



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 6AGK / pdb_00006agk
Title : The structure of CH-II-77-tubulin complex
Authors : Chen, H.; Arnst, K.; Wang, Y.; Miller, D.; Li, W.
Deposited on : 2018-08-13
Resolution : 2.80 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

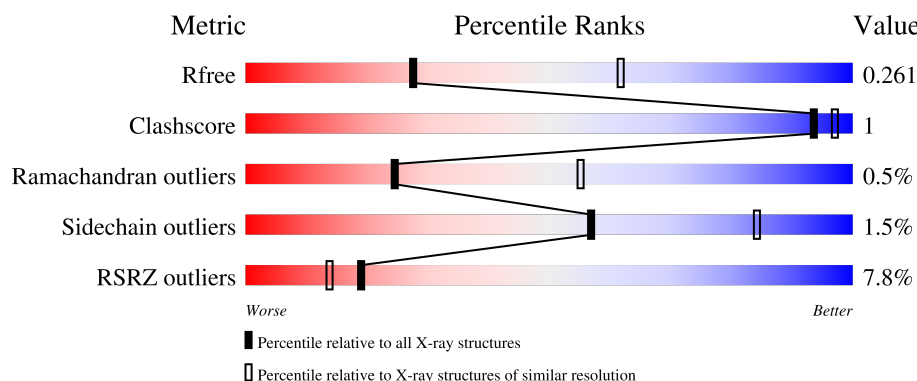
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	450	 2% 92% 5% •
1	C	450	 2% 92% 6% •
2	B	445	 2% 90% • • 5%
2	D	445	 15% 92% • 5%
3	E	143	 9% 83% • 16%

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Mol	Chain	Length	Quality of chain
4	F	384	16% 77% • 20%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17398 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	4	0
			3441	2179	586	652	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- 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	2	0
			3353	2107	574	645	27			
2	D	421	Total	C	N	O	S	0	1	0
			3306	2079	562	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	2	0
			1004	621	181	196	6			

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

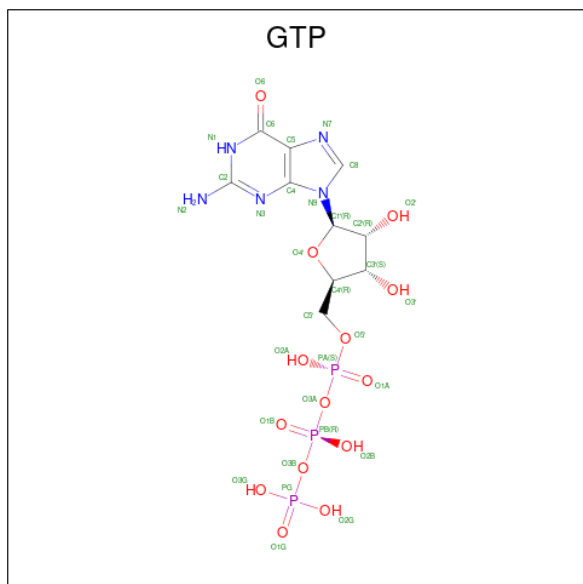
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	3	0
			2553	1645	438	455	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		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

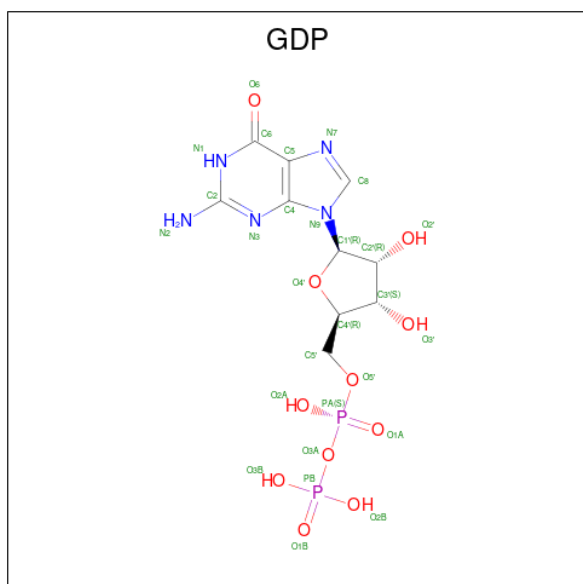
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

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

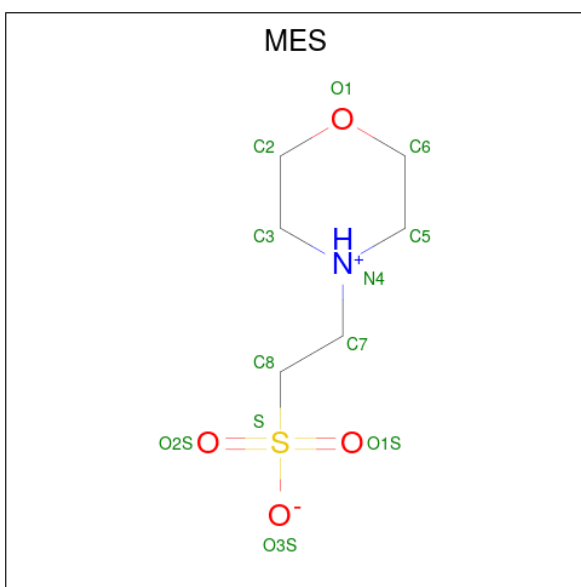
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



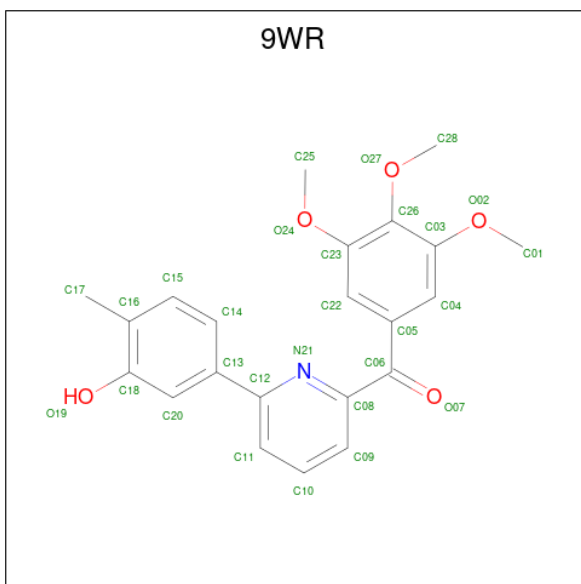
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is [6-(3-hydroxy-4-methylphenyl)pyridin-2-yl](3,4,5-trimethoxyphenyl)methanone (CCD ID: 9WR) (formula: $C_{22}H_{21}NO_5$).



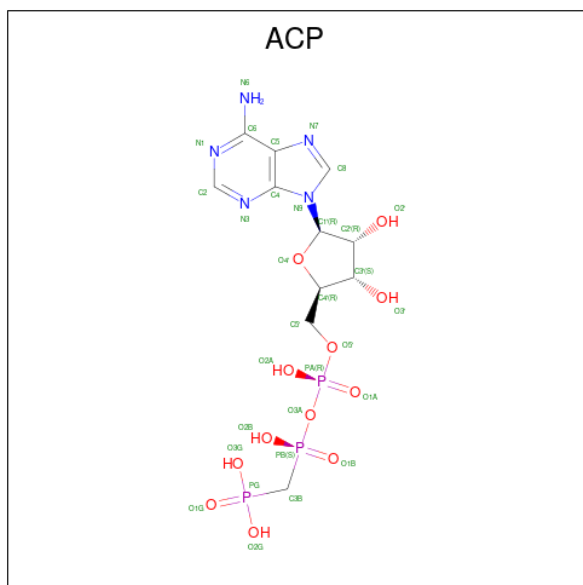
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			28	22	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			28	22	1	5		

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



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

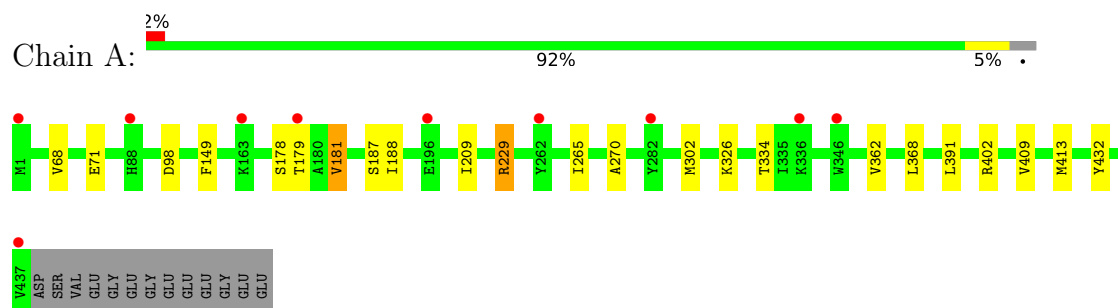
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	5	Total	O	0	0
			5	5		
12	B	4	Total	O	0	0
			4	4		
12	C	8	Total	O	0	0
			8	8		
12	D	1	Total	O	0	0
			1	1		

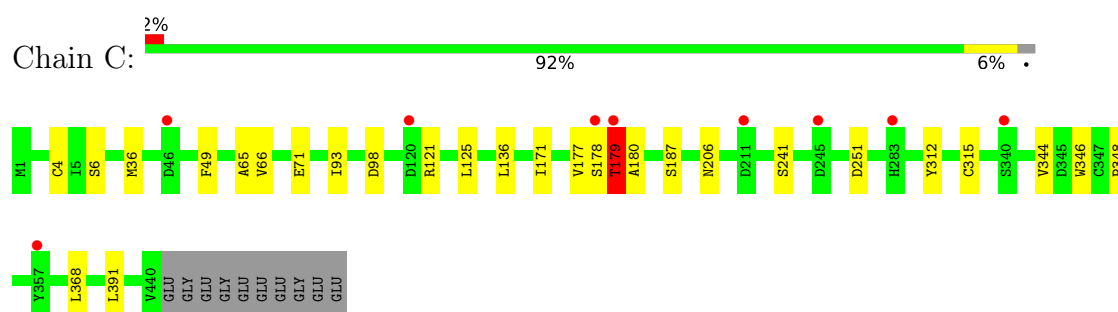
3 Residue-property plots [i](#)

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.

