



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:12 am BST

PDB ID : 6S9E
Title : Tubulin-GDP.AIF complex
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Deposited on : 2019-07-12
Resolution : 2.25 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

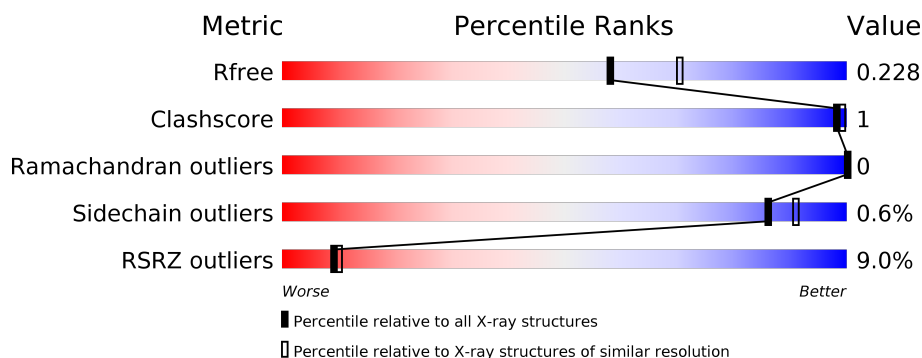
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	440	<div> <div>6%</div> <div> <div></div> <div>97%</div> <div>..</div> </div> </div>
1	C	440	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
2	D	445	<div> <div>9%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
3	E	189	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>37%</div> </div> </div>
4	F	378	<div> <div>22%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> </div>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 34744 atoms, of which 17043 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	435	Total	C	H	N	O	S	0	7	0
			6789	2172	3361	580	651	25			
1	C	440	Total	C	H	N	O	S	0	13	0
			6926	2216	3430	589	665	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	423	Total	C	H	N	O	S	0	8	0
			6627	2119	3258	573	651	26			
2	D	423	Total	C	H	N	O	S	0	6	0
			6591	2107	3238	567	651	28			

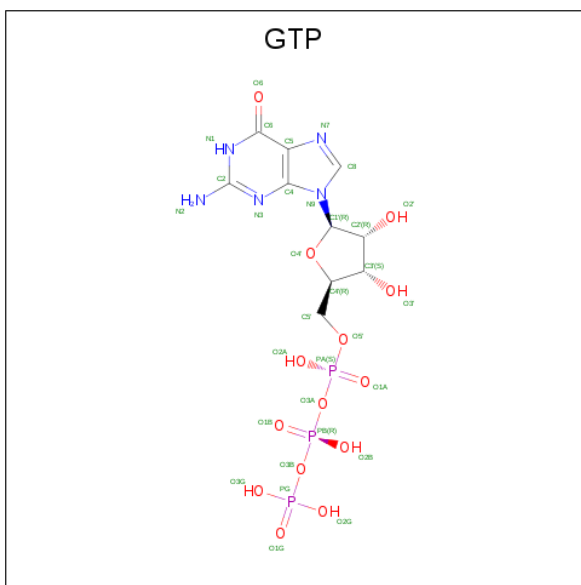
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	120	Total	C	H	N	O	S	0	5	0
			2064	631	1044	184	199	6			

- Molecule 4 is a protein called Tubulin Tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	319	Total	C	H	N	O	S	0	1	0
			5207	1686	2594	437	475	15			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			41	10	9	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		
6	F	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		

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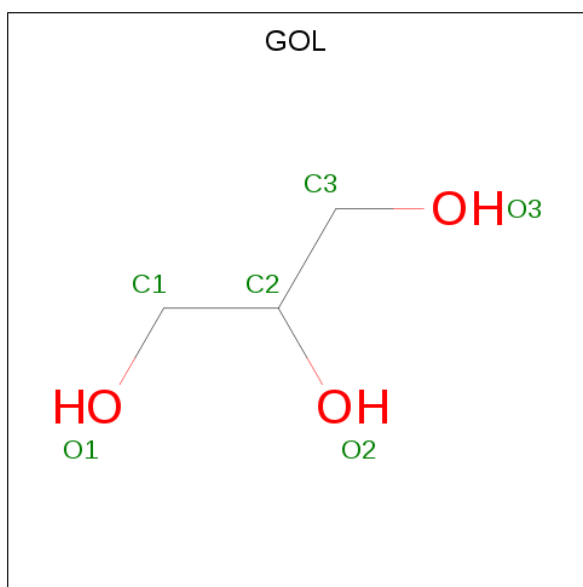
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

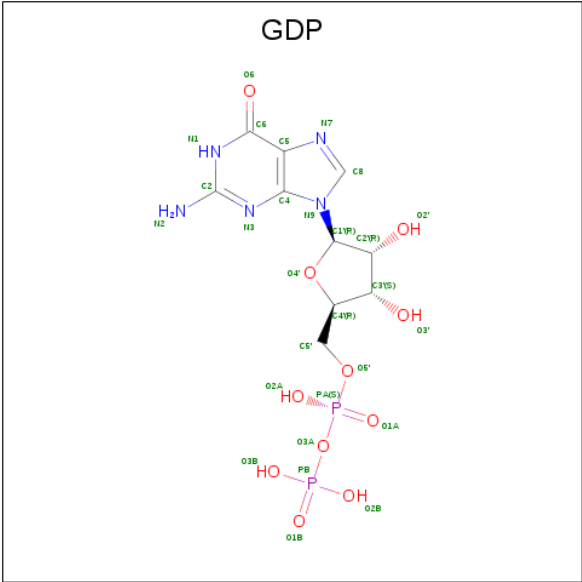
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



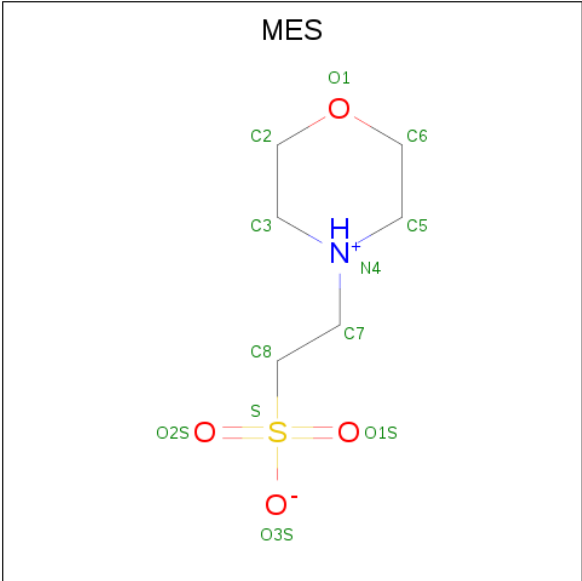
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			14	3	8	3		
9	A	1	Total	C	H	O	0	0
			14	3	8	3		
9	A	1	Total	C	H	O	0	0
			14	3	8	3		
9	B	1	Total	C	H	O	0	0
			12	3	6	3		
9	B	1	Total	C	H	O	0	0
			13	3	7	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	P	0	0
			37	10	9	5	11	2		
10	D	1	Total	C	H	N	O	P	0	0
			37	10	9	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



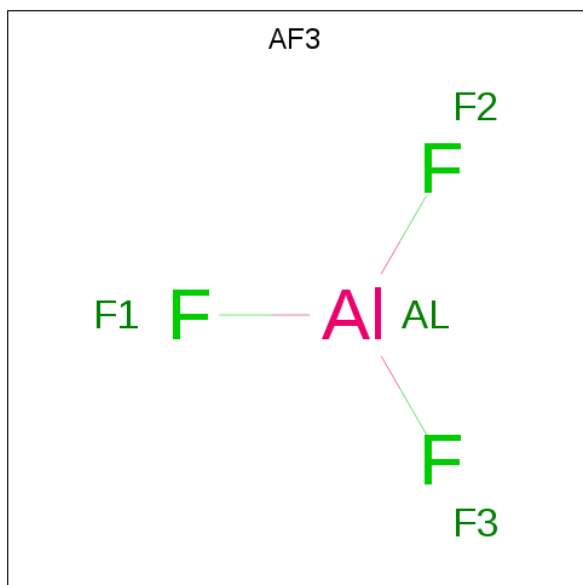
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

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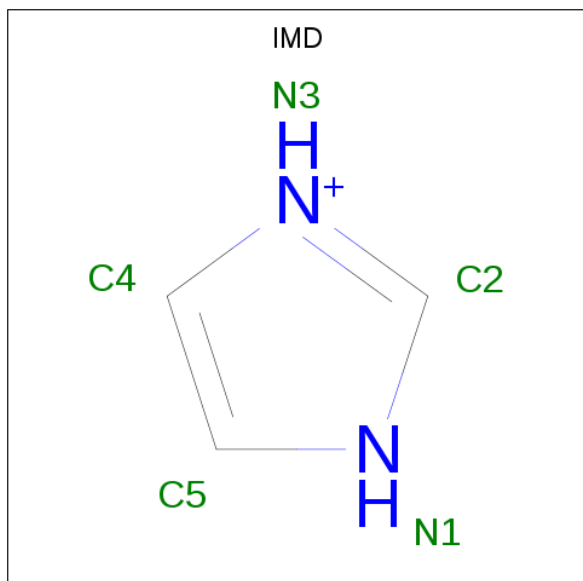
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 12 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by author).



