



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:17 PM UTC

PDB ID : 5YL2 / pdb_00005yl2
Title : Crystal structure of T2R-TTL-Y28 complex
Authors : Yang, J.H.; Yang, T.; Wen, J.L.; Chen, L.J.
Deposited on : 2017-10-16
Resolution : 2.09 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

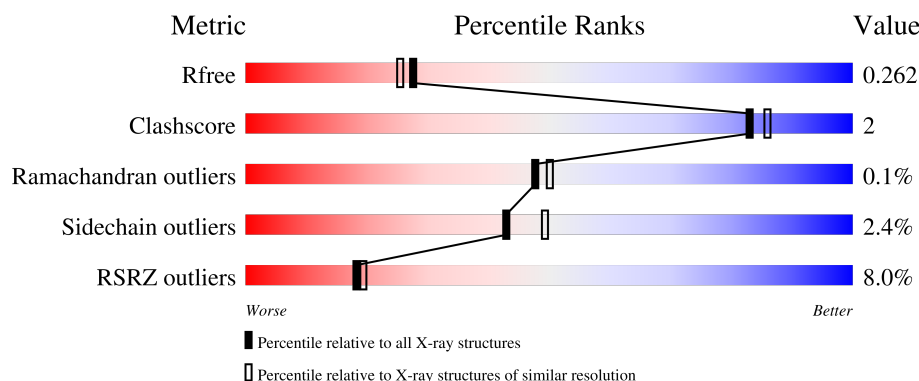
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	2% 88% 8% .
1	C	451	2% 89% 8% ..
2	B	445	2% 89% 7% .
2	D	445	13% 86% 9% 5%
3	E	143	14% 80% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	19% 80% 6% 13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18366 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	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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		
5	D	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		

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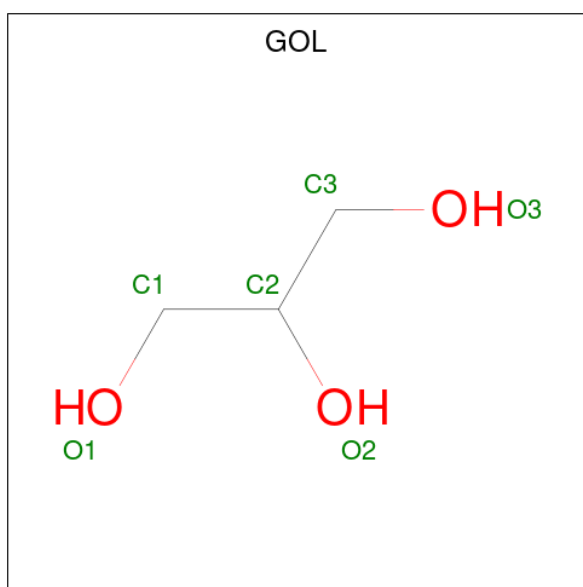
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

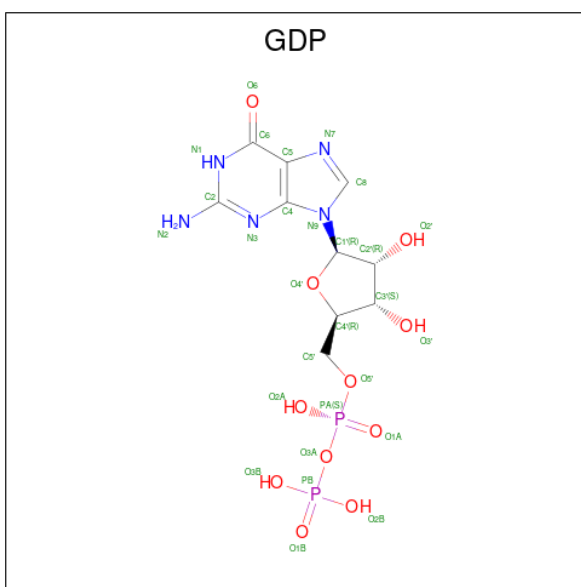
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



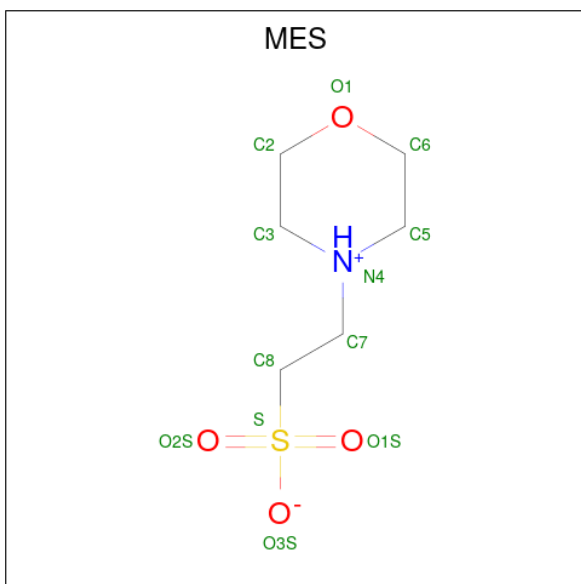
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



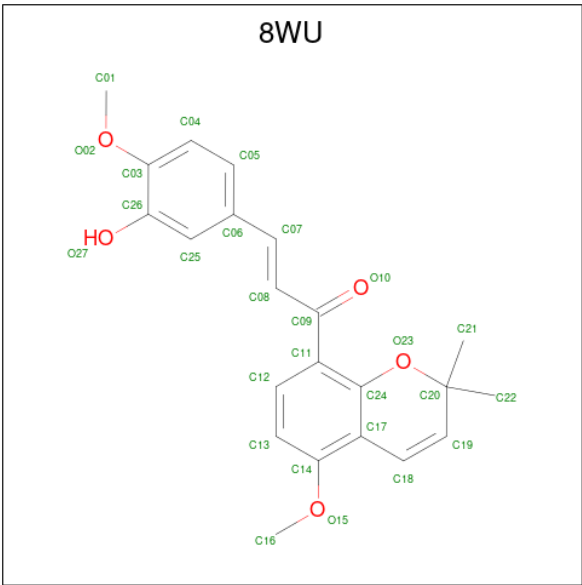
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



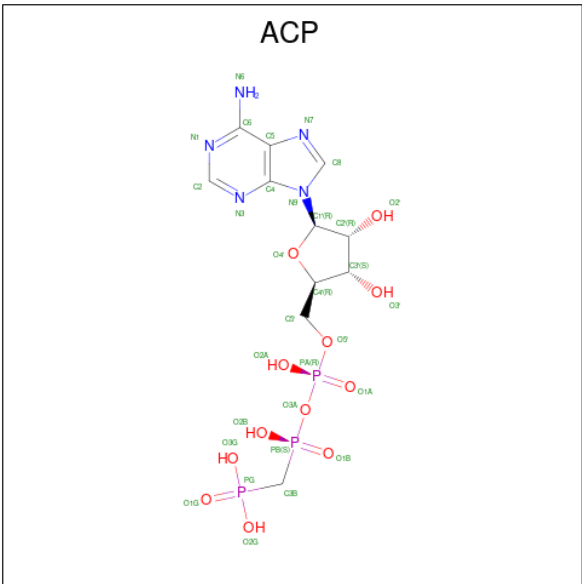
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (E)-1-(5-methoxy-2,2-dimethyl-chromen-8-yl)-3-(4-methoxy-3-oxidanyl-phenyl)prop-2-en-1-one (CCD ID: 8WU) (formula: C₂₂H₂₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			27	22	5		
11	D	1	Total	C	O	0	0
			27	22	5		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

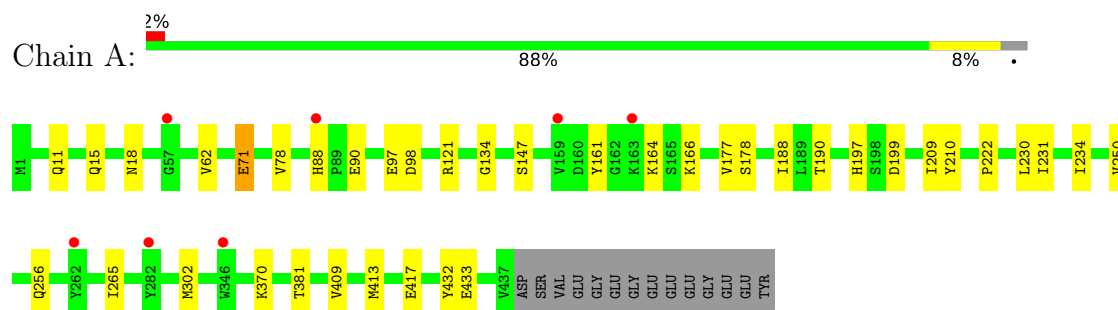
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	204	Total 204	O 204	0	0
13	B	145	Total 145	O 145	0	0
13	C	292	Total 292	O 292	0	0
13	D	81	Total 81	O 81	0	0
13	E	37	Total 37	O 37	0	0
13	F	99	Total 99	O 99	0	0

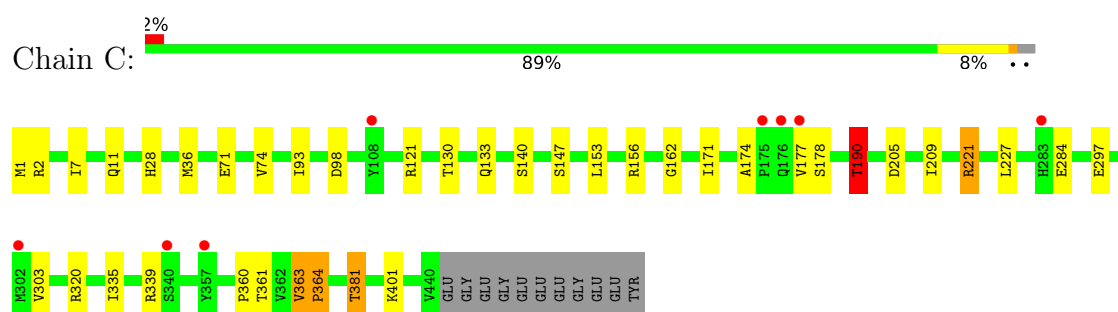
3 Residue-property plots [i](#)

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.

