



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:31 AM UTC

PDB ID : 7Z2P / pdb_00007z2p
Title : Tubulin-nocodazole complex
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Deposited on : 2022-02-28
Resolution : 2.00 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

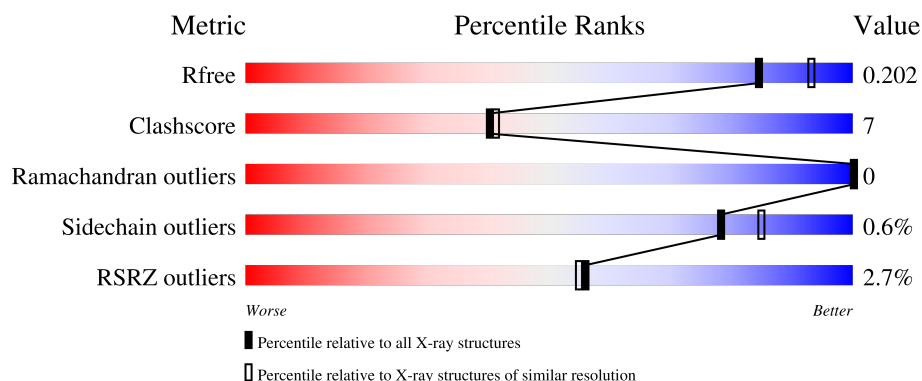
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	0% 85% 12% •
1	C	451	2% 82% 16% •
2	B	445	2% 79% 16% 5%
2	D	445	3% 79% 15% • 5%
3	E	143	5% 78% 8% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	3% 77% 12% 10%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18454 atoms, of which 22 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	439	Total	C	N	O	S	0	8	0
			3462	2199	583	655	25			
1	C	440	Total	C	N	O	S	0	10	0
			3473	2203	585	660	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	4	0
			3339	2101	565	646	27			
2	D	421	Total	C	N	O	S	0	3	0
			3320	2088	562	642	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	1	0
			1021	630	185	201	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

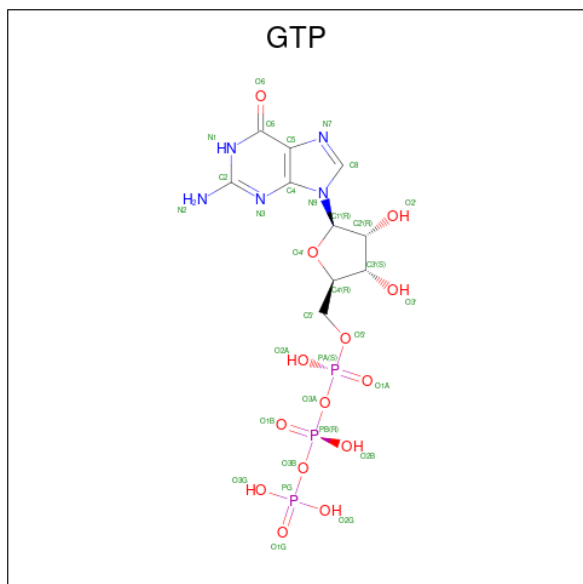
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	344	Total	C	N	O	S	0	0	0
			2818	1807	479	518	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		

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

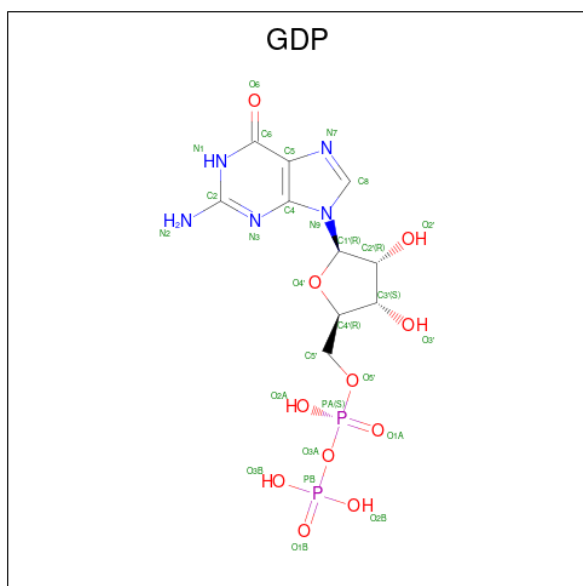
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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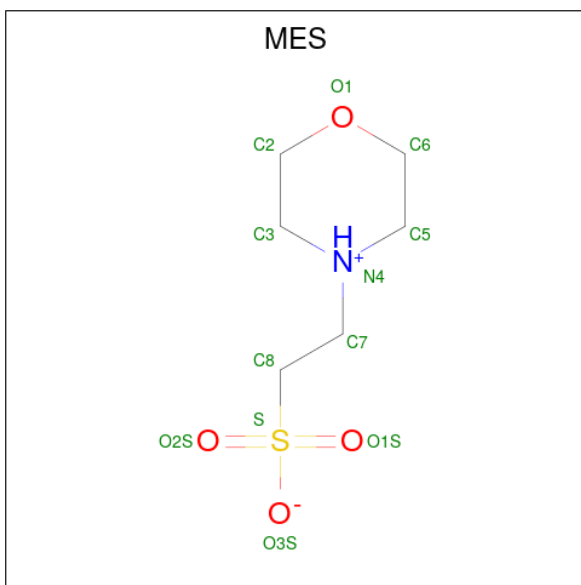
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



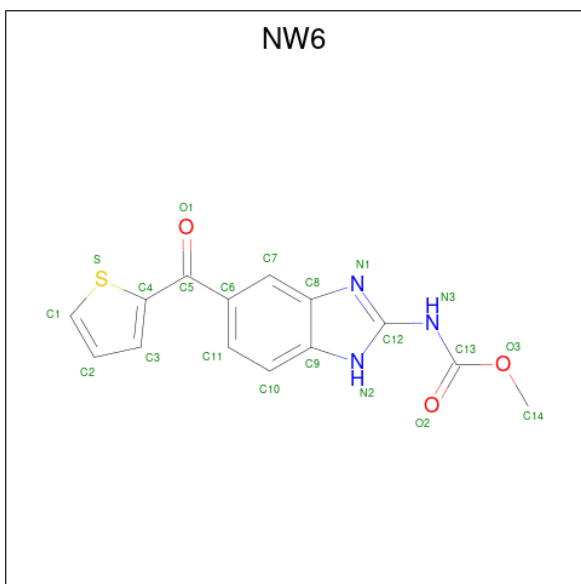
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 9 is nocodazole (CCD ID: NW6) (formula: $C_{14}H_{11}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



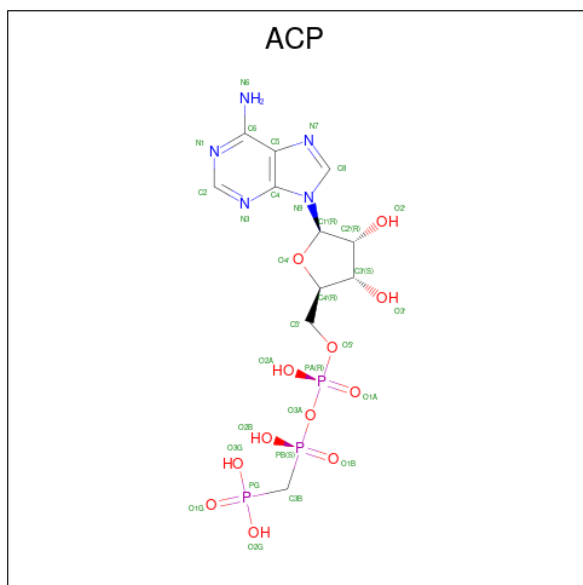
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0
			32	14	11	3	3	1	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	H	N	O	S	
			32	14	11	3	3	1	
								0	0

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

- Molecule 11 is water.

