



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:13 AM UTC

PDB ID : 9MLF / pdb_00009mlf
Title : TUBULIN-RB3_SLD IN COMPLEX WITH COMPOUND QW-4-183-llb
Authors : Miller, D.J.
Deposited on : 2024-12-19
Resolution : 2.40 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

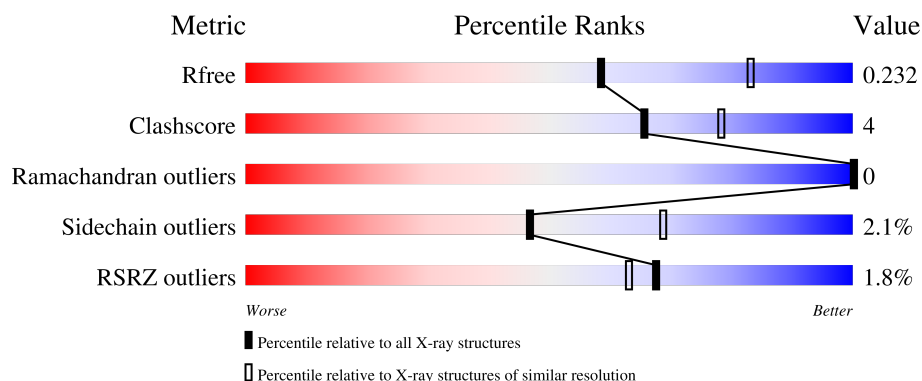
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	438	% 87% 9% .
1	C	438	2% 86% 10% ..
2	B	433	2% 88% 10% .
2	D	433	3% 85% 14% ..
3	E	143	% 83% 14%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14678 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	423	Total	C	N	O	S	0	0	0
			3290	2085	556	627	22			
1	C	424	Total	C	N	O	S	0	0	0
			3303	2092	560	629	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3304	2076	564	638	26			
2	D	430	Total	C	N	O	S	0	0	0
			3359	2107	577	648	27			

- 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
			1001	620	180	197	4			

There are 4 discrepancies between the modelled and reference sequences:

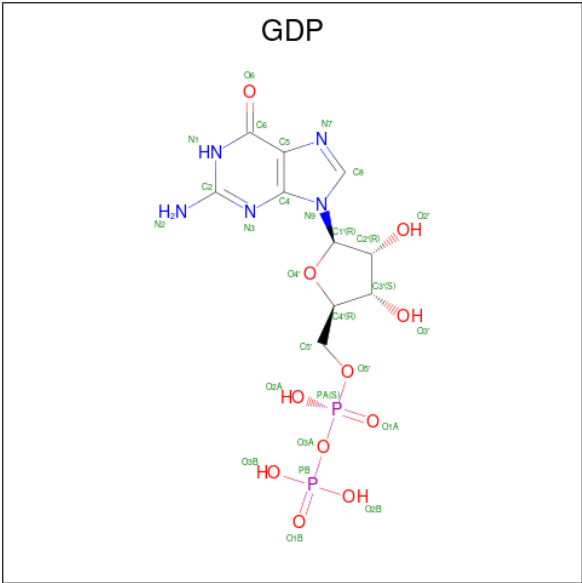
Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	conflict	UNP P63043
E	20	TRP	PHE	conflict	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



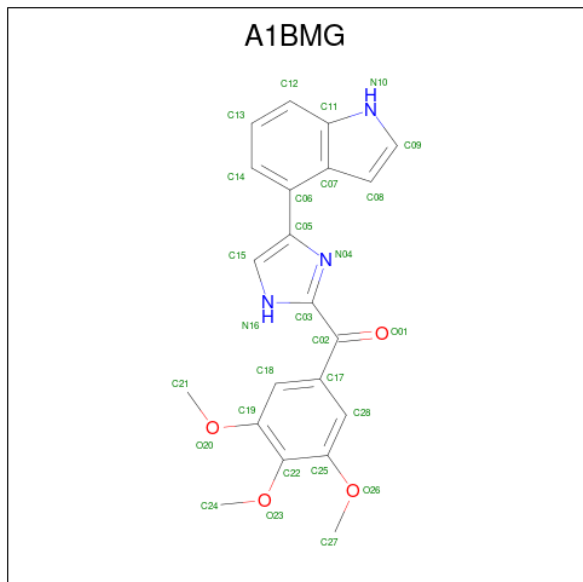
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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



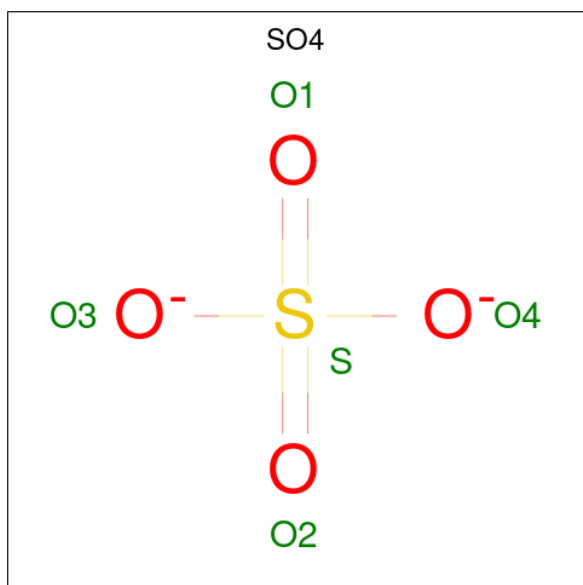
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
5	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is [(4M)-4-(1H-indol-4-yl)-1H-imidazol-2-yl](3,4,5-trimethoxyphenyl)methanone (CCD ID: A1BMG) (formula: C₂₁H₁₉N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			28	21	3	4		
6	D	1	Total	C	N	O	0	0
			28	21	3	4		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg	0	0
			1	1		

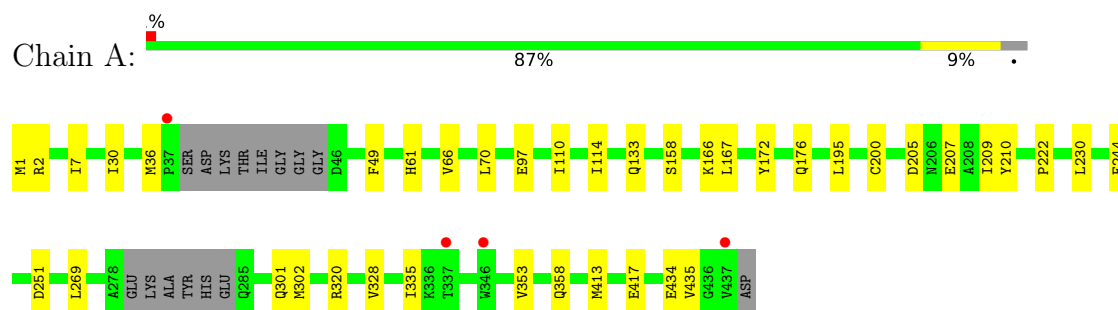
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	67	Total	O	0	0
			67	67		
9	B	44	Total	O	0	0
			44	44		
9	C	59	Total	O	0	0
			59	59		
9	D	62	Total	O	0	0
			62	62		
9	E	7	Total	O	0	0
			7	7		

