



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 PM UTC

PDB ID : 5NFZ / pdb_00005nfz
Title : TUBULIN-MTC complex
Authors : Field, J.J.; Pera, B.; Estevez Gallego, J.; Calvo, E.; Rodriguez-Salarichs, J.; Saez-Calvo, G.; Zuverra, D.; Jordi, M.; Prota, A.E.; Menchon, G.; Miller, J.H.; Altmann, K.-H.; Diaz, J.F.
Deposited on : 2017-03-16
Resolution : 2.10 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:

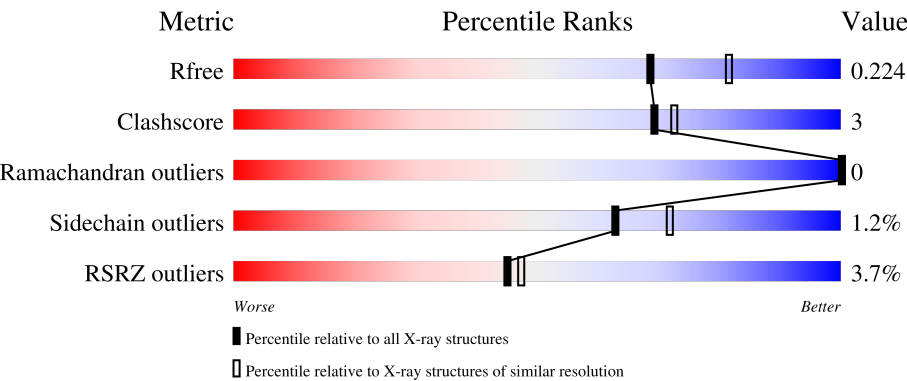
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	% 90%8%
1	C	451	2% 89%8%
2	B	445	3% 84%10%5%
2	D	445	5% 82%13%

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Mol	Chain	Length	Quality of chain
3	E	143	6% 85% 13%
4	F	384	6% 81% 9% 10%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 18133 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	440	Total	C	N	O	S	0	3	0
			3452	2185	587	657	23			
1	C	440	Total	C	N	O	S	0	4	0
			3453	2185	585	660	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3338	2098	569	645	26			
2	D	426	Total	C	N	O	S	0	0	0
			3344	2098	571	649	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	125	Total	C	N	O	S	0	1	0
			1038	639	190	204	5			

There are 2 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

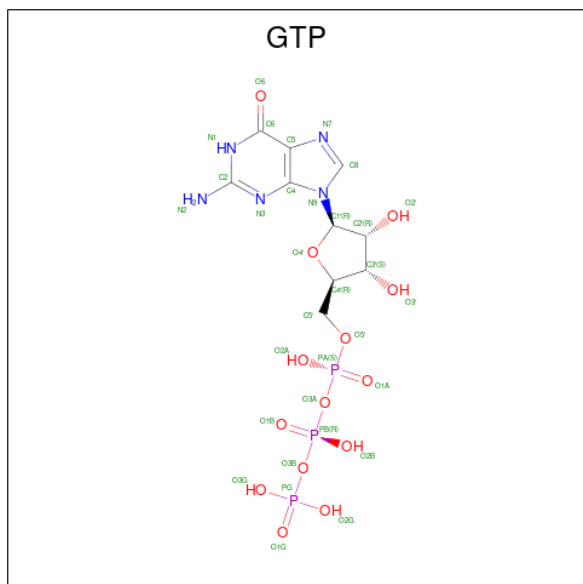
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	347	Total	C	N	O	S	0	1	0
			2837	1819	484	519	15			

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

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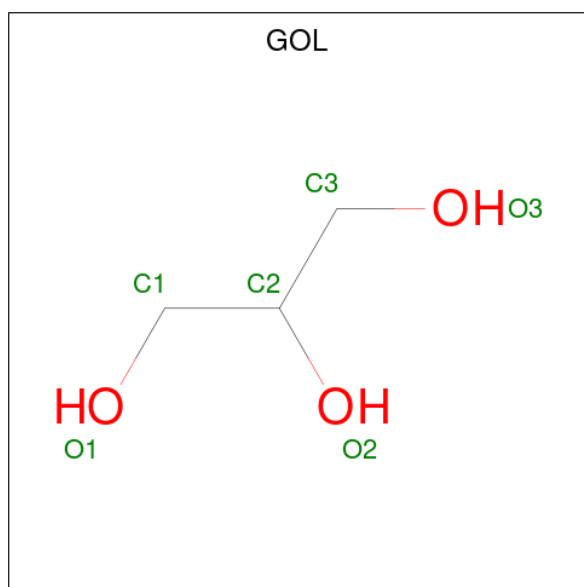
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

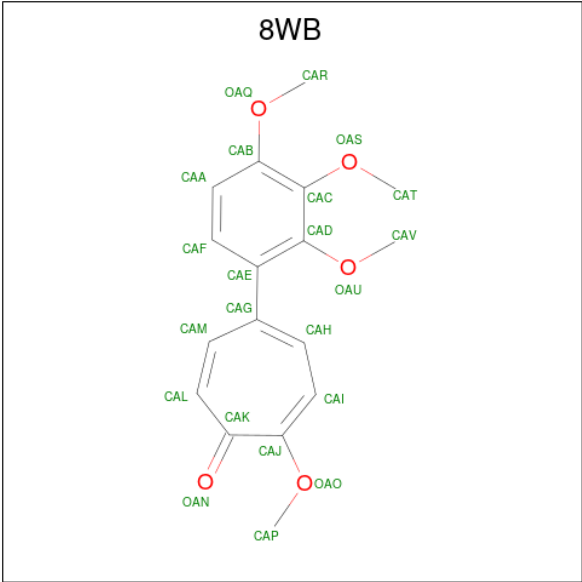
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



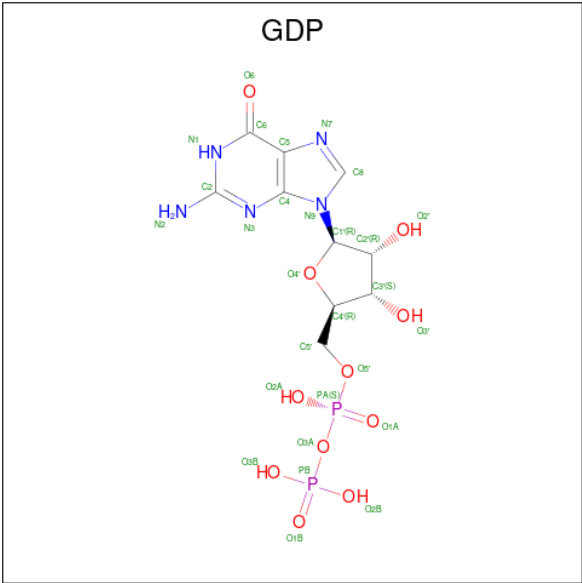
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-methoxy-5-(2,3,4-trimethoxyphenyl)cyclohepta-2,4,6-trien-1-one (CCD ID: 8WB) (formula: C₁₇H₁₈O₅).



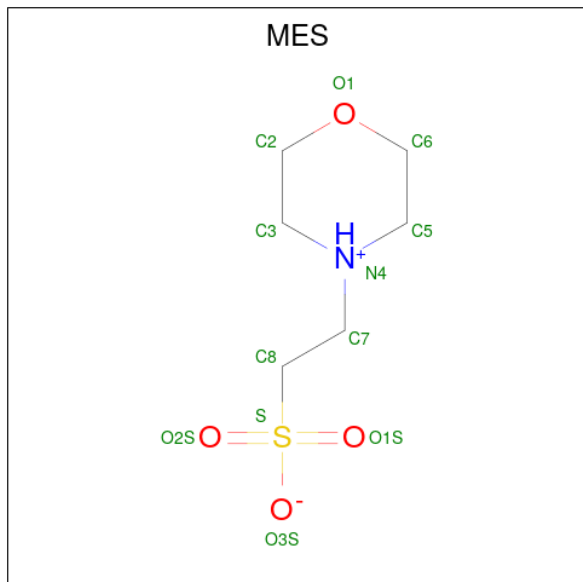
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			22	17	5		
9	D	1	Total	C	O	0	0
			22	17	5		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



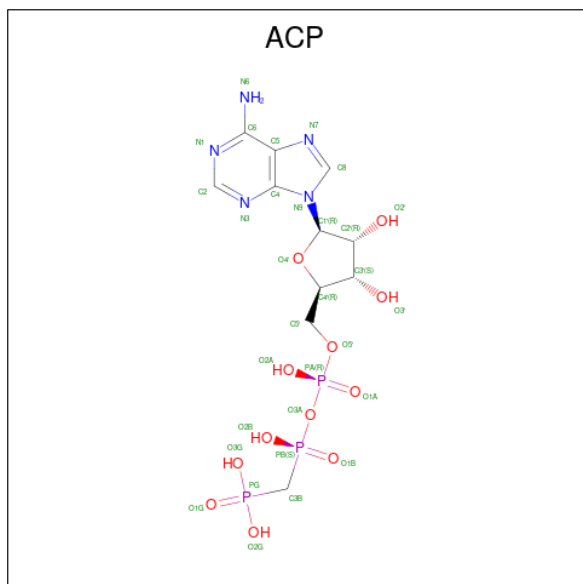
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	D	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