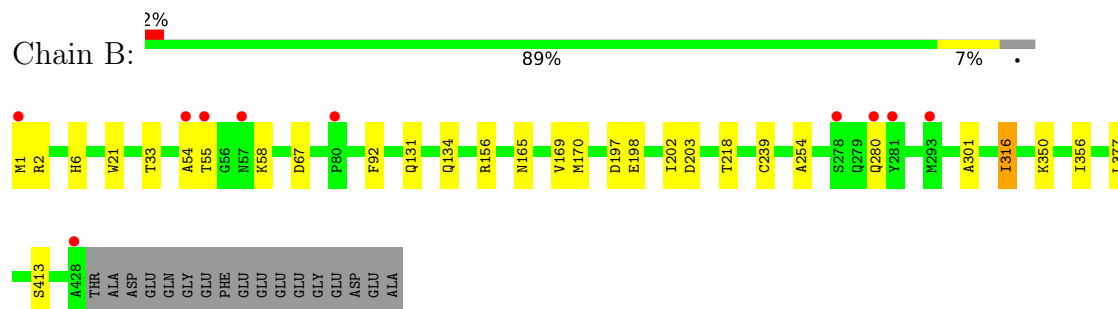
- Molecule 1: Tubulin alpha-1B chain



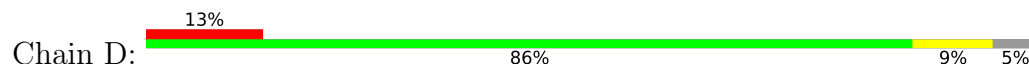
- Molecule 1: Tubulin alpha-1B chain

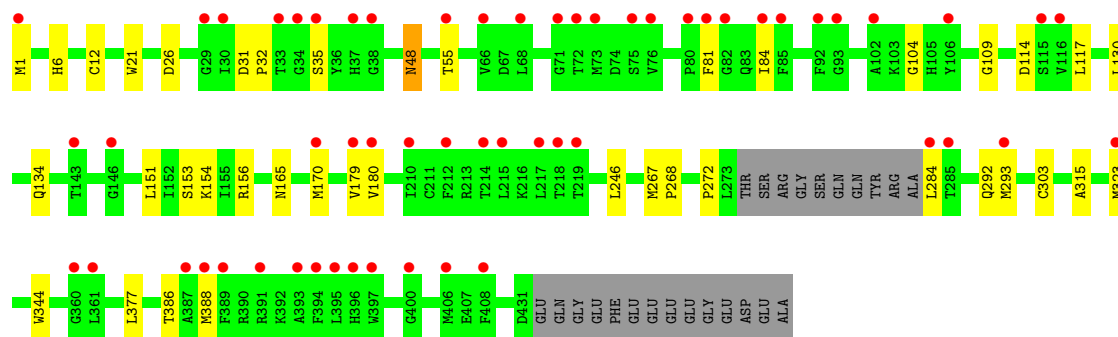


- Molecule 2: Tubulin beta chain

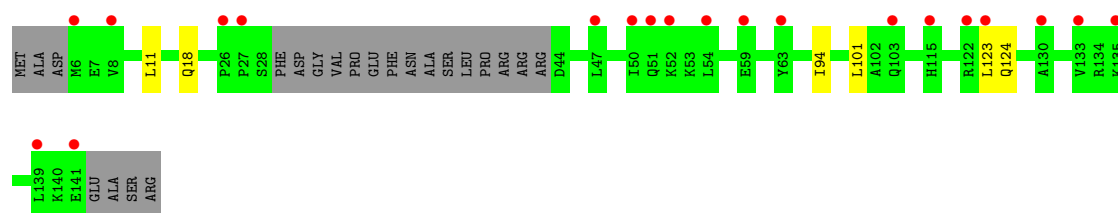
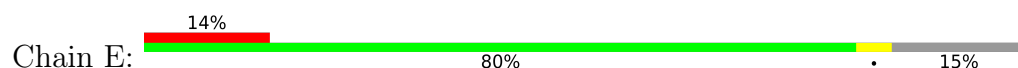


- Molecule 2: Tubulin beta chain

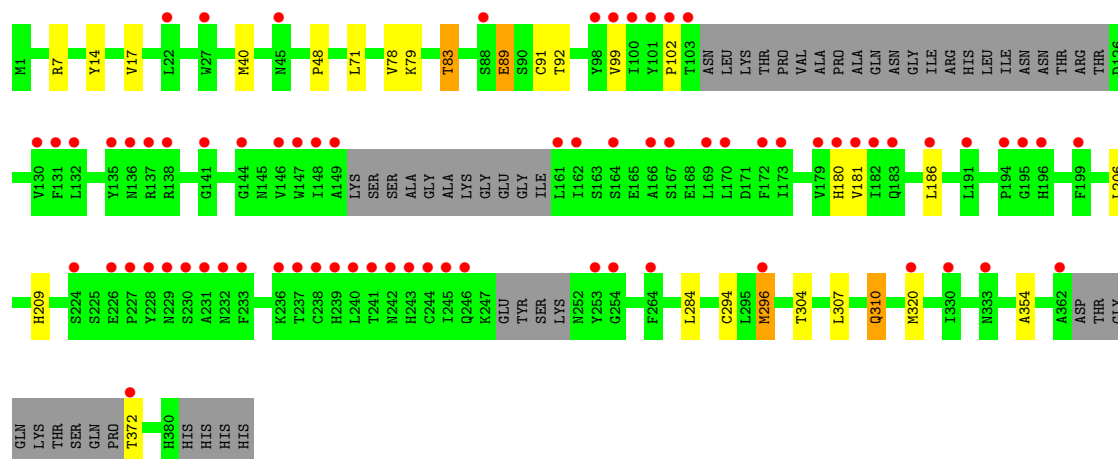
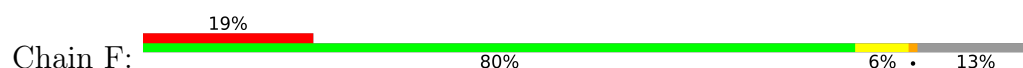




• Molecule 3: Stathmin-4



• 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	105.54Å 158.20Å 181.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.09 50.01 – 2.09	Depositor EDS
% Data completeness (in resolution range)	57.7 (50.01-2.09) 57.7 (50.01-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.209 , 0.254 (Not available) , 0.262	Depositor DCC
R_{free} test set	5217 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.4	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	0.94	EDS
Total number of atoms	18366	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: GTP, MG, MES, GOL, ACP, GDP, 8WU, CA

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	0.57	0/3494	0.97	1/4743 (0.0%)
1	C	0.57	0/3515	0.96	3/4772 (0.1%)
2	B	0.59	0/3444	0.94	1/4664 (0.0%)
2	D	0.56	0/3382	0.98	0/4581
3	E	0.50	0/1008	0.99	0/1337
4	F	0.63	0/2806	0.91	1/3791 (0.0%)
All	All	0.58	0/17649	0.96	6/23888 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	THR	CB-CA-C	-5.92	100.78	110.85
1	C	363	VAL	CA-C-N	5.86	127.17	119.84
1	C	363	VAL	C-N-CA	5.86	127.17	119.84
4	F	92	THR	N-CA-C	5.44	119.02	112.38
1	A	134	GLY	N-CA-C	5.25	117.67	110.58
2	B	54	ALA	N-CA-C	5.15	118.09	109.96

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	3416	0	3331	19	0
1	C	3437	0	3348	23	0
2	B	3369	0	3250	13	0
2	D	3309	0	3189	18	0
3	E	1000	0	1018	5	0
4	F	2744	0	2709	13	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	2	0
11	B	27	0	0	0	0
11	D	27	0	0	0	0
12	F	31	0	14	0	0
13	A	204	0	0	2	0
13	B	145	0	0	0	0
13	C	292	0	0	3	0
13	D	81	0	0	1	0
13	E	37	0	0	0	0
13	F	99	0	0	0	0
All	All	18366	0	16928	83	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 2.