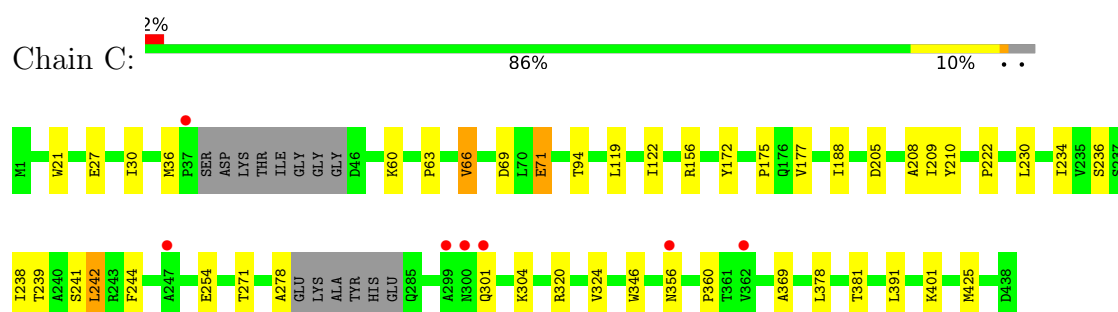
3 Residue-property plots [i](#)

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.

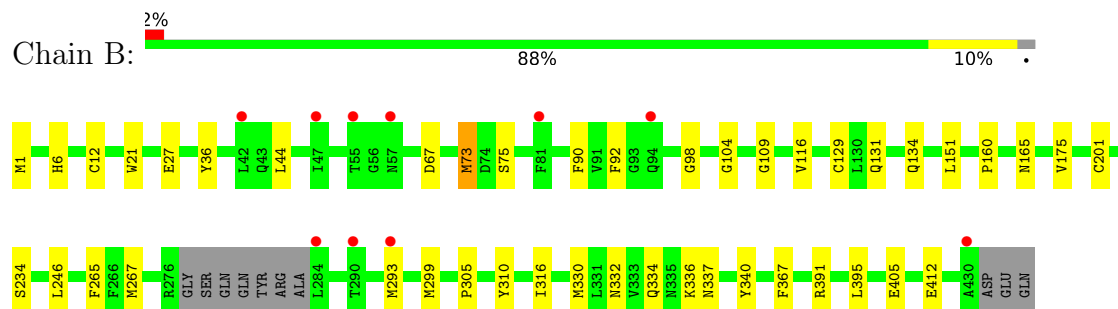
- Molecule 1: Tubulin alpha-1B chain



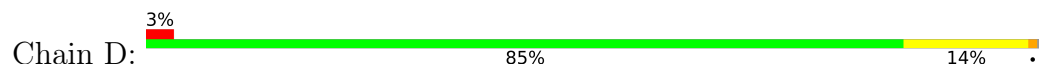
- Molecule 1: Tubulin alpha-1B chain

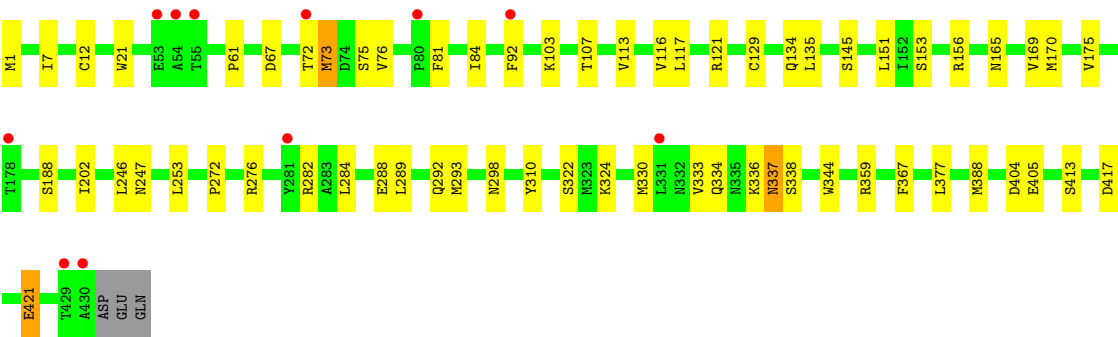


- Molecule 2: Tubulin beta chain

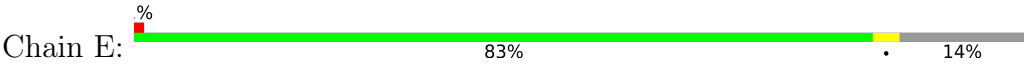


- Molecule 2: Tubulin beta chain





● Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.48Å 126.97Å 252.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.35 – 2.40 34.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.35-2.40) 99.7 (34.35-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.233 0.198 , 0.232	Depositor DCC
R_{free} test set	4217 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14678	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: A1BMG, GDP, SO4, MG, GTP

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	0.17	0/3364	0.37	0/4573
1	C	0.16	0/3376	0.35	0/4585
2	B	0.17	0/3377	0.34	0/4577
2	D	0.18	0/3433	0.37	0/4651
3	E	0.13	0/1012	0.25	0/1350
All	All	0.17	0/14562	0.35	0/19736