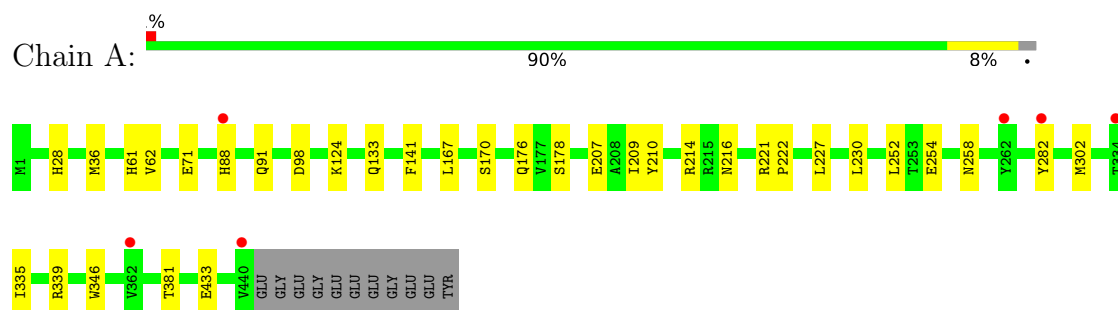
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	96	Total 96	O 96	0	0
13	B	92	Total 92	O 92	0	0
13	C	180	Total 180	O 180	0	0
13	D	36	Total 36	O 36	0	0
13	E	15	Total 15	O 15	0	0
13	F	30	Total 30	O 30	0	0

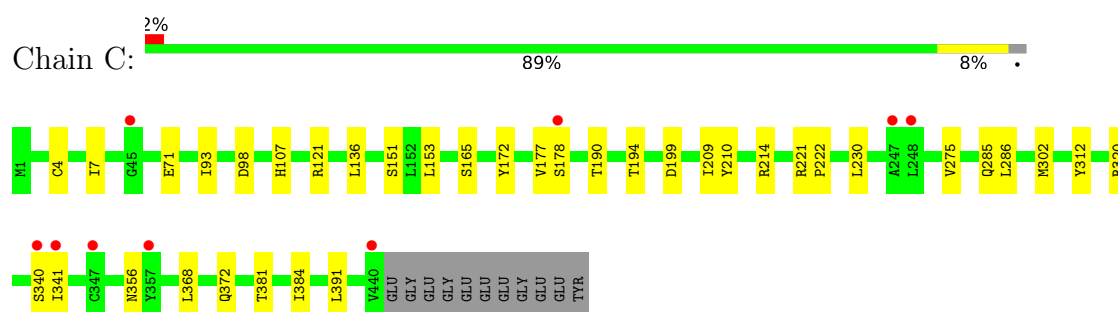
3 Residue-property plots [i](#)

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.

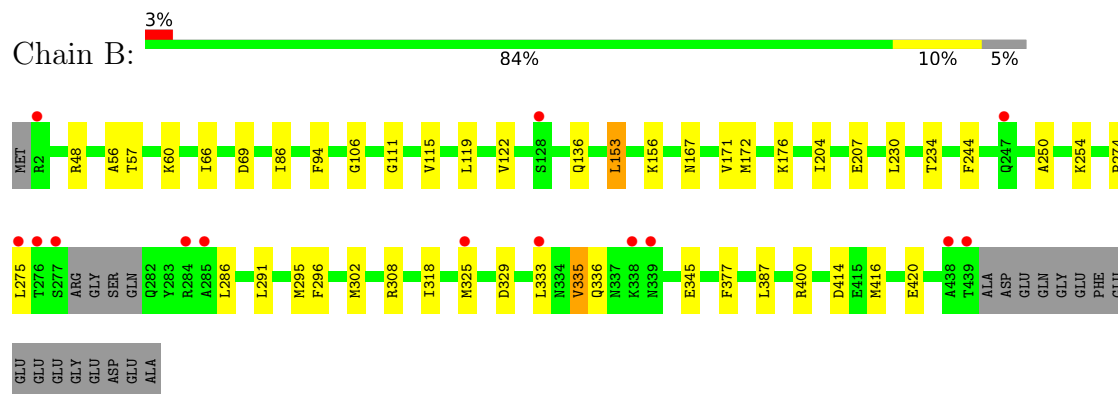
- Molecule 1: Tubulin alpha-1B chain



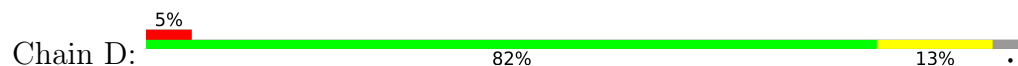
- Molecule 1: Tubulin alpha-1B chain

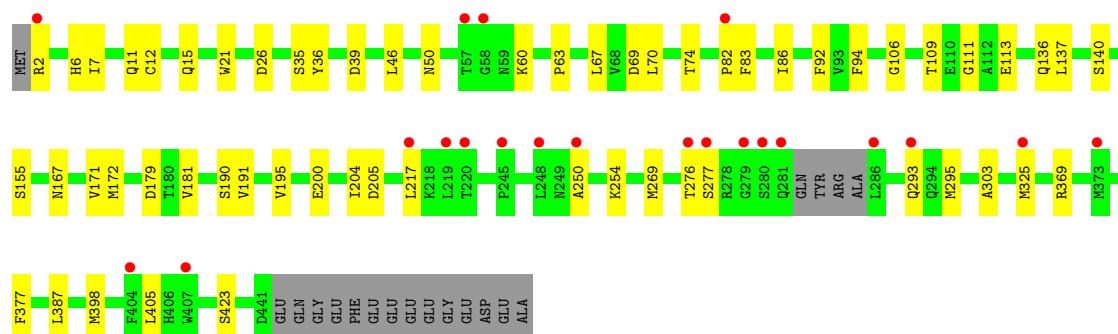


- Molecule 2: Tubulin beta-2B chain

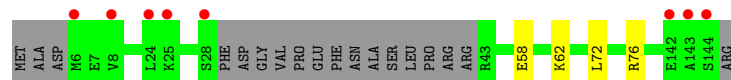
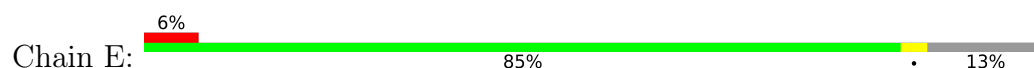


- Molecule 2: Tubulin beta-2B chain

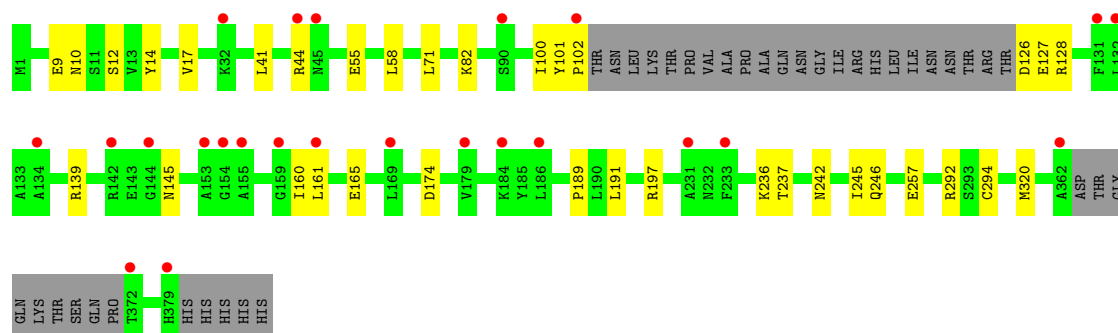
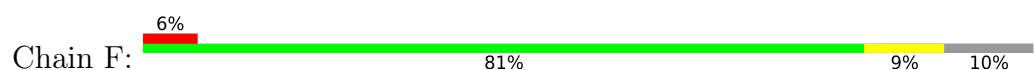




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.16Å 158.79Å 180.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.78 – 2.10 59.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.78-2.10) 100.0 (59.78-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.182 , 0.218 0.190 , 0.224	Depositor DCC
R_{free} test set	8796 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18133	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, GTP, GOL, CA, MES, MG, 8WB, ACP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.31	0/3539	0.50	0/4804
1	C	0.43	0/3543	0.57	0/4810
2	B	0.35	0/3412	0.53	0/4622
2	D	0.28	0/3417	0.45	0/4628
3	E	0.29	0/1050	0.42	0/1393
4	F	0.22	0/2904	0.42	0/3921
All	All	0.33	0/17865	0.50	0/24178

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	3452	0	3374	21	0
1	C	3453	0	3368	21	0
2	B	3338	0	3215	30	0
2	D	3344	0	3218	31	0
3	E	1038	0	1054	2	0
4	F	2837	0	2811	19	0
5	A	32	0	12	0	0

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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
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	1	0
9	B	22	0	0	1	0
9	D	22	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	12	0	12	0	0
12	F	31	0	14	0	0
13	A	96	0	0	1	0
13	B	92	0	0	3	0
13	C	180	0	0	0	0
13	D	36	0	0	0	0
13	E	15	0	0	0	0
13	F	30	0	0	0	0
All	All	18133	0	17122	121	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 3.