All (83) 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)
4:F:79:LYS:O	4:F:83:THR:OG1	1.72	1.07
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.60	0.84
1:A:209:ILE:HD11	1:A:302:MET:SD	2.27	0.75
2:B:1:MET:HB2	2:B:131:GLN:HB3	1.76	0.66
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.79	0.65
1:A:97:GLU:HB2	2:B:1:MET:HE2	1.79	0.64
1:C:381:THR:CG2	13:C:615:HOH:O	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:GLU:HG2	1:C:339:ARG:HH22	1.68	0.58
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.86	0.58
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.86	0.57
2:D:1:MET:HG3	2:D:48:ASN:HB2	1.85	0.56
1:C:221:ARG:HH11	2:D:323:MET:HB3	1.70	0.56
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.86	0.56
1:C:381:THR:HG23	13:C:615:HOH:O	2.05	0.56
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.89	0.53
1:C:147:SER:O	1:C:190:THR:HG23	2.09	0.53
1:C:1:MET:HB3	1:C:130:THR:OG1	2.09	0.53
4:F:296:MET:HE3	4:F:296:MET:HA	1.90	0.52
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.92	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
2:B:197:ASP:OD1	10:B:503:MES:H32	2.11	0.51
2:B:156:ARG:HG3	10:B:503:MES:H62	1.93	0.50
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.94	0.50
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.93	0.50
1:C:320:ARG:HG3	1:C:360:PRO:HD3	1.94	0.49
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.77	0.49
1:A:231:ILE:HD11	13:A:672:HOH:O	2.13	0.49
1:C:156:ARG:HD2	3:E:101:LEU:HD21	1.95	0.48
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.96	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.48
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.15	0.47
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.97	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.47
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.97	0.47
1:A:178:SER:O	2:B:350:LYS:HE2	2.15	0.47
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.98	0.46
4:F:14:TYR:HA	4:F:17:VAL:HB	1.98	0.46
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.96	0.45
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.99	0.45
2:D:267:MET:HA	2:D:268:PRO:HD3	1.85	0.45
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.99	0.44
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.98	0.44
2:D:117:LEU:HD21	2:D:154:LYS:HB3	1.99	0.44
4:F:99:VAL:HA	4:F:181:VAL:HG22	2.00	0.44
1:A:88:HIS:HD2	1:A:90:GLU:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:CD	3:E:101:LEU:HD21	2.48	0.44
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.43
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.01	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.43
2:B:239:CYS:SG	2:B:316:ILE:HD13	2.59	0.43
2:D:272:PRO:HB3	2:D:284:LEU:HD12	2.00	0.43
4:F:40:MET:HE1	4:F:48:PRO:HD2	2.01	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
1:A:88:HIS:HE1	13:A:666:HOH:O	2.00	0.43
1:C:174:ALA:O	1:C:178:SER:HB3	2.19	0.42
2:D:293:MET:HE1	2:D:315:ALA:HB1	2.00	0.42
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.84	0.42
2:B:170:MET:HG3	2:B:377:LEU:HD11	2.01	0.42
1:C:360:PRO:HB2	13:C:758:HOH:O	2.19	0.42
2:D:31:ASP:HB2	2:D:35:SER:H	1.83	0.42
1:C:28:HIS:O	1:C:36:MET:HE3	2.20	0.42
2:D:12:CYS:HB2	5:D:501:GTP:C8	2.55	0.42
2:D:284:LEU:HD13	2:D:292:GLN:HE22	1.84	0.42
1:C:363:VAL:HA	1:C:364:PRO:HD2	1.80	0.42
4:F:7:ARG:HD3	4:F:40:MET:HE3	2.01	0.42
2:B:198:GLU:OE2	2:B:254:ALA:HB2	2.20	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.41
1:A:11:GLN:O	1:A:15:GLN:HG3	2.21	0.41
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.56	0.41
2:D:267:MET:HE1	2:D:303:CYS:HB2	2.03	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.20	0.41
2:B:203:ASP:HB2	2:B:301:ALA:HA	2.02	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.21	0.40
4:F:89:GLU:C	4:F:91:CYS:H	2.28	0.40
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.03	0.40
2:D:32:PRO:HB3	13:D:605:HOH:O	2.20	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.22	0.40
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.57	0.40
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.40
2:D:104:GLY:O	2:D:109:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	424 (98%)	11 (2%)	0	100	100
1	C	438/451 (97%)	428 (98%)	9 (2%)	1 (0%)	43	44
2	B	426/445 (96%)	409 (96%)	17 (4%)	0	100	100
2	D	417/445 (94%)	406 (97%)	11 (3%)	0	100	100
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	308 (95%)	15 (5%)	1 (0%)	36	36
All	All	2157/2319 (93%)	2090 (97%)	65 (3%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	102	PRO
1	C	364	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	359 (98%)	9 (2%)	43	49
1	C	371/379 (98%)	363 (98%)	8 (2%)	45	53
2	B	370/383 (97%)	361 (98%)	9 (2%)	43	49
2	D	364/383 (95%)	352 (97%)	12 (3%)	33	37
3	E	109/127 (86%)	108 (99%)	1 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	F	301/342 (88%)	294 (98%)	7 (2%)	44 51
All	All	1883/1993 (94%)	1837 (98%)	46 (2%)	43 49

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	71	GLU
1	A	177	VAL
1	A	188	ILE
1	A	234	ILE
1	A	250	VAL
1	A	370	LYS
1	A	381	THR
1	A	433	GLU
2	B	2	ARG
2	B	33	THR
2	B	55	THR
2	B	58	LYS
2	B	218	THR
2	B	280	GLN
2	B	316	ILE
2	B	356	ILE
2	B	413	SER
1	C	2	ARG
1	C	133	GLN
1	C	177	VAL
1	C	190	THR
1	C	221	ARG
1	C	284	GLU
1	C	361	THR
1	C	381	THR
2	D	26	ASP
2	D	48	ASN
2	D	55	THR
2	D	114	ASP
2	D	130	LEU
2	D	151	LEU
2	D	153	SER
2	D	179	VAL
2	D	180	VAL
2	D	246	LEU

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Mol	Chain	Res	Type
2	D	386	THR
2	D	388	MET
3	E	124	GLN
4	F	83	THR
4	F	89	GLU
4	F	180	HIS
4	F	284	LEU
4	F	296	MET
4	F	310	GLN
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	309	HIS
1	A	342	GLN
1	A	356	ASN
1	A	358	GLN
1	A	393	HIS
2	B	43	GLN
2	B	48	ASN
2	B	83	GLN
2	B	165	ASN
2	B	227	HIS
2	B	245	GLN
2	B	329	GLN
2	B	332	ASN
2	B	384	GLN
2	B	426	GLN
1	C	11	GLN
1	C	85	GLN
1	C	128	GLN
1	C	372	GLN
2	D	292	GLN
2	D	329	GLN
2	D	332	ASN
2	D	347	ASN
2	D	416	ASN
3	E	18	GLN
3	E	90	ASN
3	E	92	ASN

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Mol	Chain	Res	Type
4	F	45	ASN
4	F	229	ASN
4	F	232	ASN
4	F	252	ASN
4	F	260	ASN
4	F	333	ASN
4	F	379	HIS

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 15 ligands modelled in this entry, 6 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	$\# Z > 2$
10	MES	B	503	-	12,12,12	2.11	2 (16%)	15,16,16	6.18	8 (53%)
8	GOL	A	504	-	5,5,5	0.29	0	5,5,5	0.23	0
12	ACP	F	401	-	31,33,33	2.05	10 (32%)	47,52,52	1.79	9 (19%)
5	GTP	A	501	6	33,34,34	1.35	5 (15%)	50,54,54	1.59	7 (14%)
5	GTP	D	501	6	33,34,34	1.37	6 (18%)	50,54,54	1.62	5 (10%)
11	8WU	B	504	-	29,29,29	2.87	12 (41%)	42,42,42	1.61	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GDP	B	501	6	29,30,30	1.14	3 (10%)	45,47,47	1.80	6 (13%)
5	GTP	C	501	6	33,34,34	1.35	6 (18%)	50,54,54	1.61	5 (10%)
11	8WU	D	503	-	29,29,29	2.95	13 (44%)	42,42,42	1.55	8 (19%)