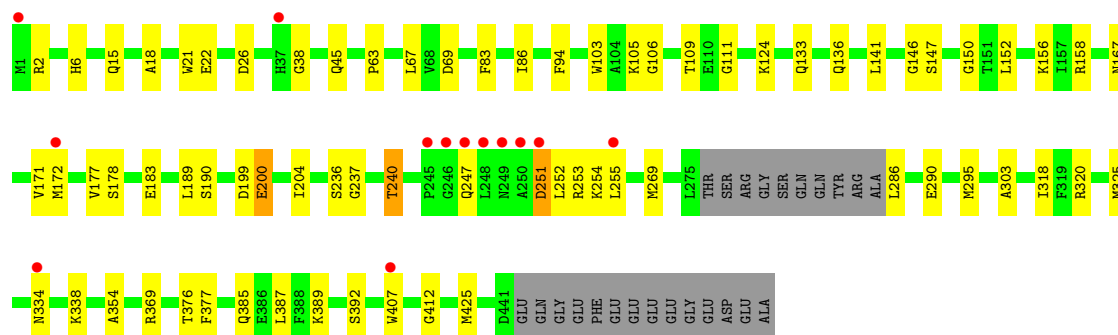
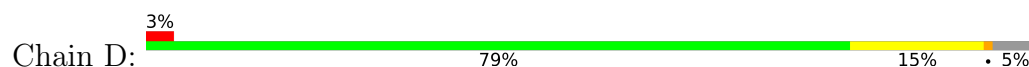
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	150	Total	O		
			150	150	0	0
11	B	169	Total	O		
			169	169	0	0
11	C	280	Total	O		
			280	280	0	0
11	D	85	Total	O		
			85	85	0	0
11	E	34	Total	O		
			34	34	0	0
11	F	59	Total	O		
			59	59	0	0

- Molecule 1: Tubulin alpha-1B chain

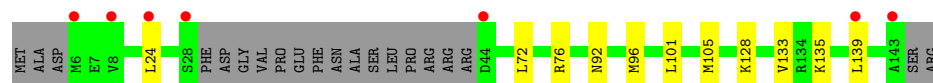
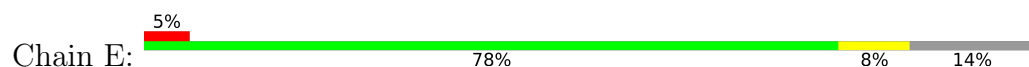




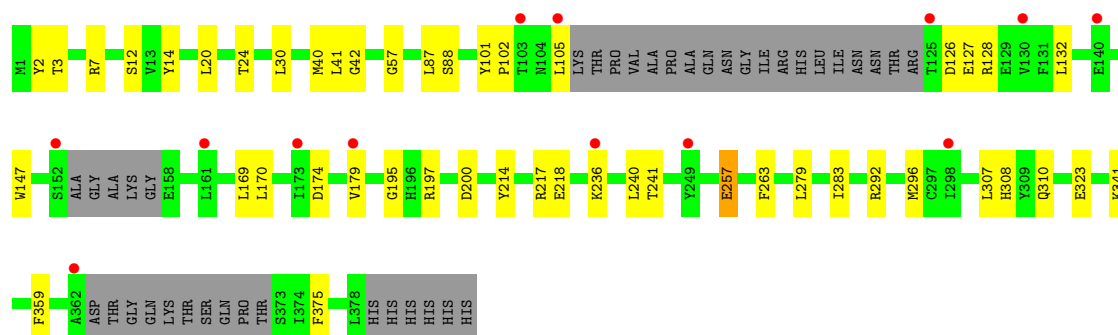
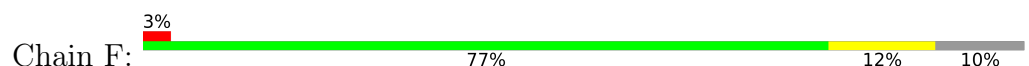
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.73Å 158.09Å 179.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.00 49.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.37-2.00) 99.8 (49.37-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.178 , 0.209 (Not available) , 0.202	Depositor DCC
R_{free} test set	10017 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18454	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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, NW6, ACP, MES, GTP, GDP

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	0.13	0/3564	0.30	0/4839
1	C	0.16	0/3582	0.34	0/4865
2	B	0.15	0/3425	0.33	0/4639
2	D	0.13	0/3402	0.30	0/4608
3	E	0.13	0/1033	0.24	0/1371
4	F	0.10	0/2880	0.28	0/3890
All	All	0.14	0/17886	0.31	0/24212