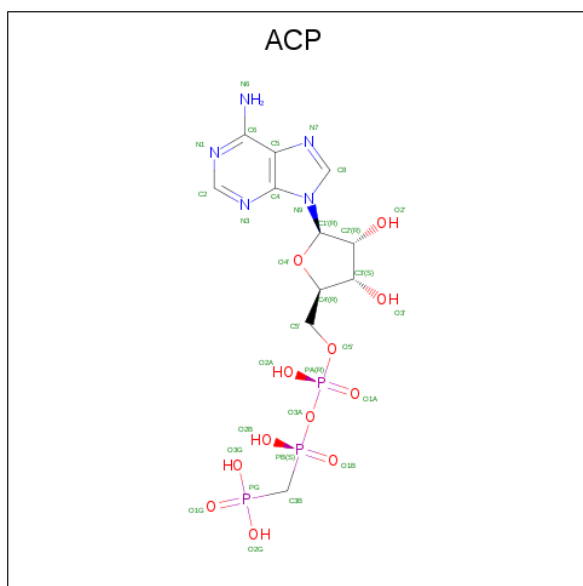
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Al	F	0	0
			4	1	3		

- Molecule 13 is IMIDAZOLE (three-letter code: IMD) (formula: $\text{C}_3\text{H}_5\text{N}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	H	N	0	0
			10	3	5	2		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

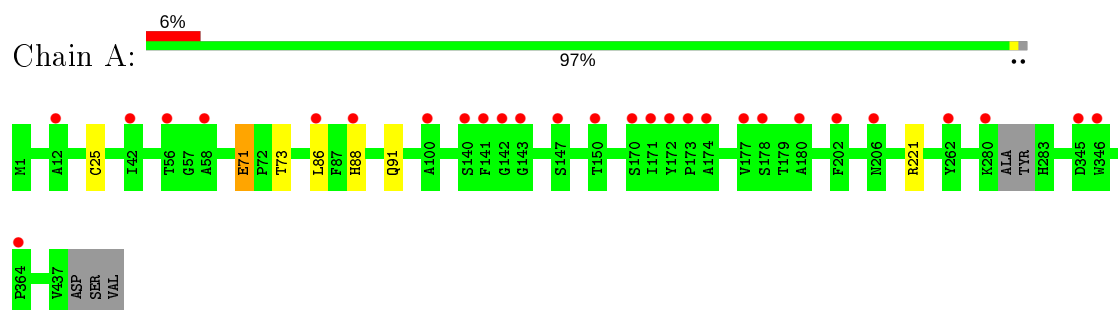
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	39	Total	O	0	0
			39	39		
15	B	40	Total	O	0	0
			40	40		
15	C	99	Total	O	0	0
			99	99		
15	D	14	Total	O	0	0
			14	14		
15	E	4	Total	O	0	0
			4	4		
15	F	3	Total	O	0	0
			3	3		

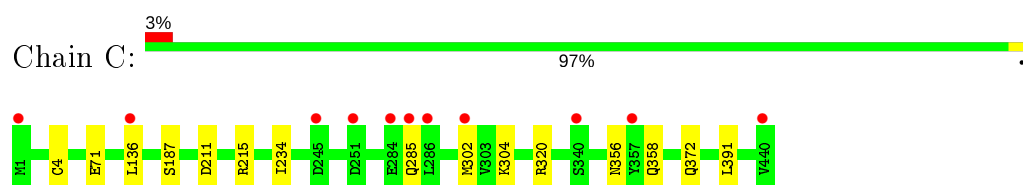
3 Residue-property plots [i](#)

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

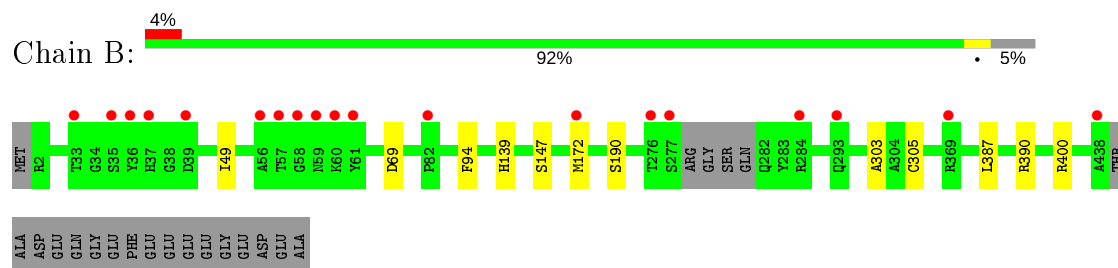
- Molecule 1: Tubulin alpha-1B chain



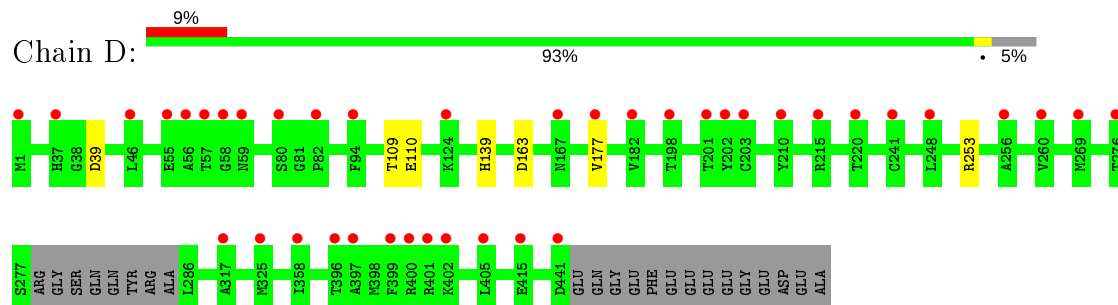
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain



- Molecule 2: Tubulin beta-2B chain



Chain E:

7% 63% 37%

Met Thr Leu Ala Tyr Lys Glu Lys Glu Pro Val Ser Leu Phe Cys Ser Cys Phe Leu Ser Asp Pro Leu Asn Lys Ser Ser Tyr Lys Tyr Glu Ala Asp Thr Val Asp Leu Asn Trp Cys Val Ile Ser Asp M6 E7 I23 L24 R25 P26 P27 Ser Phe Asn

Gly Val Pro Glu Phe Asn Ala Leu Leu Pro Arg Arg D44 P45 E46 E59 R80 E121 K128 I139 K140 E141 Glu Ala Ser Arg

Chain F:

22%

83%

16%

N229 N230 N231 A231 PHE Q234 D235 K236 T237 C238 H239 L240 T241 H242 K243 C244 L245 Q246 K247 E248 TYR SER LYS N252 Y253 G254 R255 Y256 E257 E258 G259 N260 F263 E331 Q340 K341 L342 Y343 A344 L361 A362 ASP THR GLN LYS THR SER GLN PRO THR S373 L378

ARG GLU ARG G144 N145 N146 N147 S149 A150 A151 LYS GLU GLY ILE LEU I162 S163 S164 A165 A166 S167 E168 L169 L170 D171 F172 Y173 ASP GLU GLN GLY G179 H190 V181 I182 Q183 L191 P194 R197 K198 F199 D200 Y211 T223 S224 S225 E226 P227 Y258