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
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
8	GOL	A	504	-	-	1/4/4/4	-
12	ACP	F	401	-	-	3/19/38/38	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
5	GTP	D	501	6	-	5/22/38/38	0/3/3/3
11	8WU	B	504	-	-	6/13/24/24	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
11	8WU	D	503	-	-	8/13/24/24	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	8WU	C18-C19	8.79	1.44	1.33
11	B	504	8WU	C18-C19	8.39	1.43	1.33
11	D	503	8WU	O23-C24	7.28	1.49	1.37
11	B	504	8WU	O23-C24	7.26	1.49	1.37
10	B	503	MES	C8-S	-6.38	1.68	1.77
12	F	401	ACP	PG-O1G	5.65	1.61	1.50
12	F	401	ACP	C5-C4	5.12	1.48	1.39
11	D	503	8WU	C11-C09	4.22	1.56	1.48
11	B	504	8WU	C11-C09	4.09	1.56	1.48
11	D	503	8WU	C13-C12	3.78	1.44	1.38
11	D	503	8WU	O15-C14	3.61	1.43	1.37
11	B	504	8WU	C13-C12	3.50	1.44	1.38
5	D	501	GTP	C5-C4	3.36	1.48	1.38
5	A	501	GTP	C5-C4	3.32	1.47	1.38
11	D	503	8WU	C11-C24	3.31	1.48	1.40
11	B	504	8WU	C08-C09	3.29	1.53	1.47
11	B	504	8WU	C11-C24	3.27	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	8WU	C05-C04	3.20	1.44	1.38
5	C	501	GTP	PA-O3A	3.15	1.62	1.59
9	B	501	GDP	C5-C4	3.14	1.47	1.38
12	F	401	ACP	PB-O3A	3.11	1.61	1.58
5	A	501	GTP	PB-O3B	3.11	1.62	1.59
5	C	501	GTP	C5-C4	3.10	1.47	1.38
11	D	503	8WU	C08-C09	3.07	1.52	1.47
12	F	401	ACP	C5-C6	3.02	1.49	1.41
5	D	501	GTP	PA-O3A	2.97	1.62	1.59
5	D	501	GTP	PB-O3B	2.93	1.62	1.59
12	F	401	ACP	PG-O2G	-2.86	1.48	1.55
12	F	401	ACP	PG-O3G	2.85	1.61	1.55
5	C	501	GTP	PB-O3B	2.78	1.62	1.59
11	B	504	8WU	O15-C14	2.77	1.41	1.37
11	D	503	8WU	C17-C14	2.75	1.45	1.41
12	F	401	ACP	PA-O3A	2.73	1.62	1.59
5	D	501	GTP	PB-O3A	2.62	1.62	1.59
11	D	503	8WU	C05-C04	2.58	1.43	1.38
11	B	504	8WU	C17-C14	2.57	1.45	1.41
11	D	503	8WU	C06-C07	2.56	1.54	1.47
5	A	501	GTP	PB-O3A	2.52	1.62	1.59
11	B	504	8WU	C06-C07	2.45	1.54	1.47
5	A	501	GTP	PA-O3A	2.41	1.62	1.59
11	B	504	8WU	C08-C07	2.41	1.39	1.33
12	F	401	ACP	C8-N7	2.39	1.36	1.31
9	B	501	GDP	C6-N1	-2.36	1.34	1.38
12	F	401	ACP	C5-N7	-2.36	1.34	1.39
11	D	503	8WU	C08-C07	2.34	1.39	1.33
10	B	503	MES	O2S-S	2.32	1.51	1.45
5	C	501	GTP	PB-O3A	2.28	1.62	1.59
11	D	503	8WU	C20-C19	2.27	1.54	1.50
11	D	503	8WU	O10-C09	-2.26	1.19	1.24
11	B	504	8WU	C20-C19	2.25	1.54	1.50
5	A	501	GTP	C6-N1	-2.24	1.34	1.38
5	C	501	GTP	C6-N1	-2.10	1.34	1.38
9	B	501	GDP	C5-N7	-2.08	1.34	1.39
12	F	401	ACP	PB-O2B	2.06	1.61	1.56
5	C	501	GTP	C4-N9	-2.05	1.32	1.38
5	D	501	GTP	C5-N7	-2.02	1.35	1.39
5	D	501	GTP	C6-N1	-2.00	1.35	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O1S-S-C8	-14.95	84.14	106.73
10	B	503	MES	O3S-S-O1S	-10.65	84.75	111.40
10	B	503	MES	O2S-S-O1S	-9.17	84.01	113.82
10	B	503	MES	O2S-S-C8	8.95	120.25	106.73
10	B	503	MES	O3S-S-C8	6.50	118.72	106.00
9	B	501	GDP	C5-C4-N3	-6.08	118.72	128.39
12	F	401	ACP	C5-C4-N3	-5.98	118.48	126.72
5	D	501	GTP	C5-C4-N3	-5.82	119.13	128.39
9	B	501	GDP	C2-N3-C4	5.39	121.58	112.30
5	C	501	GTP	C5-C4-N3	-5.32	119.93	128.39
5	D	501	GTP	C2-N3-C4	5.05	121.00	112.30
5	A	501	GTP	C5-C4-N3	-5.04	120.37	128.39
12	F	401	ACP	N3-C4-N9	4.72	135.20	127.17
5	C	501	GTP	C2-N3-C4	4.61	120.23	112.30
11	B	504	8WU	C22-C20-C21	-4.56	99.16	111.30
5	A	501	GTP	C2-N3-C4	4.53	120.11	112.30
9	B	501	GDP	N9-C4-N3	4.39	134.74	125.95
5	D	501	GTP	N9-C4-N3	4.36	134.67	125.95
5	C	501	GTP	N9-C4-N3	4.23	134.42	125.95
11	B	504	8WU	C16-O15-C14	-4.10	111.49	117.51
12	F	401	ACP	C2-N3-C4	3.87	121.29	111.83
11	D	503	8WU	C22-C20-C21	-3.86	101.02	111.30
9	B	501	GDP	C6-C5-N7	3.80	137.21	130.29
5	A	501	GTP	C6-C5-N7	3.80	137.20	130.29
5	A	501	GTP	N9-C4-N3	3.71	133.37	125.95
12	F	401	ACP	C4-C5-N7	-3.51	106.57	110.58
12	F	401	ACP	N3-C2-N1	-3.49	123.29	128.58
5	C	501	GTP	C6-C5-N7	3.46	136.58	130.29
5	D	501	GTP	C6-C5-N7	3.45	136.56	130.29
11	D	503	8WU	C16-O15-C14	-3.36	112.59	117.51
11	D	503	8WU	O02-C03-C26	3.17	119.31	114.55
10	B	503	MES	C5-N4-C3	3.07	115.45	108.84
11	B	504	8WU	O15-C14-C13	-3.07	119.13	124.30
11	D	503	8WU	O15-C14-C17	3.03	120.61	115.23
11	B	504	8WU	O15-C14-C17	2.82	120.24	115.23
9	B	501	GDP	C4-C5-N7	-2.77	106.29	110.67
10	B	503	MES	O3S-S-O2S	2.68	118.11	111.40
11	D	503	8WU	O15-C14-C13	-2.62	119.89	124.30
11	B	504	8WU	O02-C03-C26	2.56	118.38	114.55
12	F	401	ACP	C5-N7-C8	2.55	107.45	103.45
5	D	501	GTP	C4-C5-N7	-2.49	106.72	110.67
11	D	503	8WU	C06-C25-C26	-2.48	119.04	120.79
5	A	501	GTP	C4-C5-N7	-2.47	106.75	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C4-C5-N7	-2.45	106.78	110.67
11	B	504	8WU	C20-O23-C24	-2.33	114.07	118.04
11	D	503	8WU	C24-C11-C09	-2.30	120.82	124.07
12	F	401	ACP	C3'-C2'-C1'	2.27	105.76	101.46
12	F	401	ACP	C4-N9-C8	2.22	108.07	105.74
11	B	504	8WU	C20-C19-C18	-2.20	118.57	121.52
5	A	501	GTP	O3G-PG-O2G	2.14	115.84	107.80
10	B	503	MES	C6-C5-N4	2.13	113.36	110.12
11	D	503	8WU	C07-C08-C09	-2.11	118.17	121.61
12	F	401	ACP	C6-C5-N7	2.09	136.12	132.09
5	A	501	GTP	O6-C6-C5	-2.08	121.05	126.53
9	B	501	GDP	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (47) 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
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	C7-C8-S-O2S
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O3A
11	D	503	8WU	C07-C08-C09-O10
11	D	503	8WU	C07-C08-C09-C11
11	B	504	8WU	C13-C14-O15-C16
11	D	503	8WU	C13-C14-O15-C16
11	D	503	8WU	C17-C14-O15-C16
11	B	504	8WU	C17-C14-O15-C16
11	D	503	8WU	C26-C03-O02-C01
11	B	504	8WU	C07-C08-C09-C11
10	B	503	MES	C8-C7-N4-C3
11	D	503	8WU	C04-C03-O02-C01

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Mol	Chain	Res	Type	Atoms
11	B	504	8WU	C07-C08-C09-O10
11	D	503	8WU	O10-C09-C11-C24
10	B	503	MES	C7-C8-S-O1S
5	C	501	GTP	PB-O3B-PG-O1G
11	B	504	8WU	O10-C09-C11-C24
5	D	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O2A
8	A	504	GOL	O1-C1-C2-O2
11	D	503	8WU	C08-C09-C11-C24
11	B	504	8WU	C08-C09-C11-C24

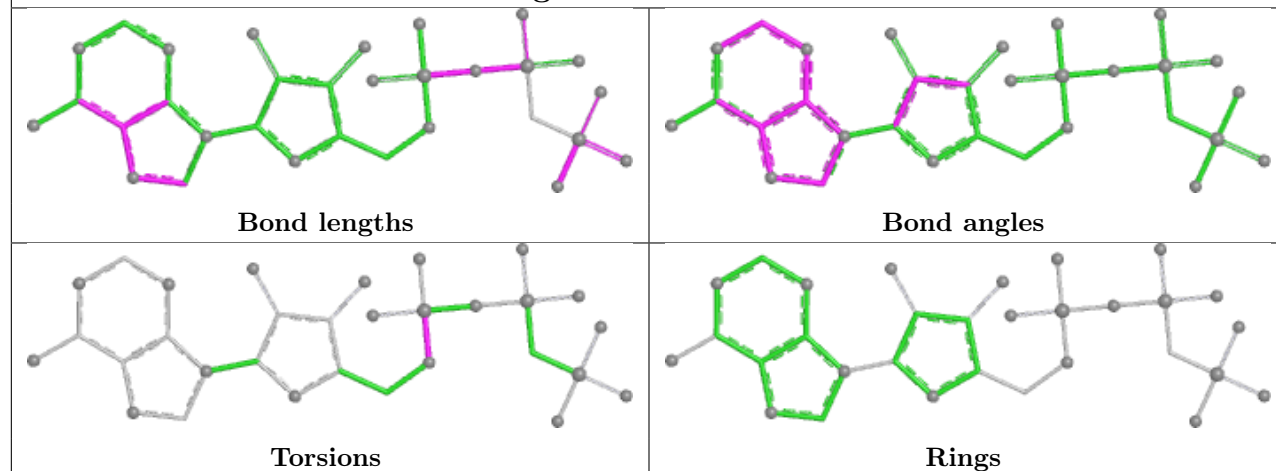
There are no ring outliers.

2 monomers are involved in 3 short contacts:

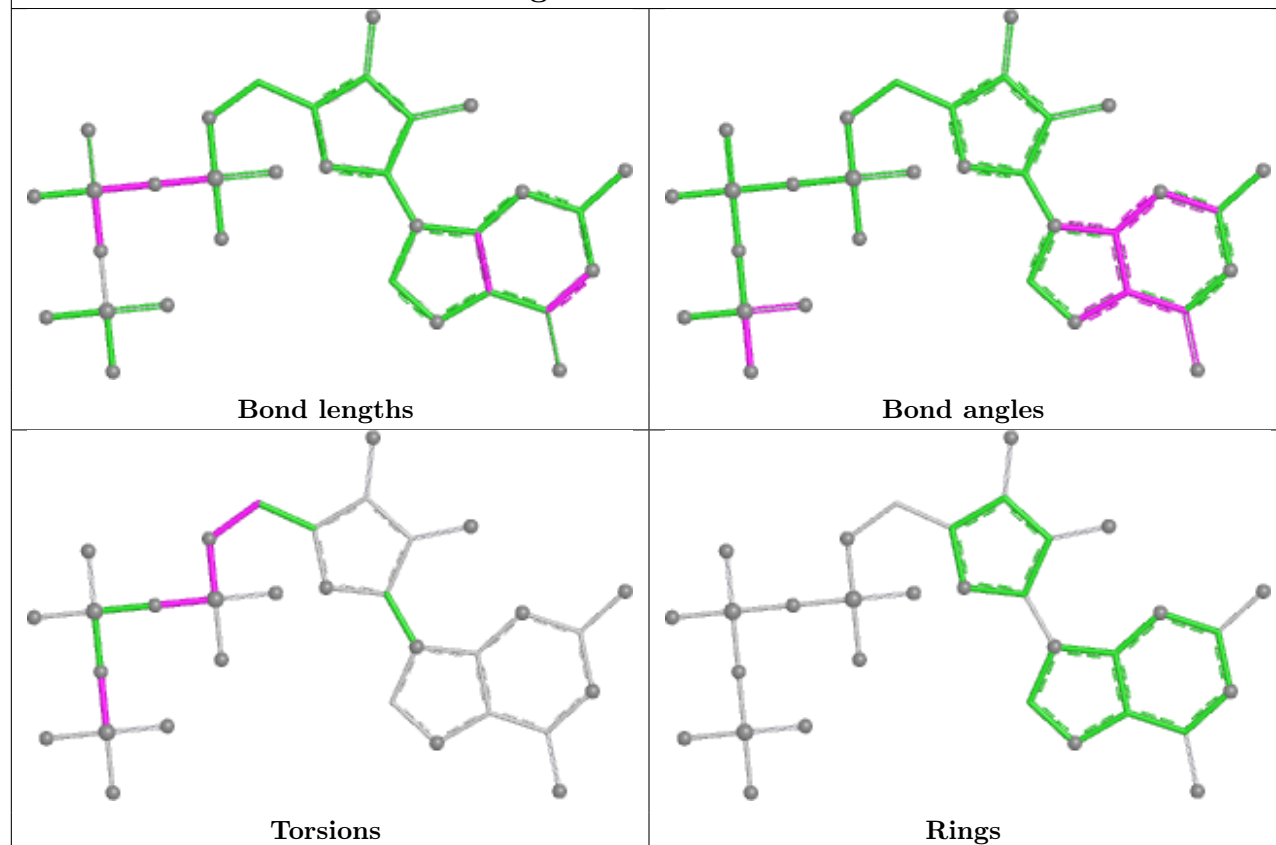
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	2	0
5	D	501	GTP	1	0