All (121) 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:176:LYS:HD3	2:B:207:GLU:HG3	1.64	0.80
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.19	0.73
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.24	0.69
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.32	0.69
4:F:102:PRO:HB3	4:F:174:ASP:HA	1.77	0.66
4:F:9:GLU:H	4:F:9:GLU:CD	2.04	0.66
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.32	0.64
1:A:221:ARG:HG2	2:B:325:MET:HG2	1.79	0.64
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.61
2:B:234:THR:OG1	2:B:302:MET:HE2	2.00	0.61
2:B:329:ASP:O	2:B:333:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.59
1:A:62:VAL:HG11	1:A:88:HIS:CE1	2.38	0.58
2:D:50:ASN:HD22	2:D:50:ASN:H	1.52	0.57
4:F:161:LEU:HA	4:F:236:LYS:HZ1	1.68	0.57
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.20	0.57
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.70	0.57
1:A:216:ASN:ND2	8:A:505:GOL:H2	2.20	0.57
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.87	0.55
4:F:160:ILE:O	4:F:236:LYS:NZ	2.39	0.54
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.89	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.08	0.54
4:F:139:ARG:HB2	4:F:145:ASN:ND2	2.22	0.54
1:C:98:ASP:H	2:D:2:ARG:NH2	2.07	0.52
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.42	0.51
1:C:221:ARG:HG2	2:D:325:MET:HB3	1.92	0.51
2:B:414:ASP:OD2	13:B:601:HOH:O	2.19	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.11	0.50
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.93	0.50
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.50
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.77	0.50
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.92	0.50
2:D:136:GLN:HA	2:D:167:ASN:O	2.13	0.49
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.93	0.49
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.47	0.49
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.47	0.48
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.95	0.48
2:B:318:ILE:HD11	9:B:501:8WB:CAT	2.43	0.48
2:B:230:LEU:HB3	2:B:302:MET:HE1	1.95	0.48
1:A:346:TRP:CD1	1:A:346:TRP:H	2.29	0.48
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.95	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.13	0.48
4:F:237:THR:O	4:F:246:GLN:NE2	2.47	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.55	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.50	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.14	0.47
2:D:11:GLN:HA	2:D:74:THR:HG21	1.97	0.47
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.96	0.47
2:B:295:MET:CG	2:B:377:PHE:HB2	2.44	0.47
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.96	0.47
2:B:416:MET:HE3	2:B:420:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.50	0.46
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.96	0.46
1:A:209:ILE:HD11	1:A:302:MET:SD	2.55	0.46
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.98	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.83	0.46
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.98	0.46
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.97	0.45
4:F:14:TYR:HA	4:F:17:VAL:HB	1.97	0.45
1:A:176:GLN:HE22	1:A:207:GLU:HG3	1.81	0.45
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.52	0.45
2:B:336:GLN:NE2	13:B:605:HOH:O	2.48	0.45
2:D:50:ASN:H	2:D:50:ASN:ND2	2.13	0.45
4:F:101:TYR:N	4:F:126:ASP:OD1	2.42	0.45
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.98	0.45
2:B:345:GLU:H	2:B:345:GLU:CD	2.22	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.45
2:D:181:VAL:O	2:D:398:MET:HE1	2.16	0.45
1:A:88:HIS:N	1:A:91:GLN:OE1	2.42	0.45
1:C:177:VAL:O	1:C:178:SER:C	2.60	0.45
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.43	0.44
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.53	0.44
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	1.99	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.99	0.44
2:D:109:THR:O	2:D:113:GLU:HG3	2.18	0.44
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.44
4:F:320:MET:HE3	4:F:320:MET:HB3	1.80	0.43
2:B:308:ARG:NH1	13:B:608:HOH:O	2.52	0.43
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.43
2:B:250:ALA:HA	2:B:254:LYS:HD2	2.01	0.43
2:B:286:LEU:HD23	2:B:291:LEU:HD13	2.00	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.43
2:D:217:LEU:HA	2:D:277:SER:HB3	2.00	0.43
1:A:282:TYR:HA	13:A:644:HOH:O	2.19	0.43
2:D:205:ASP:HB3	2:D:303:ALA:HA	2.01	0.42
2:B:296:PHE:CE2	2:B:335:VAL:HG11	2.53	0.42
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.02	0.42
2:D:35:SER:OG	2:D:60:LYS:HE2	2.19	0.42
2:B:48:ARG:NH2	2:B:244:PHE:O	2.52	0.42
1:C:151[B]:SER:HA	1:C:194:THR:HG22	2.00	0.42
2:D:69:ASP:O	2:D:94:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.02	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.20	0.42
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.55	0.41
2:B:115:VAL:HG23	2:B:153:LEU:HD13	2.01	0.41
2:B:295:MET:HB3	2:B:295:MET:HE2	1.79	0.41
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.03	0.41
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.41
2:B:400:ARG:HE	2:B:400:ARG:HB3	1.55	0.41
4:F:55:GLU:HB3	4:F:58:LEU:HD12	2.03	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.41
1:C:190:THR:O	1:C:194:THR:HG23	2.20	0.41
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.02	0.41
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.56	0.41
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.21	0.41
2:D:250:ALA:HA	2:D:254:LYS:HD2	2.03	0.41
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.91	0.41
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.56	0.41
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.03	0.41
1:C:286:LEU:HD23	1:C:286:LEU:HA	1.94	0.40
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	0.40
2:D:7:ILE:O	2:D:137:LEU:HA	2.20	0.40
1:A:176:GLN:NE2	1:A:207:GLU:HG3	2.36	0.40
2:B:345:GLU:OE1	2:B:345:GLU:N	2.47	0.40
2:D:39:ASP:OD1	2:D:39:ASP:N	2.53	0.40
2:D:82:PRO:O	2:D:83:PHE:HB2	2.21	0.40
1:A:28:HIS:O	1:A:36:MET:HE3	2.22	0.40
2:D:69:ASP:OD1	2:D:70:LEU:N	2.54	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	441/451 (98%)	430 (98%)	11 (2%)	0	100	100
1	C	442/451 (98%)	430 (97%)	12 (3%)	0	100	100
2	B	420/445 (94%)	412 (98%)	8 (2%)	0	100	100
2	D	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
3	E	122/143 (85%)	122 (100%)	0	0	100	100
4	F	342/384 (89%)	337 (98%)	5 (2%)	0	100	100
All	All	2189/2319 (94%)	2145 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	374/379 (99%)	370 (99%)	4 (1%)	65	74
1	C	375/379 (99%)	372 (99%)	3 (1%)	73	81
2	B	367/383 (96%)	362 (99%)	5 (1%)	59	67
2	D	368/383 (96%)	359 (98%)	9 (2%)	43	49
3	E	113/127 (89%)	113 (100%)	0	100	100
4	F	310/342 (91%)	308 (99%)	2 (1%)	78	86
All	All	1907/1993 (96%)	1884 (99%)	23 (1%)	63	72

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	178	SER
1	A	381	THR
1	A	433	GLU
2	B	57	THR
2	B	86	ILE
2	B	153	LEU

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Mol	Chain	Res	Type
2	B	275	LEU
2	B	335	VAL
1	C	340	SER
1	C	381	THR
1	C	384	ILE
2	D	15	GLN
2	D	86	ILE
2	D	155	SER
2	D	179	ASP
2	D	190	SER
2	D	200	GLU
2	D	276	THR
2	D	293	GLN
2	D	423	SER
4	F	12	SER
4	F	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	101	ASN
1	A	258	ASN
1	A	301	GLN
1	A	393	HIS
2	B	192	HIS
2	B	249	ASN
2	B	258	ASN
2	B	282	GLN
2	B	436	GLN
1	C	15	GLN
1	C	133	GLN
1	C	256	GLN
1	C	356	ASN
1	C	393	HIS
2	D	15	GLN
2	D	50	ASN
2	D	247	GLN
2	D	349	ASN
2	D	406	HIS
3	E	12	ASN
4	F	242	ASN

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Mol	Chain	Res	Type
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\# Z > 2$
12	ACP	F	402	6	31,33,33	1.74	8 (25%)	47,52,52	1.97	10 (21%)
8	GOL	A	505	-	5,5,5	0.32	0	5,5,5	0.55	0
9	8WB	D	500	-	22,23,23	1.96	3 (13%)	27,31,31	1.65	4 (14%)
5	GTP	A	501	6	33,34,34	1.75	7 (21%)	50,54,54	1.55	6 (12%)
10	GDP	B	502	6	29,30,30	1.44	5 (17%)	45,47,47	1.71	7 (15%)
10	GDP	D	501	6	29,30,30	1.52	6 (20%)	45,47,47	1.70	8 (17%)
9	8WB	B	501	-	22,23,23	2.03	3 (13%)	27,31,31	1.49	5 (18%)
5	GTP	C	501	6	33,34,34	1.70	9 (27%)	50,54,54	1.43	6 (12%)
11	MES	B	505	-	12,12,12	2.00	1 (8%)	15,16,16	1.67	4 (26%)