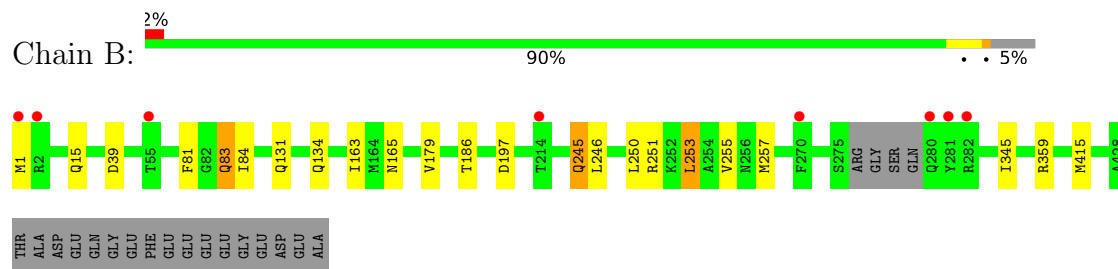
- Molecule 1: Tubulin alpha-1B chain



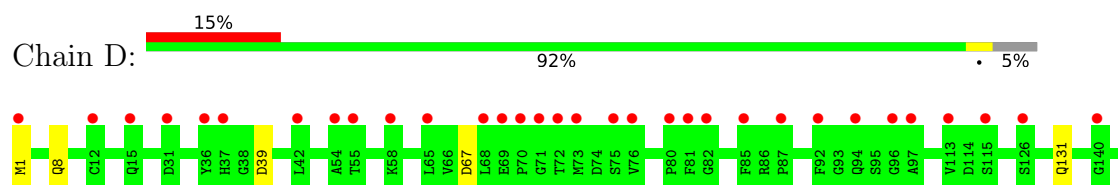
- Molecule 1: Tubulin alpha-1B chain

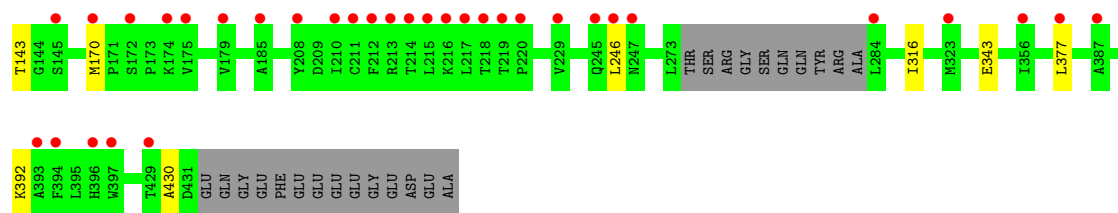


- Molecule 2: Tubulin beta-2B chain

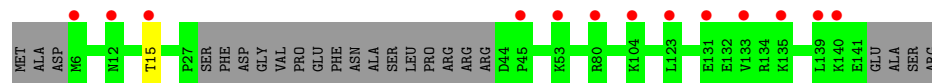
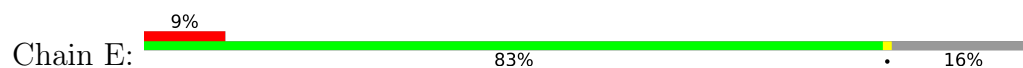


- Molecule 2: Tubulin beta-2B chain

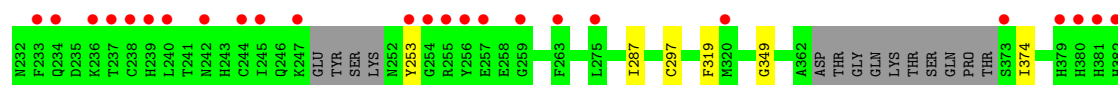
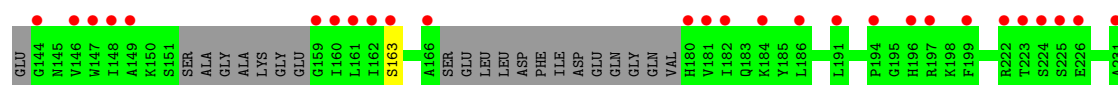
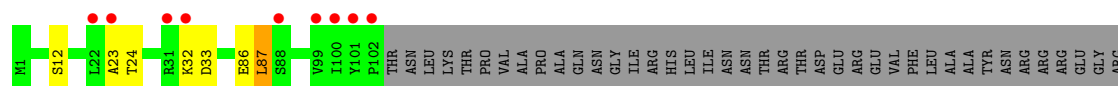
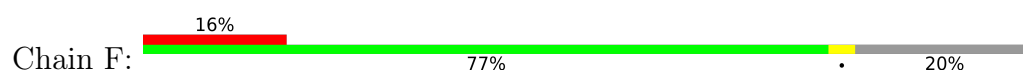




● Molecule 3: Stathmin-4



● 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	105.08Å 157.06Å 182.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.80) 99.2 (50.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.211 , 0.264 0.213 , 0.261	Depositor DCC
R_{free} test set	3787 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17398	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: MG, ACP, GTP, 9WR, GDP, MES, 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	0.63	0/3525	0.85	0/4784
1	C	0.63	0/3572	0.87	2/4850 (0.0%)
2	B	0.62	0/3427	0.84	0/4640
2	D	0.63	0/3379	0.86	0/4577
3	E	0.67	0/1018	0.83	0/1350
4	F	0.61	0/2618	0.76	0/3537
All	All	0.63	0/17539	0.84	2/23738 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	THR	CA-C-N	6.36	133.15	121.70
1	C	179	THR	C-N-CA	6.36	133.15	121.70

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	3441	0	3363	15	0
1	C	3482	0	3384	13	0
2	B	3353	0	3228	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3306	0	3181	5	0
3	E	1004	0	1028	0	0
4	F	2553	0	2519	3	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	3	0
10	B	28	0	0	0	0
10	D	28	0	0	1	0
11	F	31	0	14	0	0
12	A	5	0	0	0	0
12	B	4	0	0	0	0
12	C	8	0	0	0	0
12	D	1	0	0	0	0
All	All	17398	0	16791	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (49) 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)
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.17	1.05
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.70	1.04
2:B:197:ASP:OD1	9:B:503:MES:H32	1.61	1.00
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.89	0.75
2:B:251:ARG:NH1	9:B:503:MES:O2S	2.22	0.73
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.76	0.67
2:B:1:MET:HE3	2:B:131:GLN:HB2	1.76	0.66
2:B:197:ASP:CG	9:B:503:MES:H32	2.22	0.65
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:N	2.17	0.59
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:H	1.68	0.57
1:C:177:VAL:O	1:C:179:THR:N	2.36	0.56
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:HG3	1.68	0.55
2:B:1:MET:HE3	2:B:131:GLN:CB	2.37	0.54
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.90	0.53
4:F:87:LEU:HD21	4:F:297:CYS:HB2	1.91	0.53
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.45	0.52
1:A:209:ILE:HD11	1:A:302:MET:SD	2.50	0.51
2:B:83:GLN:HE21	2:B:83:GLN:HA	1.75	0.51
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.93	0.51
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.92	0.51
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.92	0.51
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.50
2:B:253:LEU:HD22	2:B:257:MET:HG3	1.92	0.49
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.49	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.49	0.48
1:C:177:VAL:HG21	1:C:206:ASN:HD22	1.78	0.48
1:A:181:VAL:HG11	2:B:345:ILE:CG2	2.46	0.46
1:A:409:VAL:HA	1:A:413:MET:O	2.16	0.45
2:B:251:ARG:O	2:B:255:VAL:HG23	2.17	0.45
2:B:81:PHE:O	2:B:84:ILE:HG22	2.18	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.99	0.43
2:D:316:ILE:HD11	10:D:502:9WR:C28	2.49	0.43
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.43
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.00	0.43
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.01	0.43
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.00	0.42
2:D:67:ASP:HA	2:D:143:THR:HG21	2.00	0.42
1:A:270:ALA:HB3	1:A:302:MET:HG3	2.01	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.21	0.41
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.55	0.41
2:B:253:LEU:HD22	2:B:257:MET:CG	2.51	0.41
1:C:171:ILE:N	1:C:171:ILE:HD12	2.36	0.41
1:C:312:TYR:CD1	1:C:315[B]:CYS:SG	3.14	0.41
2:B:186:THR:HG23	2:B:415:MET:HE2	2.02	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.03	0.41
2:D:1:MET:HE3	2:D:131:GLN:HB2	2.03	0.41
1:C:6:SER:O	1:C:65:ALA:HA	2.22	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	439/450 (98%)	427 (97%)	11 (2%)	1 (0%)	43	72
1	C	446/450 (99%)	433 (97%)	11 (2%)	2 (0%)	30	60
2	B	422/445 (95%)	403 (96%)	17 (4%)	2 (0%)	24	55
2	D	417/445 (94%)	400 (96%)	15 (4%)	2 (0%)	24	55
3	E	118/143 (82%)	113 (96%)	5 (4%)	0	100	100
4	F	300/384 (78%)	286 (95%)	11 (4%)	3 (1%)	12	38
All	All	2142/2317 (92%)	2062 (96%)	70 (3%)	10 (0%)	24	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
2	B	245	GLN
1	C	178	SER
2	D	39	ASP
2	B	39	ASP
1	C	180	ALA
4	F	253	TYR
2	D	392	LYS
4	F	163	SER
4	F	23	ALA