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	3462	0	3406	38	0
1	C	3473	0	3412	50	0
2	B	3339	0	3224	56	0
2	D	3320	0	3208	54	0
3	E	1021	0	1036	10	0
4	F	2818	0	2789	32	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	B	28	0	12	0	0
7	D	28	0	12	0	0
8	B	12	0	12	1	0
8	D	12	0	12	3	0
9	B	21	11	0	0	0
9	D	21	11	0	4	0
10	F	31	0	14	1	0
11	A	150	0	0	3	0
11	B	169	0	0	6	0
11	C	280	0	0	6	0
11	D	85	0	0	1	0
11	E	34	0	0	1	0
11	F	59	0	0	1	0
All	All	18432	22	17161	230	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 7.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:GLN:HE21	2:D:354:ALA:HA	1.41	0.84
1:A:77:GLU:OE1	11:A:601:HOH:O	1.99	0.81
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.63	0.80
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.63	0.80
2:D:167:ASN:OD1	2:D:200:GLU:HG3	1.82	0.79
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.64	0.79
2:D:236:SER:O	2:D:240:THR:HG22	1.82	0.78
1:C:339:ARG:O	11:C:601:HOH:O	2.03	0.76
2:B:323:MET:HE2	2:B:373:MET:HE2	1.66	0.76
2:B:323:MET:HB3	2:B:373:MET:HE1	1.68	0.75
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.70	0.73
2:D:247:GLN:NE2	2:D:354:ALA:HA	2.04	0.73
1:C:101:ASN:ND2	1:C:180:ALA:HB2	2.04	0.73
2:D:255:LEU:HD13	9:D:504:NW6:C8	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.30	0.71
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.24	0.70
2:D:237:GLY:O	2:D:240:THR:HG23	1.92	0.70
2:B:1:MET:HG3	2:B:130:ASP:OD2	1.91	0.69
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.75	0.68
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.28	0.68
2:B:294:GLN:OE1	11:B:601:HOH:O	2.11	0.67
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.34	0.67
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.30	0.66
2:B:329:ASP:O	2:B:333:LEU:HG	1.95	0.66
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.76	0.66
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.26	0.65
1:C:360:PRO:HB2	11:C:807:HOH:O	1.97	0.65
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.79	0.65
2:B:301:MET:HE2	2:B:301:MET:HA	1.79	0.64
2:B:420:GLU:OE1	11:B:602:HOH:O	2.14	0.64
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.34	0.62
1:C:286:LEU:HB2	11:C:621:HOH:O	1.98	0.62
2:D:147[B]:SER:HG	2:D:190:SER:HG	1.27	0.62
1:C:178:SER:HB2	1:C:183:GLU:OE1	2.00	0.62
2:B:323:MET:HB3	2:B:373:MET:CE	2.30	0.61
2:D:167:ASN:ND2	2:D:252:LEU:HD22	2.14	0.61
2:B:332:MET:HG3	2:B:353:THR:HG21	1.82	0.61
1:C:179:THR:HG22	11:C:837:HOH:O	2.00	0.60
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.83	0.59
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.37	0.59
2:D:2:ARG:HB3	2:D:133:GLN:HE21	1.68	0.59
2:D:318:ILE:CG2	2:D:376:THR:HB	2.32	0.59
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.84	0.59
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.85	0.59
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.85	0.58
2:B:1:MET:HB2	2:B:3:GLU:OE2	2.03	0.58
3:E:72:LEU:O	3:E:76:ARG:HG2	2.03	0.58
2:B:181:VAL:HG12	1:C:348[A]:PRO:HG2	1.86	0.58
4:F:241:THR:OG1	10:F:401:ACP:O3'	2.19	0.58
2:D:2:ARG:HB3	2:D:133:GLN:NE2	2.19	0.57
2:B:141:LEU:HD12	2:B:172:MET:SD	2.44	0.57
2:D:124:LYS:C	2:D:124:LYS:HD3	2.30	0.56
2:D:255:LEU:HB3	9:D:504:NW6:C10	2.35	0.56
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.20	0.56
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:126:ASP:OD1	4:F:127:GLU:N	2.39	0.56
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.41	0.56
2:B:337:ASN:OD1	2:B:338:LYS:N	2.38	0.56
1:C:415:GLU:OE2	11:C:602:HOH:O	2.18	0.56
2:D:240:THR:OG1	2:D:318:ILE:HD11	2.05	0.56
1:C:320:ARG:HA	1:C:356:ASN:O	2.06	0.56
1:C:359:PRO:HB2	11:C:667:HOH:O	2.06	0.55
2:D:106:GLY:O	2:D:111:GLY:HA3	2.06	0.55
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.89	0.55
1:C:174:ALA:O	1:C:178:SER:HB3	2.07	0.55
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.89	0.55
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.89	0.55
2:D:69:ASP:O	2:D:94:PHE:HA	2.06	0.55
2:B:69:ASP:O	2:B:94:PHE:HA	2.07	0.54
2:D:177:VAL:HG12	2:D:177:VAL:O	2.06	0.54
2:B:215:ARG:NH1	11:B:606:HOH:O	2.40	0.54
3:E:92:ASN:HD21	3:E:96:MET:HE2	1.73	0.54
3:E:135:LYS:NZ	3:E:139:LEU:HD11	2.22	0.54
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.43	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.53
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.43	0.53
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.38	0.53
2:D:392:SER:HB2	2:D:425:MET:HE3	1.90	0.53
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.51	0.53
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.36	0.52
2:B:2:ARG:HA	2:B:133:GLN:HG3	1.92	0.52
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.92	0.52
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.09	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.45	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.45	0.52
2:B:282:GLN:N	11:B:609:HOH:O	2.43	0.52
2:B:301:MET:HE1	2:B:377:PHE:CD1	2.45	0.52
1:A:261:PRO:HD2	11:A:710:HOH:O	2.10	0.51
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.38	0.51
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.10	0.51
1:A:264:ARG:NH1	11:A:604:HOH:O	2.31	0.51
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.51
2:D:83:PHE:O	2:D:86:ILE:HG22	2.10	0.51
2:D:152:LEU:O	2:D:156:LYS:HG2	2.10	0.51
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.51
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.46	0.50
2:D:141:LEU:HD12	2:D:172:MET:SD	2.50	0.50
2:B:333:LEU:CD1	4:F:57:GLY:HA3	2.41	0.50
4:F:7:ARG:CD	4:F:40:MET:HE3	2.38	0.50
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.52	0.50
2:D:158:ARG:NE	8:D:503:MES:O1	2.43	0.50
2:D:240:THR:HG21	2:D:320:ARG:HD2	1.94	0.50
4:F:323:GLU:OE2	11:F:501:HOH:O	2.20	0.50
2:B:296:PHE:CG	2:B:335:VAL:HG11	2.46	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.12	0.50
1:C:234:ILE:HD13	1:C:302:MET:SD	2.52	0.50
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.76	0.49
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.94	0.49
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.95	0.49
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.47	0.49
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.95	0.49
2:B:292:THR:HG22	2:B:335:VAL:CG2	2.40	0.49
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.48	0.49
2:D:407:TRP:NE1	11:D:610:HOH:O	2.46	0.49
3:E:135:LYS:HZ2	3:E:139:LEU:HD11	1.78	0.49
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.13	0.48
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.95	0.48
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.43	0.48
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.44	0.48
2:B:304:ALA:N	11:B:611:HOH:O	2.46	0.48
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.49	0.48
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.48	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.43	0.48
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.14	0.48
1:C:97:GLU:OE2	2:D:253:ARG:NH1	2.47	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.48
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.95	0.47
1:C:297:GLU:OE2	1:C:339:ARG:NH2	2.36	0.47
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.95	0.47
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.95	0.47
1:A:79:ARG:O	1:A:84:ARG:HB2	2.14	0.47
2:B:275:LEU:O	2:B:276:THR:C	2.57	0.47
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.30	0.47
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.97	0.47
2:D:251:ASP:OD1	2:D:251:ASP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.32	0.47
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.46
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.46
1:C:108:TYR:O	1:C:112:LYS:HG2	2.16	0.46
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	1.98	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.15	0.46
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.46
2:B:2:ARG:CA	2:B:133:GLN:HG3	2.45	0.46
1:C:1:MET:HG2	1:C:130:THR:OG1	2.15	0.46
4:F:236:LYS:HB3	4:F:240:LEU:HG	1.98	0.46
1:C:165[B]:SER:HA	1:C:199:ASP:OD2	2.15	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.96	0.46
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.31	0.45
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.98	0.45
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.50	0.45
1:C:419:SER:O	1:C:423:GLU:HG3	2.17	0.45
2:D:105:LYS:HA	2:D:109:THR:OG1	2.17	0.45
4:F:40:MET:HE2	4:F:42:GLY:HA3	1.98	0.45
2:B:349:ASN:O	2:B:352:LYS:HE2	2.17	0.45
2:D:167:ASN:HD21	2:D:252:LEU:HD22	1.80	0.45
2:D:158:ARG:HE	8:D:503:MES:C2	2.30	0.45
4:F:40:MET:HE2	4:F:42:GLY:CA	2.47	0.45
2:B:424:ASN:HB3	11:B:621:HOH:O	2.17	0.45
1:C:165[A]:SER:HA	1:C:199:ASP:OD2	2.16	0.45
1:C:112:LYS:HE2	11:E:233:HOH:O	2.16	0.45
2:D:178:SER:OG	2:D:183:GLU:OE2	2.29	0.45
1:C:100:ALA:HA	2:D:254:LYS:CG	2.47	0.45
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.99	0.45
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.45
2:B:28:HIS:HB3	2:B:49:ILE:HD13	1.99	0.45
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.81	0.44
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.48	0.44
1:C:2:ARG:HD2	1:C:2:ARG:N	2.32	0.44
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.52	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.44
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.53	0.44
2:D:325:MET:HE2	2:D:325:MET:HB2	1.83	0.44
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.00	0.43
2:D:255:LEU:HB3	9:D:504:NW6:C9	2.48	0.43
3:E:128:LYS:HD3	3:E:128:LYS:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:263:PHE:CE2	4:F:341:LYS:HE2	2.53	0.43
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	2.00	0.43
4:F:292:ARG:O	4:F:296:MET:HG2	2.18	0.43
1:C:302:MET:HE3	1:C:302:MET:HA	2.00	0.43
2:D:199:ASP:OD1	8:D:503:MES:H62	2.18	0.43
4:F:87:LEU:O	4:F:88:SER:OG	2.25	0.43
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.53	0.43
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.49	0.43
2:B:181:VAL:HG12	1:C:348[A]:PRO:CG	2.47	0.43
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.01	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.42
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.18	0.42
3:E:101:LEU:O	3:E:105:MET:HG2	2.20	0.42
2:B:123:ARG:O	2:B:127:GLU:HG3	2.19	0.42
2:D:255:LEU:HD13	9:D:504:NW6:C9	2.50	0.42
2:D:387:LEU:HD23	2:D:387:LEU:C	2.45	0.42
4:F:20:LEU:O	4:F:24:THR:HG23	2.19	0.42
3:E:92:ASN:O	3:E:96:MET:HG2	2.20	0.42
2:B:288:VAL:N	2:B:289:PRO:CD	2.83	0.42
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.54	0.42
2:D:18:ALA:O	2:D:22:GLU:HG3	2.19	0.42
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.20	0.42
4:F:3:THR:HB	4:F:30:LEU:HD11	2.02	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.41
2:B:55:GLU:HG2	2:B:61:TYR:CE2	2.55	0.41
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.03	0.41
1:C:141:PHE:HB3	1:C:187:SER:OG	2.19	0.41
1:C:181[B]:VAL:HG11	1:C:404:PHE:CZ	2.56	0.41
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.02	0.41
2:B:387:LEU:C	2:B:387:LEU:HD23	2.46	0.41
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.85	0.41
1:A:28:HIS:O	1:A:36:MET:HE3	2.20	0.41
1:A:184:PRO:O	1:A:188:ILE:HD13	2.20	0.41
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.34	0.41
1:A:346:TRP:CD1	1:A:346:TRP:H	2.37	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
1:A:187:SER:CB	1:A:391:LEU:HD21	2.51	0.41
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.03	0.41
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.03	0.40
2:B:164:ARG:O	8:B:503:MES:H31	2.22	0.40
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:GLN:OE1	2:D:389:LYS:HE3	2.21	0.40
1:A:1:MET:HE3	1:A:1:MET:HB3	2.01	0.40
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.47	0.40
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.21	0.40
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.56	0.40
2:D:146:GLY:O	2:D:150:GLY:HA3	2.21	0.40
2:D:412:GLY:C	3:E:133:VAL:HG13	2.47	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	445/451 (99%)	437 (98%)	8 (2%)	0	100	100
1	C	448/451 (99%)	441 (98%)	7 (2%)	0	100	100
2	B	423/445 (95%)	418 (99%)	5 (1%)	0	100	100
2	D	420/445 (94%)	409 (97%)	11 (3%)	0	100	100
3	E	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
4	F	336/384 (88%)	328 (98%)	8 (2%)	0	100	100
All	All	2192/2319 (94%)	2150 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/379 (100%)	376 (100%)	2 (0%)	81	87
1	C	381/379 (100%)	379 (100%)	2 (0%)	81	87
2	B	369/383 (96%)	369 (100%)	0	100	100
2	D	367/383 (96%)	363 (99%)	4 (1%)	65	73
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	310/342 (91%)	307 (99%)	3 (1%)	68	75
All	All	1916/1993 (96%)	1905 (99%)	11 (1%)	78	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	381	THR
1	C	2	ARG
1	C	361	THR
2	D	15	GLN
2	D	200	GLU
2	D	240	THR
2	D	251	ASP
4	F	12	SER
4	F	257	GLU
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	HIS
2	B	15	GLN
2	B	37	HIS
2	B	167	ASN
2	B	192	HIS
1	C	85	GLN
1	C	107	HIS
1	C	133	GLN
1	C	356	ASN
1	C	393	HIS
2	D	15	GLN