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.00 Å 157.36 Å 180.26 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.25 48.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.00-2.25) 98.8 (48.00-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.24 Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.203 , 0.228 0.203 , 0.228	Depositor DCC
R_{free} test set	6924 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.0	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	34744	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, IMD, CL, CA, GTP, ACP, MES, AF3

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	0.25	0/3525	0.42	0/4783
1	C	0.25	0/3614	0.43	0/4909
2	B	0.25	0/3474	0.43	0/4705
2	D	0.25	0/3439	0.42	0/4660
3	E	0.25	0/1043	0.35	0/1384
4	F	0.25	0/2672	0.40	0/3606
All	All	0.25	0/17767	0.42	0/24047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3428	3361	3360	3	0
1	C	3496	3430	3430	7	0
2	B	3369	3258	3249	5	0
2	D	3353	3238	3228	4	0
3	E	1020	1044	1048	1	0
4	F	2613	2594	2594	1	0
5	A	32	9	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	9	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	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	A	18	24	24	0	0
9	B	12	13	16	0	0
10	B	28	9	12	0	0
10	D	28	9	12	0	0
11	B	24	26	26	0	0
12	B	4	0	0	0	0
13	C	5	5	5	0	0
14	F	31	14	13	0	0
15	A	39	0	0	0	0
15	B	40	0	0	1	0
15	C	99	0	0	0	0
15	D	14	0	0	0	0
15	E	4	0	0	0	0
15	F	3	0	0	0	0
All	All	17701	17043	17041	21	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 1.

All (21) 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:147[A]:SER:HG	2:B:190:SER:HG	1.41	0.66
1:A:88:HIS:N	1:A:91:GLN:OE1	2.35	0.58
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.24	0.52
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.43	0.51
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.52	0.49
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.39	0.49
3:E:48:GLU:OE1	3:E:48:GLU:N	2.46	0.49
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.33	0.47
2:D:163:ASP:O	2:D:253:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.56	0.45
2:B:390:ARG:NH1	15:B:609:HOH:O	2.48	0.44
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.43
2:D:39:ASP:N	2:D:39:ASP:OD1	2.51	0.43
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.01	0.43
1:C:234:ILE:HD13	1:C:302[B]:MET:SD	2.60	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.20	0.42
2:B:303:ALA:O	2:B:305:CYS:N	2.49	0.42
2:B:172:MET:HG3	2:B:387:LEU:HD21	2.03	0.41
2:D:177:VAL:HG12	2:D:177:VAL:O	2.21	0.41
1:C:356[B]:ASN:ND2	1:C:358[B]:GLN:OE1	2.55	0.40

There are no symmetry-related clashes.

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	438/440 (100%)	431 (98%)	7 (2%)	0	100	100
1	C	451/440 (102%)	441 (98%)	10 (2%)	0	100	100
2	B	427/445 (96%)	417 (98%)	10 (2%)	0	100	100
2	D	425/445 (96%)	415 (98%)	10 (2%)	0	100	100
3	E	121/189 (64%)	120 (99%)	1 (1%)	0	100	100
4	F	304/378 (80%)	295 (97%)	9 (3%)	0	100	100
All	All	2166/2337 (93%)	2119 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	374/371 (101%)	372 (100%)	2 (0%)	88	92
1	C	384/371 (104%)	382 (100%)	2 (0%)	88	92
2	B	374/383 (98%)	371 (99%)	3 (1%)	81	88
2	D	372/383 (97%)	371 (100%)	1 (0%)	92	95
3	E	113/171 (66%)	113 (100%)	0	100	100
4	F	289/336 (86%)	285 (99%)	4 (1%)	67	76
All	All	1906/2015 (95%)	1894 (99%)	12 (1%)	86	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
2	B	49	ILE
2	B	139	HIS
2	B	400	ARG
1	C	71	GLU
1	C	215	ARG
2	D	139	HIS
4	F	172	PHE
4	F	183	GLN
4	F	211	TYR
4	F	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 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
9	GOL	A	506	-	5,5,5	0.89	0	5,5,5	0.99	0
12	AF3	B	507	6	0,3,3	0.00	-	-		
11	MES	B	505	-	12,12,12	2.29	1 (8%)	14,16,16	1.44	3 (21%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.81	7 (21%)
10	GDP	B	501	6	24,30,30	1.11	2 (8%)	31,47,47	2.01	8 (25%)
5	GTP	C	501	6	26,34,34	0.94	1 (3%)	33,54,54	1.75	6 (18%)
9	GOL	A	507	-	5,5,5	0.91	0	5,5,5	1.00	0
9	GOL	B	506	-	5,5,5	0.93	0	5,5,5	0.94	0
13	IMD	C	504	-	3,5,5	0.39	0	4,5,5	0.59	0
14	ACP	F	501	6	27,33,33	4.49	11 (40%)	32,52,52	1.86	5 (15%)
11	MES	B	504	-	12,12,12	2.23	1 (8%)	14,16,16	1.46	4 (28%)
9	GOL	A	505	-	5,5,5	0.90	0	5,5,5	0.99	0
9	GOL	B	508	-	5,5,5	0.92	0	5,5,5	0.93	0
10	GDP	D	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.95	8 (25%)

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
9	GOL	A	506	-	-	0/4/4/4	-
11	MES	B	505	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	GDP	B	501	6	-	4/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
9	GOL	A	507	-	-	0/4/4/4	-
9	GOL	B	506	-	-	1/4/4/4	-
13	IMD	C	504	-	-	-	0/1/1/1
14	ACP	F	501	6	-	3/15/38/38	0/3/3/3
11	MES	B	504	-	-	3/6/14/14	0/1/1/1
9	GOL	A	505	-	-	0/4/4/4	-
9	GOL	B	508	-	-	0/4/4/4	-
10	GDP	D	501	6	-	4/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	501	ACP	O4'-C1'	15.28	1.62	1.41
14	F	501	ACP	C2'-C1'	-13.13	1.33	1.53
11	B	505	MES	C8-S	-7.67	1.66	1.77
11	B	504	MES	C8-S	-7.46	1.66	1.77
14	F	501	ACP	O4'-C4'	-5.69	1.32	1.45
14	F	501	ACP	C6-N6	4.38	1.50	1.34
14	F	501	ACP	PB-O2B	-4.27	1.46	1.56
10	D	501	GDP	C6-C5	3.96	1.48	1.41
10	B	501	GDP	C6-C5	3.86	1.48	1.41
14	F	501	ACP	O3'-C3'	-3.50	1.34	1.43
14	F	501	ACP	PB-O3A	3.45	1.62	1.58
14	F	501	ACP	C2-N3	3.24	1.37	1.32
5	A	501	GTP	C6-N1	3.09	1.38	1.33
14	F	501	ACP	PA-O5'	2.96	1.71	1.59
5	C	501	GTP	C6-N1	2.96	1.38	1.33
10	D	501	GDP	C5-C4	2.41	1.47	1.40
10	B	501	GDP	C5-C4	2.27	1.46	1.40
14	F	501	ACP	PG-O2G	-2.26	1.49	1.54
14	F	501	ACP	C5-C4	-2.12	1.35	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	501	ACP	C5-C6-N6	5.86	129.25	120.35
14	F	501	ACP	N3-C2-N1	-5.60	119.93	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.53	119.84	127.22
5	C	501	GTP	N3-C2-N1	-5.45	119.95	127.22
10	B	501	GDP	C6-C5-C4	-5.00	116.02	120.80
10	B	501	GDP	C6-N1-C2	4.94	123.77	115.93
10	D	501	GDP	C2-N3-C4	4.56	120.56	115.36
10	D	501	GDP	C6-N1-C2	4.33	122.81	115.93
5	A	501	GTP	C2-N3-C4	4.26	120.23	115.36
10	D	501	GDP	C6-C5-C4	-4.23	116.76	120.80
10	B	501	GDP	C5-C6-N1	-4.12	117.79	123.43
10	B	501	GDP	C2-N3-C4	4.10	120.03	115.36
5	C	501	GTP	C2-N3-C4	4.03	119.95	115.36
10	D	501	GDP	C5-C6-N1	-3.96	118.02	123.43
10	B	501	GDP	N3-C2-N1	-3.87	122.07	127.22
14	F	501	ACP	N6-C6-N1	-3.58	111.14	118.57
10	D	501	GDP	N3-C2-N1	-3.49	122.57	127.22
5	C	501	GTP	PB-O3B-PG	-3.31	121.45	132.83
5	A	501	GTP	PA-O3A-PB	-3.13	122.07	132.83
5	A	501	GTP	PB-O3B-PG	-3.12	122.11	132.83
10	D	501	GDP	PA-O3A-PB	-3.10	122.20	132.83
5	C	501	GTP	C5-C6-N1	-3.08	119.22	123.43
5	A	501	GTP	C5-C6-N1	-3.08	119.22	123.43
14	F	501	ACP	C3'-C2'-C1'	3.00	105.49	100.98
5	C	501	GTP	C6-N1-C2	2.91	120.55	115.93
5	A	501	GTP	C6-N1-C2	2.81	120.39	115.93
11	B	504	MES	C5-N4-C3	2.80	115.12	108.83
10	B	501	GDP	PA-O3A-PB	-2.72	123.49	132.83
11	B	505	MES	C5-N4-C3	2.71	114.92	108.83
14	F	501	ACP	PA-O3A-PB	-2.61	124.30	132.56
11	B	504	MES	O1S-S-C8	2.38	109.78	106.92
10	D	501	GDP	C4-C5-N7	-2.35	106.94	109.40
10	D	501	GDP	C3'-C2'-C1'	2.33	104.49	100.98
5	C	501	GTP	PA-O3A-PB	-2.33	124.84	132.83
11	B	505	MES	O3S-S-C8	2.21	109.34	105.77
11	B	504	MES	O3S-S-C8	2.16	109.27	105.77
11	B	505	MES	O1S-S-C8	2.09	109.43	106.92
10	B	501	GDP	C1'-N9-C4	-2.08	122.99	126.64
10	B	501	GDP	C4-C5-N7	-2.07	107.24	109.40
11	B	504	MES	O2S-S-C8	2.05	109.38	106.92
5	A	501	GTP	N2-C2-N1	2.04	120.43	117.25