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	372/378 (98%)	363 (98%)	9 (2%)	43	77
1	C	379/378 (100%)	374 (99%)	5 (1%)	61	86
2	B	367/383 (96%)	361 (98%)	6 (2%)	55	83
2	D	362/383 (94%)	360 (99%)	2 (1%)	78	92
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	89
4	F	281/342 (82%)	275 (98%)	6 (2%)	47	79
All	All	1871/1991 (94%)	1842 (98%)	29 (2%)	57	84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	THR
1	A	181	VAL
1	A	188	ILE
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	326	LYS
1	A	334	THR
1	A	362	VAL
1	A	402	ARG
2	B	15	GLN
2	B	83	GLN
2	B	245	GLN
2	B	246	LEU
2	B	253	LEU
2	B	359	ARG
1	C	179	THR
1	C	241	SER
1	C	251[A]	ASP
1	C	251[B]	ASP
1	C	368	LEU
2	D	8	GLN
2	D	246	LEU
3	E	15	THR
4	F	12	SER
4	F	24	THR
4	F	32	LYS
4	F	33	ASP
4	F	86	GLU
4	F	87	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	61	HIS
1	A	101	ASN
1	A	301	GLN
2	B	83	GLN
2	B	191	GLN
2	B	292	GLN
2	B	332	ASN
1	C	11	GLN
1	C	88	HIS
1	C	128	GLN
1	C	133	GLN
1	C	249	ASN
1	C	256	GLN
1	C	283	HIS
2	D	8	GLN
2	D	14	ASN
2	D	329	GLN
2	D	334	GLN
2	D	337	ASN
3	E	90	ASN
3	E	136	ASN
4	F	180	HIS
4	F	333	ASN
4	F	384	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
5	GTP	C	501	6	33,34,34	1.22	5 (15%)	50,54,54	1.62	10 (20%)
10	9WR	B	506	-	30,30,30	1.40	3 (10%)	42,42,42	1.43	9 (21%)
5	GTP	D	501	-	33,34,34	1.16	4 (12%)	50,54,54	1.69	7 (14%)
9	MES	B	503	-	12,12,12	2.69	1 (8%)	15,16,16	6.09	7 (46%)
8	GDP	B	501	6	29,30,30	1.23	3 (10%)	45,47,47	1.67	6 (13%)
9	MES	B	505	-	12,12,12	2.12	1 (8%)	15,16,16	5.53	8 (53%)
11	ACP	F	401	-	31,33,33	2.08	11 (35%)	47,52,52	1.81	11 (23%)
5	GTP	A	501	6	33,34,34	1.28	5 (15%)	50,54,54	1.78	9 (18%)
10	9WR	D	502	-	30,30,30	1.43	5 (16%)	42,42,42	1.46	10 (23%)

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	GTP	C	501	6	-	7/22/38/38	0/3/3/3
10	9WR	B	506	-	-	4/18/18/18	0/3/3/3
5	GTP	D	501	-	-	7/22/38/38	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
9	MES	B	505	-	-	3/6/14/14	0/1/1/1
11	ACP	F	401	-	-	6/19/38/38	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
10	9WR	D	502	-	-	4/18/18/18	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-9.12	1.64	1.77
9	B	505	MES	C8-S	-6.80	1.68	1.77
11	F	401	ACP	PG-O1G	5.67	1.61	1.50
10	B	506	9WR	C13-C12	-4.88	1.41	1.49
11	F	401	ACP	C5-C4	4.86	1.47	1.39
10	D	502	9WR	C13-C12	-4.72	1.41	1.49
11	F	401	ACP	PB-O3A	3.93	1.62	1.58
5	D	501	GTP	C5-C4	3.24	1.47	1.38
5	C	501	GTP	C5-C4	3.09	1.47	1.38
5	A	501	GTP	C5-C4	3.04	1.47	1.38
8	B	501	GDP	C5-C4	2.99	1.47	1.38
5	A	501	GTP	PB-O3B	2.96	1.62	1.59
11	F	401	ACP	C5-C6	2.93	1.49	1.41
5	C	501	GTP	PB-O3B	2.92	1.62	1.59
11	F	401	ACP	PG-O2G	-2.89	1.48	1.55
11	F	401	ACP	PA-O3A	2.87	1.62	1.59
11	F	401	ACP	PG-O3G	2.83	1.61	1.55
8	B	501	GDP	PA-O3A	2.58	1.62	1.59
10	D	502	9WR	C05-C06	2.52	1.53	1.49
10	B	506	9WR	O24-C23	2.52	1.41	1.37
10	B	506	9WR	C05-C06	2.50	1.53	1.49
5	A	501	GTP	C6-N1	-2.46	1.34	1.38
10	D	502	9WR	O24-C23	2.40	1.41	1.37
5	C	501	GTP	C6-N1	-2.39	1.34	1.38
11	F	401	ACP	C8-N7	2.39	1.36	1.31
5	D	501	GTP	PB-O3B	2.28	1.62	1.59
11	F	401	ACP	C5-N7	-2.28	1.34	1.39
8	B	501	GDP	C6-N1	-2.24	1.34	1.38
5	A	501	GTP	C4-N9	-2.22	1.32	1.38
10	D	502	9WR	O07-C06	-2.22	1.18	1.22
5	C	501	GTP	C4-N9	-2.19	1.32	1.38
5	A	501	GTP	C5-N7	-2.14	1.34	1.39
5	D	501	GTP	C5-N7	-2.08	1.34	1.39
5	D	501	GTP	C4-N9	-2.07	1.32	1.38
5	C	501	GTP	PA-O3A	2.06	1.61	1.59
11	F	401	ACP	PB-O2B	2.03	1.61	1.56
11	F	401	ACP	C4-N9	-2.02	1.33	1.37
10	D	502	9WR	O19-C18	2.02	1.40	1.36