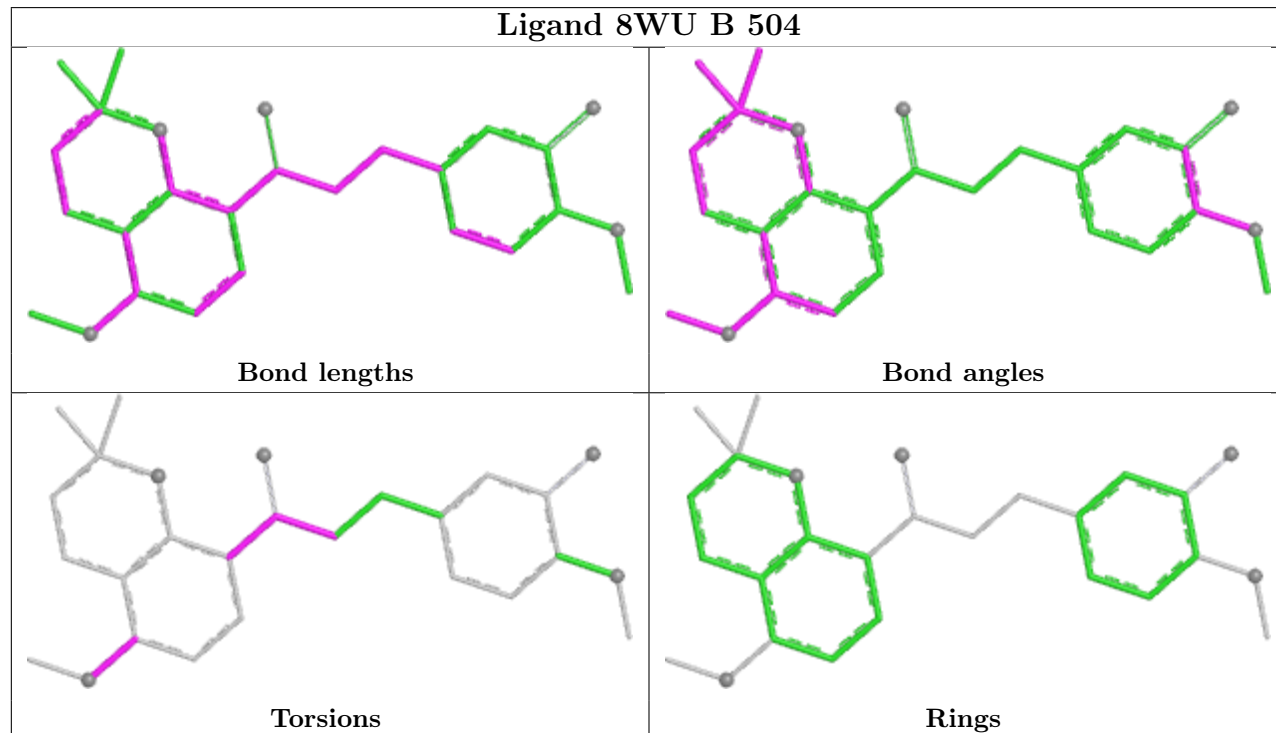
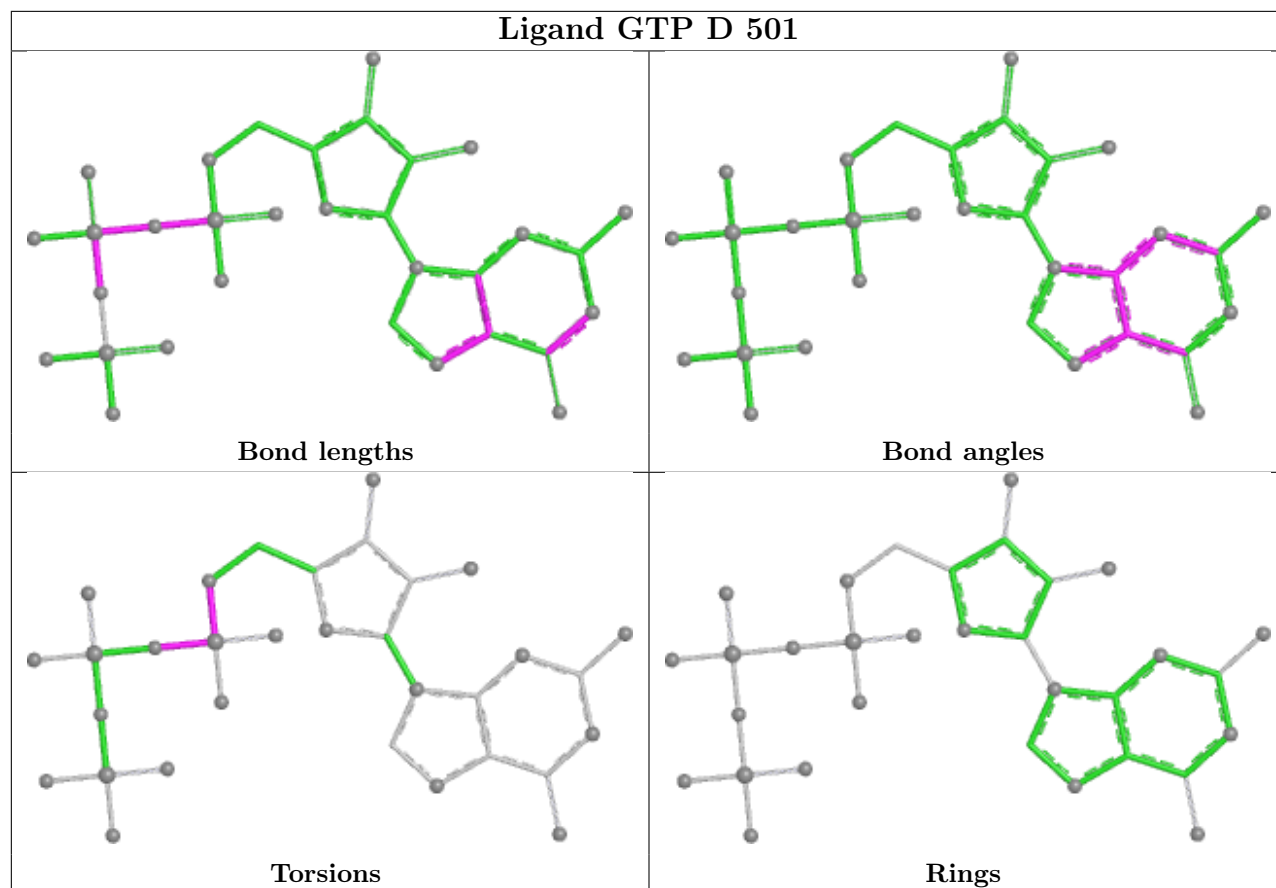
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