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
12	ACP	F	402	6	-	3/19/38/38	0/3/3/3
8	GOL	A	505	-	-	2/4/4/4	-
9	8WB	D	500	-	-	2/12/12/12	0/2/2/2
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
10	GDP	B	502	6	-	5/16/32/32	0/3/3/3
10	GDP	D	501	6	-	5/16/32/32	0/3/3/3
9	8WB	B	501	-	-	2/12/12/12	0/2/2/2
5	GTP	C	501	6	-	5/22/38/38	0/3/3/3
11	MES	B	505	-	-	1/6/14/14	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	8WB	CAE-CAG	-6.88	1.39	1.48
9	D	500	8WB	CAE-CAG	-6.87	1.39	1.48
11	B	505	MES	C8-S	-6.56	1.68	1.77
5	C	501	GTP	C6-N1	-4.53	1.30	1.38
9	B	501	8WB	CAJ-CAK	-4.46	1.40	1.47
5	A	501	GTP	C6-N1	-4.21	1.31	1.38
9	D	500	8WB	CAJ-CAK	-4.09	1.41	1.47
12	F	402	ACP	PB-O1B	3.57	1.60	1.51
10	D	501	GDP	C6-N1	-3.52	1.32	1.38
5	C	501	GTP	PG-O3G	-3.43	1.42	1.54
10	D	501	GDP	C5-N7	-3.42	1.32	1.39
5	A	501	GTP	C5-N7	-3.36	1.32	1.39
12	F	402	ACP	PB-O2B	-3.31	1.48	1.56
5	A	501	GTP	C4-N9	-3.27	1.29	1.38
12	F	402	ACP	C5-N7	-3.18	1.33	1.39
12	F	402	ACP	C5-C4	3.17	1.44	1.39
10	B	502	GDP	C5-N7	-3.16	1.32	1.39
10	B	502	GDP	C6-N1	-3.11	1.33	1.38
10	B	502	GDP	C4-N9	-3.01	1.30	1.38
5	A	501	GTP	PG-O3G	-3.00	1.43	1.54
5	A	501	GTP	C8-N9	-2.97	1.30	1.37
12	F	402	ACP	C4-N9	-2.78	1.31	1.37
5	A	501	GTP	PB-O3A	-2.76	1.56	1.59
12	F	402	ACP	C8-N9	-2.75	1.32	1.37
10	D	501	GDP	C4-N9	-2.74	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C4-N9	-2.72	1.31	1.38
10	D	501	GDP	C2-N1	-2.70	1.31	1.37
5	A	501	GTP	C2-N1	-2.68	1.31	1.37
5	C	501	GTP	PB-O3A	-2.64	1.56	1.59
12	F	402	ACP	PG-O2G	2.60	1.60	1.55
5	C	501	GTP	C5-N7	-2.55	1.34	1.39
12	F	402	ACP	PG-O3G	2.49	1.60	1.55
10	B	502	GDP	C8-N9	-2.42	1.32	1.37
5	C	501	GTP	C8-N9	-2.41	1.32	1.37
10	B	502	GDP	C2-N1	-2.35	1.31	1.37
10	D	501	GDP	C5-C4	2.27	1.44	1.38
9	B	501	8WB	OAU-CAD	-2.25	1.34	1.38
5	C	501	GTP	PA-O2A	-2.21	1.45	1.55
5	C	501	GTP	C5-C4	2.10	1.44	1.38
9	D	500	8WB	CAM-CAG	-2.09	1.39	1.44
5	C	501	GTP	C2-N1	-2.04	1.32	1.37
10	D	501	GDP	C8-N9	-2.02	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	C5-C4-N3	-5.93	118.55	126.72
10	D	501	GDP	C5-C4-N3	-5.59	119.49	128.39
10	B	502	GDP	C5-C4-N3	-5.43	119.75	128.39
12	F	402	ACP	N3-C4-N9	5.37	136.30	127.17
5	A	501	GTP	C5-C4-N3	-4.93	120.55	128.39
9	D	500	8WB	OAO-CAJ-CAK	4.90	114.11	109.60
5	C	501	GTP	C5-C4-N3	-4.64	121.00	128.39
10	B	502	GDP	C2-N3-C4	4.45	119.96	112.30
10	D	501	GDP	C2-N3-C4	4.40	119.87	112.30
11	B	505	MES	C5-N4-C3	4.29	118.08	108.84
12	F	402	ACP	C4-N9-C8	4.26	110.21	105.74
5	C	501	GTP	N9-C4-N3	4.19	134.34	125.95
5	A	501	GTP	C2-N3-C4	4.18	119.50	112.30
9	B	501	8WB	OAO-CAJ-CAK	4.06	113.33	109.60
12	F	402	ACP	C2-N3-C4	3.96	121.51	111.83
12	F	402	ACP	N3-C2-N1	-3.90	122.67	128.58
5	A	501	GTP	C6-C5-N7	3.87	137.32	130.29
10	B	502	GDP	N9-C4-N3	3.83	133.62	125.95
5	A	501	GTP	N9-C4-N3	3.83	133.61	125.95
10	D	501	GDP	C6-C5-N7	3.74	137.09	130.29
10	D	501	GDP	N9-C4-N3	3.63	133.21	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	502	GDP	C6-C5-N7	3.45	136.56	130.29
9	D	500	8WB	CAL-CAK-CAJ	3.31	126.77	121.64
9	B	501	8WB	CAL-CAK-CAJ	3.30	126.75	121.64
5	C	501	GTP	C2-N3-C4	3.25	117.90	112.30
12	F	402	ACP	PB-O3A-PA	-3.21	121.89	132.37
5	C	501	GTP	C6-C5-N7	3.07	135.88	130.29
9	D	500	8WB	CAR-OAQ-CAB	-3.04	113.05	117.51
10	B	502	GDP	O6-C6-C5	-2.98	118.66	126.53
12	F	402	ACP	N9-C8-N7	-2.90	109.82	113.94
10	D	501	GDP	C4-C5-N7	-2.88	106.11	110.67
11	B	505	MES	O1S-S-C8	2.87	111.06	106.73
12	F	402	ACP	C4-C5-N7	-2.77	107.42	110.58
5	C	501	GTP	C8-N9-C4	2.57	110.83	106.03
5	A	501	GTP	C4-C5-N7	-2.55	106.63	110.67
10	B	502	GDP	C4-C5-N7	-2.53	106.67	110.67
12	F	402	ACP	C5-N7-C8	2.51	107.39	103.45
11	B	505	MES	O2S-S-C8	2.44	110.42	106.73
10	D	501	GDP	O2A-PA-O3A	2.33	113.57	107.27
9	B	501	8WB	CAP-OAO-CAJ	2.27	121.38	116.96
10	B	502	GDP	O4'-C1'-N9	-2.27	103.21	108.36
10	D	501	GDP	O4'-C1'-N9	-2.20	103.36	108.36
5	C	501	GTP	C4-C5-N7	-2.15	107.27	110.67
9	D	500	8WB	CAP-OAO-CAJ	2.13	121.11	116.96
10	D	501	GDP	C2'-C1'-N9	2.12	119.14	113.25
9	B	501	8WB	CAR-OAQ-CAB	-2.11	114.42	117.51
9	B	501	8WB	CAE-CAG-CAM	2.10	119.02	117.11
11	B	505	MES	C7-N4-C5	2.08	116.77	111.24
5	A	501	GTP	C8-N9-C4	2.04	109.84	106.03
12	F	402	ACP	C5-C6-N6	-2.01	118.31	123.29

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	505	GOL	O1-C1-C2-C3
9	B	501	8WB	CAD-CAE-CAG-CAM

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Mol	Chain	Res	Type	Atoms
9	D	500	8WB	CAD-CAE-CAG-CAM
10	B	502	GDP	C5'-O5'-PA-O3A
10	B	502	GDP	C5'-O5'-PA-O1A
10	B	502	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O1A
11	B	505	MES	C8-C7-N4-C5
8	A	505	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O3G
10	D	501	GDP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O3A
9	B	501	8WB	CAD-CAE-CAG-CAH
9	D	500	8WB	CAD-CAE-CAG-CAH
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
10	B	502	GDP	PB-O3A-PA-O1A
10	B	502	GDP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O1A
10	D	501	GDP	PB-O3A-PA-O2A

