	All	2197/2319 (94%)	0.08	110 (5%) 28 30	24, 49, 95, 136	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	104	ASN	7.7
3	E	143	ALA	6.9
4	F	177	GLY	5.3
1	A	282	TYR	5.2
4	F	139	ARG	5.0
4	F	133	ALA	5.0
2	D	400	ARG	4.5
4	F	169	LEU	4.3
2	D	404	PHE	4.3
4	F	101	TYR	4.3
4	F	362	ALA	4.3
4	F	140	GLU	4.2
4	F	173	ILE	4.1
2	D	218	LYS	4.0
4	F	175	GLU	4.0
2	D	407	TRP	4.0
4	F	137	ARG	4.0
4	F	232	ASN	4.0
4	F	149	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	3.9
4	F	171	ASP	3.8
2	D	1	MET	3.7
4	F	100	ILE	3.7
1	A	438	ASP	3.7
2	D	37	HIS	3.6
1	A	439	SER	3.6
4	F	233	PHE	3.5
4	F	103	THR	3.5
4	F	372	THR	3.4
4	F	167	SER	3.4
4	F	172	PHE	3.4
1	A	281	ALA	3.3
4	F	176	GLN	3.2
3	E	139	LEU	3.2
1	C	440	VAL	3.2
2	B	59	ASN	3.2
1	A	262	TYR	3.1
2	B	281	GLN	3.1
4	F	381	HIS	3.1
4	F	234	GLN	3.1
4	F	235	ASP	3.1
3	E	140	LYS	3.1
4	F	178	GLN	3.0
4	F	361	LEU	3.0
2	D	401	ARG	3.0
2	B	1	MET	3.0
3	E	24	LEU	2.9
4	F	363	ASP	2.9
2	B	283	TYR	2.9
4	F	99	VAL	2.9
4	F	170	LEU	2.9
3	E	8	VAL	2.8
4	F	249	TYR	2.8
2	D	216	THR	2.7
3	E	27	PRO	2.7
2	D	94	PHE	2.7
3	E	28	SER	2.7
3	E	25	LYS	2.6
1	C	340	SER	2.6
2	D	276	THR	2.6
4	F	136	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	137	LEU	2.6
3	E	26	PRO	2.6
2	D	169	PHE	2.5
3	E	142	GLU	2.5
4	F	231	ALA	2.5
4	F	182	ILE	2.5
2	D	168	THR	2.5
4	F	141	GLY	2.5
4	F	161	LEU	2.5
2	D	201	THR	2.5
4	F	134	ALA	2.4
4	F	179	VAL	2.4
4	F	255	ARG	2.4
4	F	174	ASP	2.4
4	F	194	PRO	2.4
4	F	125	THR	2.4
2	D	147	SER	2.4
3	E	51	GLN	2.4
1	A	365	GLY	2.4
2	D	179	ASP	2.3
2	D	138	THR	2.3
3	E	23	ILE	2.3
1	A	235	VAL	2.3
2	D	217	LEU	2.3
2	B	56	ALA	2.3
2	D	220	THR	2.3
2	D	406	HIS	2.2
2	D	7	ILE	2.2
4	F	166	ALA	2.2
4	F	130	VAL	2.2
1	A	169	PHE	2.2
2	D	219	LEU	2.2
2	D	286	LEU	2.2
3	E	6	MET	2.2
4	F	9	GLU	2.2
2	D	399	PHE	2.2
4	F	25	GLY	2.2
4	F	384	HIS	2.2
3	E	141	GLU	2.2
4	F	143	GLU	2.2
2	D	57	ALA	2.1
2	D	397	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	202	PHE	2.1
2	D	139	HIS	2.1
1	A	346	TRP	2.1
2	D	441	ASP	2.0
4	F	22	LEU	2.0
4	F	145	ASN	2.0
2	D	369	ARG	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(Å ²)	Q<0.9
6	MG	B	502	1/1	0.54	0.33	74,74,74,74	0
8	GOL	C	505	6/6	0.63	0.67	81,96,107,130	0
8	GOL	A	504	6/6	0.76	0.22	70,74,80,86	0
8	GOL	A	506	6/6	0.80	0.29	56,64,70,71	0
8	GOL	C	504	6/6	0.84	0.35	55,69,70,72	0
8	GOL	B	506	6/6	0.84	0.23	80,84,88,88	0
6	MG	D	502	1/1	0.87	0.43	53,53,53,53	0
10	MES	B	504	12/12	0.91	0.17	53,63,74,82	0
8	GOL	A	505	6/6	0.92	0.13	61,65,68,69	0
12	ACP	F	401	31/31	0.92	0.14	72,85,113,115	0
8	GOL	C	506	6/6	0.93	0.21	49,62,65,74	0
10	MES	B	505	12/12	0.95	0.14	65,71,76,76	0
9	GDP	D	501	28/28	0.95	0.13	44,48,60,67	0
11	VLB	C	507	59/59	0.96	0.12	28,35,44,49	0
7	CA	B	503	1/1	0.98	0.07	76,76,76,76	0
6	MG	C	502	1/1	0.98	0.07	28,28,28,28	0

Continued on next page...