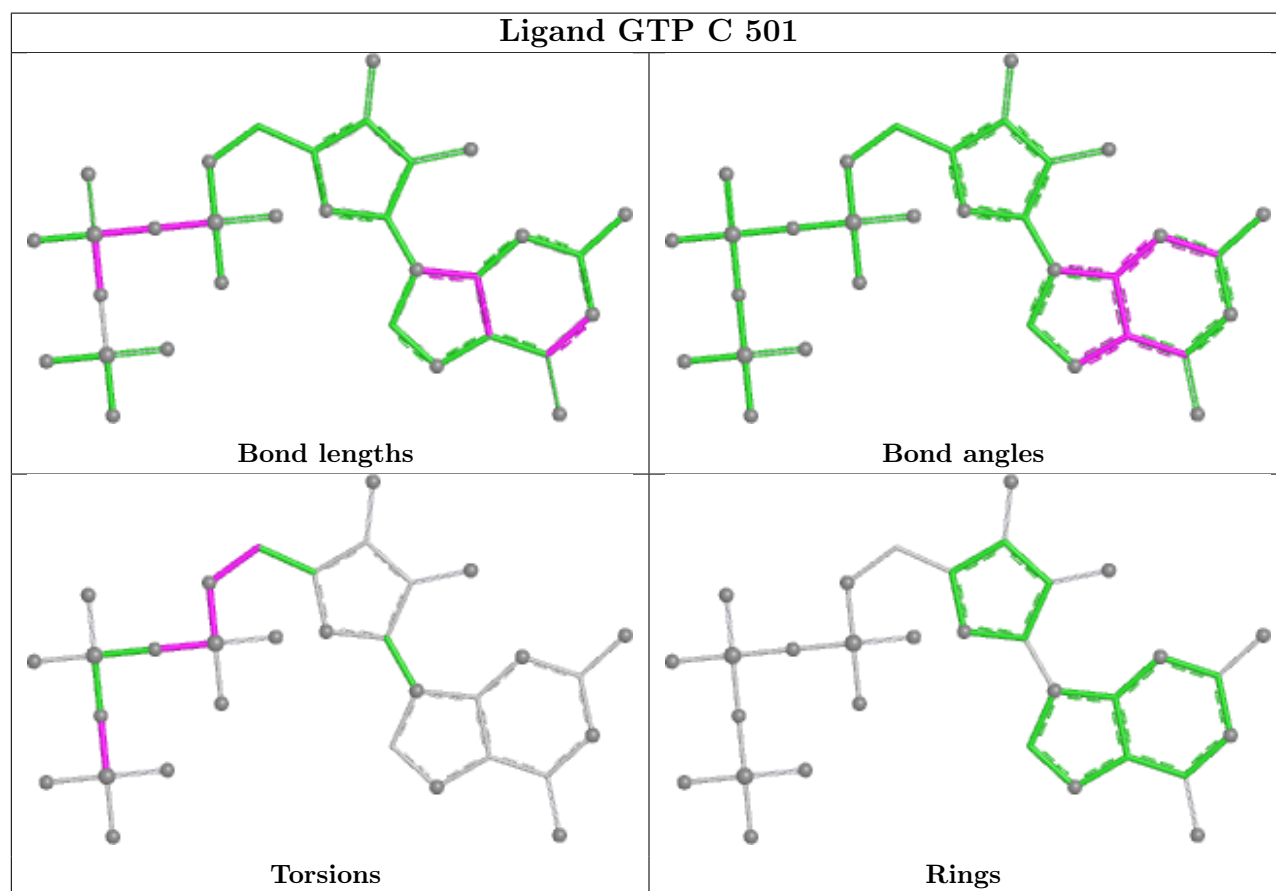
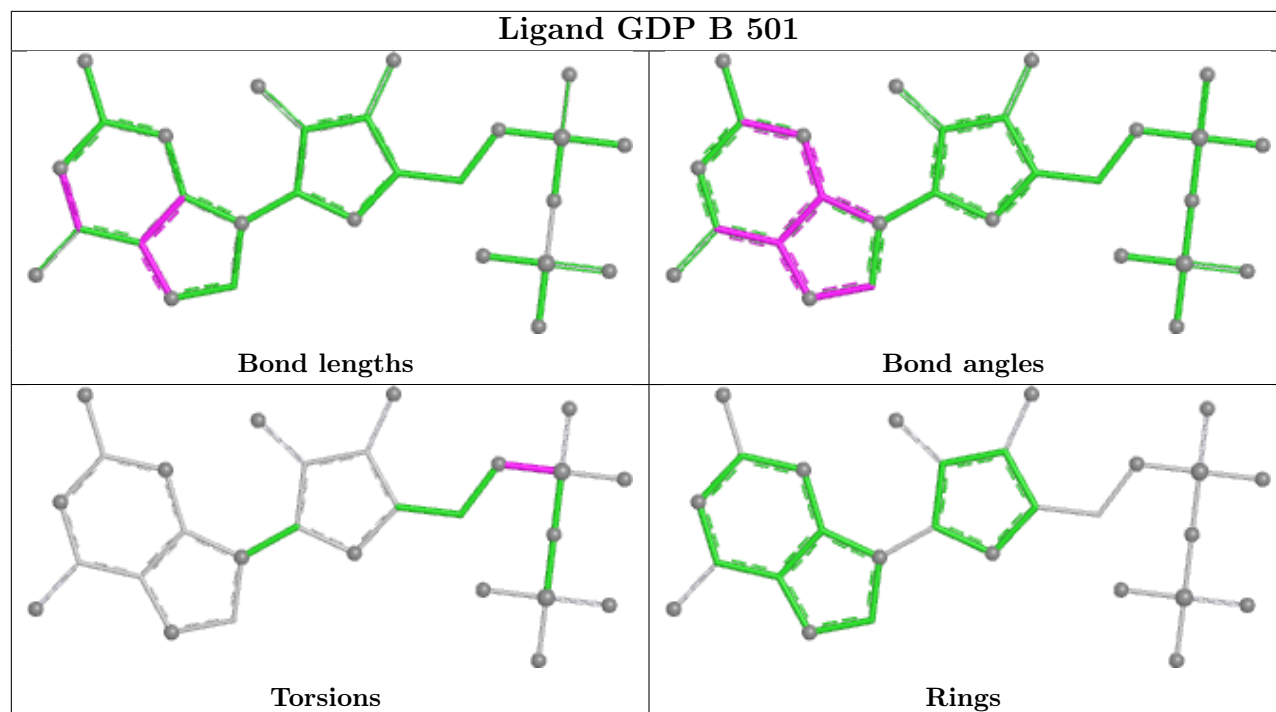
Ligand ACP F 401

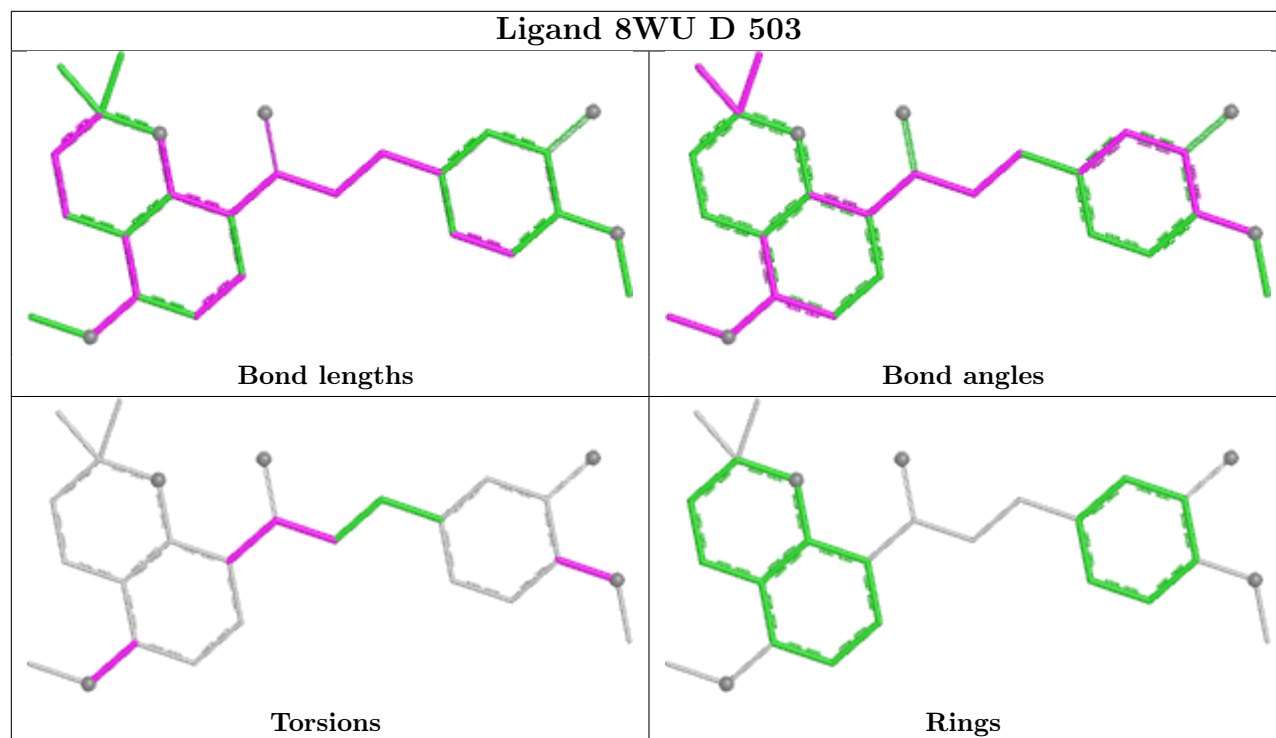


Ligand GTP A 501









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	437/451 (96%)	0.13	7 (1%) 70 73	13, 26, 45, 65	0
1	C	440/451 (97%)	-0.14	8 (1%) 67 70	8, 20, 39, 50	0
2	B	428/445 (96%)	0.19	10 (2%) 61 64	11, 27, 51, 87	0
2	D	421/445 (94%)	0.98	57 (13%) 7 7	14, 42, 69, 84	0
3	E	121/143 (84%)	1.14	20 (16%) 4 4	23, 44, 72, 92	0
4	F	334/384 (86%)	1.21	72 (21%) 2 2	19, 46, 108, 123	0
All	All	2181/2319 (94%)	0.47	174 (7%) 18 19	8, 30, 71, 123	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	6.8
2	B	1	MET	5.8
2	B	55	THR	5.4
4	F	169	LEU	5.3
4	F	172	PHE	5.1
4	F	100	ILE	4.9
2	D	1	MET	4.8
4	F	130	VAL	4.6
4	F	144	GLY	4.6
4	F	181	VAL	4.6
4	F	149	ALA	4.6
4	F	166	ALA	4.5
4	F	132	LEU	4.5
4	F	173	ILE	4.5
4	F	162	ILE	4.4
4	F	170	LEU	4.4
4	F	236	LYS	4.3
2	D	284	LEU	4.3
4	F	103	THR	4.3