There are no chirality outliers.

All (30) torsion outliers are listed below:

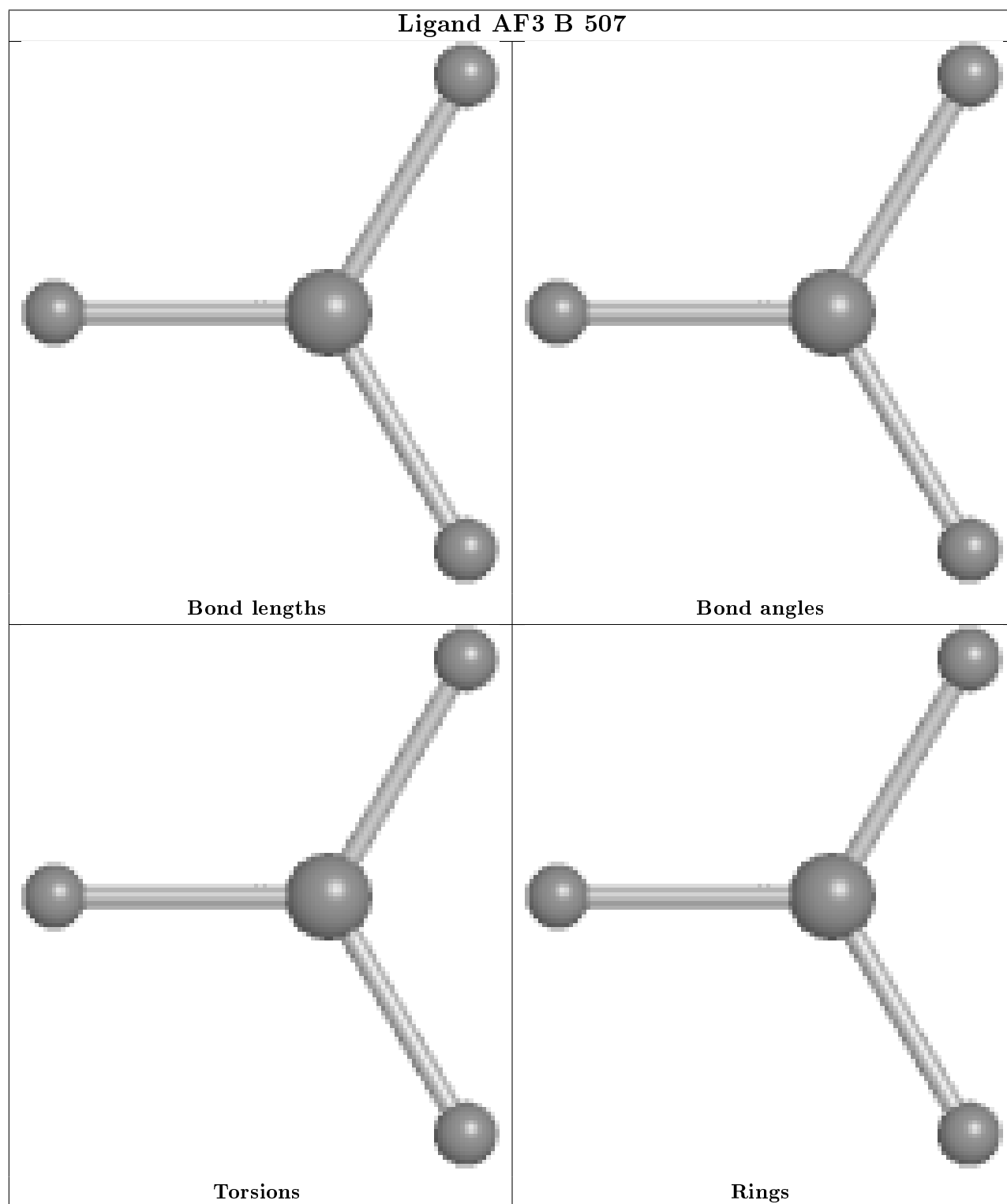
Mol	Chain	Res	Type	Atoms
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O2A
14	F	501	ACP	C5'-O5'-PA-O1A
14	F	501	ACP	O4'-C4'-C5'-O5'
9	B	506	GOL	O1-C1-C2-C3
11	B	504	MES	C8-C7-N4-C3
11	B	504	MES	C8-C7-N4-C5
10	B	501	GDP	PB-O3A-PA-O2A
11	B	505	MES	C8-C7-N4-C5
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
10	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O3A
14	F	501	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C4'-C5'-O5'-PA
10	D	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
11	B	504	MES	C7-C8-S-O1S