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Mol	Chain	Res	Type
2	D	247	GLN
2	D	334	ASN
2	D	339	ASN
2	D	436	GLN
3	E	92	ASN
3	E	103	GLN
4	F	180	HIS
4	F	269	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 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	A	501	6	33,34,34	0.91	0	50,54,54	1.45	8 (16%)
9	NW6	D	504	-	23,23,23	1.48	4 (17%)	32,32,32	1.44	7 (21%)
7	GDP	D	501	6	29,30,30	1.15	2 (6%)	45,47,47	1.70	5 (11%)
7	GDP	B	501	6	29,30,30	1.11	2 (6%)	45,47,47	1.72	8 (17%)
8	MES	D	503	-	12,12,12	2.23	1 (8%)	15,16,16	1.84	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NW6	B	504	-	23,23,23	1.36	4 (17%)	32,32,32	1.38	7 (21%)
5	GTP	C	501	6	33,34,34	0.93	2 (6%)	50,54,54	1.50	8 (16%)
10	ACP	F	401	6	31,33,33	1.66	8 (25%)	47,52,52	1.81	9 (19%)
8	MES	B	503	-	12,12,12	2.00	1 (8%)	15,16,16	1.75	3 (20%)

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	A	501	6	-	8/22/38/38	0/3/3/3
9	NW6	D	504	-	-	2/14/14/14	0/3/3/3
7	GDP	D	501	6	-	4/16/32/32	0/3/3/3
7	GDP	B	501	6	-	5/16/32/32	0/3/3/3
8	MES	D	503	-	-	4/6/14/14	0/1/1/1
9	NW6	B	504	-	-	2/14/14/14	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
10	ACP	F	401	6	-	3/19/38/38	0/3/3/3
8	MES	B	503	-	-	0/6/14/14	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	MES	C8-S	-7.43	1.67	1.77
8	B	503	MES	C8-S	-6.66	1.68	1.77
10	F	401	ACP	C5-C4	4.80	1.47	1.39
9	D	504	NW6	C12-N2	3.84	1.41	1.35
9	B	504	NW6	C12-N2	3.39	1.41	1.35
7	D	501	GDP	C5-C4	3.09	1.47	1.38
9	D	504	NW6	C12-N3	3.03	1.44	1.37
10	F	401	ACP	PG-O3G	3.01	1.61	1.55
10	F	401	ACP	PG-O2G	2.92	1.61	1.55
7	B	501	GDP	C5-C4	2.86	1.46	1.38
9	D	504	NW6	C13-N3	2.83	1.42	1.37
10	F	401	ACP	C5-C6	2.74	1.48	1.41
9	B	504	NW6	C12-N3	2.60	1.43	1.37
10	F	401	ACP	PB-O3A	2.55	1.61	1.58
9	D	504	NW6	C11-C6	2.54	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	NW6	C11-C6	2.51	1.43	1.39
7	D	501	GDP	C6-N1	-2.35	1.34	1.38
7	B	501	GDP	C6-N1	-2.26	1.34	1.38
10	F	401	ACP	C8-N7	2.26	1.36	1.31
10	F	401	ACP	C5-N7	-2.18	1.35	1.39
9	B	504	NW6	C13-N3	2.10	1.41	1.37
10	F	401	ACP	PB-O2B	2.08	1.61	1.56
5	C	501	GTP	C2-N3	2.08	1.38	1.33
5	C	501	GTP	PA-O3A	2.01	1.61	1.59

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	401	ACP	C5-C4-N3	-5.83	118.69	126.72
7	D	501	GDP	C5-C4-N3	-5.83	119.11	128.39
7	B	501	GDP	C5-C4-N3	-5.58	119.51	128.39
7	D	501	GDP	C2-N3-C4	4.92	120.78	112.30
10	F	401	ACP	N3-C4-N9	4.74	135.23	127.17
7	B	501	GDP	C2-N3-C4	4.74	120.46	112.30
5	C	501	GTP	C5-C4-N3	-4.63	121.02	128.39
8	B	503	MES	C5-N4-C3	4.49	118.50	108.84
5	C	501	GTP	C2-N3-C4	4.45	119.97	112.30
5	A	501	GTP	C5-C4-N3	-4.38	121.42	128.39
7	B	501	GDP	N9-C4-N3	4.28	134.51	125.95
7	D	501	GDP	N9-C4-N3	4.25	134.44	125.95
5	A	501	GTP	C2-N3-C4	4.24	119.60	112.30
10	F	401	ACP	C2-N3-C4	3.63	120.69	111.83
9	D	504	NW6	O3-C13-N3	3.56	113.24	109.15
8	D	503	MES	C5-N4-C3	3.49	116.35	108.84
10	F	401	ACP	PB-O3A-PA	-3.48	121.00	132.37
7	D	501	GDP	C6-C5-N7	3.44	136.55	130.29
10	F	401	ACP	C4-C5-N7	-3.37	106.73	110.58
7	B	501	GDP	C6-C5-N7	3.29	136.28	130.29
10	F	401	ACP	N3-C2-N1	-3.10	123.89	128.58
5	C	501	GTP	N9-C4-N3	3.01	131.97	125.95
9	D	504	NW6	N3-C12-N1	2.99	128.60	122.77
9	B	504	NW6	O3-C13-N3	2.91	112.50	109.15
5	C	501	GTP	N9-C8-N7	-2.86	108.10	113.40
5	A	501	GTP	N9-C8-N7	-2.82	108.17	113.40
8	D	503	MES	C6-C5-N4	-2.82	105.84	110.12
10	F	401	ACP	C4-N9-C8	2.77	108.65	105.74
8	D	503	MES	O2S-S-C8	2.75	110.88	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	NW6	C9-N2-C12	-2.73	103.15	107.60
9	D	504	NW6	N2-C12-N3	-2.63	116.80	123.05
5	A	501	GTP	C2-N1-C6	-2.61	120.38	125.11
9	B	504	NW6	N2-C12-N3	-2.60	116.87	123.05
8	B	503	MES	O1S-S-C8	2.60	110.65	106.73
7	D	501	GDP	C4-C5-N7	-2.59	106.56	110.67
9	B	504	NW6	N3-C12-N1	2.55	127.74	122.77
5	C	501	GTP	C2-N1-C6	-2.54	120.50	125.11
5	C	501	GTP	C8-N7-C5	2.54	108.79	104.26
5	A	501	GTP	C8-N7-C5	2.53	108.78	104.26
9	D	504	NW6	C9-N2-C12	-2.53	103.48	107.60
7	B	501	GDP	O6-C6-C5	-2.51	119.89	126.53
5	A	501	GTP	N9-C4-N3	2.50	130.96	125.95
10	F	401	ACP	C5-N7-C8	2.47	107.33	103.45
9	B	504	NW6	C9-C8-N1	2.37	112.66	109.42
9	D	504	NW6	C6-C5-C4	2.34	123.49	120.10
5	A	501	GTP	C5-C6-N1	2.29	119.08	113.25
5	C	501	GTP	C5-C6-N1	2.28	119.05	113.25
7	B	501	GDP	C4-C5-N7	-2.28	107.06	110.67
9	D	504	NW6	O3-C13-O2	-2.21	121.40	124.62
10	F	401	ACP	C3'-C2'-C1'	2.21	105.64	101.46
7	B	501	GDP	O2A-PA-O3A	2.20	113.23	107.27
9	D	504	NW6	C9-C8-N1	2.19	112.42	109.42
5	C	501	GTP	O6-C6-C5	-2.19	120.76	126.53
8	B	503	MES	O3S-S-C8	2.12	110.15	106.00
5	A	501	GTP	O6-C6-C5	-2.09	121.03	126.53
8	D	503	MES	C7-N4-C5	2.06	116.74	111.24
9	B	504	NW6	C10-C9-C8	2.05	124.36	122.10
7	B	501	GDP	C5-C6-N1	2.04	118.46	113.25
9	B	504	NW6	C6-C5-C4	2.01	123.01	120.10

There are no chirality outliers.