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	3290	0	3179	22	0
1	C	3303	0	3209	26	0
2	B	3304	0	3169	28	0
2	D	3359	0	3230	36	0
3	E	1001	0	996	4	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	B	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	28	0	12	1	0
6	B	28	0	0	0	0
6	D	28	0	0	1	0
7	B	5	0	0	0	0
8	C	1	0	0	0	0
9	A	67	0	0	0	0
9	B	44	0	0	0	0
9	C	59	0	0	3	0
9	D	62	0	0	2	0
9	E	7	0	0	0	0
All	All	14678	0	13831	108	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 4.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:N	2:D:129:CYS:SG	2.55	0.76
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.69	0.73
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.74	0.70
9:C:658:HOH:O	2:D:129:CYS:SG	2.50	0.68
1:A:158:SER:OG	1:A:166:LYS:NZ	2.25	0.68
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.75	0.68
2:B:1:MET:N	2:B:129:CYS:SG	2.67	0.67
1:A:30:ILE:HG12	1:A:36:MET:HE2	1.77	0.66
1:C:30:ILE:HG12	1:C:36:MET:HE2	1.75	0.66
2:B:1:MET:HE3	2:B:131:GLN:HG3	1.80	0.63
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.81	0.63
2:B:73:MET:HG3	2:B:90:PHE:HD2	1.63	0.63
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.81	0.62
1:A:176:GLN:HE22	1:A:207:GLU:HG3	1.65	0.61
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.82	0.61
2:B:299:MET:HE3	2:B:305:PRO:HG3	1.83	0.61
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.81	0.61
1:C:238:ILE:HD12	1:C:378:LEU:HD11	1.87	0.57
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.86	0.57
1:C:60:LYS:NZ	9:C:603:HOH:O	2.39	0.54
1:A:97:GLU:HG2	2:B:1:MET:HG2	1.90	0.54
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.89	0.53
2:B:160:PRO:HG3	3:E:69:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:CYS:HB2	5:D:502:GDP:C8	2.44	0.52
2:B:104:GLY:O	2:B:109:GLY:HA3	2.10	0.52
2:B:134:GLN:HA	2:B:165:ASN:O	2.10	0.51
2:D:276:ARG:HG2	9:D:633:HOH:O	2.10	0.51
1:A:2:ARG:HB3	1:A:133:GLN:CD	2.36	0.50
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.47	0.50
1:C:71:GLU:OE2	2:D:247:ASN:ND2	2.45	0.50
2:D:145:SER:HB2	2:D:188:SER:OG	2.11	0.50
2:B:12:CYS:HB2	5:B:501:GDP:C8	2.47	0.49
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.94	0.49
2:D:67:ASP:OD2	2:D:72:THR:OG1	2.21	0.49
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.48
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.95	0.48
2:B:310:TYR:CE1	2:B:367:PHE:HZ	2.31	0.48
2:D:156:ARG:HD3	3:E:119:MET:HE2	1.95	0.48
1:A:70:LEU:HD21	1:A:114:ILE:HD13	1.94	0.48
2:B:391:ARG:HG3	1:C:346:TRP:CD1	2.48	0.48
2:D:282:ARG:HH22	2:D:288:GLU:CD	2.22	0.48
1:A:2:ARG:HB3	1:A:133:GLN:NE2	2.29	0.47
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.49	0.47
2:D:72:THR:O	2:D:76:VAL:HG23	2.15	0.47
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.15	0.47
2:D:337:ASN:N	2:D:337:ASN:OD1	2.47	0.47
1:C:69:ASP:O	1:C:94:THR:HA	2.15	0.46
2:D:116:VAL:HG11	2:D:151:LEU:HD21	1.97	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.46
2:B:27:GLU:OE2	2:B:234:SER:OG	2.29	0.46
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.49	0.46
2:B:36:TYR:CD1	2:B:44:LEU:HD21	2.50	0.46
1:C:239:THR:HA	1:C:242:LEU:HD12	1.98	0.46
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.51	0.46
2:D:330:MET:O	2:D:334:GLN:HG3	2.15	0.46
1:C:66:VAL:HG21	1:C:122:ILE:HG12	1.98	0.46
2:D:117:LEU:O	2:D:121:ARG:HG3	2.17	0.45
2:D:324:LYS:NZ	9:D:613:HOH:O	2.48	0.45
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.34	0.45
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.98	0.45
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.99	0.45
2:B:337:ASN:HB3	2:B:340:TYR:HD2	1.82	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.99	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
1:C:320:ARG:HD3	1:C:360:PRO:HB3	1.99	0.44
2:B:332:ASN:O	2:B:336:LYS:HG2	2.18	0.44
2:D:292:GLN:HG2	2:D:298:ASN:ND2	2.33	0.44
1:C:175:PRO:HG3	9:C:611:HOH:O	2.17	0.44
1:A:7:ILE:HG23	1:A:66:VAL:HG13	1.99	0.44
2:B:134:GLN:HB2	2:B:165:ASN:HD22	1.83	0.43
2:B:98:GLY:HA2	1:C:254:GLU:HG3	2.00	0.43
1:C:208:ALA:HB2	1:C:304:LYS:HG2	2.01	0.43
2:D:72:THR:O	2:D:75:SER:OG	2.34	0.43
2:B:395:LEU:HD21	2:B:405:GLU:HG2	2.01	0.43
2:B:73:MET:HG2	2:B:92:PHE:CD2	2.54	0.42
2:D:289:LEU:O	2:D:293:MET:HB2	2.19	0.42
2:D:388:MET:HE2	2:D:388:MET:HB3	1.91	0.42
2:D:272:PRO:HB3	2:D:284:LEU:HD22	2.02	0.42
1:A:320:ARG:HG3	1:A:358:GLN:O	2.20	0.42
2:B:1:MET:CE	2:B:131:GLN:HG3	2.48	0.42
2:D:113:VAL:HG23	2:D:151:LEU:HD13	2.02	0.42
3:E:6:MET:HE3	3:E:6:MET:HB2	1.90	0.42
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.02	0.42
2:D:7:ILE:O	2:D:135:LEU:HA	2.20	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.42
2:B:330:MET:O	2:B:334:GLN:HG3	2.19	0.41
1:C:234:ILE:O	1:C:238:ILE:HG12	2.20	0.41
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.54	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.41
1:C:27:GLU:OE2	1:C:236:SER:OG	2.35	0.41
1:A:36:MET:HE3	1:A:61:HIS:CD2	2.56	0.41
2:B:151:LEU:HD23	2:B:151:LEU:HA	1.90	0.41
1:C:27:GLU:HB3	1:C:244:PHE:HZ	1.85	0.41
2:D:134:GLN:HA	2:D:165:ASN:O	2.20	0.41
2:D:404:ASP:OD1	2:D:405:GLU:N	2.53	0.41
1:A:1:MET:HE3	1:A:1:MET:HA	2.02	0.41
1:A:244:PHE:CG	1:A:358:GLN:HG3	2.56	0.41
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.60	0.41
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.03	0.41
2:D:103:LYS:HA	2:D:107:THR:OG1	2.21	0.40
1:C:271:THR:HG22	1:C:301:GLN:HG2	2.02	0.40
2:D:417:ASP:O	2:D:421:GLU:HG2	2.21	0.40
1:C:230:LEU:O	1:C:234:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:MET:HE2	2:D:92:PHE:HB3	2.03	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.21	0.40
2:D:253:LEU:HD13	6:D:501:A1BMG:C28	2.52	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	417/438 (95%)	408 (98%)	9 (2%)	0	100	100
1	C	418/438 (95%)	408 (98%)	10 (2%)	0	100	100
2	B	419/433 (97%)	408 (97%)	11 (3%)	0	100	100
2	D	428/433 (99%)	422 (99%)	6 (1%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
All	All	1801/1885 (96%)	1763 (98%)	38 (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	353/369 (96%)	348 (99%)	5 (1%)	59	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	356/369 (96%)	348 (98%)	8 (2%)	45 67
2	B	360/374 (96%)	353 (98%)	7 (2%)	50 71
2	D	366/374 (98%)	354 (97%)	12 (3%)	33 55
3	E	106/126 (84%)	105 (99%)	1 (1%)	70 85
All	All	1541/1612 (96%)	1508 (98%)	33 (2%)	47 69