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Mol	Chain	Res	Type	RSRZ
4	F	186	LEU	4.2
2	D	30	ILE	4.2
4	F	182	ILE	4.2
4	F	179	VAL	4.2
4	F	233	PHE	4.1
4	F	180	HIS	4.1
4	F	245	ILE	4.1
2	D	73	MET	4.0
2	D	81	PHE	4.0
4	F	231	ALA	3.9
4	F	362	ALA	3.9
1	C	357	TYR	3.8
2	D	72	THR	3.7
4	F	131	PHE	3.7
2	D	388	MET	3.7
2	D	55	THR	3.7
1	A	262	TYR	3.6
4	F	146	VAL	3.5
4	F	237	THR	3.5
4	F	101	TYR	3.5
1	C	177	VAL	3.5
2	B	57	ASN	3.5
4	F	239	HIS	3.4
2	D	219	THR	3.4
4	F	228	TYR	3.4
4	F	238	CYS	3.3
4	F	194	PRO	3.3
2	D	180	VAL	3.3
3	E	8	VAL	3.3
4	F	167	SER	3.2
2	D	179	VAL	3.2
3	E	139	LEU	3.2
3	E	59	GLU	3.2
2	D	360	GLY	3.2
2	B	278	SER	3.1
2	D	394	PHE	3.1
2	D	406	MET	3.1
2	D	80	PRO	3.1
4	F	164	SER	3.1
3	E	26	PRO	3.1
2	B	281	TYR	3.0
4	F	148	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	99	VAL	3.0
4	F	102	PRO	3.0
4	F	135	TYR	2.9
3	E	135	LYS	2.9
2	D	215	LEU	2.9
2	B	428	ALA	2.9
4	F	199	PHE	2.8
1	A	346	TRP	2.8
3	E	27	PRO	2.8
2	D	387	ALA	2.8
1	C	340	SER	2.8
2	D	389	PHE	2.8
2	D	323	MET	2.7
3	E	47	LEU	2.7
2	D	218	THR	2.7
2	D	92	PHE	2.7
2	D	116	VAL	2.7
4	F	240	LEU	2.7
2	D	115	SER	2.7
2	B	54	ALA	2.6
1	A	282	TYR	2.6
2	D	106	TYR	2.6
4	F	254	GLY	2.6
3	E	50	ILE	2.6
4	F	320	MET	2.6
2	D	217	LEU	2.6
4	F	227	PRO	2.6
3	E	6	MET	2.5
4	F	141	GLY	2.5
4	F	195	GLY	2.5
1	A	88	HIS	2.5
4	F	45	ASN	2.5
2	D	82	GLY	2.5
2	D	84	ILE	2.5
2	B	80	PRO	2.5
4	F	243	HIS	2.5
4	F	333	ASN	2.5
4	F	372	THR	2.5
2	D	361	LEU	2.5
1	C	176	GLN	2.4
4	F	244	CYS	2.4
2	D	212	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	136	ASN	2.4
4	F	147	TRP	2.4
1	A	159	VAL	2.4
1	C	175	PRO	2.4
1	C	283	HIS	2.4
2	D	393	ALA	2.4
4	F	224	SER	2.4
2	D	102	ALA	2.3
4	F	183	GLN	2.3
2	D	29	GLY	2.3
2	D	170	MET	2.3
4	F	138	ARG	2.3
4	F	27	TRP	2.3
3	E	123	LEU	2.3
2	B	293	MET	2.3
2	D	396	HIS	2.3
3	E	130	ALA	2.3
4	F	191	LEU	2.3
4	F	226	GLU	2.2
2	D	85	PHE	2.2
4	F	253	TYR	2.2
3	E	115	HIS	2.2
4	F	232	ASN	2.2
2	D	66	VAL	2.2
2	D	93	GLY	2.2
2	D	37	HIS	2.2
3	E	103	GLN	2.2
1	C	108	TYR	2.2
1	C	302	MET	2.2
2	D	210	ILE	2.2
2	D	214	THR	2.2
4	F	330	ILE	2.2
3	E	133	VAL	2.2
3	E	51	GLN	2.2
2	D	397	TRP	2.2
4	F	241	THR	2.2
4	F	230	SER	2.1
4	F	242	ASN	2.1
4	F	296	MET	2.1
2	D	285	THR	2.1
1	A	57	GLY	2.1
2	D	38	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	196	HIS	2.1
4	F	137	ARG	2.1
3	E	54	LEU	2.1
4	F	22	LEU	2.1
4	F	88	SER	2.1
2	D	143	THR	2.1
2	D	71	GLY	2.1
2	D	408	PHE	2.1
2	D	76	VAL	2.1
2	D	68	LEU	2.1
2	D	293	MET	2.1
2	B	280	GLN	2.1
4	F	246	GLN	2.1
2	D	391	ARG	2.1
3	E	63	TYR	2.1
3	E	122	ARG	2.1
2	D	146	GLY	2.1
4	F	264	PHE	2.1
2	D	35	SER	2.1
3	E	141	GLU	2.0
2	D	395	LEU	2.0
4	F	229	ASN	2.0
2	D	33	THR	2.0
2	D	34	GLY	2.0
4	F	98	TYR	2.0
2	D	75	SER	2.0
1	A	163	LYS	2.0
3	E	52	LYS	2.0
2	D	400	GLY	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 oligosaccharides in this entry.

6.4 Ligands

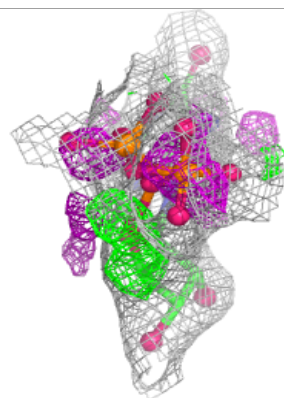
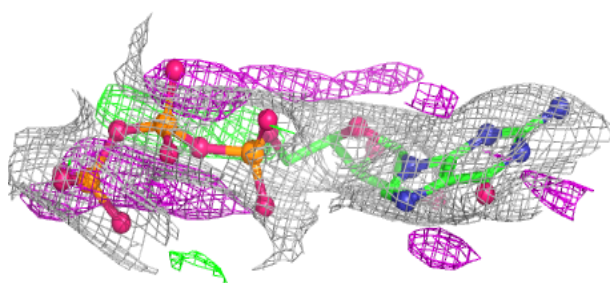
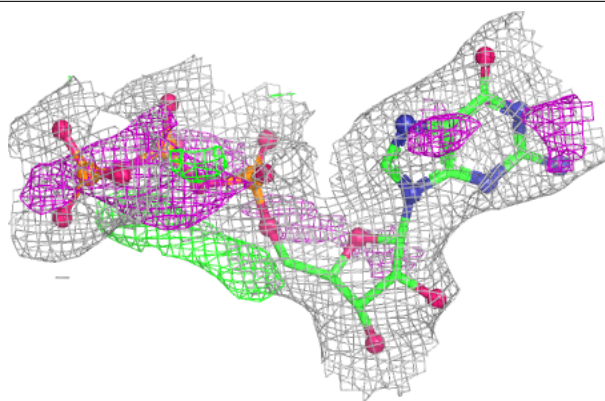
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MES	B	503	12/12	0.88	0.15	58,59,61,61	0
5	GTP	D	501	32/32	0.89	0.10	29,34,39,41	0
12	ACP	F	401	31/31	0.89	0.11	66,68,74,75	0
8	GOL	A	504	6/6	0.92	0.10	35,36,38,39	0
11	8WU	D	503	27/27	0.94	0.10	24,31,36,37	0
6	MG	D	502	1/1	0.94	0.07	22,22,22,22	0
11	8WU	B	504	27/27	0.95	0.09	24,26,27,28	0
6	MG	B	502	1/1	0.96	0.05	12,12,12,12	0
5	GTP	A	501	32/32	0.98	0.05	12,13,14,14	0
9	GDP	B	501	28/28	0.98	0.05	14,16,17,17	0
7	CA	C	503	1/1	0.98	0.04	24,24,24,24	0
7	CA	A	503	1/1	0.99	0.02	28,28,28,28	0
5	GTP	C	501	32/32	0.99	0.04	10,12,13,13	0
6	MG	C	502	1/1	0.99	0.01	10,10,10,10	0
6	MG	A	502	1/1	0.99	0.03	17,17,17,17	0

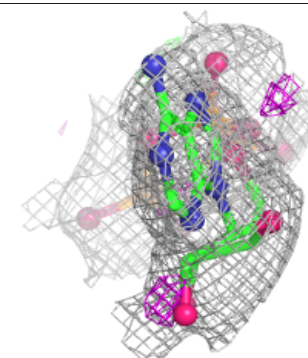
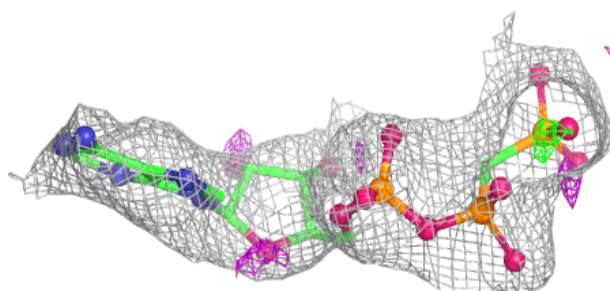
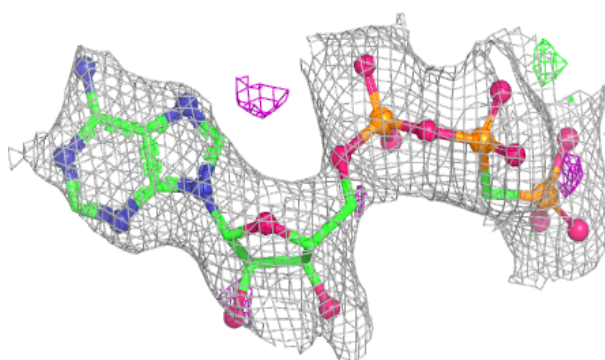
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