All (37) 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
7	B	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
7	D	501	GDP	C5'-O5'-PA-O3A
7	D	501	GDP	C5'-O5'-PA-O1A
8	D	503	MES	C8-C7-N4-C5
8	D	503	MES	C7-C8-S-O1S
8	D	503	MES	C7-C8-S-O3S
8	D	503	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O1G
7	D	501	GDP	C5'-O5'-PA-O2A
10	F	401	ACP	C5'-O5'-PA-O1A
10	F	401	ACP	C5'-O5'-PA-O2A
10	F	401	ACP	C5'-O5'-PA-O3A
9	B	504	NW6	N1-C12-N3-C13
9	D	504	NW6	N1-C12-N3-C13
7	D	501	GDP	PB-O3A-PA-O2A
9	B	504	NW6	N2-C12-N3-C13
9	D	504	NW6	N2-C12-N3-C13
5	A	501	GTP	PB-O3B-PG-O1G
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	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
7	B	501	GDP	PB-O3A-PA-O1A
7	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A

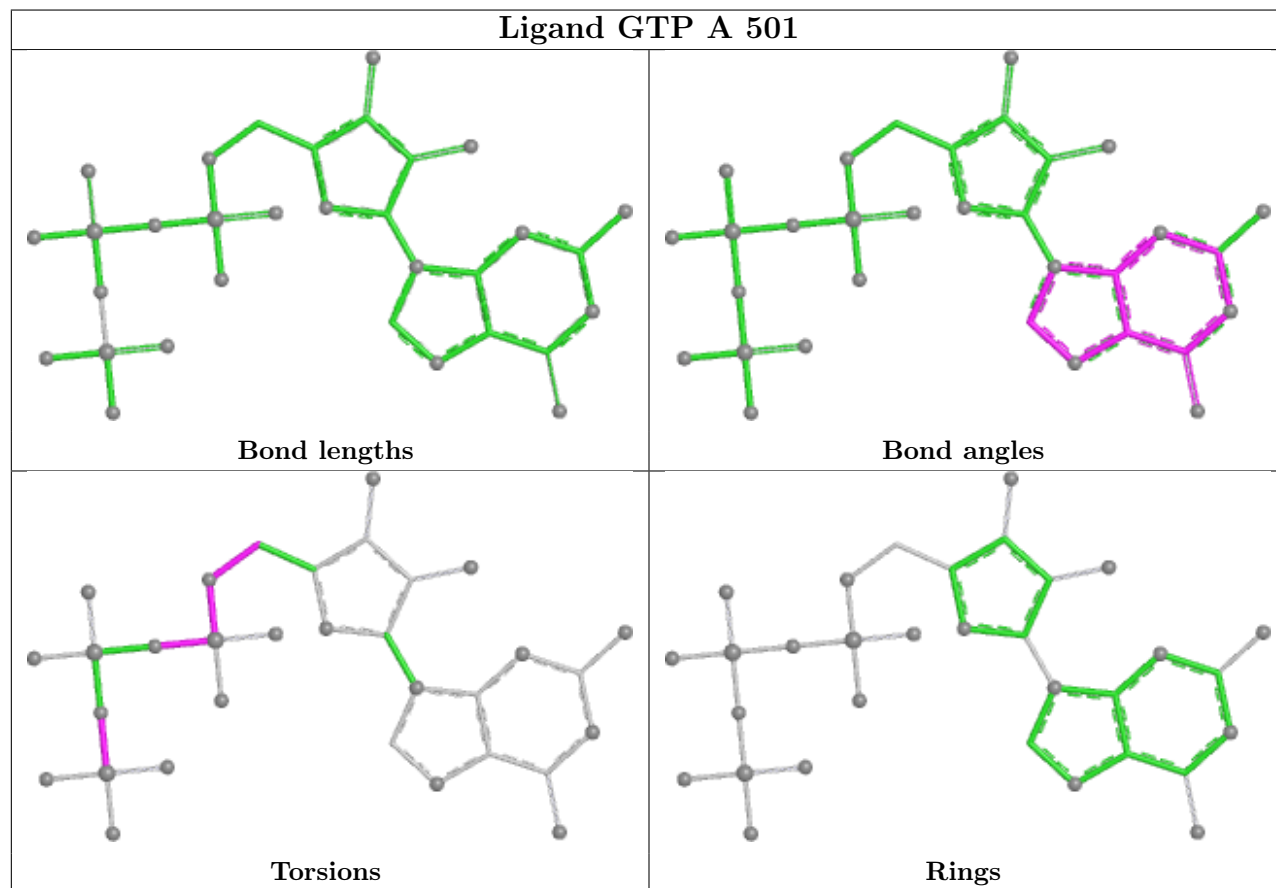
There are no ring outliers.

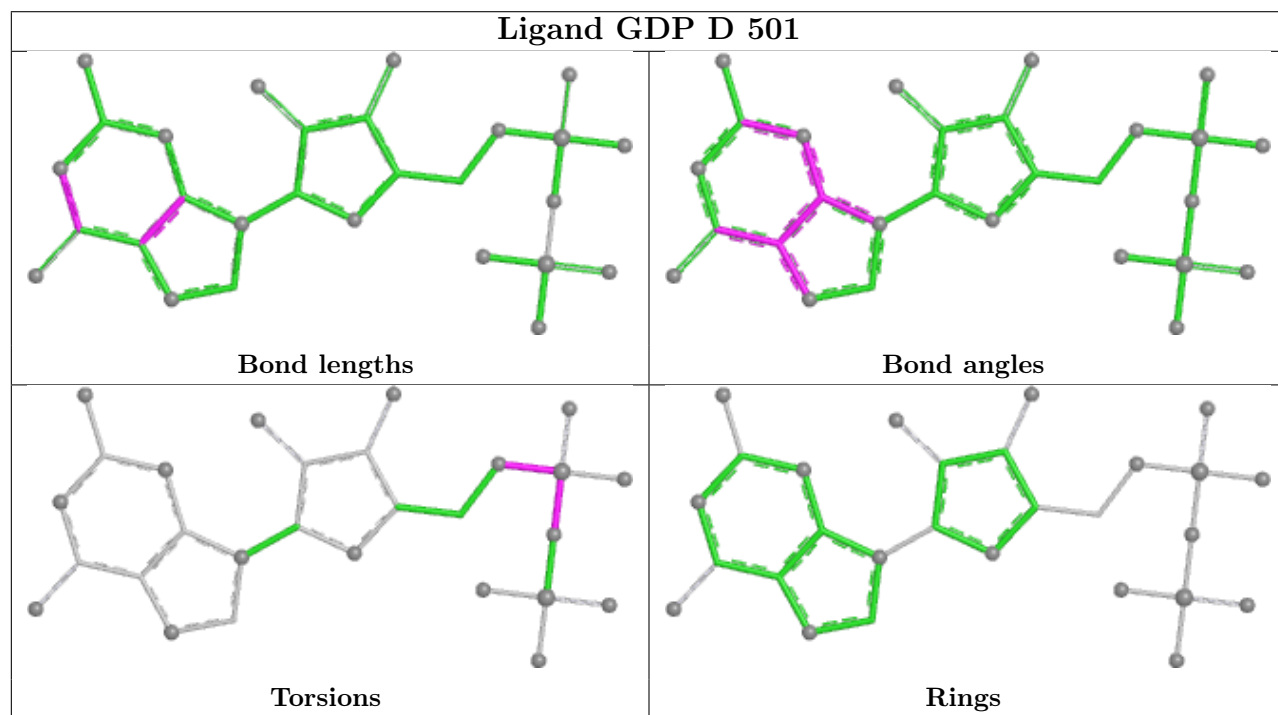
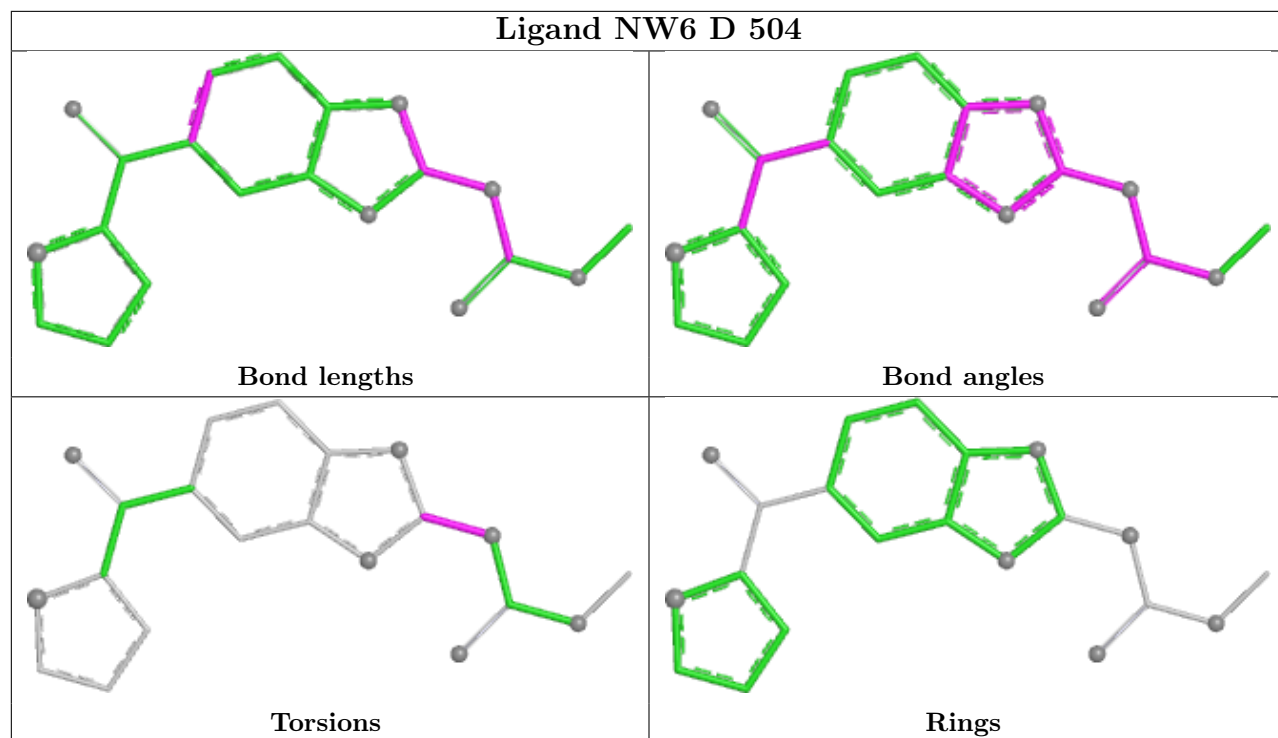
4 monomers are involved in 9 short contacts:

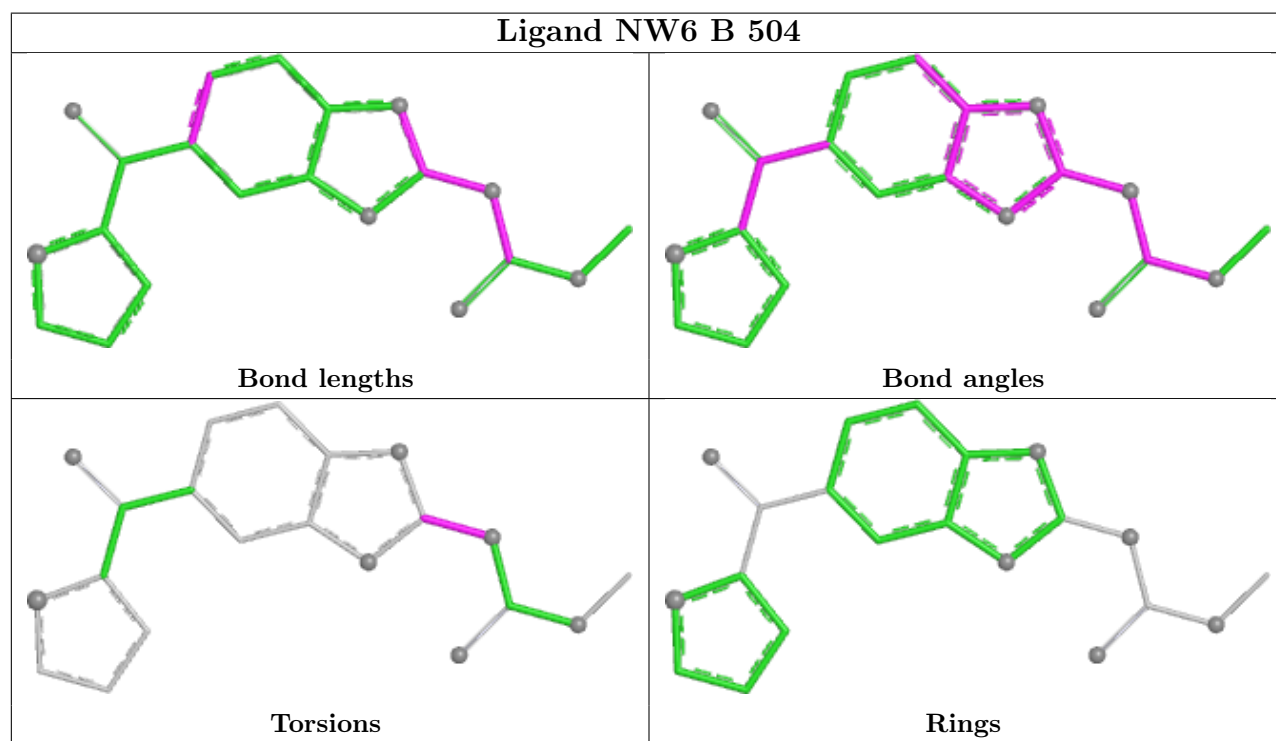
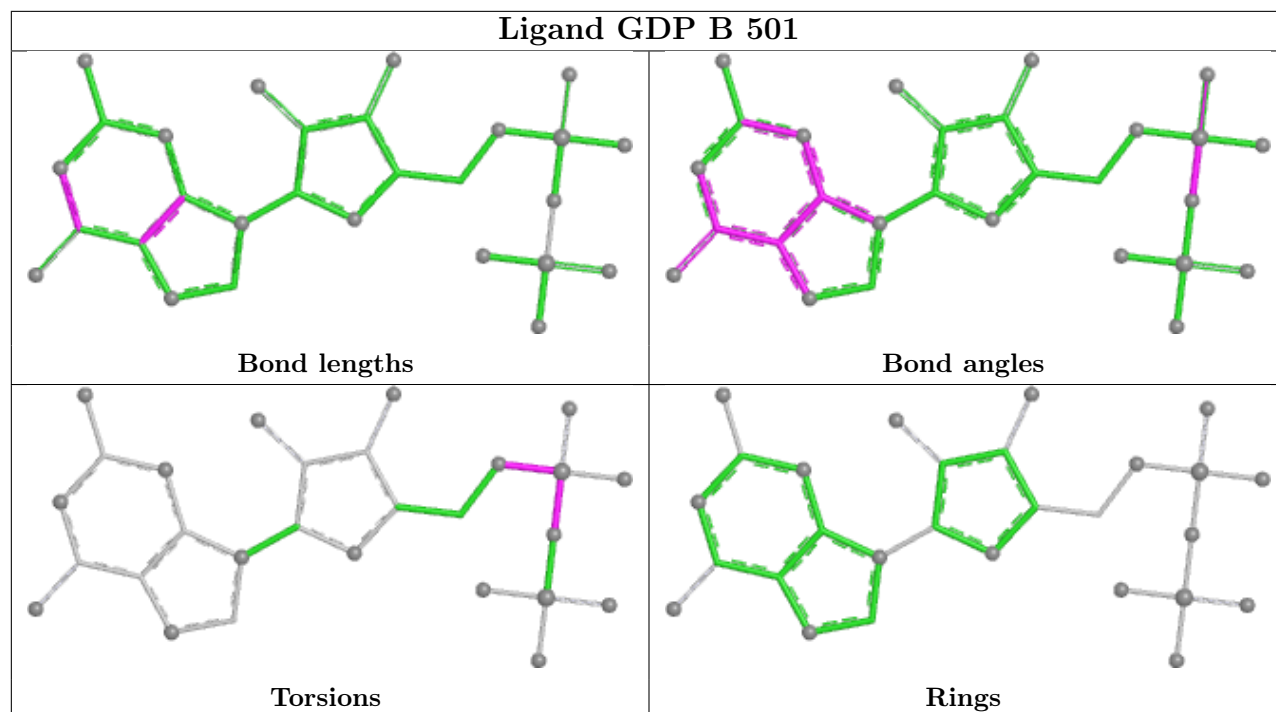
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	504	NW6	4	0
8	D	503	MES	3	0
10	F	401	ACP	1	0
8	B	503	MES	1	0