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	505	MES	O3S-S-O1S	-12.23	80.79	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O3S-S-O1S	-11.97	81.45	111.40
9	B	503	MES	O3S-S-C8	-11.71	83.10	106.00
9	B	503	MES	O3S-S-O2S	-11.30	83.12	111.40
9	B	505	MES	O3S-S-O2S	-10.10	86.14	111.40
9	B	503	MES	O2S-S-C8	8.78	120.00	106.73
9	B	505	MES	O1S-S-C8	8.41	119.43	106.73
9	B	505	MES	O3S-S-C8	-7.90	90.55	106.00
9	B	503	MES	O1S-S-C8	6.99	117.29	106.73
9	B	505	MES	O2S-S-C8	6.97	117.25	106.73
5	A	501	GTP	C5-C4-N3	-5.69	119.34	128.39
11	F	401	ACP	C5-C4-N3	-5.68	118.90	126.72
5	D	501	GTP	C5-C4-N3	-5.59	119.50	128.39
8	B	501	GDP	C5-C4-N3	-5.10	120.28	128.39
5	D	501	GTP	C2-N3-C4	4.92	120.77	112.30
8	B	501	GDP	C2-N3-C4	4.76	120.50	112.30
5	A	501	GTP	C2-N3-C4	4.74	120.47	112.30
5	C	501	GTP	C5-C4-N3	-4.74	120.84	128.39
8	B	501	GDP	N9-C4-N3	4.47	134.88	125.95
11	F	401	ACP	N3-C4-N9	4.46	134.75	127.17
5	C	501	GTP	C2-N3-C4	4.35	119.79	112.30
5	D	501	GTP	N9-C4-N3	4.24	134.43	125.95
11	F	401	ACP	C2-N3-C4	3.87	121.27	111.83
5	A	501	GTP	N9-C4-N3	3.81	133.56	125.95
5	A	501	GTP	C6-C5-N7	3.80	137.21	130.29
11	F	401	ACP	N3-C2-N1	-3.78	122.86	128.58
5	C	501	GTP	N9-C4-N3	3.74	133.44	125.95
11	F	401	ACP	C4-C5-N7	-3.70	106.35	110.58
5	D	501	GTP	C6-C5-N7	3.63	136.89	130.29
5	C	501	GTP	C6-C5-N7	3.58	136.80	130.29
10	B	506	9WR	O02-C03-C26	3.51	121.15	115.14
8	B	501	GDP	C6-C5-N7	3.29	136.28	130.29
5	A	501	GTP	C4-C5-N7	-3.14	105.69	110.67
10	B	506	9WR	O02-C03-C04	-3.10	118.73	124.08
10	D	502	9WR	O02-C03-C26	2.90	120.11	115.14
11	F	401	ACP	C4-N9-C8	2.90	108.78	105.74
10	D	502	9WR	C06-C08-N21	2.79	120.86	116.96
11	F	401	ACP	C5-N7-C8	2.72	107.73	103.45
10	D	502	9WR	C11-C12-N21	-2.67	118.45	121.97
10	D	502	9WR	C12-N21-C08	2.66	122.84	118.22
10	B	506	9WR	C12-N21-C08	2.66	122.83	118.22
5	D	501	GTP	C4-C5-N7	-2.60	106.55	110.67
10	B	506	9WR	C11-C12-N21	-2.58	118.56	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	C6-O1-C2	2.55	118.12	109.88
11	F	401	ACP	C3'-C2'-C1'	2.45	106.09	101.46
5	D	501	GTP	O6-C6-C5	-2.44	120.08	126.53
9	B	505	MES	O2S-S-O1S	2.42	121.68	113.82
10	D	502	9WR	O24-C23-C26	2.37	119.20	115.14
10	B	506	9WR	C06-C08-N21	2.36	120.25	116.96
10	D	502	9WR	O19-C18-C16	2.32	122.08	117.60
10	B	506	9WR	C09-C08-N21	-2.32	120.22	122.92
5	C	501	GTP	O2A-PA-O3A	2.32	113.53	107.27
11	F	401	ACP	C6-C5-N7	2.31	136.54	132.09
10	B	506	9WR	O24-C23-C26	2.27	119.03	115.14
9	B	505	MES	C7-N4-C5	-2.27	105.20	111.24
9	B	503	MES	C7-N4-C5	-2.26	105.22	111.24
5	A	501	GTP	O3G-PG-O3B	-2.24	97.12	104.64
10	D	502	9WR	C09-C08-N21	-2.24	120.31	122.92
11	F	401	ACP	N9-C8-N7	-2.22	110.79	113.94
9	B	505	MES	C2-C3-N4	2.22	113.49	110.12
8	B	501	GDP	O6-C6-C5	-2.21	120.71	126.53
8	B	501	GDP	C8-N9-C4	2.19	110.13	106.03
5	C	501	GTP	O2G-PG-O1G	2.18	119.34	110.83
5	A	501	GTP	O3G-PG-O2G	2.18	115.97	107.80
10	D	502	9WR	C13-C20-C18	2.17	122.48	120.72
5	C	501	GTP	O6-C6-C5	-2.15	120.85	126.53
5	A	501	GTP	O6-C6-C5	-2.15	120.86	126.53
10	D	502	9WR	C11-C10-C09	-2.12	117.52	120.24
5	A	501	GTP	C8-N7-C5	2.08	107.97	104.26
10	D	502	9WR	O02-C03-C04	-2.08	120.50	124.08
11	F	401	ACP	C2-N1-C6	2.04	122.09	118.73
10	B	506	9WR	C13-C20-C18	2.04	122.38	120.72
5	C	501	GTP	C8-N9-C4	2.04	109.86	106.03
5	C	501	GTP	C6-C5-C4	-2.04	115.76	118.83
5	C	501	GTP	C4-C5-N7	-2.04	107.44	110.67
5	D	501	GTP	C5-C6-N1	2.02	118.41	113.25
10	B	506	9WR	C11-C10-C09	-2.02	117.65	120.24

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A

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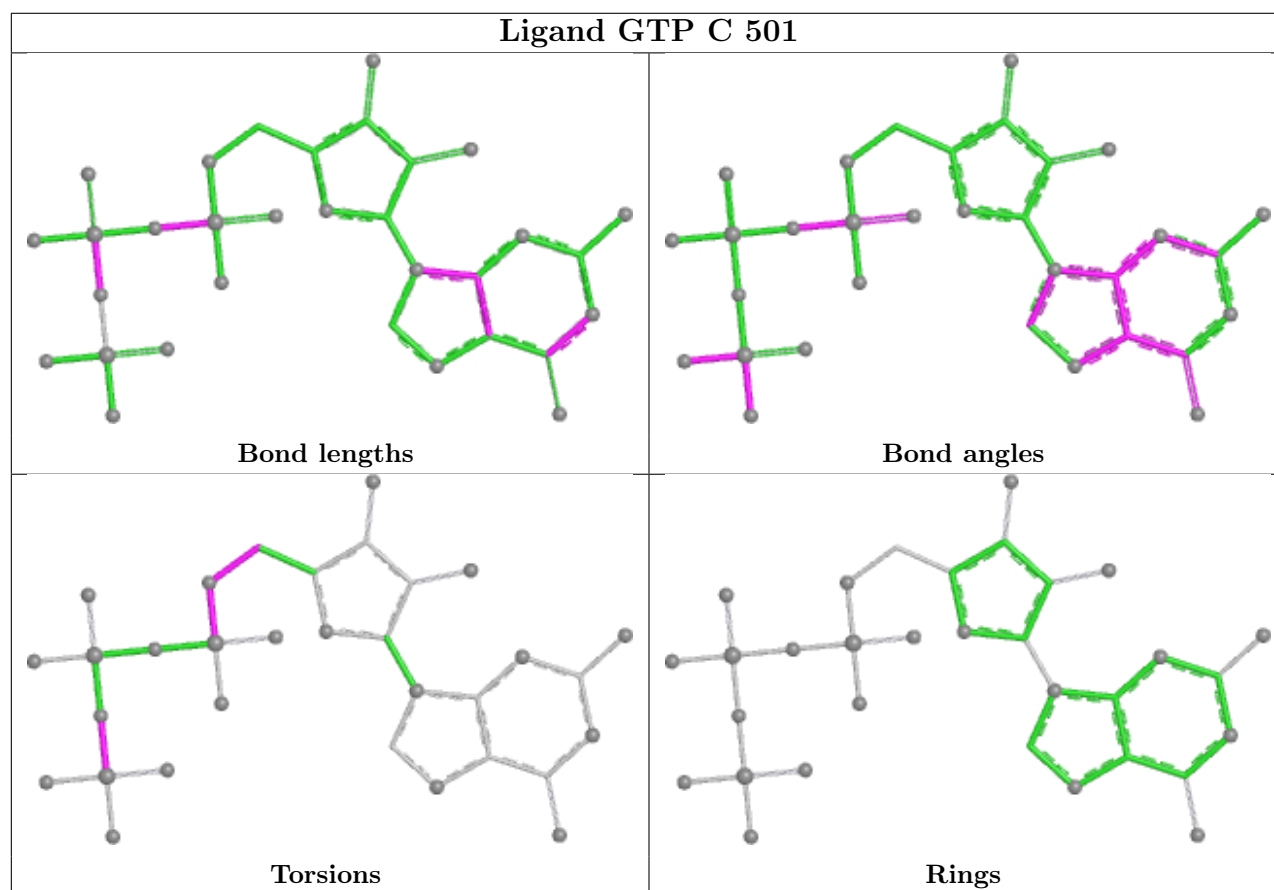
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C3
9	B	503	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O2S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
10	B	506	9WR	C26-C03-O02-C01
10	D	502	9WR	C26-C03-O02-C01
10	D	502	9WR	C26-C23-O24-C25
10	B	506	9WR	C04-C03-O02-C01
10	D	502	9WR	C22-C23-O24-C25
10	D	502	9WR	C04-C03-O02-C01
10	B	506	9WR	C26-C23-O24-C25
10	B	506	9WR	C22-C23-O24-C25
9	B	503	MES	C7-C8-S-O2S
9	B	505	MES	C7-C8-S-O1S
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	D	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-O3A-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	505	MES	N4-C7-C8-S
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PB-O3A-PA-O1A