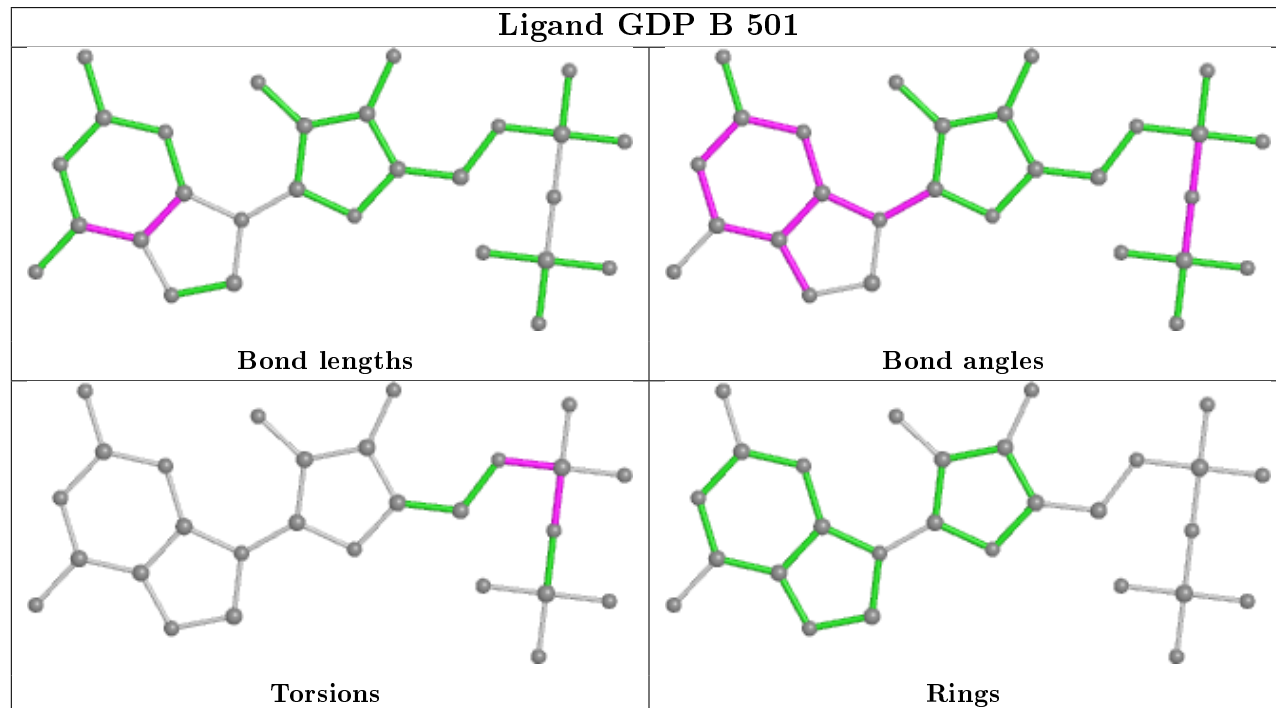
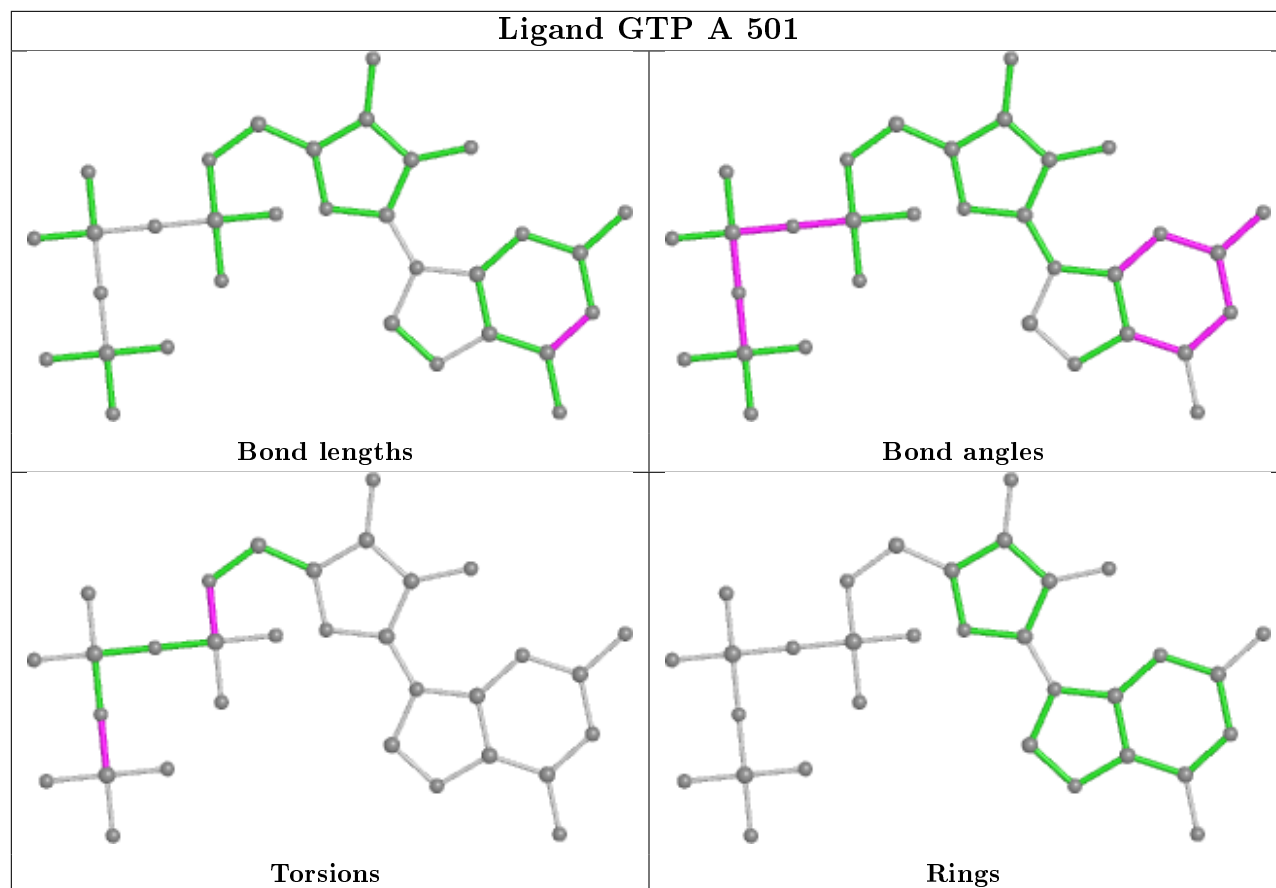
There are no ring outliers.

No monomer is involved in short contacts.

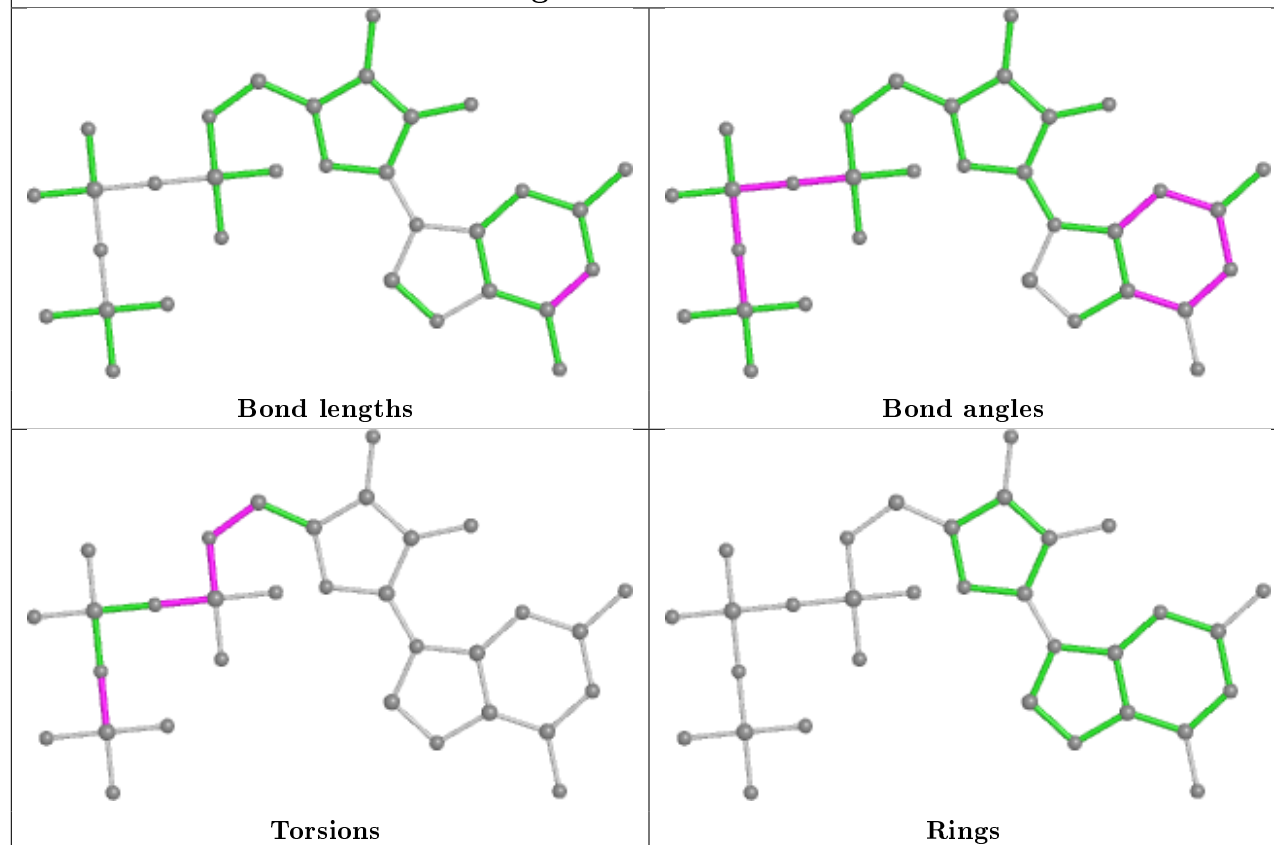
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