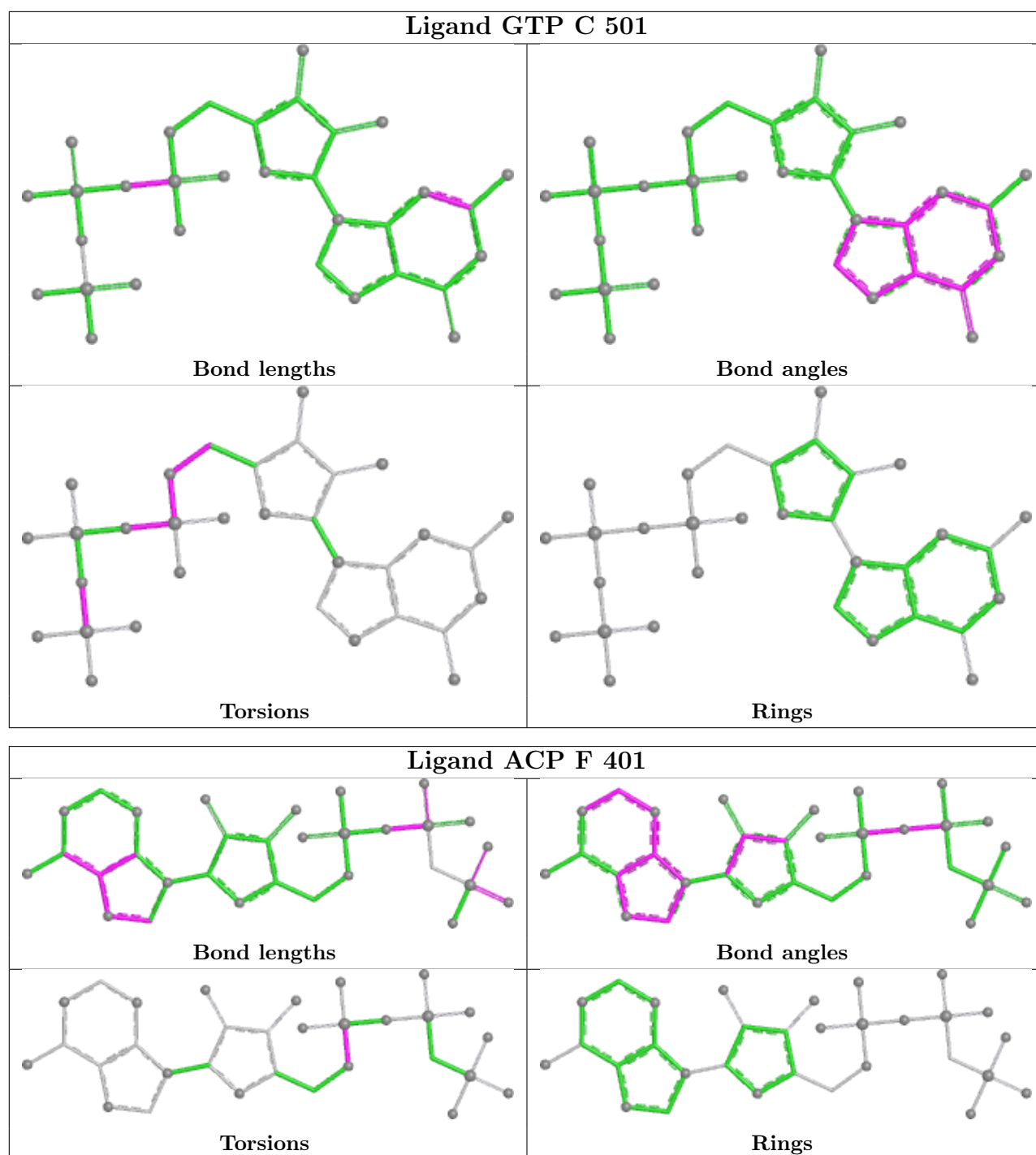
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	439/451 (97%)	-0.11	6 (1%) 73 73	20, 44, 71, 130	8 (1%)
1	C	440/451 (97%)	-0.30	11 (2%) 58 58	18, 34, 57, 89	10 (2%)
2	B	423/445 (95%)	-0.12	9 (2%) 63 63	17, 40, 70, 110	4 (0%)
2	D	421/445 (94%)	0.16	13 (3%) 51 50	25, 50, 79, 133	3 (0%)
3	E	123/143 (86%)	0.36	7 (5%) 29 28	25, 55, 93, 113	1 (0%)
4	F	344/384 (89%)	0.42	13 (3%) 44 43	36, 68, 124, 148	0
All	All	2190/2319 (94%)	0.01	59 (2%) 56 55	17, 45, 91, 148	26 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	250	ALA	10.3
1	C	179	THR	6.1
2	D	248	LEU	5.7
2	D	249	ASN	5.6
3	E	143	ALA	4.7
1	A	262	TYR	4.6
2	B	276	THR	4.4
1	C	340	SER	4.2
4	F	125	THR	3.9
2	B	249	ASN	3.8
1	A	282	TYR	3.7
2	B	333	LEU	3.5
2	D	246	GLY	3.4
1	C	357	TYR	3.4
1	C	440	VAL	3.3
1	C	1	MET	3.3
2	B	285	ALA	3.2
4	F	362	ALA	3.2
1	C	41	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	247	GLN	3.2
2	D	255	LEU	3.2
1	A	283	HIS	3.2
3	E	28	SER	3.1
2	D	407	TRP	3.0
3	E	44	ASP	3.0
1	A	346	TRP	2.9
2	D	245	PRO	2.8
4	F	152	SER	2.8
2	D	1	MET	2.8
1	A	120	ASP	2.7
4	F	105	LEU	2.7
2	B	220	THR	2.7
4	F	130	VAL	2.7
2	D	172	MET	2.6
4	F	161	LEU	2.6
4	F	179	VAL	2.5
4	F	140	GLU	2.4
3	E	6	MET	2.4
2	B	57	THR	2.4
3	E	24	LEU	2.4
1	C	178	SER	2.4
4	F	249	TYR	2.3
1	C	341	ILE	2.3
4	F	103	THR	2.3
2	B	284	ARG	2.3
2	D	251	ASP	2.3
1	C	309	HIS	2.2
1	A	439	SER	2.2
4	F	173	ILE	2.1
1	C	308	ARG	2.1
2	D	334	ASN	2.1
1	C	285	GLN	2.1
2	D	37	HIS	2.1
2	B	325	MET	2.1
3	E	8	VAL	2.1
4	F	298	ILE	2.1
2	B	438	ALA	2.0
3	E	139	LEU	2.0
4	F	236	LYS	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](#)

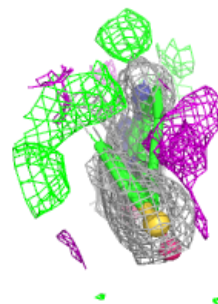
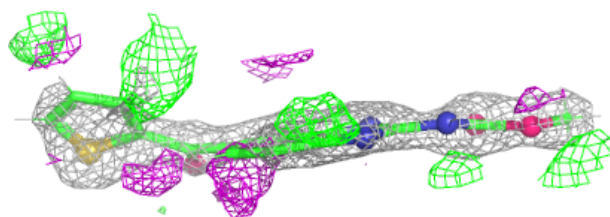
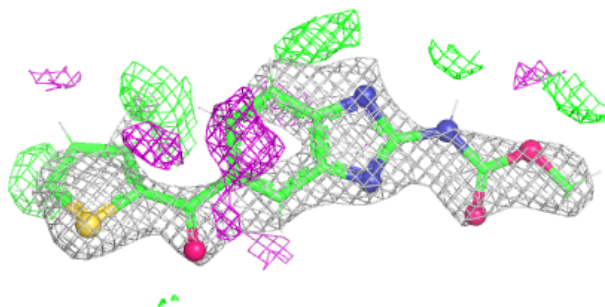
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MES	D	503	12/12	0.84	0.19	47,53,57,60	12
9	NW6	D	504	21/21	0.84	0.18	39,48,60,62	32
10	ACP	F	401	31/31	0.91	0.10	61,73,90,95	0
8	MES	B	503	12/12	0.94	0.09	34,39,48,49	0
6	MG	F	402	1/1	0.94	0.10	57,57,57,57	0
7	GDP	D	501	28/28	0.95	0.08	38,45,51,54	0
6	MG	D	502	1/1	0.96	0.07	52,52,52,52	0
7	GDP	B	501	28/28	0.98	0.05	23,29,31,32	0
9	NW6	B	504	21/21	0.98	0.05	30,36,41,46	0
5	GTP	C	501	32/32	0.99	0.04	19,25,29,30	0
6	MG	A	502	1/1	0.99	0.03	27,27,27,27	0
6	MG	C	502	1/1	0.99	0.04	26,26,26,26	0
5	GTP	A	501	32/32	0.99	0.04	23,29,34,34	0
6	MG	B	502	1/1	1.00	0.06	18,18,18,18	0