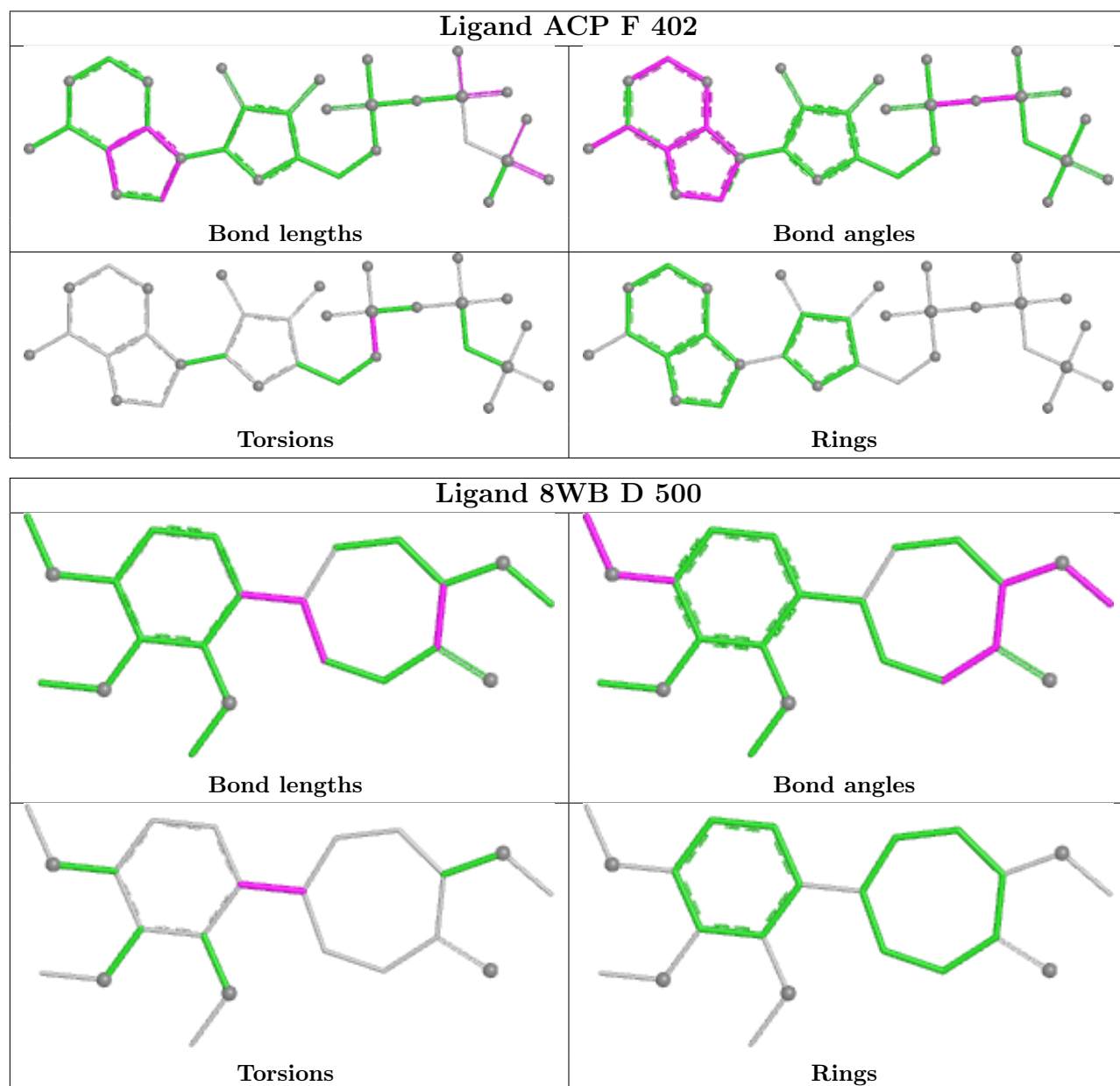
There are no ring outliers.

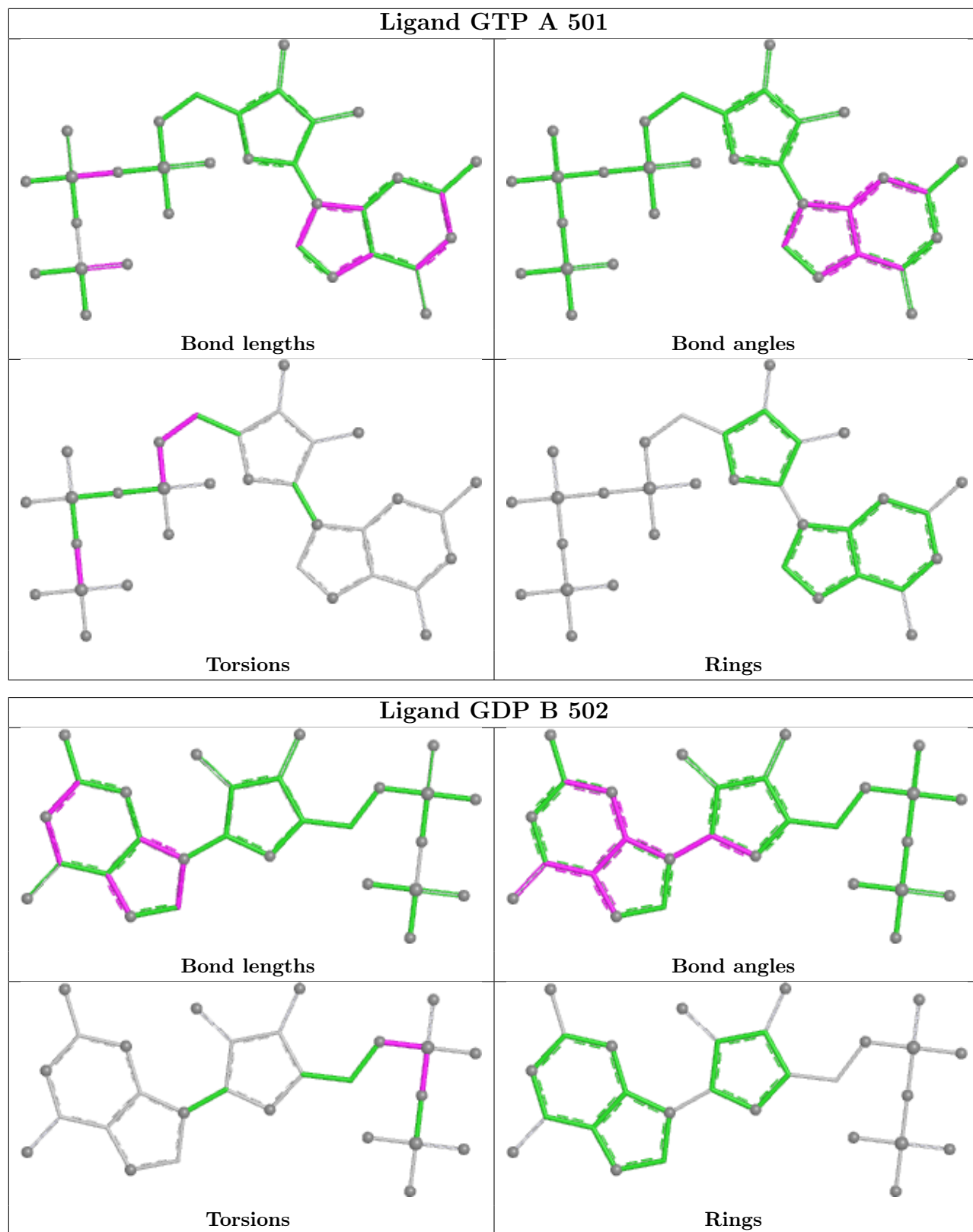
3 monomers are involved in 3 short contacts:

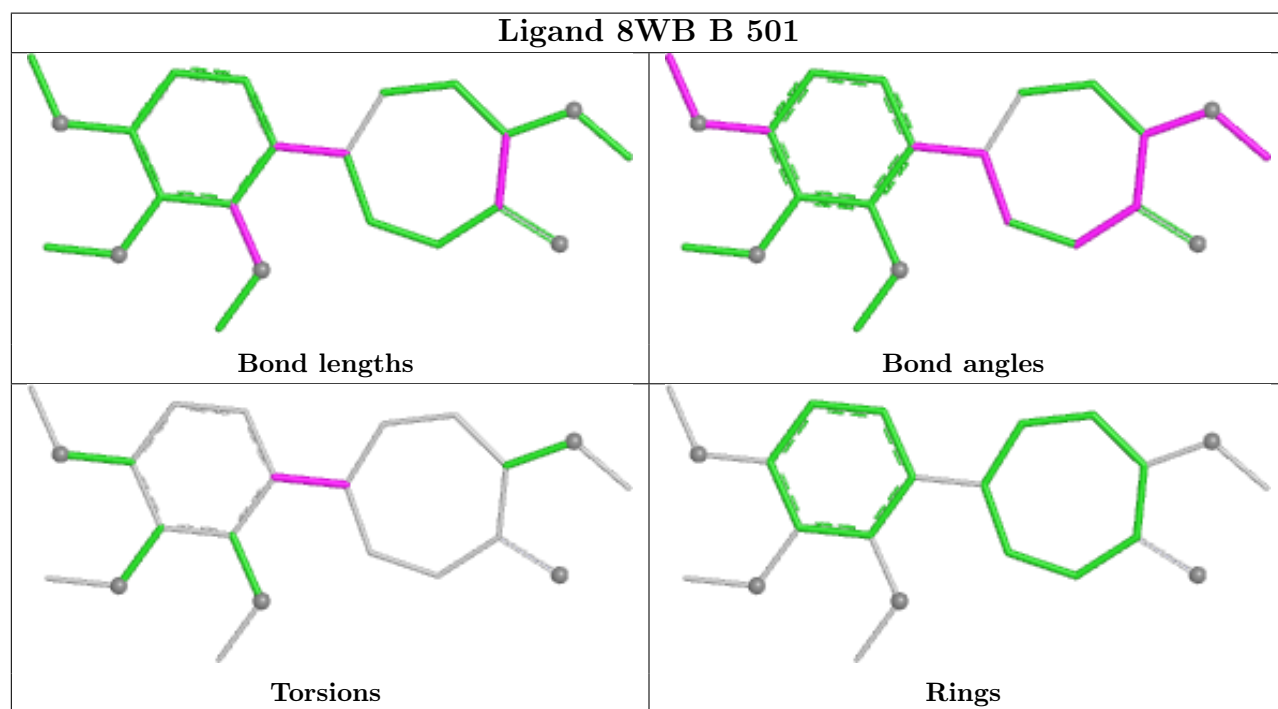
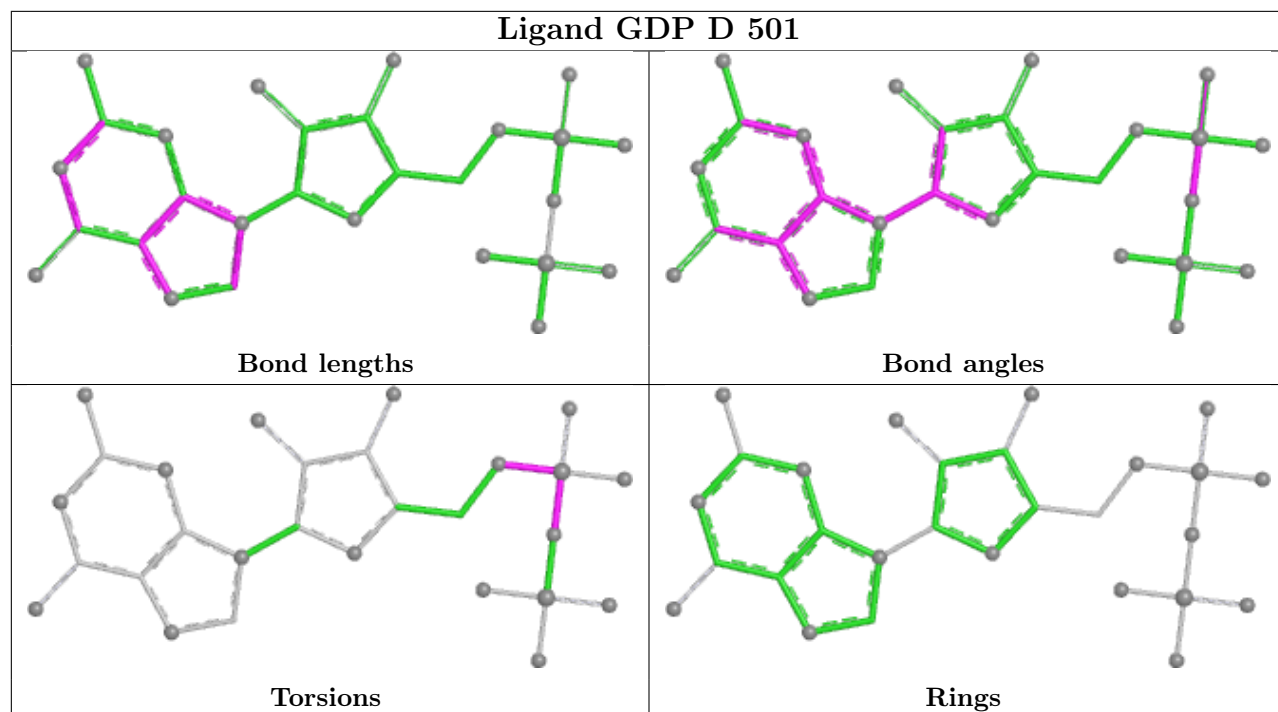
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	505	GOL	1	0
10	D	501	GDP	1	0
9	B	501	8WB	1	0

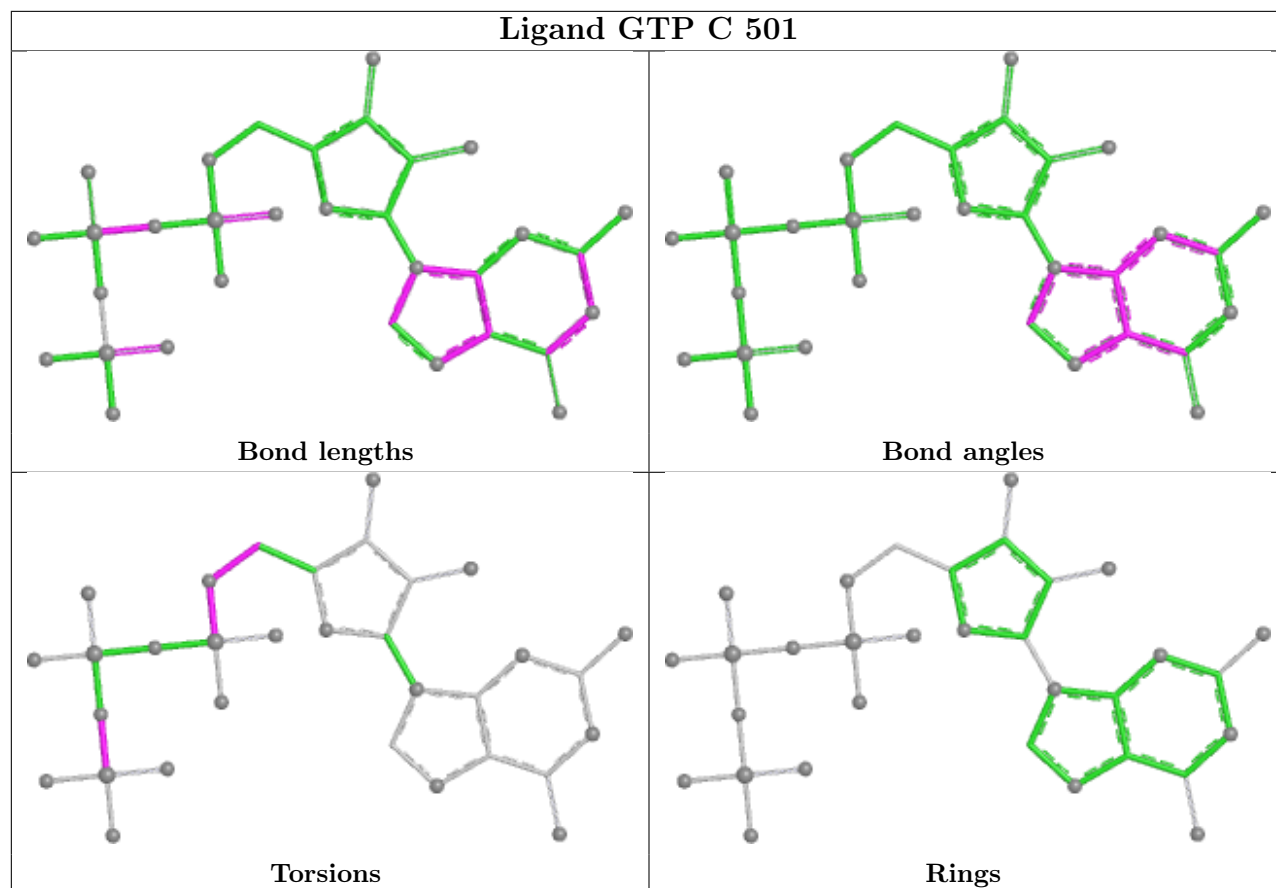
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	440/451 (97%)	-0.02	6 (1%)	73	75	29, 52, 85, 127	3 (0%)
1	C	440/451 (97%)	-0.30	9 (2%)	65	67	21, 39, 67, 113	4 (0%)
2	B	424/445 (95%)	0.03	14 (3%)	49	51	28, 49, 85, 132	2 (0%)
2	D	426/445 (95%)	0.28	21 (4%)	35	37	36, 62, 98, 131	3 (0%)
3	E	125/143 (87%)	0.49	8 (6%)	25	27	31, 66, 109, 126	1 (0%)
4	F	347/384 (90%)	0.61	24 (6%)	23	24	29, 80, 146, 172	1 (0%)
All	All	2202/2319 (94%)	0.12	82 (3%)	45	47	21, 55, 109, 172	14 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	438	ALA	4.7
2	B	276	THR	4.0
2	D	250	ALA	3.9
1	C	178	SER	3.8
4	F	179	VAL	3.7
4	F	102	PRO	3.6
4	F	90	SER	3.6
4	F	379	HIS	3.6
1	A	282	TYR	3.5
1	A	440	VAL	3.5
4	F	161	LEU	3.4
4	F	153	ALA	3.4
1	C	340	SER	3.4
2	D	281	GLN	3.4
2	D	325	MET	3.3
3	E	28	SER	3.3
2	D	279	GLY	3.3
2	D	2	ARG	3.3
1	C	440	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	439	THR	3.1
1	A	262	TYR	3.1
4	F	231	ALA	3.1
2	D	277	SER	3.0
2	D	276	THR	3.0
2	D	407	TRP	3.0
2	B	325	MET	2.8
3	E	6	MET	2.8
2	D	57	THR	2.8
4	F	32	LYS	2.8
4	F	144	GLY	2.8
2	D	286	LEU	2.8
2	D	82	PRO	2.8
1	C	247	ALA	2.7
4	F	132	LEU	2.7
4	F	372	THR	2.6
4	F	186	LEU	2.6
1	C	357	TYR	2.6
2	B	2	ARG	2.6
2	D	404	PHE	2.6
2	B	284	ARG	2.6
3	E	25	LYS	2.6
2	D	245	PRO	2.6
2	D	373	MET	2.5
1	A	362	VAL	2.5
3	E	8	VAL	2.5
2	B	275	LEU	2.4
4	F	184	LYS	2.4
3	E	144	SER	2.4
4	F	134	ALA	2.4
2	B	277	SER	2.3
2	B	333	LEU	2.3
2	D	293	GLN	2.3
3	E	143	ALA	2.3
4	F	44	ARG	2.3
4	F	233	PHE	2.3
1	A	334	THR	2.3
2	D	219	LEU	2.3
3	E	24	LEU	2.3
4	F	154	GLY	2.2
4	F	159	GLY	2.2
1	C	248	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	339	ASN	2.2
1	C	347	CYS	2.2
2	D	217	LEU	2.2
4	F	169	LEU	2.2
1	C	341	ILE	2.1
4	F	131	PHE	2.1
2	B	247	GLN	2.1
2	D	248	LEU	2.1
4	F	142	ARG	2.1
2	D	220	THR	2.1
4	F	155	ALA	2.1
2	D	280	SER	2.1
3	E	142	GLU	2.1
2	B	338	LYS	2.1
2	B	285	ALA	2.1
1	A	88	HIS	2.1
4	F	45	ASN	2.0
2	B	128	SER	2.0
4	F	362	ALA	2.0
1	C	45	GLY	2.0
2	D	58	GLY	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.