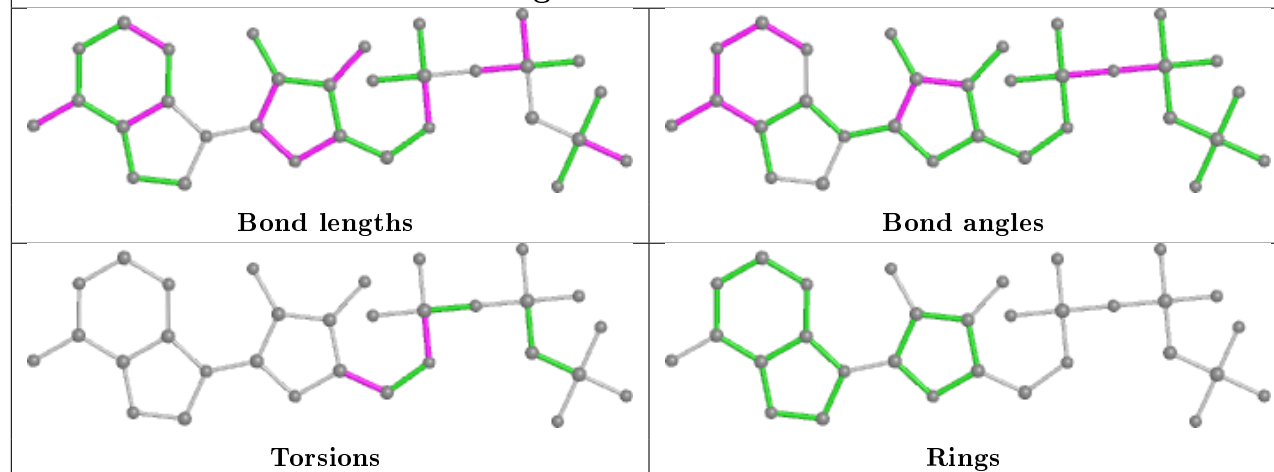


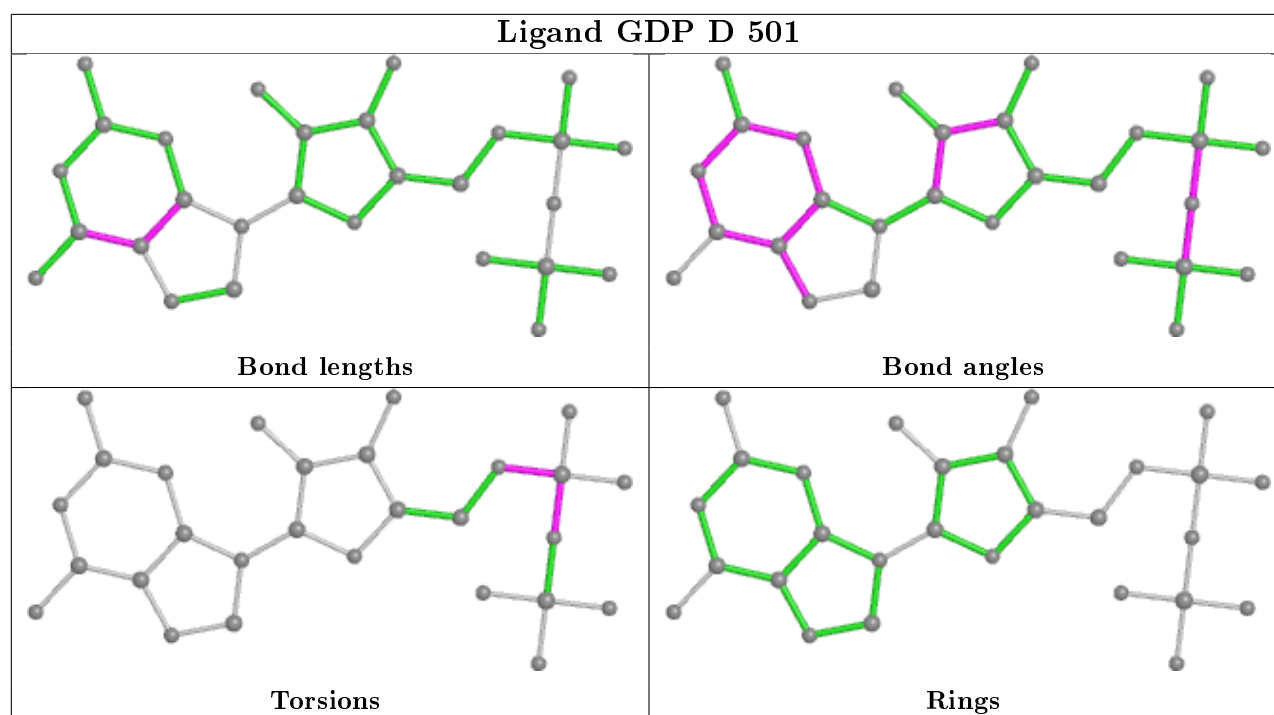


Ligand GTP C 501



Ligand ACP F 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	435/440 (98%)	0.55	28 (6%)	19 21	41, 58, 90, 120	0
1	C	440/440 (100%)	0.32	11 (2%)	57 60	34, 46, 70, 109	0
2	B	423/445 (95%)	0.46	19 (4%)	33 36	34, 55, 89, 122	2 (0%)
2	D	423/445 (95%)	0.60	40 (9%)	8 8	42, 64, 99, 131	5 (1%)
3	E	120/189 (63%)	0.65	13 (10%)	5 5	45, 70, 102, 120	0
4	F	319/378 (84%)	1.18	84 (26%)	0 0	49, 78, 130, 151	0
All	All	2160/2337 (92%)	0.59	195 (9%)	9 10	34, 60, 102, 151	7 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	9.4
4	F	130	VAL	8.3
4	F	253	TYR	7.0
4	F	131	PHE	6.8
4	F	244	CYS	6.8
4	F	169	LEU	6.5
2	B	57	THR	6.3
4	F	240	LEU	6.2
2	B	59	ASN	5.9
2	D	57	THR	5.9
4	F	135	TYR	5.8
4	F	234	GLN	5.7
4	F	133	ALA	5.7
1	A	262	TYR	5.7
4	F	170	LEU	5.7
4	F	100	ILE	5.6
3	E	26	PRO	5.6
4	F	129	GLU	5.5
2	D	400	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
4	F	134	ALA	5.3
4	F	101	TYR	5.2
2	D	1	MET	5.1
4	F	225	SER	4.8
2	B	284	ARG	4.8
4	F	256	TYR	4.7
4	F	182	ILE	4.7
4	F	247	LYS	4.7
4	F	223	THR	4.4
3	E	27	PRO	4.4
4	F	236	LYS	4.3
4	F	166	ALA	4.3
4	F	252	ASN	4.3
1	C	1	MET	4.3
2	D	37	HIS	4.2
4	F	167	SER	4.2
4	F	173	ILE	4.2
2	D	401	ARG	4.2
4	F	361	LEU	4.2
2	B	56	ALA	4.2
3	E	25	LYS	4.1
4	F	165	GLU	4.1
1	C	340	SER	4.1
4	F	254	GLY	4.1
4	F	128	ARG	4.0
4	F	243	HIS	4.0
4	F	242	ASN	4.0
4	F	340	GLN	3.9
4	F	259	GLY	3.9
4	F	163	SER	3.9
2	B	37	HIS	3.9
4	F	246	GLN	3.8
3	E	24	LEU	3.8
1	C	357	TYR	3.7
2	D	415	GLU	3.7
2	B	438	ALA	3.7
4	F	230	SER	3.7
3	E	45	PRO	3.7
4	F	248	GLU	3.7
2	D	405	LEU	3.6
4	F	19	ARG	3.6
2	B	277	SER	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	245	ILE	3.6
4	F	258	GLU	3.5
1	A	346	TRP	3.5
2	B	58	GLY	3.5
3	E	23	ILE	3.4
4	F	25	GLY	3.3
4	F	102	PRO	3.3
4	F	194	PRO	3.3
2	B	293	GLN	3.3
4	F	17	VAL	3.3
4	F	255	ARG	3.3
4	F	191	LEU	3.3
1	A	364	PRO	3.2
1	A	56	THR	3.2
2	B	36	TYR	3.2
2	B	82	PRO	3.2
4	F	20	LEU	3.1
4	F	126	ASP	3.1
4	F	147	TRP	3.1
1	C	440	VAL	3.1
1	C	284	GLU	3.1
2	D	59	ASN	3.1
4	F	227	PRO	3.1
1	A	171	ILE	3.1
1	A	42	ILE	3.0
4	F	21	LEU	3.0
1	A	172	TYR	3.0
4	F	22	LEU	3.0
4	F	362	ALA	2.9
4	F	27	TRP	2.9
2	D	399	PHE	2.9
4	F	241	THR	2.9
2	D	58	GLY	2.9
3	E	80	ARG	2.9
4	F	24	THR	2.9
2	D	94	PHE	2.9
2	D	441	ASP	2.8
4	F	26	GLN	2.8
4	F	172	PHE	2.8
2	D	202	TYR	2.8
2	D	177	VAL	2.7
1	A	178	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	241	CYS	2.7
2	D	124	LYS	2.7
4	F	127	GLU	2.7
2	B	39	ASP	2.7
4	F	179	VAL	2.7
4	F	144	GLY	2.7
2	D	80	SER	2.7
1	A	86	LEU	2.7
4	F	46	ARG	2.7
1	A	170	SER	2.6
2	D	56	ALA	2.6
1	C	251	ASP	2.6
2	D	276	THR	2.6
1	C	285	GLN	2.6