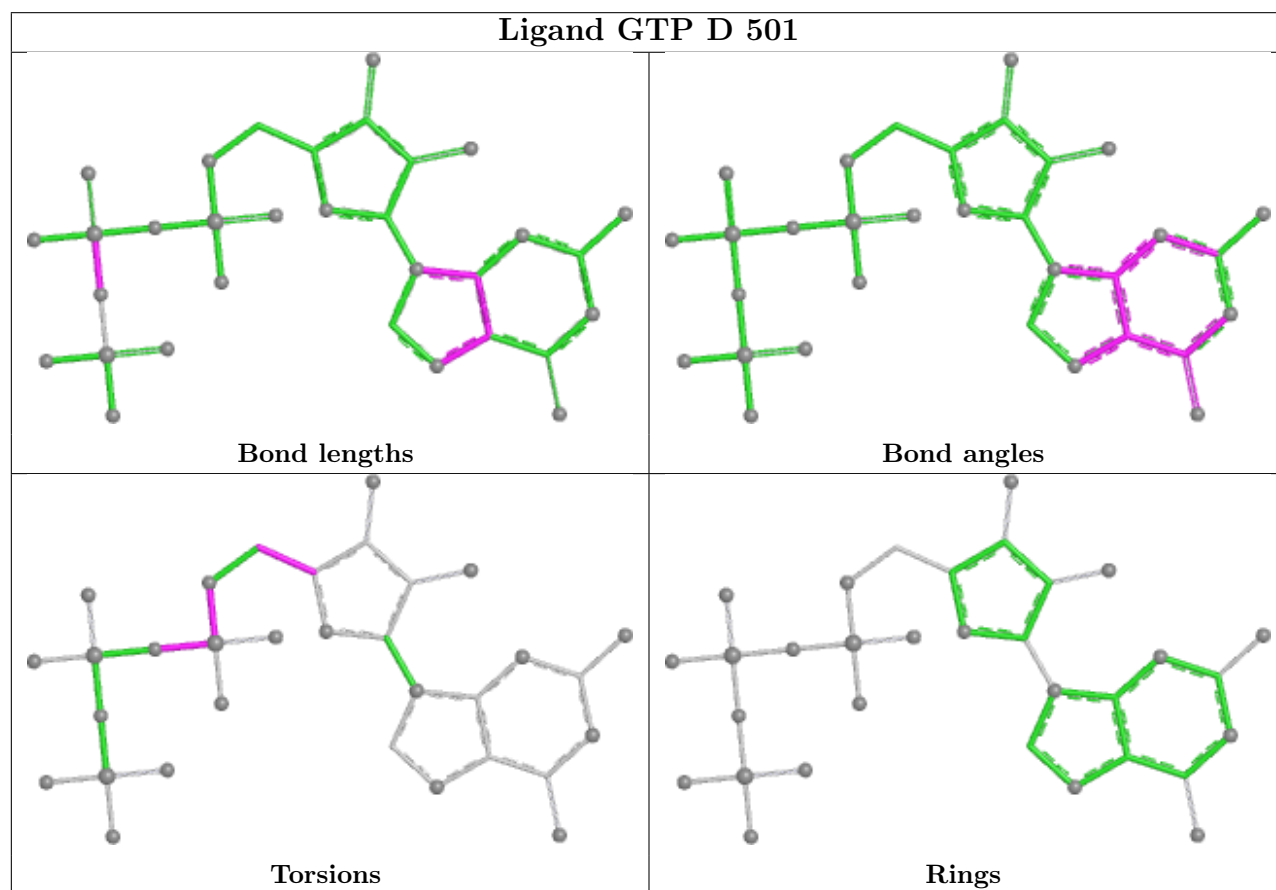
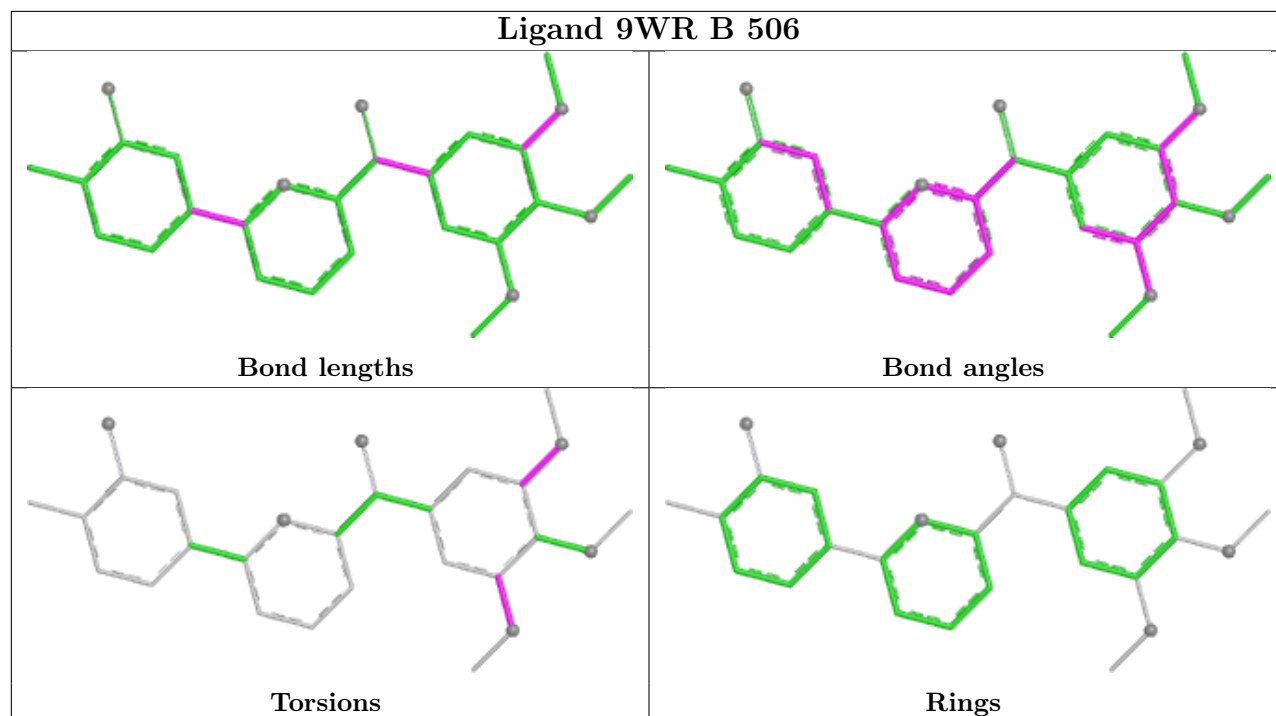
There are no ring outliers.

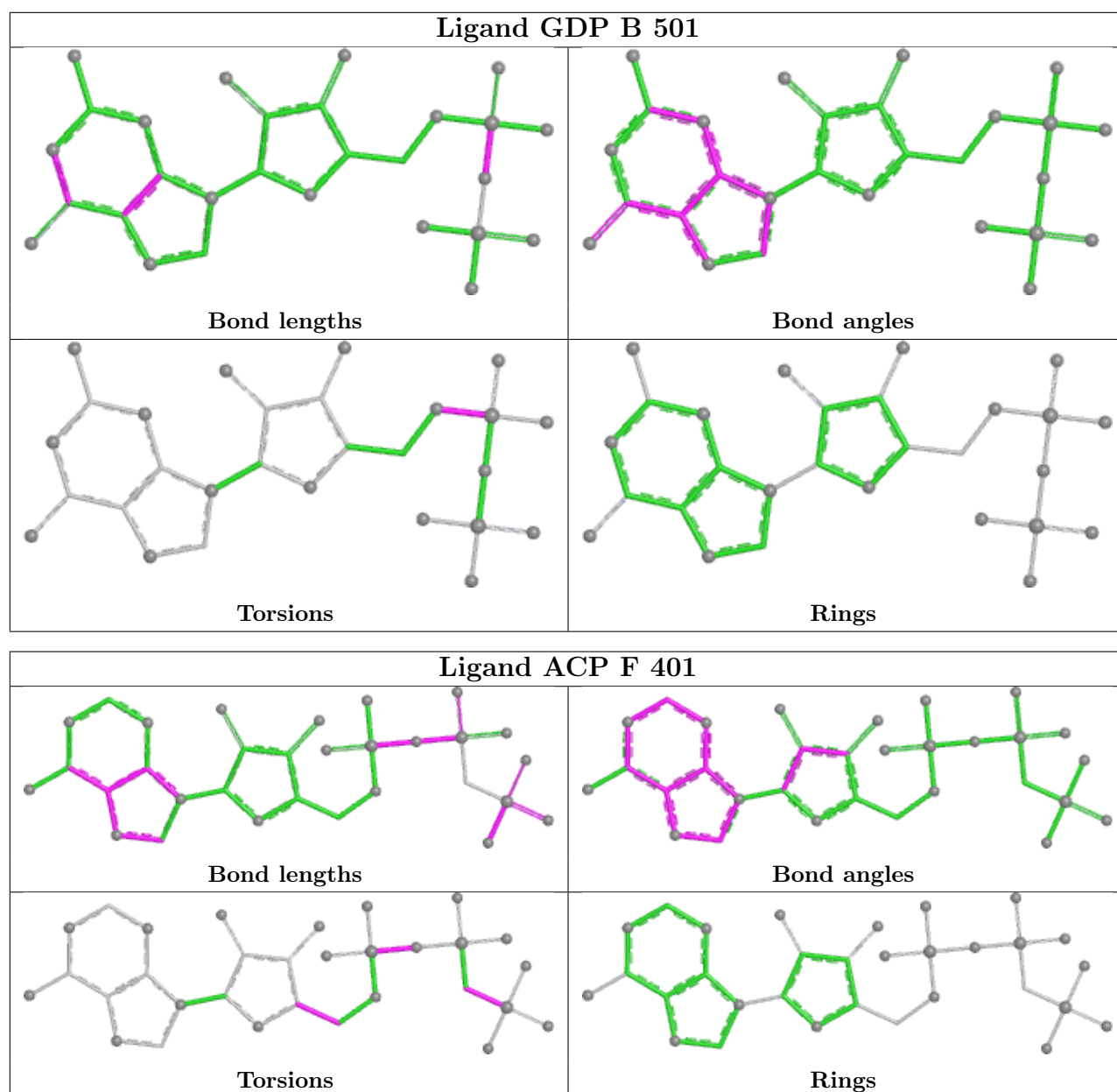
2 monomers are involved in 4 short contacts:

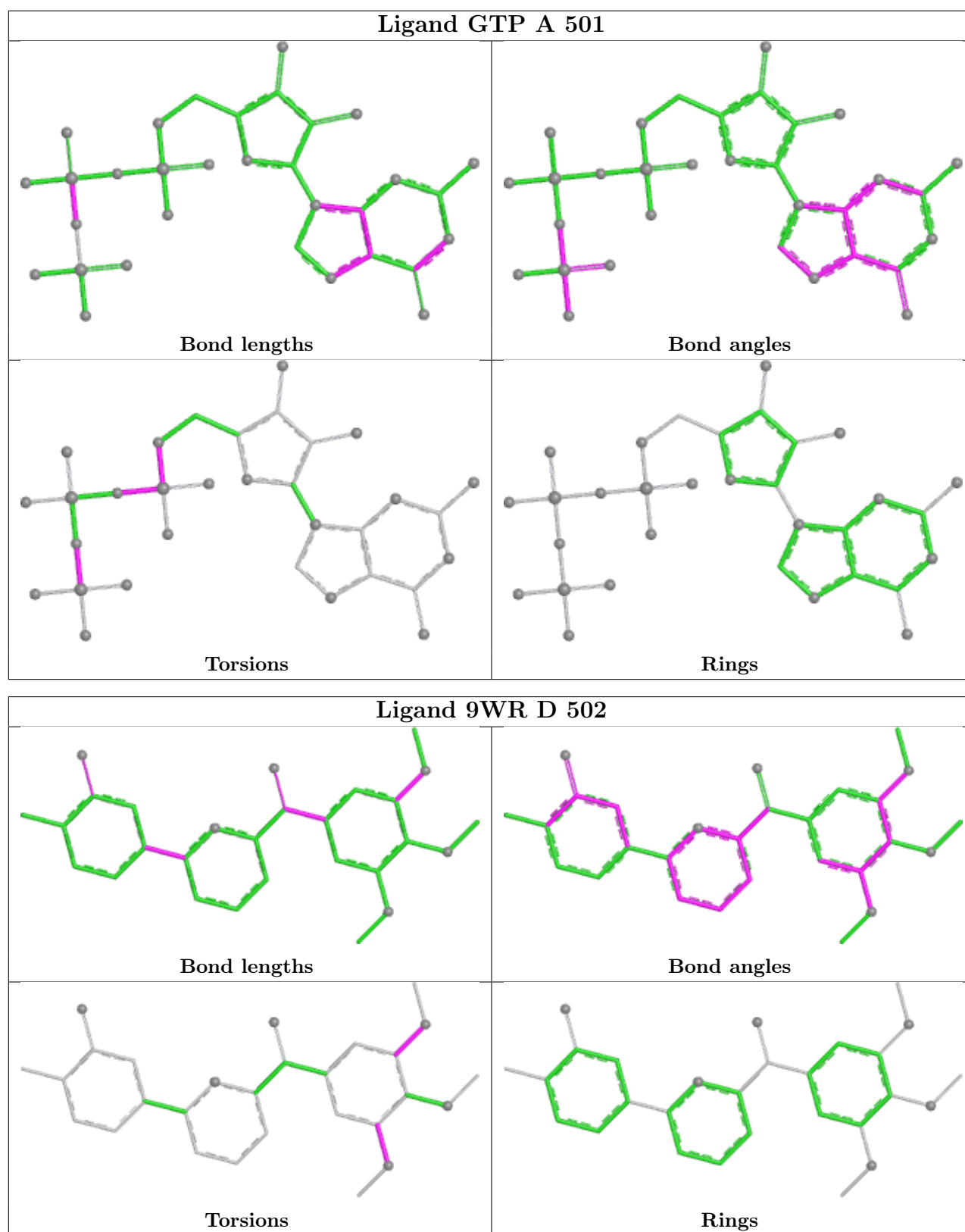
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	3	0
10	D	502	9WR	1	0

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 ⓘ

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	437/450 (97%)	0.08	10 (2%) 61 51	17, 41, 68, 94	4 (0%)
1	C	440/450 (97%)	-0.23	9 (2%) 65 56	12, 30, 58, 75	9 (2%)
2	B	424/445 (95%)	-0.01	8 (1%) 66 57	16, 39, 69, 100	3 (0%)
2	D	421/445 (94%)	1.05	65 (15%) 5 4	26, 68, 105, 134	4 (0%)
3	E	120/143 (83%)	0.91	13 (10%) 11 8	31, 60, 96, 108	2 (1%)
4	F	309/384 (80%)	1.09	63 (20%) 3 2	18, 69, 123, 147	3 (0%)
All	All	2151/2317 (92%)	0.38	168 (7%) 19 14	12, 47, 98, 147	25 (1%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	6.8
4	F	100	ILE	6.0
4	F	161	LEU	5.5
4	F	233	PHE	5.3
4	F	384	HIS	5.2
3	E	12[A]	ASN	5.2
4	F	380	HIS	5.0
4	F	225	SER	4.9
4	F	382	HIS	4.4
2	D	92	PHE	4.4
4	F	245	ILE	4.4
4	F	383	HIS	4.3
4	F	182	ILE	4.2
4	F	381	HIS	4.2
2	D	215	LEU	4.2
2	D	175	VAL	4.1
4	F	159	GLY	4.1
2	D	1	MET	4.0
2	D	396	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
4	F	237	THR	3.9
4	F	102	PRO	3.8
4	F	256	TYR	3.7
4	F	379	HIS	3.7
1	A	437	VAL	3.6
4	F	146	VAL	3.6
4	F	224	SER	3.6
4	F	197	ARG	3.6
1	C	211[A]	ASP	3.6
4	F	231	ALA	3.6
4	F	147	TRP	3.5
2	B	55	THR	3.5
1	A	262	TYR	3.5
4	F	253	TYR	3.5
4	F	160	ILE	3.4
2	D	323	MET	3.4
3	E	6	MET	3.4
2	D	55	THR	3.4
2	D	247	ASN	3.4
3	E	139	LEU	3.3
4	F	240	LEU	3.3
2	D	81	PHE	3.3
2	D	72	THR	3.3
2	D	73	MET	3.3
2	D	54	ALA	3.2
2	B	281	TYR	3.2
2	D	172	SER	3.2
1	C	283	HIS	3.1
2	D	220	PRO	3.1
2	D	217	LEU	3.1
2	D	37	HIS	3.1
2	D	85	PHE	3.0
2	B	2	ARG	3.0
3	E	45	PRO	3.0
4	F	23	ALA	3.0
4	F	186	LEU	3.0
2	D	94	GLN	2.9
1	A	196	GLU	2.9
2	D	211	CYS	2.9
1	C	46	ASP	2.9
1	A	163	LYS	2.9
4	F	236	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	394	PHE	2.9
2	D	245	GLN	2.8
4	F	162	ILE	2.8
2	D	214	THR	2.8
2	D	218	THR	2.8
4	F	247	LYS	2.8
2	D	140	GLY	2.8
4	F	163	SER	2.8
2	D	65	LEU	2.7
4	F	88	SER	2.7
2	D	377	LEU	2.7
2	B	280	GLN	2.7
4	F	99	VAL	2.7
1	A	88	HIS	2.7
2	D	210	ILE	2.7
2	D	397	TRP	2.7
1	C	178	SER	2.7
2	D	185	ALA	2.6
1	C	245	ASP	2.6
2	D	145[A]	SER	2.6
4	F	22	LEU	2.6
4	F	101	TYR	2.6
2	B	1	MET	2.5
3	E	133	VAL	2.5
4	F	257	GLU	2.5
4	F	259	GLY	2.5
1	A	346	TRP	2.5
1	A	282	TYR	2.5
3	E	104	LYS	2.5
4	F	184	LYS	2.5
4	F	194	PRO	2.5
4	F	254	GLY	2.5
2	D	97	ALA	2.5
2	D	42	LEU	2.4
2	D	212	PHE	2.4
4	F	255	ARG	2.4
2	D	219	THR	2.4
4	F	244	CYS	2.4
2	D	82	GLY	2.4
4	F	222	ARG	2.4
1	A	336	LYS	2.4
4	F	199	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	387	ALA	2.4
3	E	53	LYS	2.4
3	E	135	LYS	2.4
4	F	234	GLN	2.4
4	F	191	LEU	2.4
2	D	70	PRO	2.4
2	D	87	PRO	2.4
4	F	144	GLY	2.4
2	D	393	ALA	2.4
4	F	373	SER	2.4
4	F	239	HIS	2.3
2	D	356	ILE	2.3
4	F	263	PHE	2.3
4	F	238	CYS	2.3
4	F	180	HIS	2.3
4	F	320	MET	2.3
4	F	31	ARG	2.3
4	F	181	VAL	2.3
4	F	275	LEU	2.2
2	D	58	LYS	2.2
4	F	32	LYS	2.2
4	F	226	GLU	2.2
2	D	113	VAL	2.2
1	C	120[A]	ASP	2.2
2	D	179	VAL	2.2
2	D	75	SER	2.2
2	D	216	LYS	2.2
3	E	140	LYS	2.2
2	D	68	LEU	2.2
4	F	242	ASN	2.2
2	D	80	PRO	2.2
2	D	71	GLY	2.2
4	F	148	ILE	2.1
2	D	96	GLY	2.1
2	B	282	ARG	2.1
3	E	80	ARG	2.1
4	F	196	HIS	2.1
2	D	284	LEU	2.1
1	C	357	TYR	2.1
2	D	213	ARG	2.1
2	D	126	SER	2.1
3	E	131	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.1
2	D	174	LYS	2.1
2	D	31	ASP	2.1
4	F	223	THR	2.1
2	D	76	VAL	2.1
2	D	229	VAL	2.1
2	D	246	LEU	2.1
2	B	270	PHE	2.1
1	C	179	THR	2.1
2	B	214	THR	2.1
2	D	429	THR	2.1
2	D	69	GLU	2.1
2	D	208	TYR	2.1
1	C	340	SER	2.0
2	D	115	SER	2.0
2	D	15	GLN	2.0
1	A	179	THR	2.0
3	E	15	THR	2.0
4	F	149	ALA	2.0
2	D	170	MET	2.0
2	D	12	CYS	2.0
3	E	123	LEU	2.0
2	D	36	TYR	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.