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
1	A	302	MET
1	A	335	ILE
1	A	434	GLU
1	A	435	VAL
2	B	73	MET
2	B	75	SER
2	B	175	VAL
2	B	246	LEU
2	B	267	MET
2	B	316	ILE
2	B	412	GLU
1	C	66	VAL
1	C	71	GLU
1	C	177	VAL
1	C	241	SER
1	C	242	LEU
1	C	324	VAL
1	C	381	THR
1	C	391	LEU
2	D	73	MET
2	D	153	SER
2	D	175	VAL
2	D	246	LEU
2	D	322	SER
2	D	333	VAL
2	D	336	LYS
2	D	337	ASN
2	D	338	SER
2	D	359	ARG
2	D	413	SER
2	D	421	GLU

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Mol	Chain	Res	Type
3	E	28	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	GLN
1	A	216	ASN
1	A	356	ASN
1	A	393	HIS
1	A	406	HIS
2	B	165	ASN
2	B	334	GLN
2	B	347	ASN
2	B	416	ASN
1	C	393	HIS
2	D	8	GLN
2	D	11	GLN
2	D	14	ASN
2	D	134	GLN
2	D	247	ASN
2	D	292	GLN
2	D	298	ASN
2	D	375	GLN
2	D	423	GLN
2	D	426	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GDP	B	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.71	7 (15%)
6	A1BMG	B	502	-	31,31,31	0.42	0	37,44,44	0.50	0
4	GTP	A	501	-	33,34,34	1.07	2 (6%)	50,54,54	1.51	10 (20%)
4	GTP	C	501	8	33,34,34	0.89	1 (3%)	50,54,54	1.59	10 (20%)
6	A1BMG	D	501	-	31,31,31	0.41	0	37,44,44	0.49	0
7	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.06	0
5	GDP	D	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.80	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
5	GDP	B	501	-	-	4/16/32/32	0/3/3/3
6	A1BMG	B	502	-	-	2/18/18/18	0/4/4/4
4	GTP	A	501	-	-	7/22/38/38	0/3/3/3
4	GTP	C	501	8	-	6/22/38/38	0/3/3/3
6	A1BMG	D	501	-	-	0/18/18/18	0/4/4/4
5	GDP	D	502	-	-	3/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	PB-O3A	3.38	1.63	1.59
5	D	502	GDP	C5-C4	3.03	1.47	1.38
5	B	501	GDP	C5-C4	2.98	1.46	1.38
4	A	501	GTP	PB-O3B	2.88	1.62	1.59
5	D	502	GDP	C6-N1	-2.25	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	GDP	C5-N7	-2.13	1.34	1.39
5	B	501	GDP	C6-N1	-2.11	1.34	1.38
4	C	501	GTP	C2-N3	2.11	1.38	1.33
5	D	502	GDP	PA-O3A	2.03	1.61	1.59
5	B	501	GDP	C5-N7	-2.03	1.35	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C5-C4-N3	-5.61	119.45	128.39
5	D	502	GDP	C5-C4-N3	-5.56	119.54	128.39
5	D	502	GDP	C2-N3-C4	5.10	121.08	112.30
5	B	501	GDP	C2-N3-C4	4.76	120.49	112.30
5	D	502	GDP	N9-C4-N3	4.45	134.85	125.95
4	C	501	GTP	C5-C4-N3	-4.38	121.42	128.39
4	C	501	GTP	C2-N3-C4	4.37	119.83	112.30
5	B	501	GDP	N9-C4-N3	4.37	134.69	125.95
4	A	501	GTP	C5-C4-N3	-4.22	121.67	128.39
4	A	501	GTP	C2-N3-C4	4.04	119.25	112.30
5	D	502	GDP	C6-C5-N7	3.76	137.13	130.29
5	B	501	GDP	C6-C5-N7	3.25	136.20	130.29
4	C	501	GTP	N9-C4-N3	2.92	131.79	125.95
4	A	501	GTP	O3G-PG-O3B	2.84	114.16	104.64
4	C	501	GTP	C2-N1-C6	-2.83	119.99	125.11
4	C	501	GTP	N9-C8-N7	-2.81	108.20	113.40
4	C	501	GTP	O3B-PB-O1B	-2.81	102.27	110.70
4	A	501	GTP	O2B-PB-O3B	2.72	114.61	107.27
4	A	501	GTP	C2-N1-C6	-2.61	120.37	125.11
4	C	501	GTP	C5-C6-N1	2.61	119.90	113.25
4	A	501	GTP	N9-C4-N3	2.54	131.03	125.95
5	D	502	GDP	C4-C5-N7	-2.50	106.70	110.67
4	A	501	GTP	N9-C8-N7	-2.48	108.81	113.40
4	C	501	GTP	C8-N7-C5	2.41	108.56	104.26
4	C	501	GTP	O6-C6-C5	-2.39	120.22	126.53
5	B	501	GDP	O6-C6-C5	-2.38	120.25	126.53
5	B	501	GDP	C4-C5-N7	-2.33	106.98	110.67
4	A	501	GTP	C8-N7-C5	2.29	108.34	104.26
5	D	502	GDP	O2A-PA-O3A	2.24	113.34	107.27
4	A	501	GTP	C5-C6-N1	2.24	118.95	113.25
5	B	501	GDP	O3B-PB-O3A	2.22	112.07	104.64
5	D	502	GDP	C5-C6-N1	2.12	118.64	113.25
5	D	502	GDP	C8-N7-C5	2.11	108.03	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	GTP	O2B-PB-O3B	2.09	112.91	107.27
4	A	501	GTP	O6-C6-C5	-2.02	121.20	126.53

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O2A
5	B	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O1A
5	B	501	GDP	C5'-O5'-PA-O2A
5	D	502	GDP	C5'-O5'-PA-O3A
5	D	502	GDP	C5'-O5'-PA-O1A
5	D	502	GDP	C5'-O5'-PA-O2A
6	B	502	A1BMG	C22-C25-O26-C27
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	C5'-O5'-PA-O1A
6	B	502	A1BMG	C28-C25-O26-C27
5	B	501	GDP	PB-O3A-PA-O2A
4	A	501	GTP	C4'-C5'-O5'-PA
4	C	501	GTP	PB-O3B-PG-O1G
4	A	501	GTP	PB-O3B-PG-O2G
4	C	501	GTP	C4'-C5'-O5'-PA
4	A	501	GTP	PB-O3A-PA-O2A