2	B	60	LYS	2.6
4	F	168	GLU	2.6
4	F	164	SER	2.6
1	C	286	LEU	2.6
1	A	345	ASP	2.5
1	A	140	SER	2.5
2	D	203	CYS	2.5
3	E	7	GLU	2.5
1	A	177	VAL	2.5
4	F	224	SER	2.5
1	A	174	ALA	2.5
1	A	173	PRO	2.5
4	F	229	ASN	2.5
2	D	248	LEU	2.5
4	F	197	ARG	2.5
1	A	88	HIS	2.5
2	B	61	TYR	2.4
3	E	139	LEU	2.4
4	F	228	TYR	2.4
2	D	167	ASN	2.4
4	F	239	HIS	2.4
1	C	245	ASP	2.4
4	F	99	VAL	2.4
2	D	256	ALA	2.4
1	C	302[A]	MET	2.4
1	A	141	PHE	2.4
2	D	182	VAL	2.4
2	D	402	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	2.3
2	D	46	LEU	2.3
4	F	9	GLU	2.3
3	E	48	GLU	2.3
2	D	82	PRO	2.3
4	F	145	ASN	2.3
2	D	220	THR	2.3
1	A	142	GLY	2.3
4	F	344	ALA	2.3
4	F	263	PHE	2.3
2	D	397	ALA	2.3
4	F	31	ARG	2.2
2	B	33	THR	2.2
2	D	317	ALA	2.2
2	D	396	THR	2.2
4	F	237	THR	2.2
1	A	150	THR	2.2
2	D	201	THR	2.2
4	F	23	ALA	2.2
1	C	136	LEU	2.2
4	F	199	PHE	2.2
4	F	260	ASN	2.2
2	B	276	THR	2.2
4	F	231	ALA	2.2
2	D	325	MET	2.2
3	E	128	LYS	2.1
4	F	162	ILE	2.1
2	D	269[A]	MET	2.1
1	A	58	ALA	2.1
1	A	280	LYS	2.1
2	D	215	ARG	2.1
4	F	342	LEU	2.1
2	B	172	MET	2.1
1	A	202	PHE	2.1
2	D	210	TYR	2.1
4	F	180	HIS	2.1
1	A	147	SER	2.1
2	D	198	THR	2.0
2	B	369	ARG	2.0
4	F	341	LYS	2.0
2	D	358	ILE	2.0
1	A	206	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	E	59	GLU	2.0
1	A	143	GLY	2.0
1	A	180	ALA	2.0
2	D	260	VAL	2.0
2	D	55	GLU	2.0
3	E	121	GLU	2.0
2	B	35	SER	2.0
1	A	100	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
9	GOL	B	508	6/6	0.75	0.19	64,76,88,93	0
6	MG	D	502	1/1	0.79	0.12	62,62,62,62	0
9	GOL	B	506	6/6	0.83	0.15	83,100,117,117	0
7	CA	A	503	1/1	0.86	0.05	71,71,71,71	0
6	MG	F	502	1/1	0.86	0.11	91,91,91,91	0
9	GOL	A	506	6/6	0.87	0.19	59,80,99,107	0
13	IMD	C	504	5/5	0.88	0.17	54,66,80,87	0
14	ACP	F	501	31/31	0.89	0.12	72,92,118,138	0
6	MG	A	502	1/1	0.90	0.21	38,38,38,38	0
8	CL	A	504	1/1	0.90	0.08	67,67,67,67	0
12	AF3	B	507	4/4	0.90	0.32	63,71,78,95	4
7	CA	B	503	1/1	0.90	0.08	79,79,79,79	0
9	GOL	A	505	6/6	0.91	0.12	68,86,103,103	0
11	MES	B	505	12/12	0.91	0.21	80,99,118,118	0
7	CA	C	503	1/1	0.92	0.06	58,58,58,58	0

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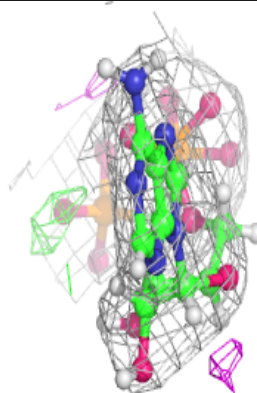
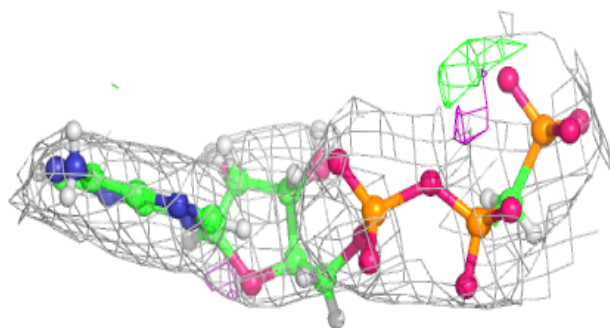
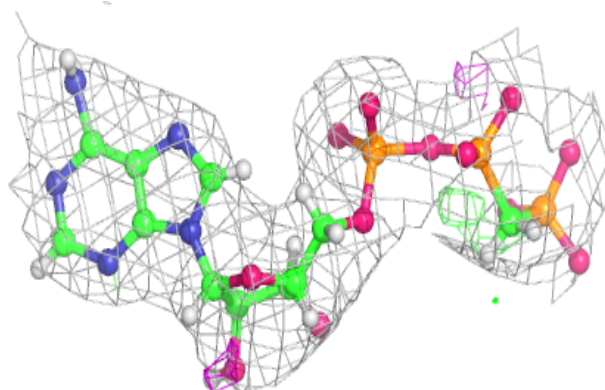
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	502	1/1	0.93	0.16	32,32,32,32	0
9	GOL	A	507	6/6	0.94	0.14	55,70,84,84	14
11	MES	B	504	12/12	0.94	0.17	46,62,70,76	25
10	GDP	D	501	28/28	0.95	0.13	46,59,75,81	0
6	MG	B	502	1/1	0.96	0.18	34,34,34,34	0
5	GTP	A	501	32/32	0.98	0.24	31,42,53,56	0
10	GDP	B	501	28/28	0.98	0.20	28,39,54,55	0
5	GTP	C	501	32/32	0.98	0.18	29,36,45,48	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.