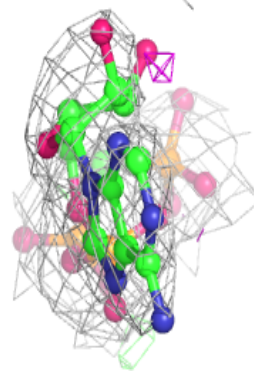
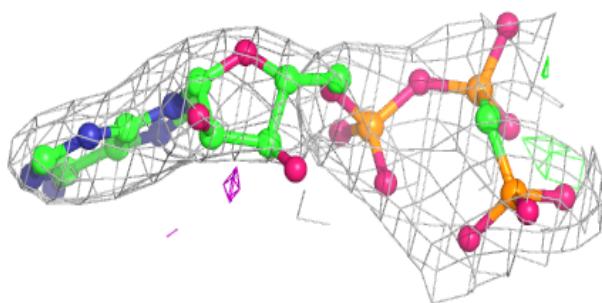
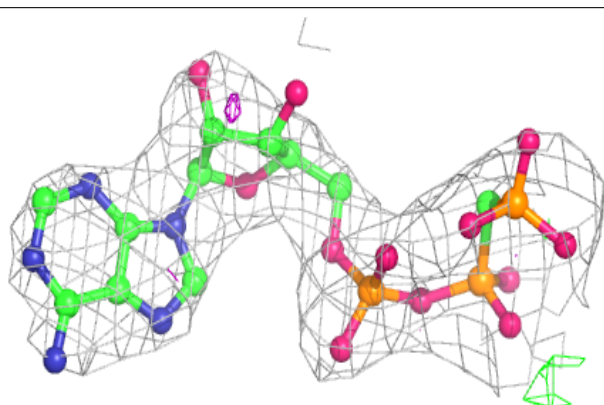
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	C	501	32/32	0.99	0.12	25,28,32,33	0
5	GTP	A	501	32/32	0.99	0.15	25,30,34,34	0
6	MG	A	502	1/1	0.99	0.07	36,36,36,36	0
9	GDP	B	501	28/28	0.99	0.14	23,26,28,29	0
7	CA	A	503	1/1	0.99	0.04	62,62,62,62	0
7	CA	C	503	1/1	0.99	0.02	49,49,49,49	0

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

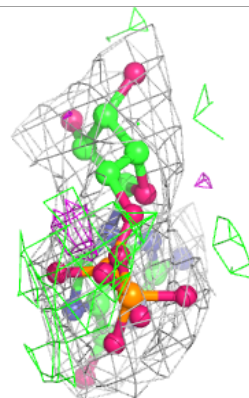
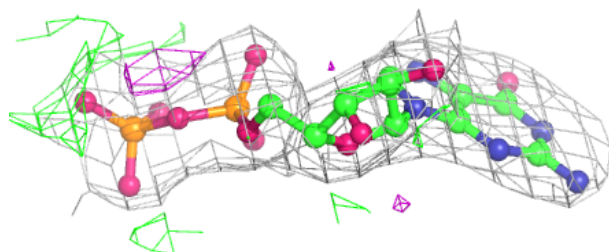
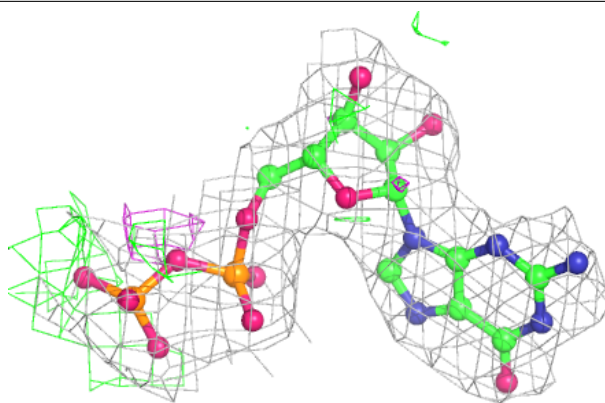
Electron density around ACP F 401:

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



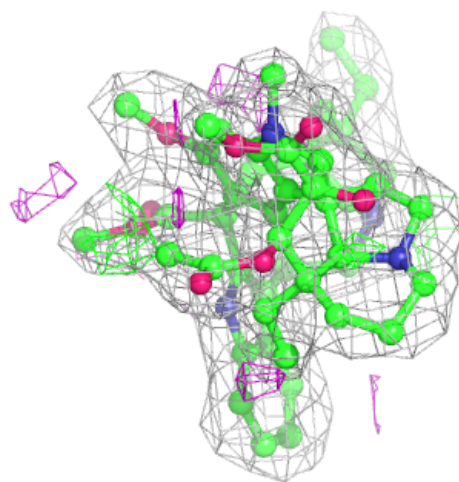
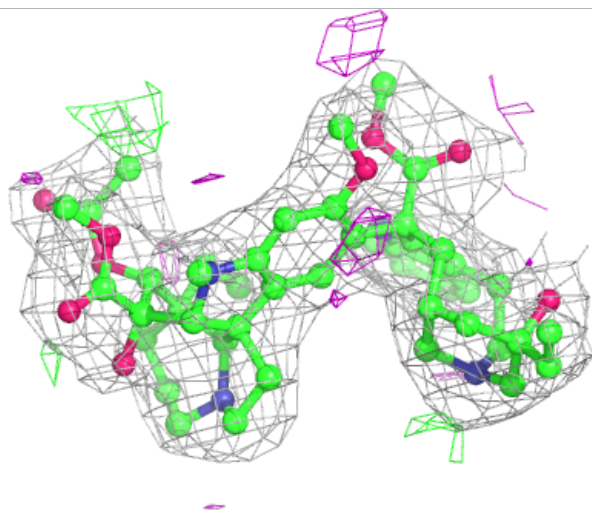
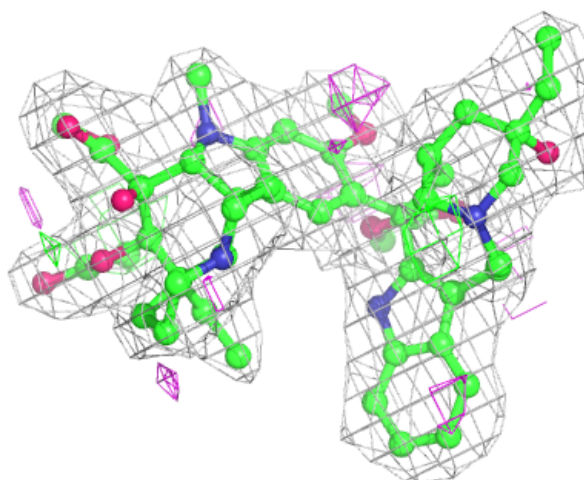
Electron density around GDP D 501:

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



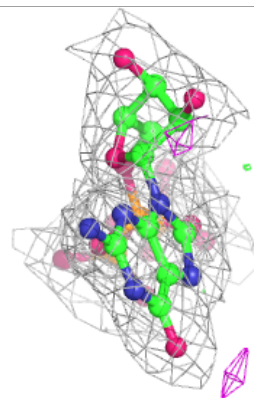
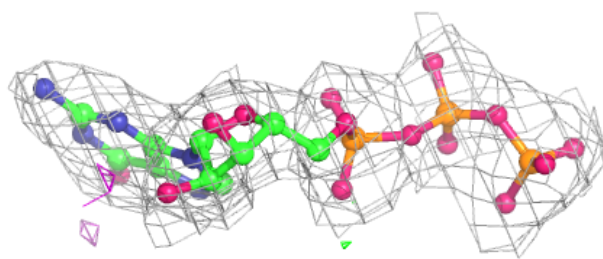
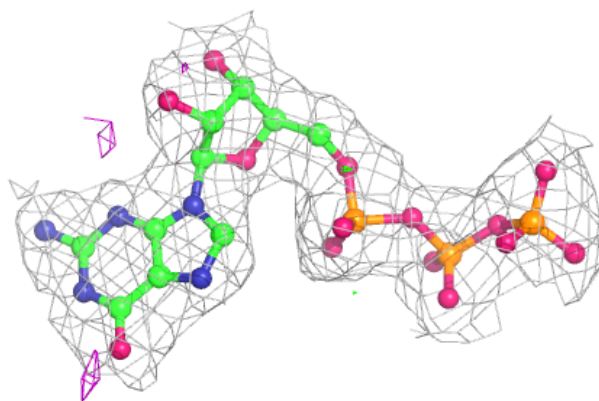
Electron density around VLB C 507:

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

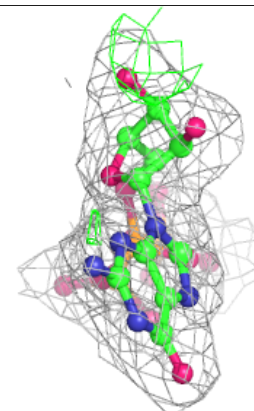
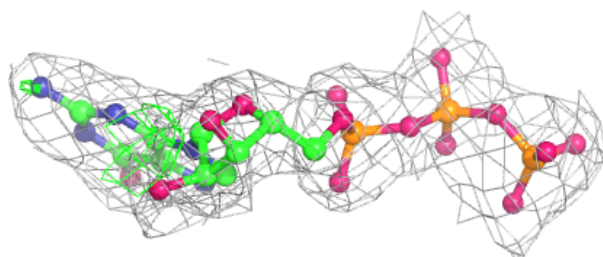
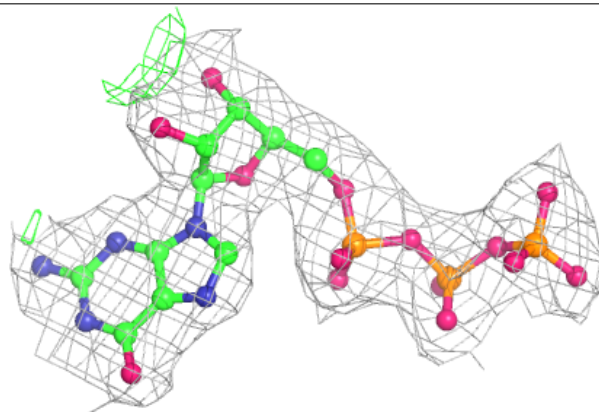


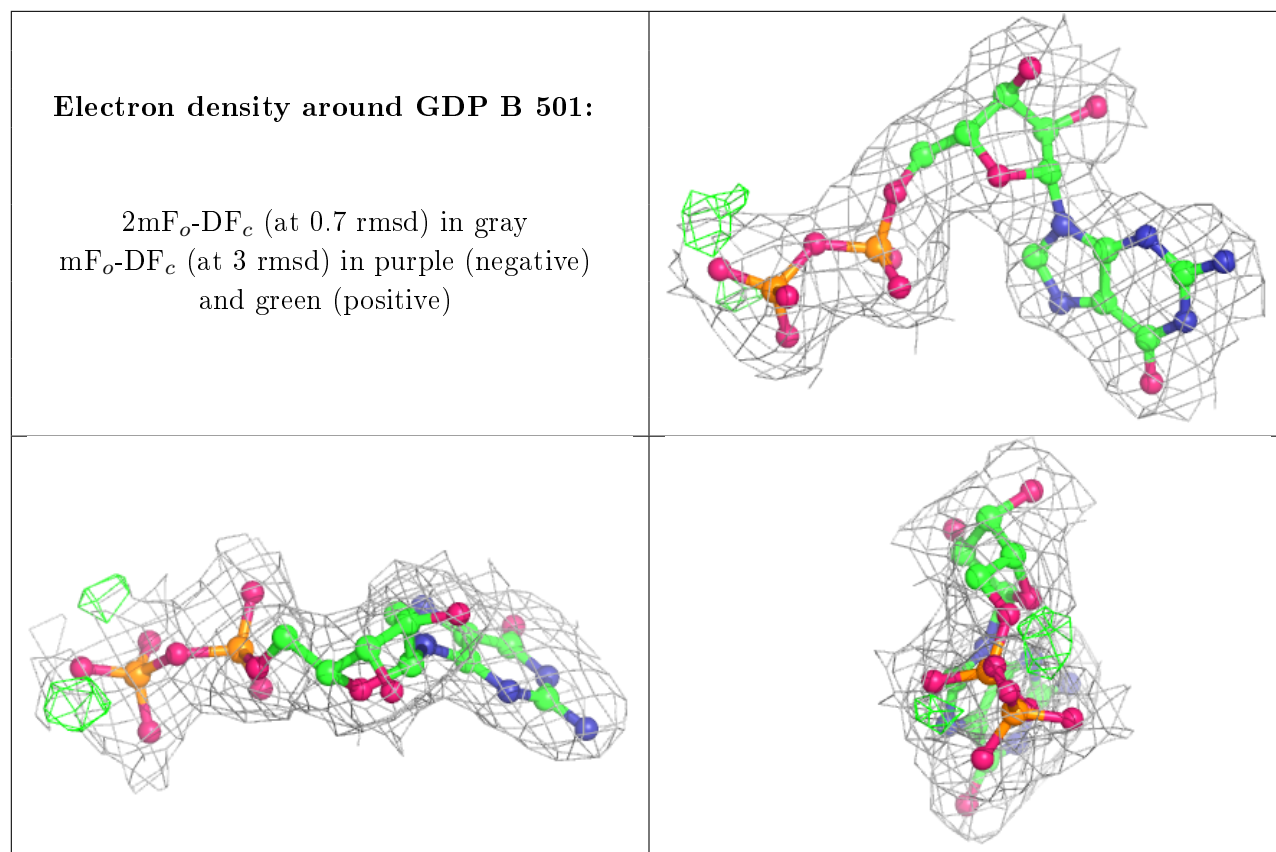
Electron density around GTP C 501:

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

**Electron density around GTP A 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.