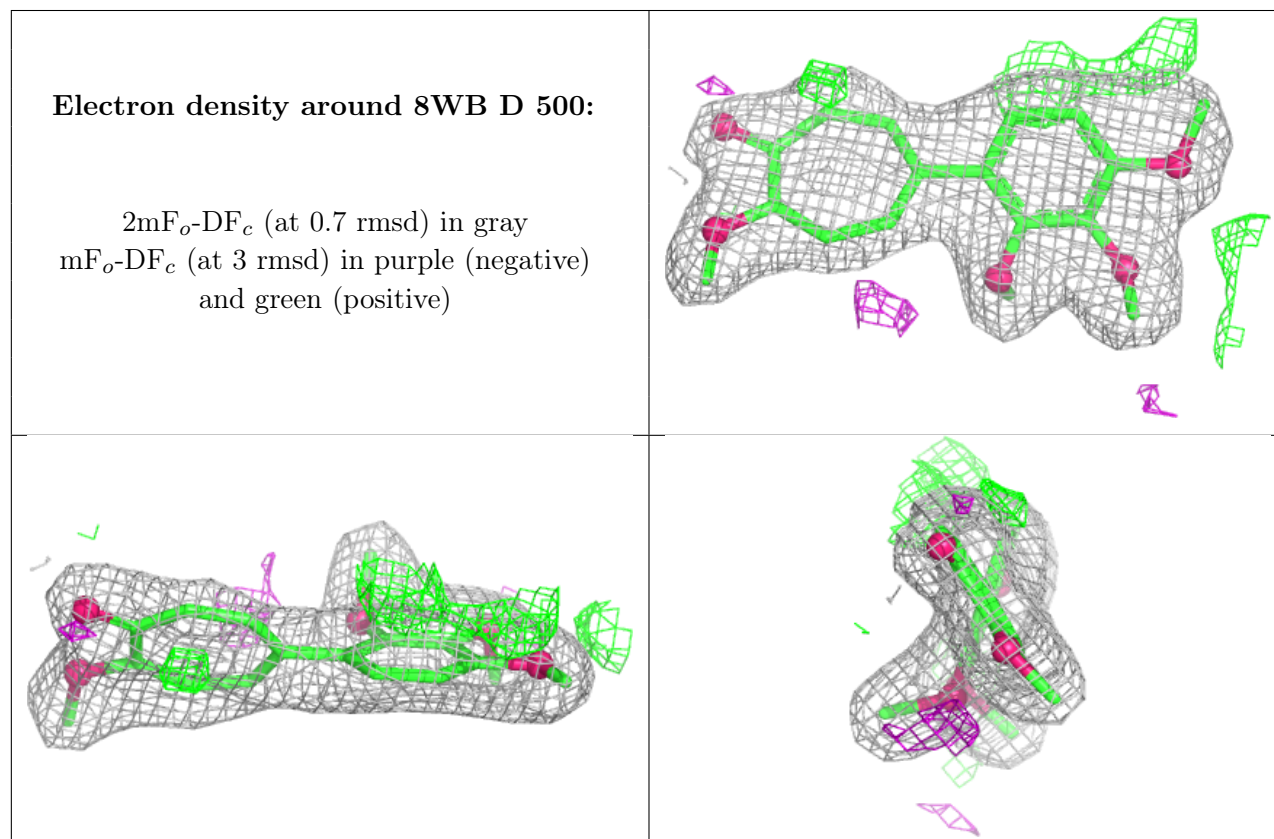
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	A	505	6/6	0.87	0.15	72,73,75,76	0
11	MES	B	505	12/12	0.90	0.12	55,61,71,82	0

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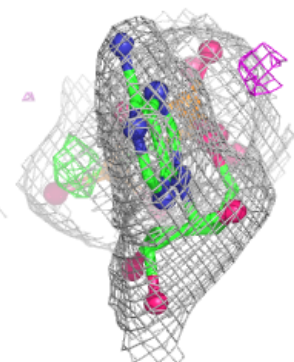
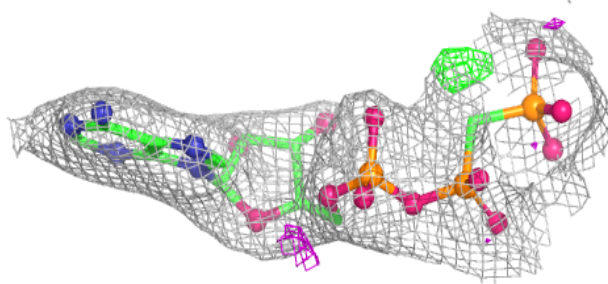
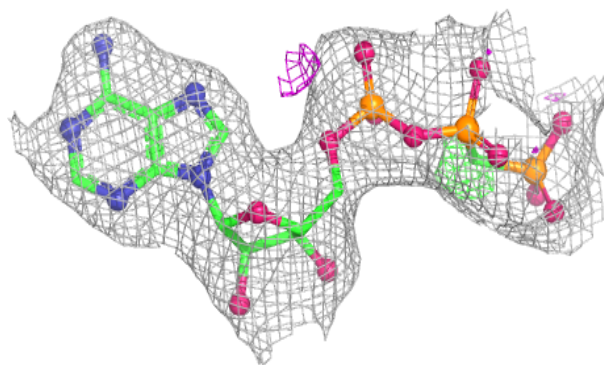
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	8WB	D	500	22/22	0.92	0.11	33,44,48,50	22
12	ACP	F	402	31/31	0.93	0.08	83,90,105,118	0
10	GDP	D	501	28/28	0.94	0.08	46,53,61,63	0
7	CA	A	504	1/1	0.95	0.08	96,96,96,96	0
6	MG	F	401	1/1	0.96	0.06	72,72,72,72	0
6	MG	D	502	1/1	0.97	0.04	58,58,58,58	0
9	8WB	B	501	22/22	0.97	0.07	33,41,48,49	0
7	CA	B	504	1/1	0.97	0.08	86,86,86,86	0
10	GDP	B	502	28/28	0.98	0.05	29,34,38,40	0
7	CA	A	503	1/1	0.98	0.05	69,69,69,69	0
6	MG	B	503	1/1	0.99	0.04	27,27,27,27	0
5	GTP	A	501	32/32	0.99	0.04	26,35,38,42	0
7	CA	C	503	1/1	0.99	0.04	54,54,54,54	0
5	GTP	C	501	32/32	0.99	0.04	27,30,34,34	0
6	MG	A	502	1/1	0.99	0.02	34,34,34,34	0
6	MG	C	502	1/1	1.00	0.04	32,32,32,32	0