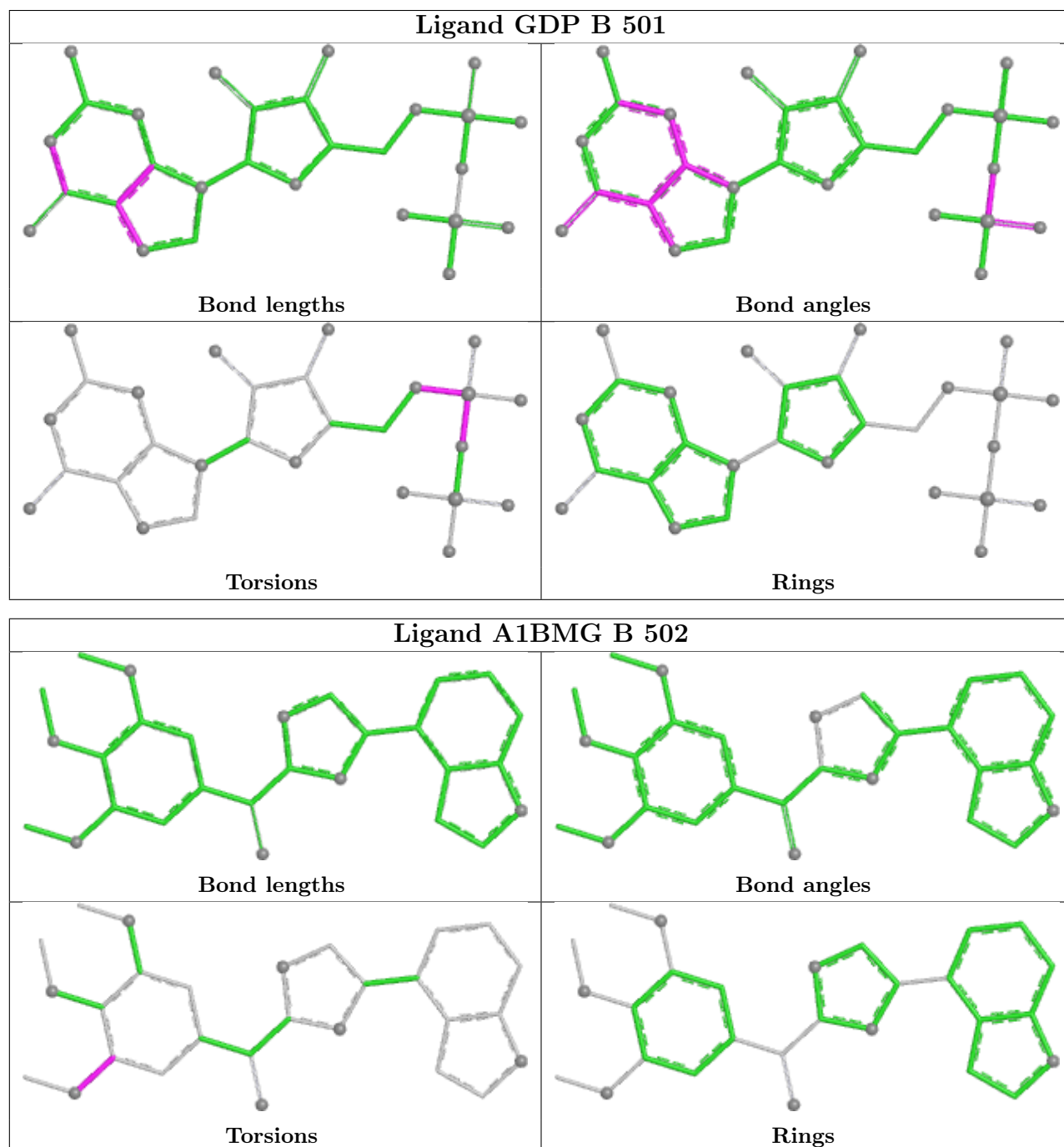
There are no ring outliers.

3 monomers are involved in 3 short contacts:

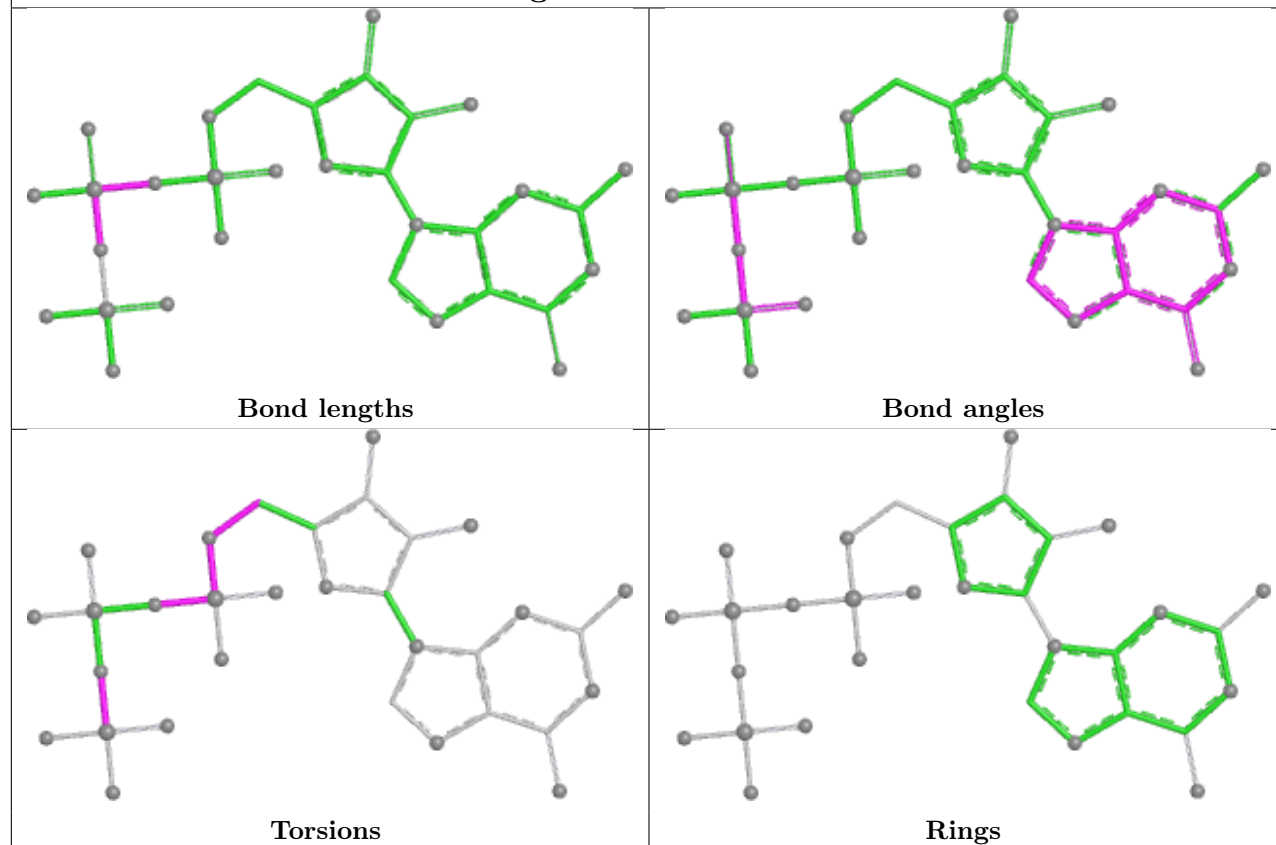
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GDP	1	0
6	D	501	A1BMG	1	0
5	D	502	GDP	1	0