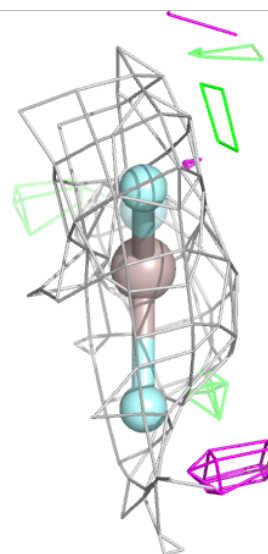
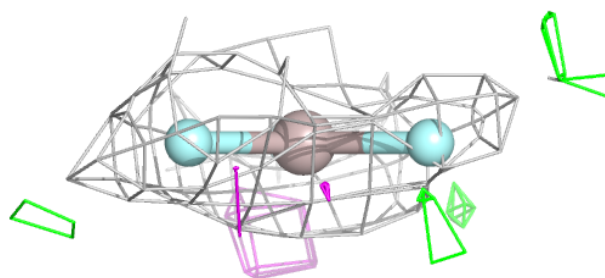
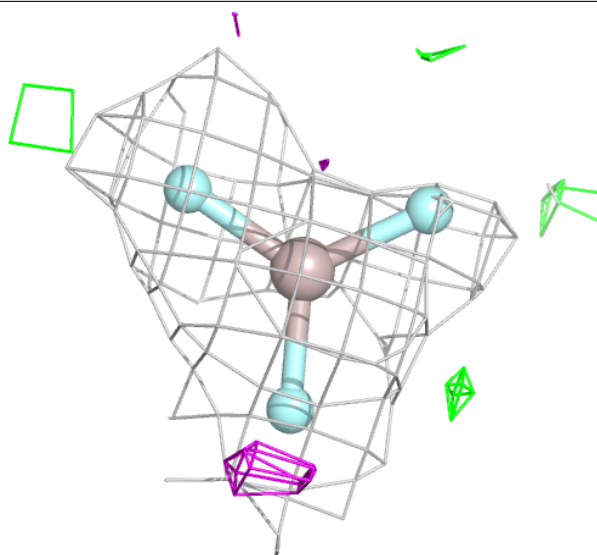
Electron density around ACP F 501:

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



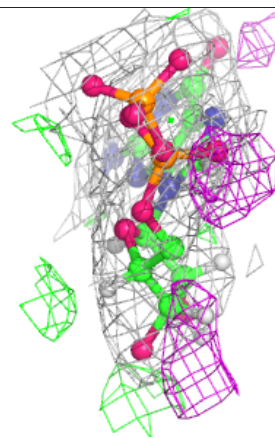
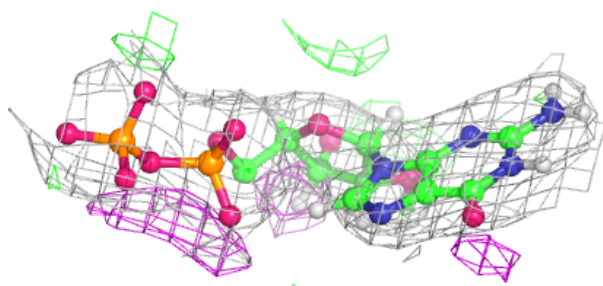
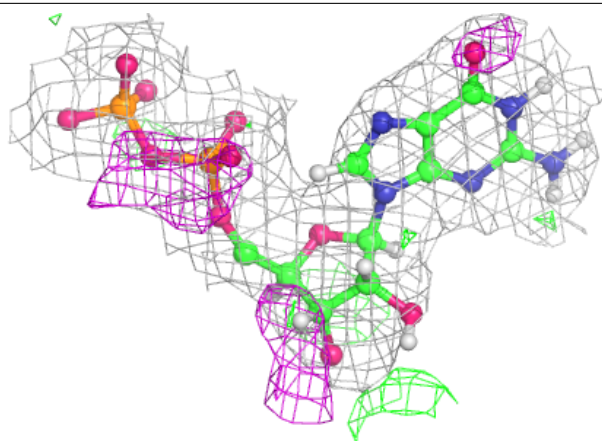
Electron density around AF3 B 507:

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

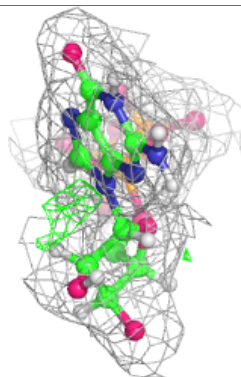
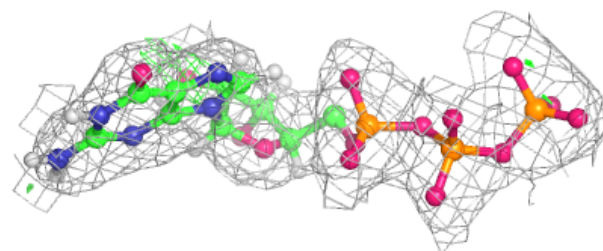
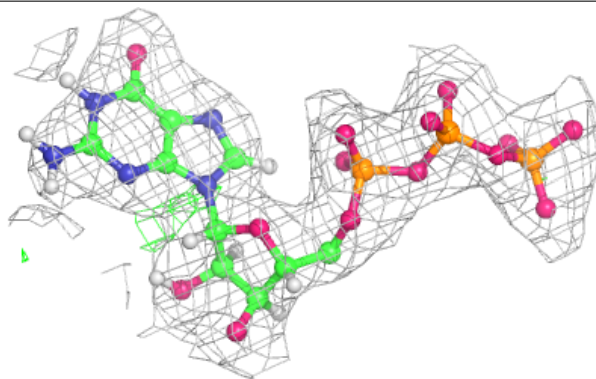


Electron density around GDP D 501:

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

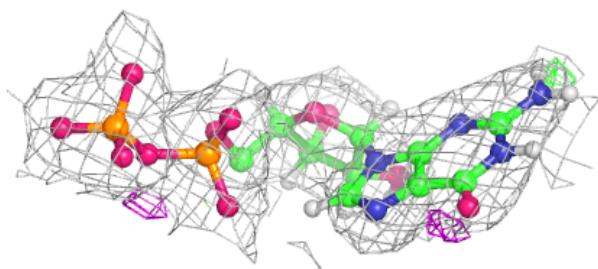
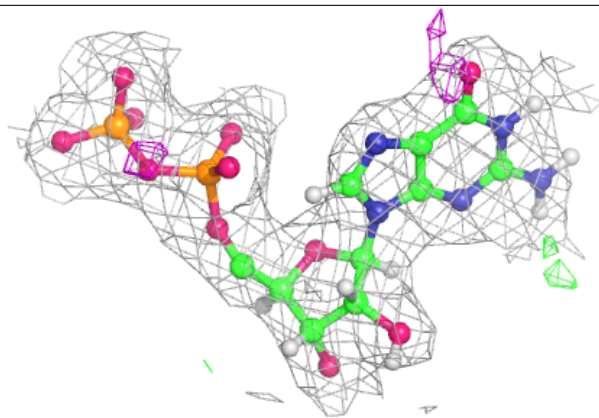
**Electron density around GTP A 501:**

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

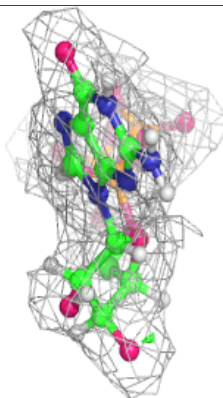
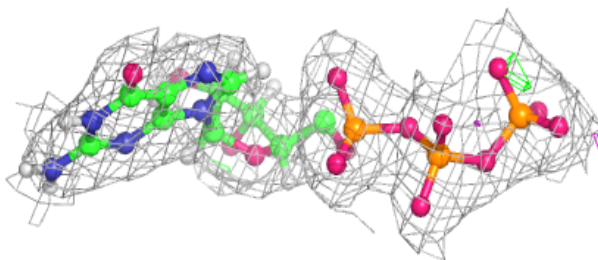
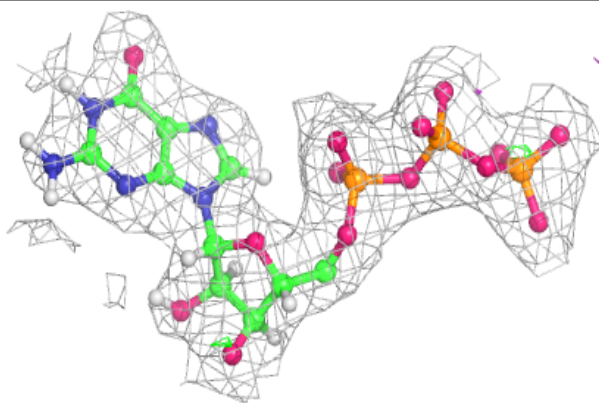


Electron density around GDP B 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.