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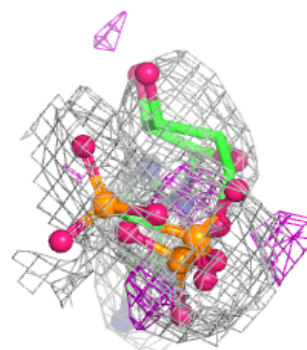
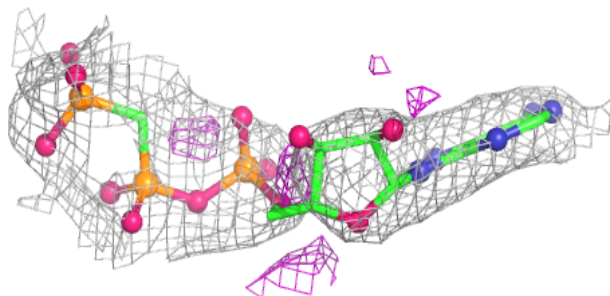
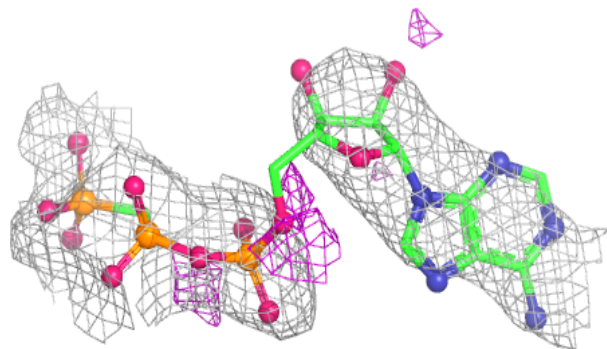
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ACP	F	401	31/31	0.77	0.15	83,93,137,139	0
5	GTP	D	501	32/32	0.84	0.14	51,60,86,92	0
9	MES	B	503	12/12	0.88	0.14	39,67,77,82	1
7	CA	B	504	1/1	0.89	0.09	67,67,67,67	0
9	MES	B	505	12/12	0.91	0.14	64,68,80,81	0
10	9WR	D	502	28/28	0.92	0.11	37,47,64,73	0
6	MG	B	502	1/1	0.94	0.17	30,30,30,30	0
10	9WR	B	506	28/28	0.94	0.09	26,29,42,44	0
7	CA	C	503	1/1	0.96	0.05	52,52,52,52	0
5	GTP	A	501	32/32	0.97	0.07	23,24,30,31	0
8	GDP	B	501	28/28	0.98	0.05	18,24,29,30	0
5	GTP	C	501	32/32	0.98	0.05	19,22,23,24	0
7	CA	A	503	1/1	0.98	0.04	58,58,58,58	0
6	MG	A	502	1/1	0.99	0.03	20,20,20,20	0
6	MG	C	502	1/1	1.00	0.01	24,24,24,24	0

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

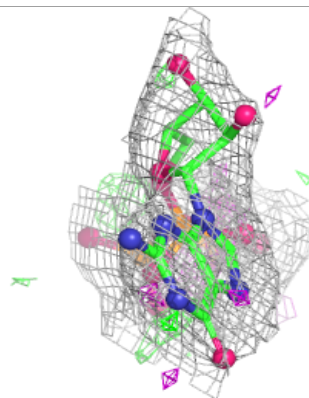
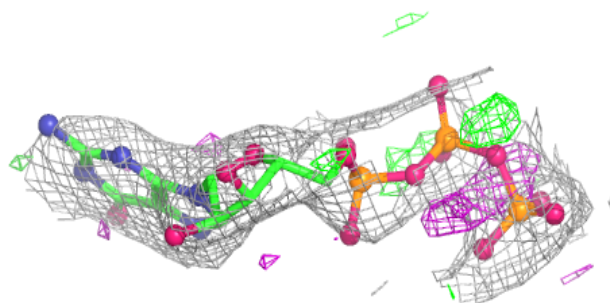
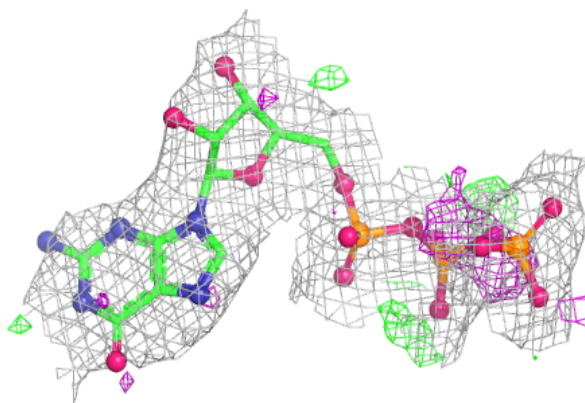
Electron density around ACP F 401:

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

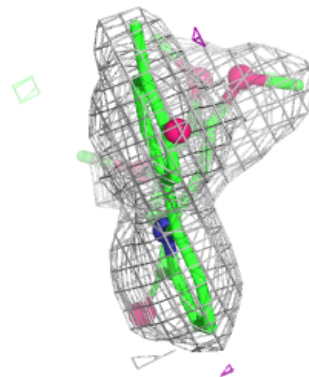
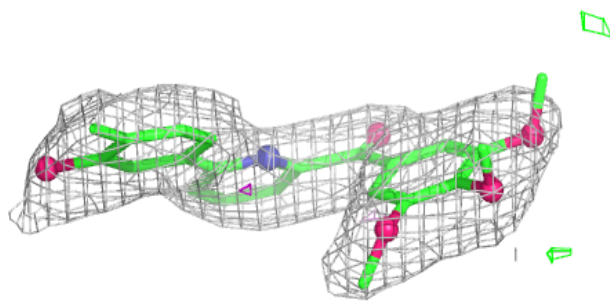
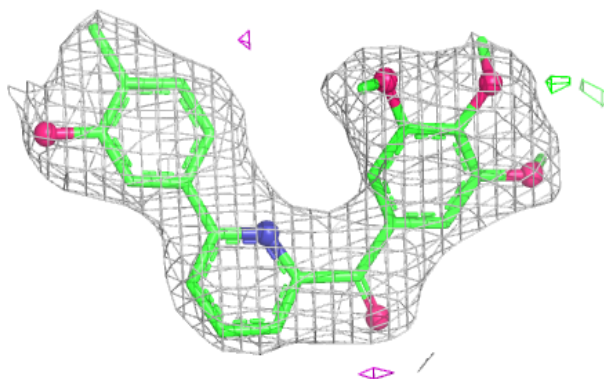


Electron density around GTP D 501:

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

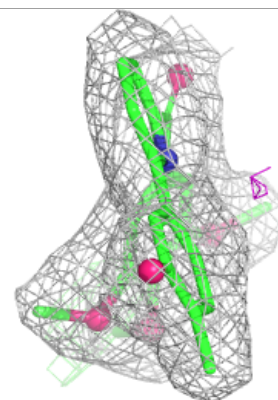
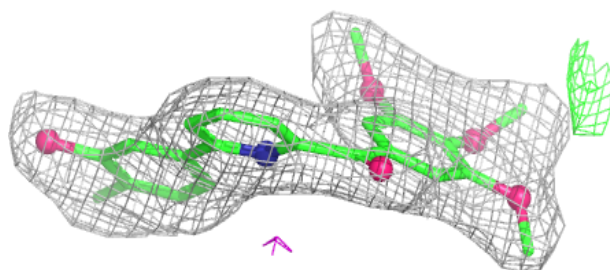
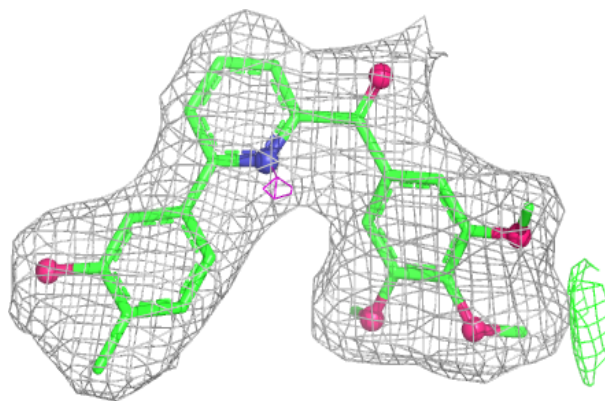
**Electron density around 9WR D 502:**

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

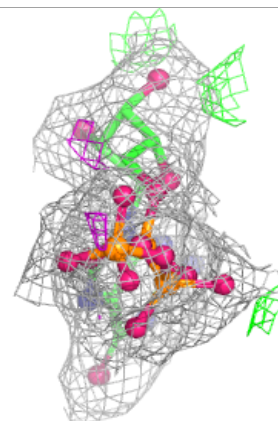
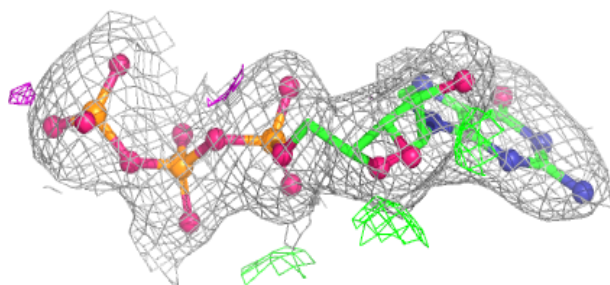
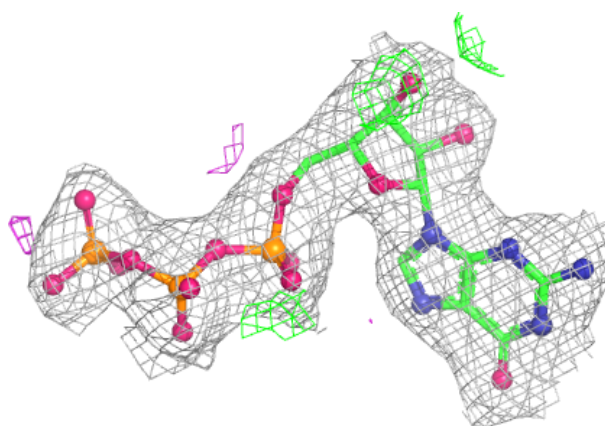


Electron density around 9WR B 506:

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

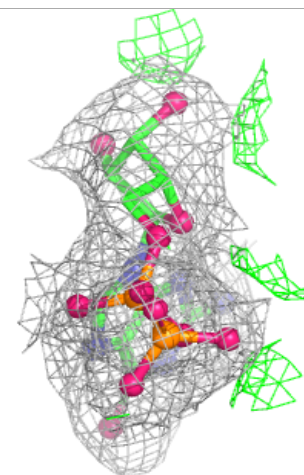
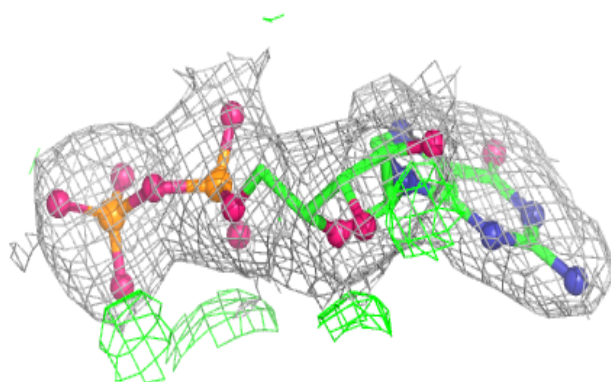
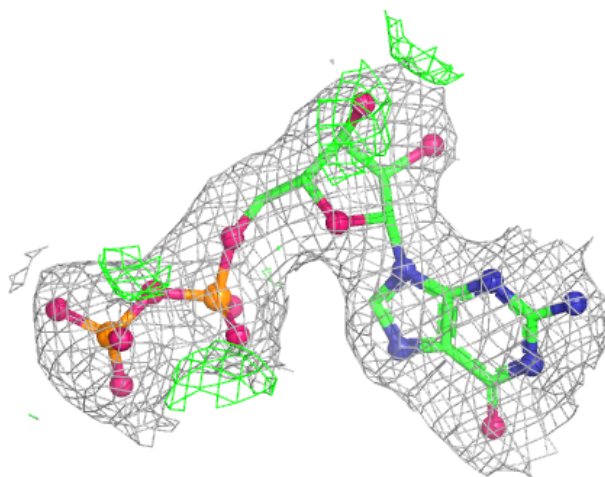
**Electron density around GTP A 501:**

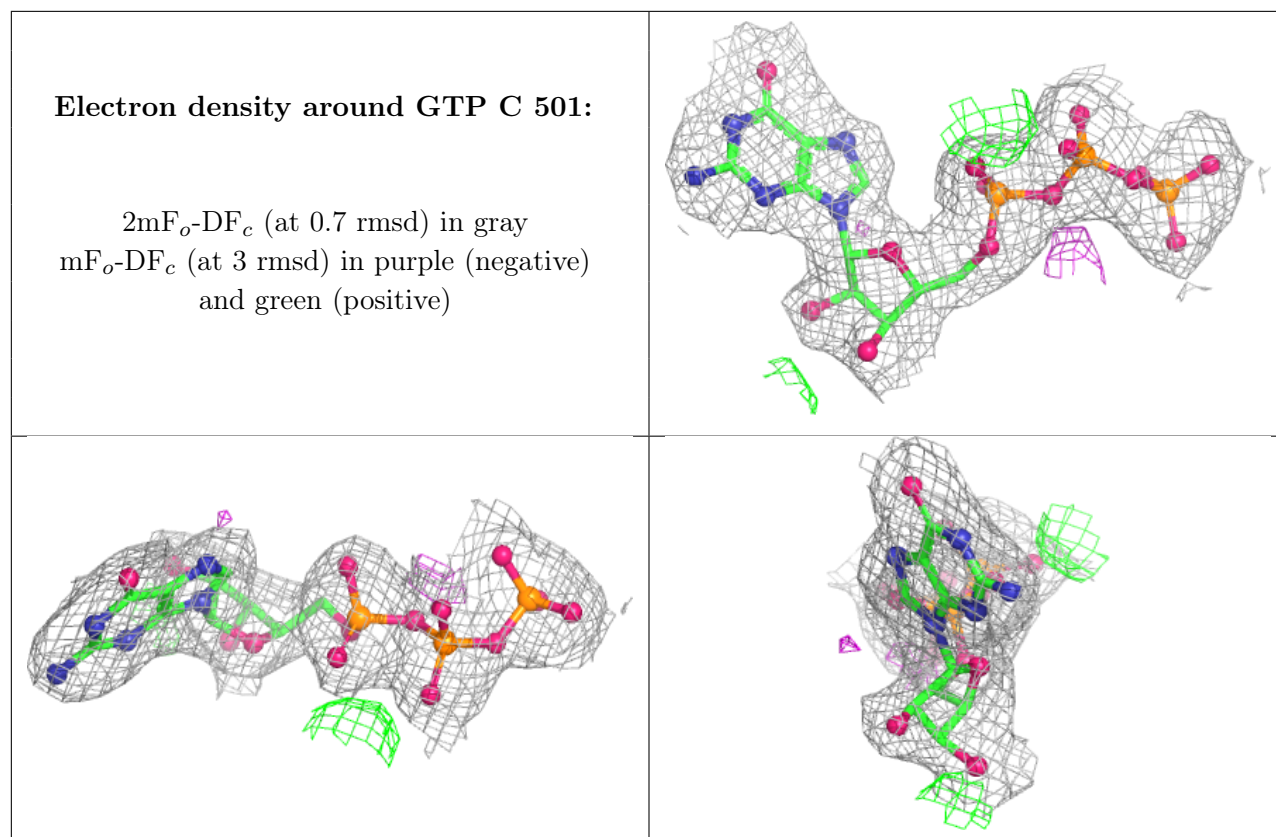
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.