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

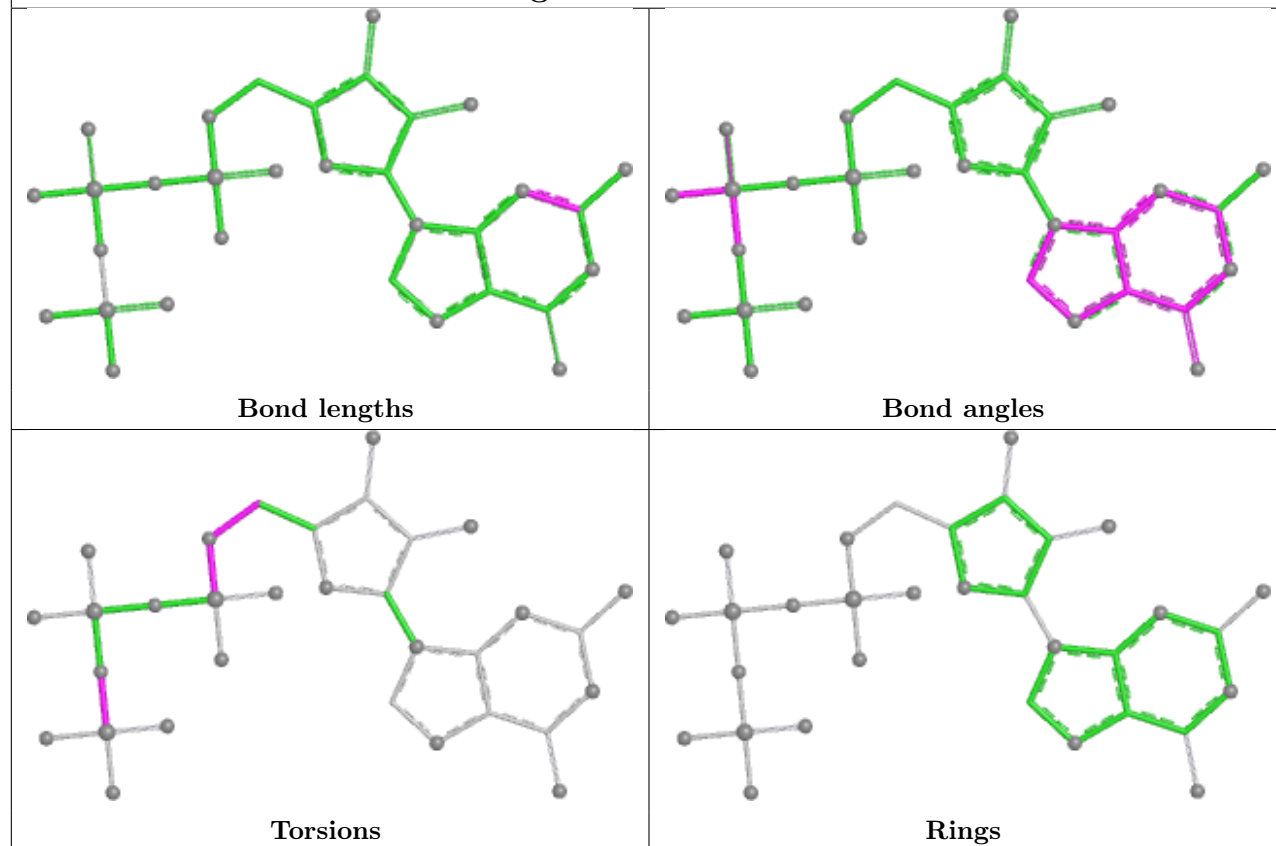
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