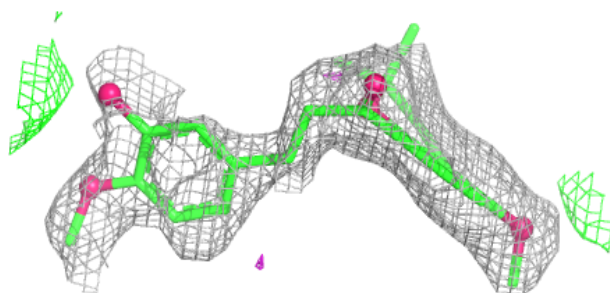
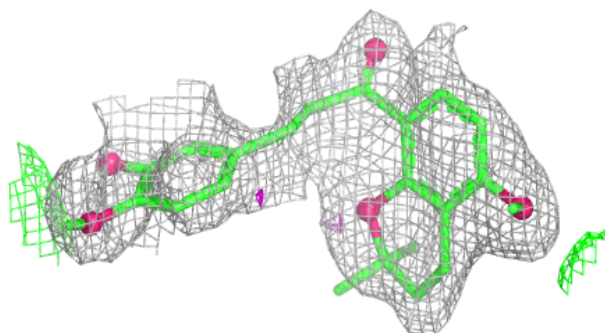
**Electron density around ACP F 401:**

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

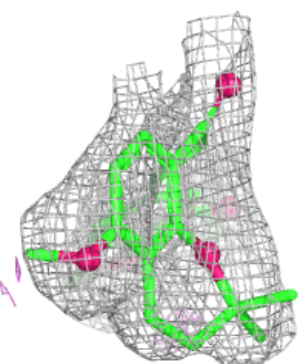
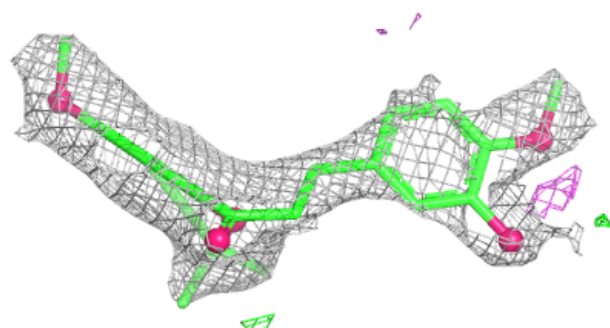
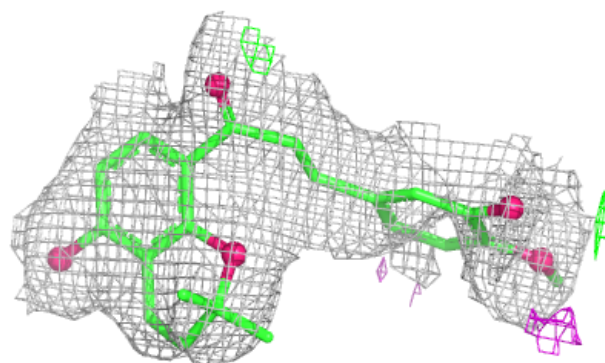


Electron density around 8WU D 503:

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

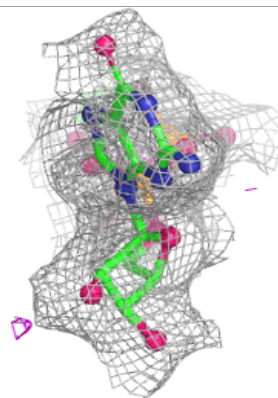
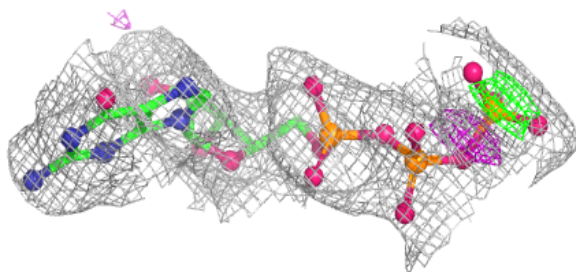
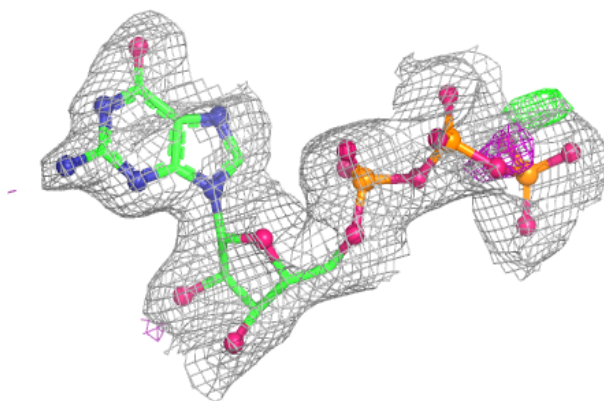
**Electron density around 8WU B 504:**

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

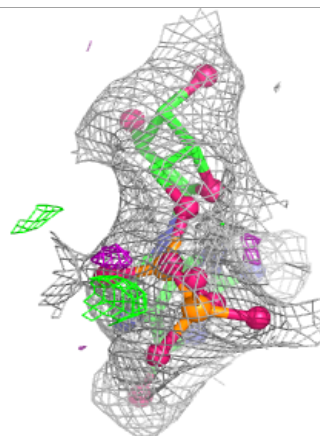
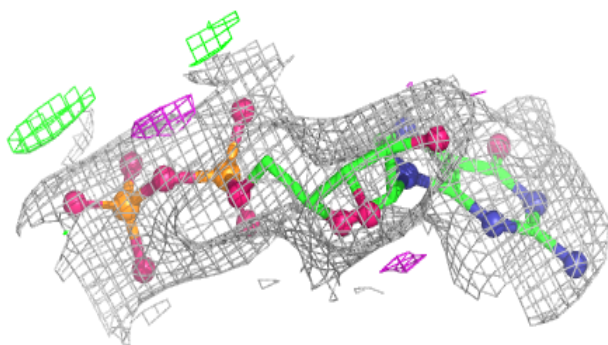
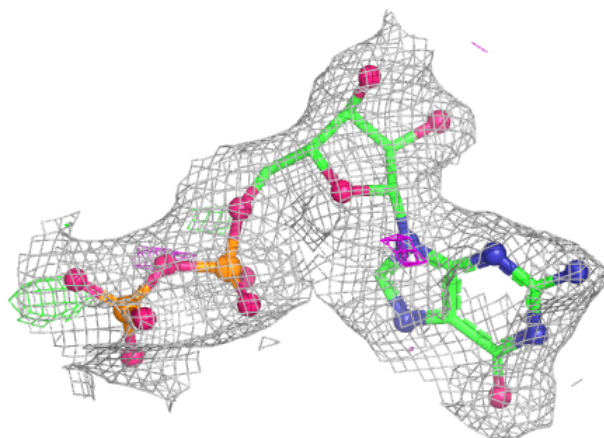


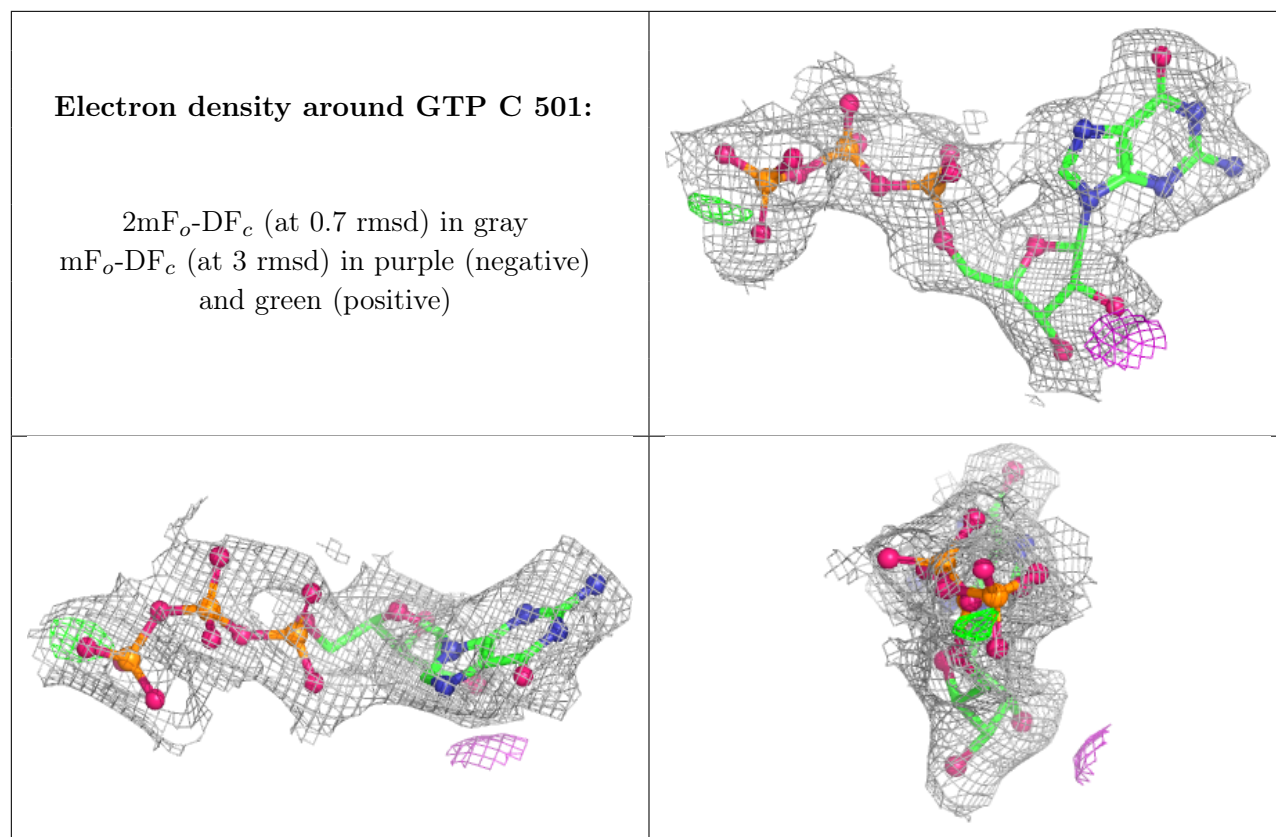
Electron density around GTP A 501:

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

**Electron density around GDP B 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.