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



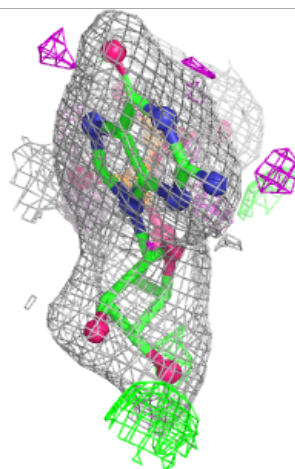
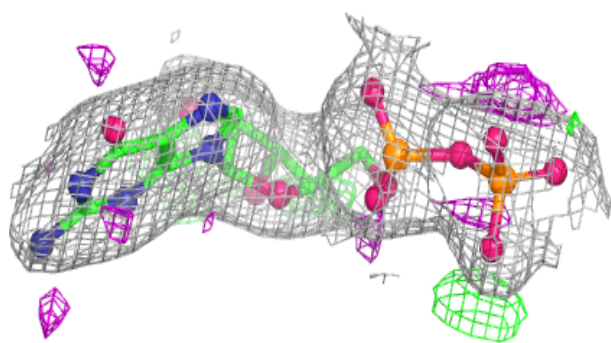
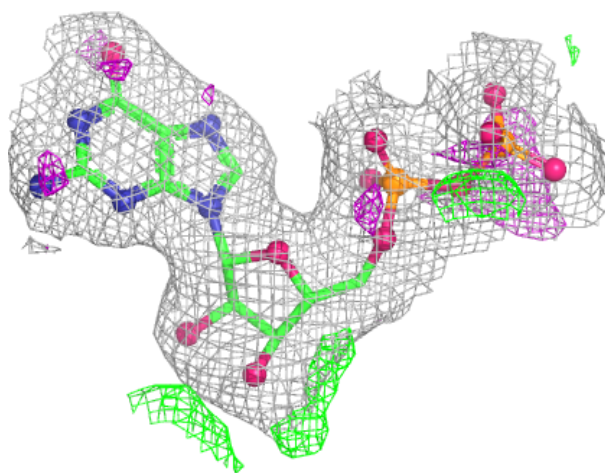
Electron density around ACP F 402:

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



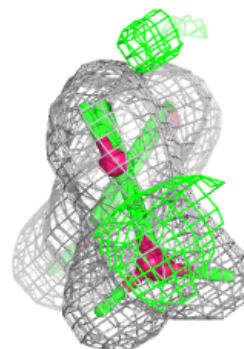
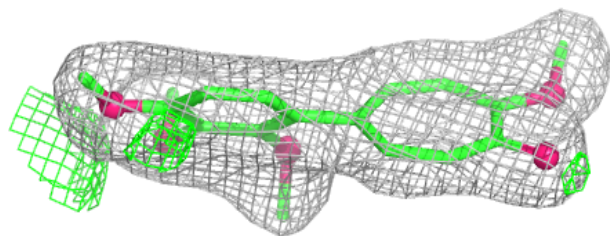
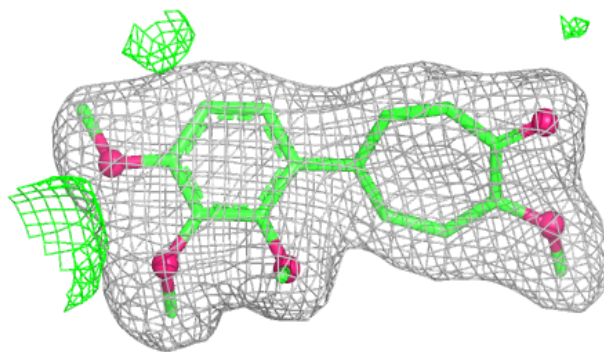
Electron density around GDP D 501:

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



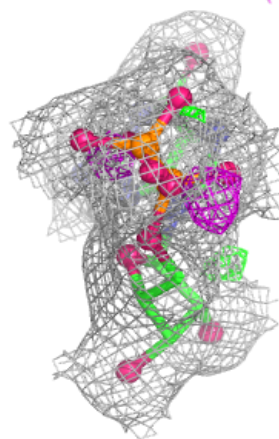
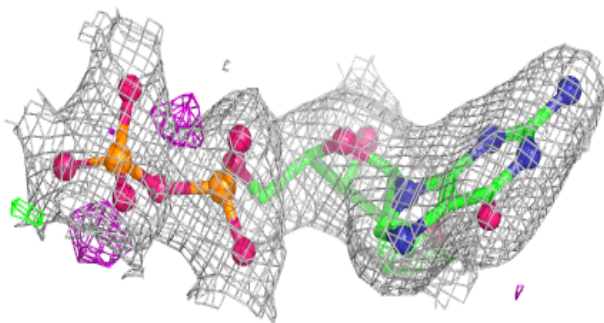
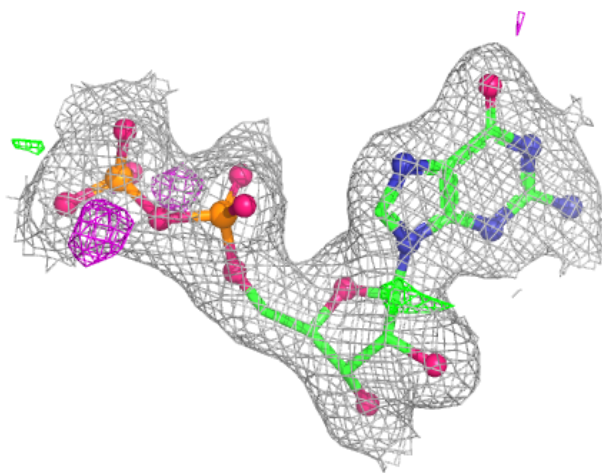
Electron density around 8WB B 501:

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



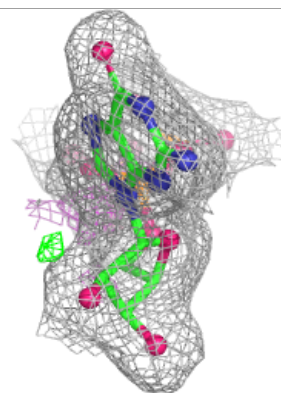
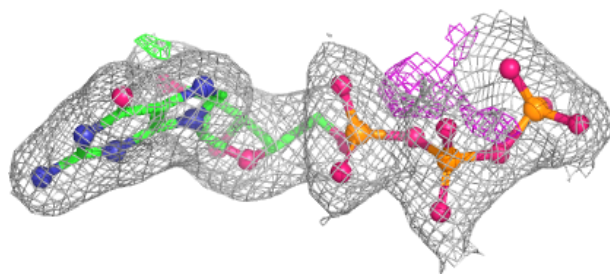
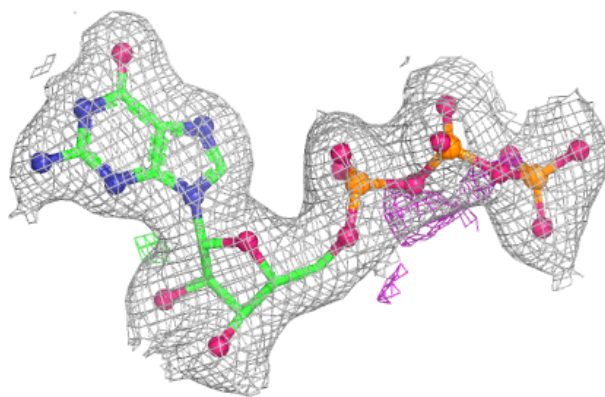
Electron density around GDP B 502:

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

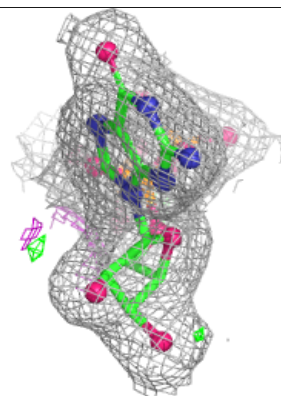
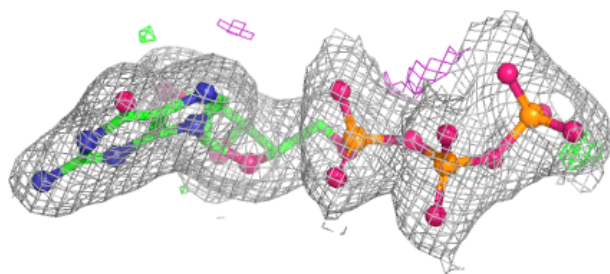
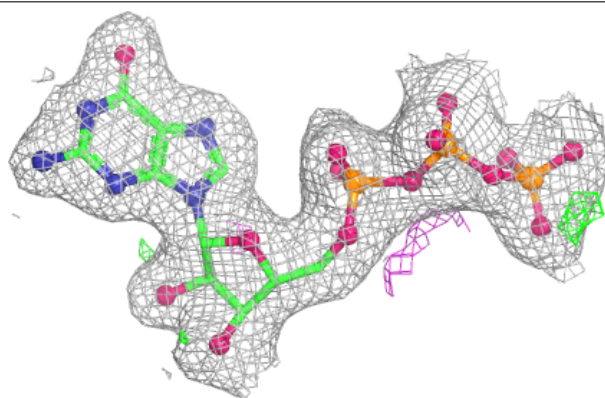


Electron density around GTP A 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.