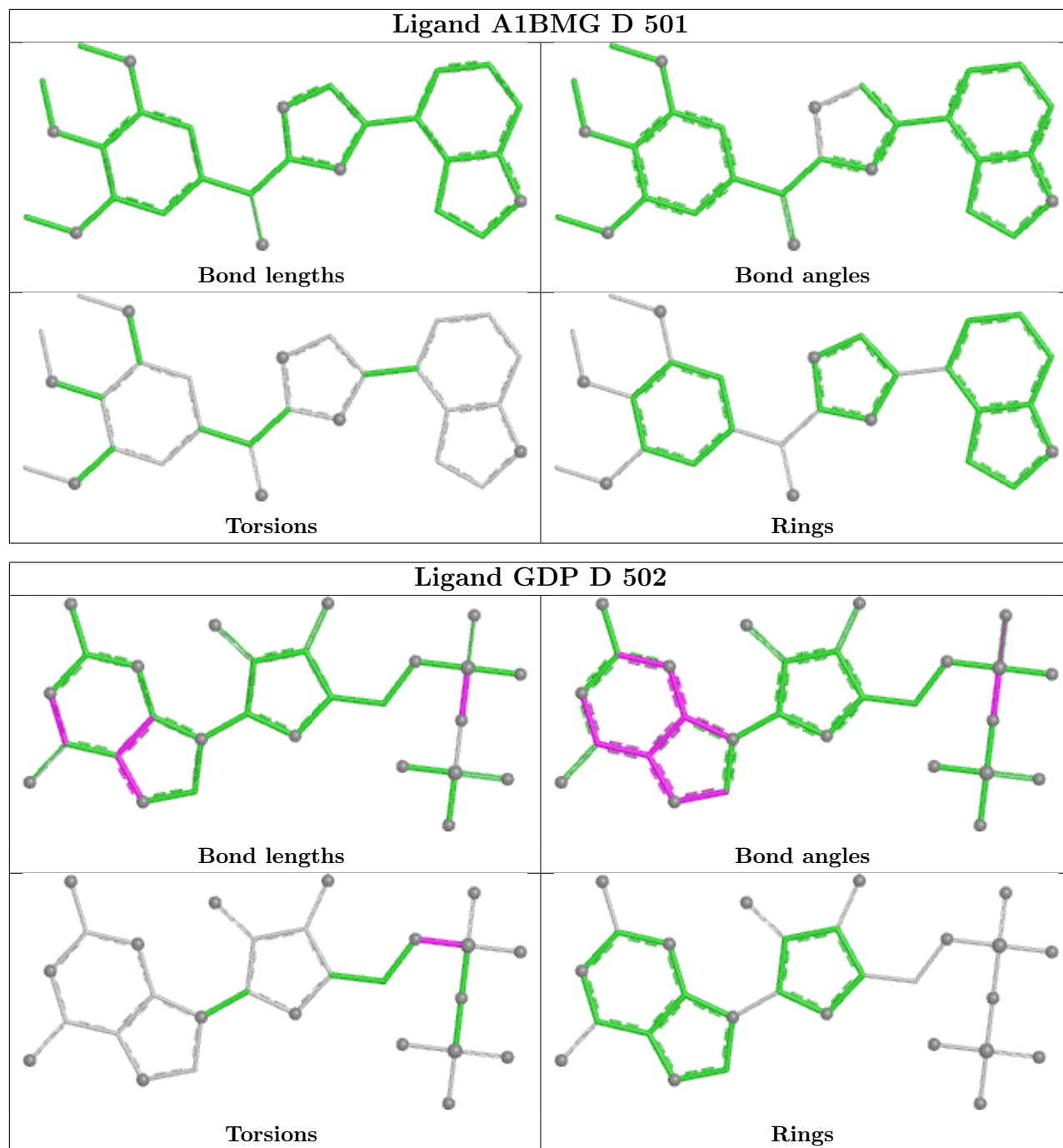


Ligand GTP A 501



Ligand GTP C 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	423/438 (96%)	-0.08	4 (0%) 81 78	27, 45, 74, 91	0
1	C	424/438 (96%)	-0.01	7 (1%) 69 65	27, 46, 74, 96	0
2	B	423/433 (97%)	0.02	10 (2%) 59 55	29, 44, 79, 113	0
2	D	430/433 (99%)	-0.01	11 (2%) 57 53	24, 40, 76, 112	0
3	E	123/143 (86%)	0.42	1 (0%) 82 80	43, 61, 83, 93	0
All	All	1823/1885 (96%)	0.01	33 (1%) 67 63	24, 46, 77, 113	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	PRO	4.3
2	D	281	TYR	4.1
2	B	57	ASN	3.7
2	D	92	PHE	3.3
1	A	437	VAL	3.3
2	B	430	ALA	3.2
3	E	139	LEU	2.9
2	B	290	THR	2.9
2	D	54	ALA	2.8
2	D	53	GLU	2.8
1	C	247	ALA	2.7
2	D	55	THR	2.7
2	B	293	MET	2.6
2	D	430	ALA	2.6
1	C	299	ALA	2.6
1	A	37	PRO	2.5
2	D	331	LEU	2.5
2	D	80	PRO	2.5
2	B	81	PHE	2.5
2	D	72	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	301	GLN	2.3
2	B	42	LEU	2.3
1	C	356	ASN	2.2
2	B	284	LEU	2.2
2	B	94	GLN	2.2
2	B	55	THR	2.2
1	A	346	TRP	2.2
1	A	337	THR	2.1
2	D	178	THR	2.1
1	C	300	ASN	2.1
1	C	362	VAL	2.1
2	B	47	ILE	2.0
2	D	429	THR	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.

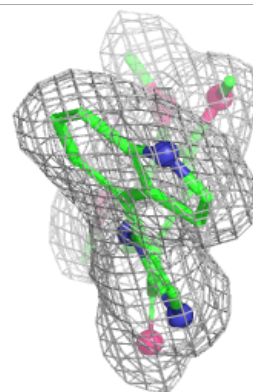
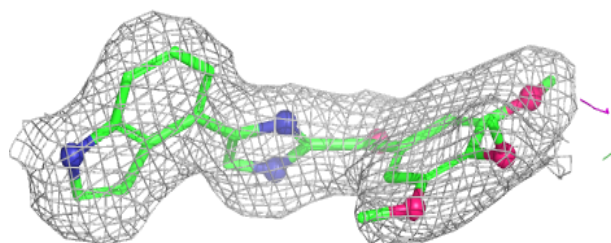
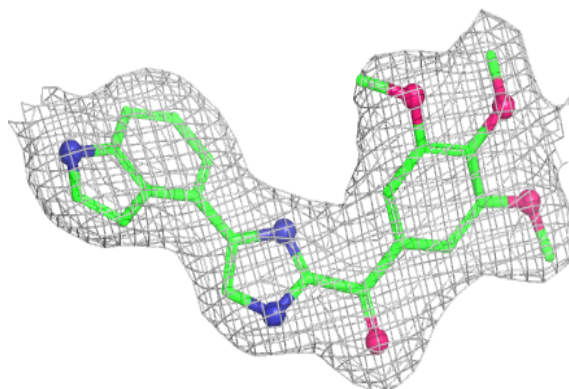
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	B	503	5/5	0.78	0.08	77,82,88,112	0
6	A1BMG	D	501	28/28	0.95	0.07	31,35,38,44	0
6	A1BMG	B	502	28/28	0.95	0.07	29,33,39,48	0
5	GDP	B	501	28/28	0.96	0.06	30,34,39,43	0
4	GTP	A	501	32/32	0.96	0.07	25,31,35,56	0
8	MG	C	502	1/1	0.96	0.05	46,46,46,46	0
4	GTP	C	501	32/32	0.97	0.07	30,35,40,44	0
5	GDP	D	502	28/28	0.97	0.06	24,30,34,35	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.

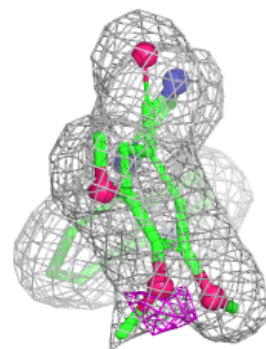
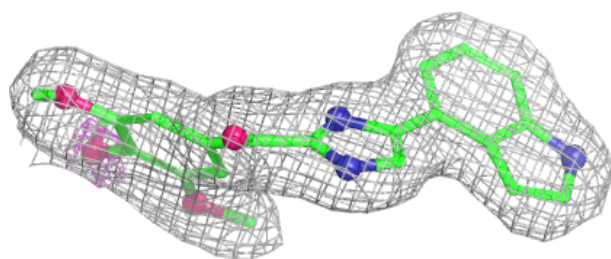
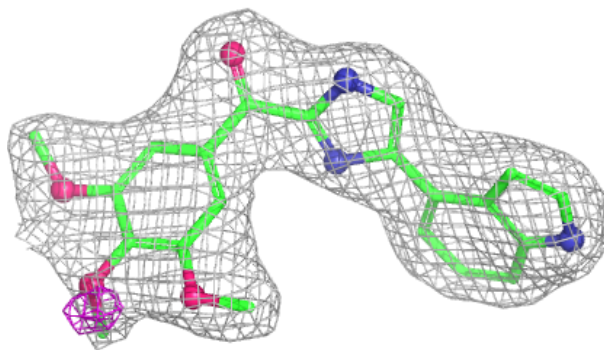
Electron density around A1BMG D 501:

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

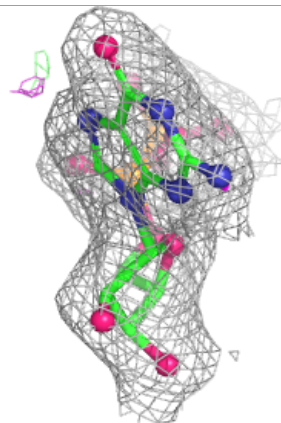
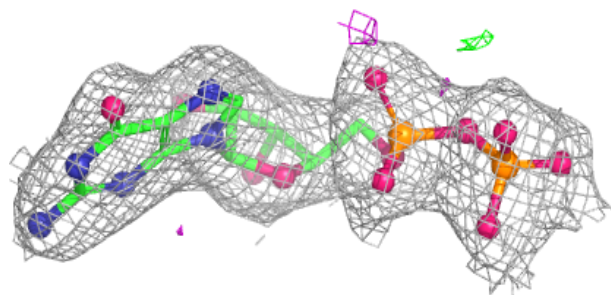
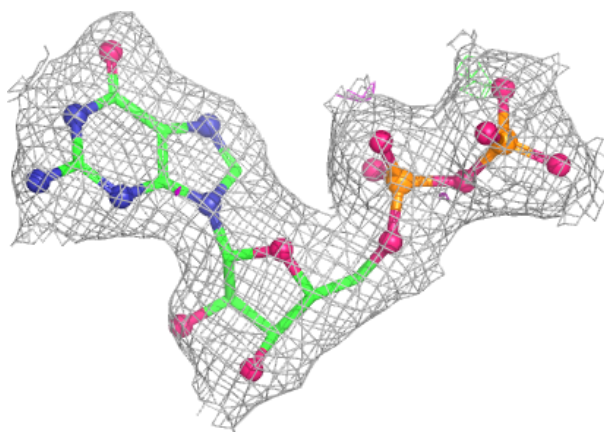


Electron density around A1BMG B 502:

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

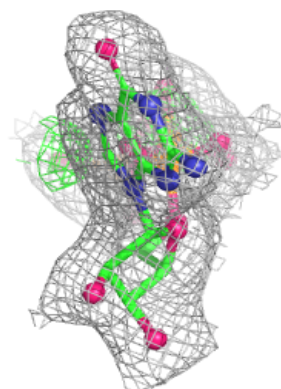
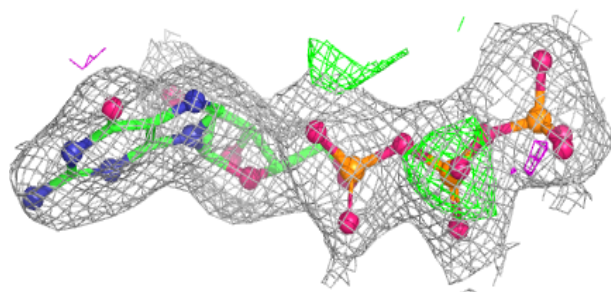
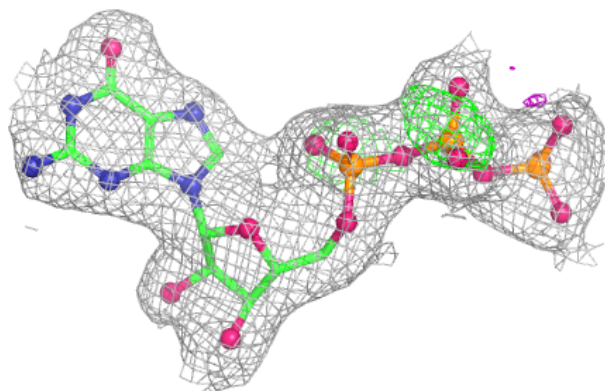
**Electron density around GDP B 501:**

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

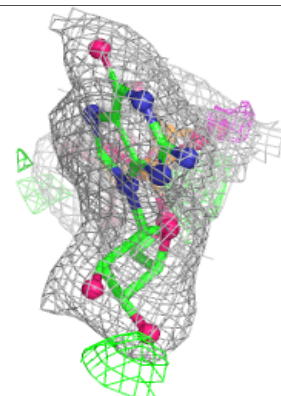
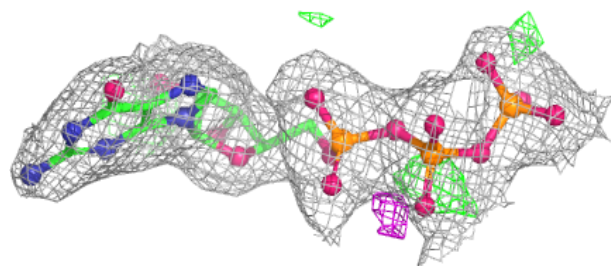
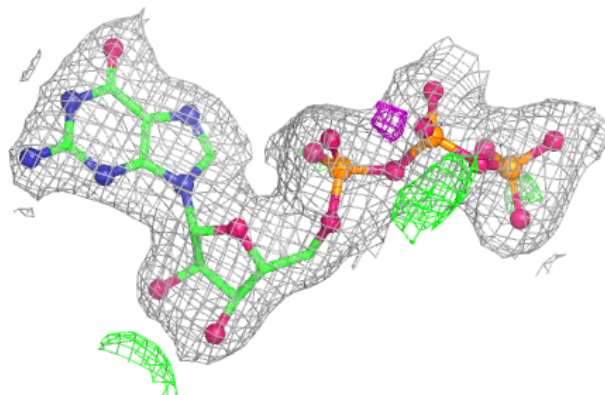


Electron density around GTP A 501:

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

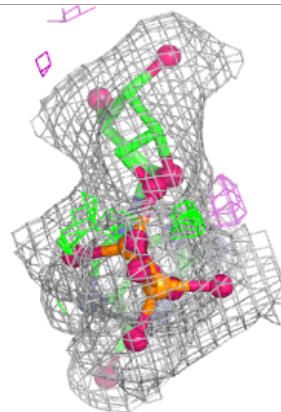
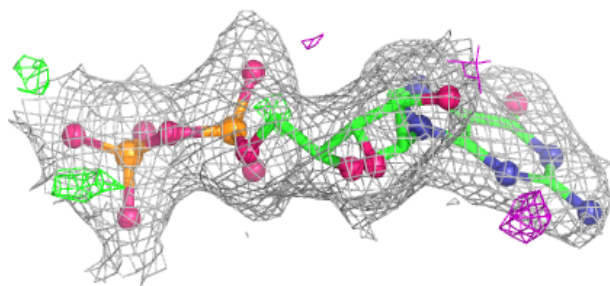
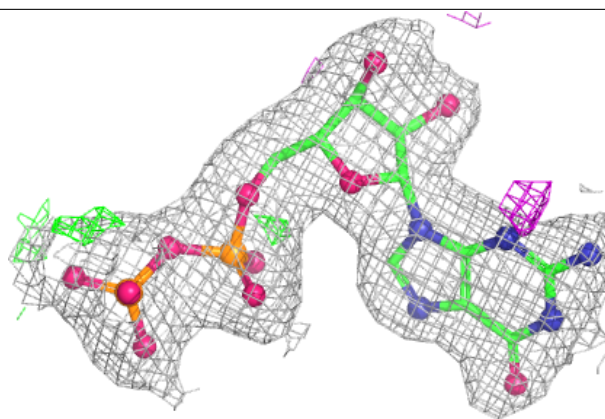
**Electron density around GTP C 501:**

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



Electron density around GDP D 502:

$2mF_o-DF_c$ (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.