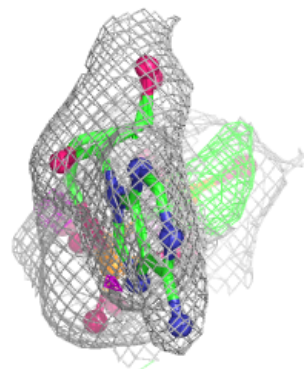
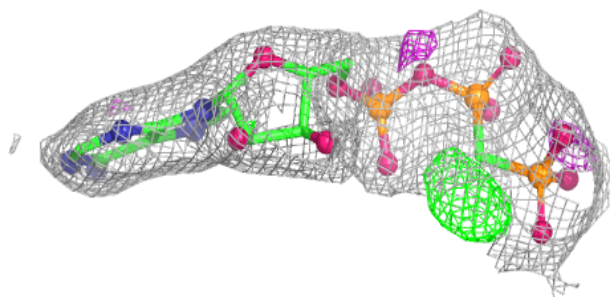
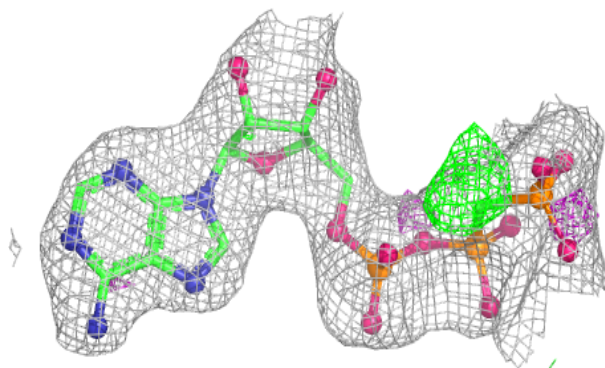
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NW6 D 504:

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

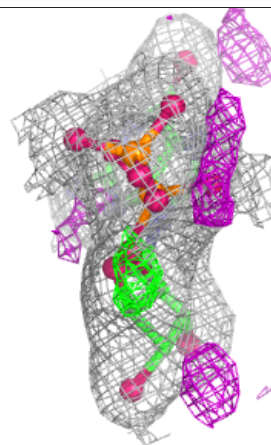
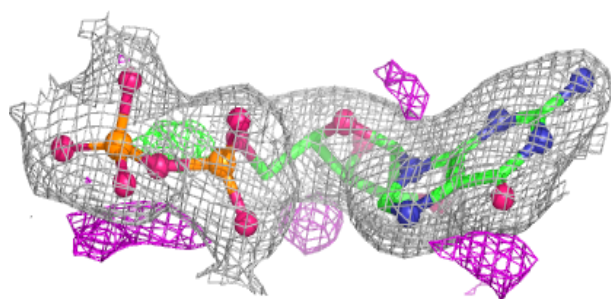
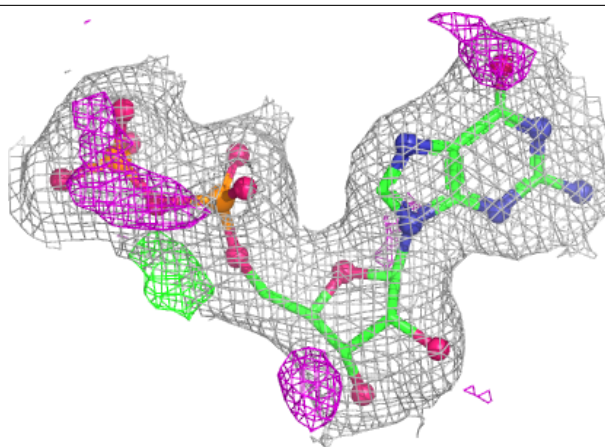
**Electron density around ACP F 401:**

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



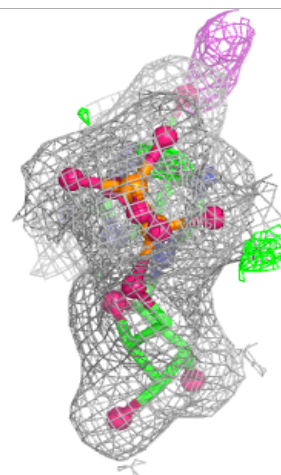
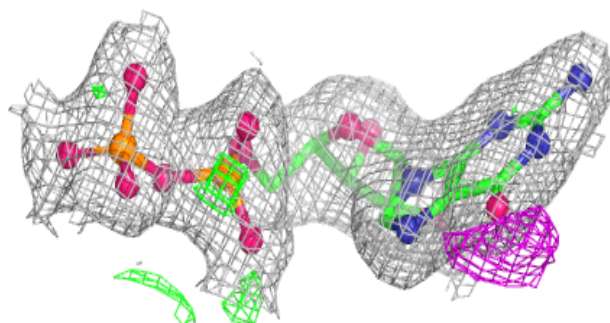
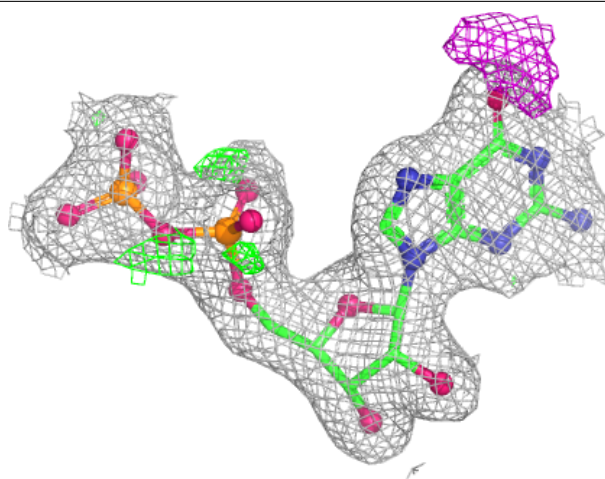
Electron density around GDP D 501:

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



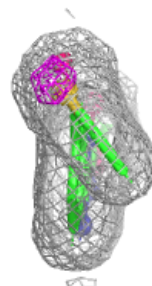
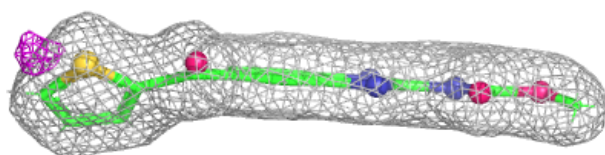
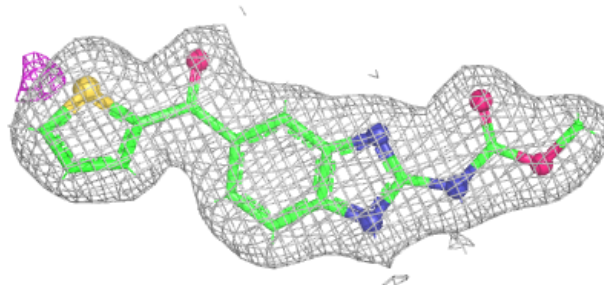
Electron density around GDP B 501:

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

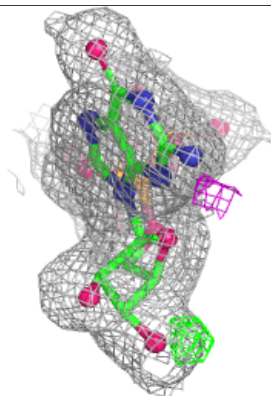
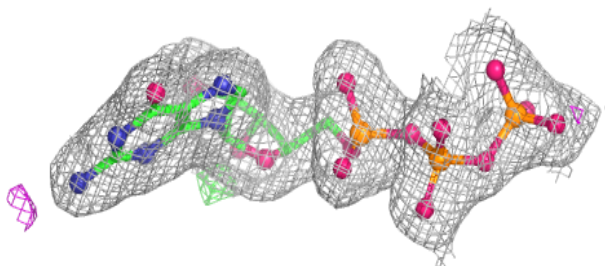
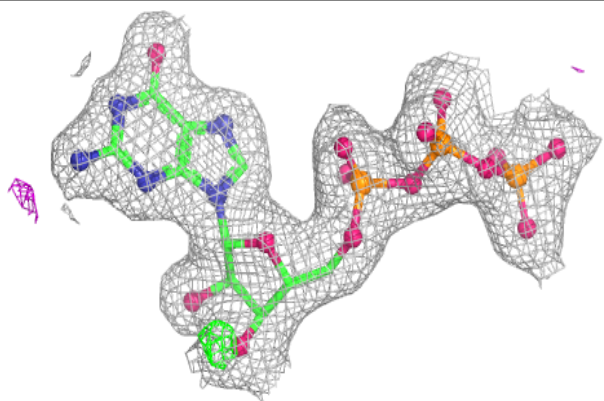


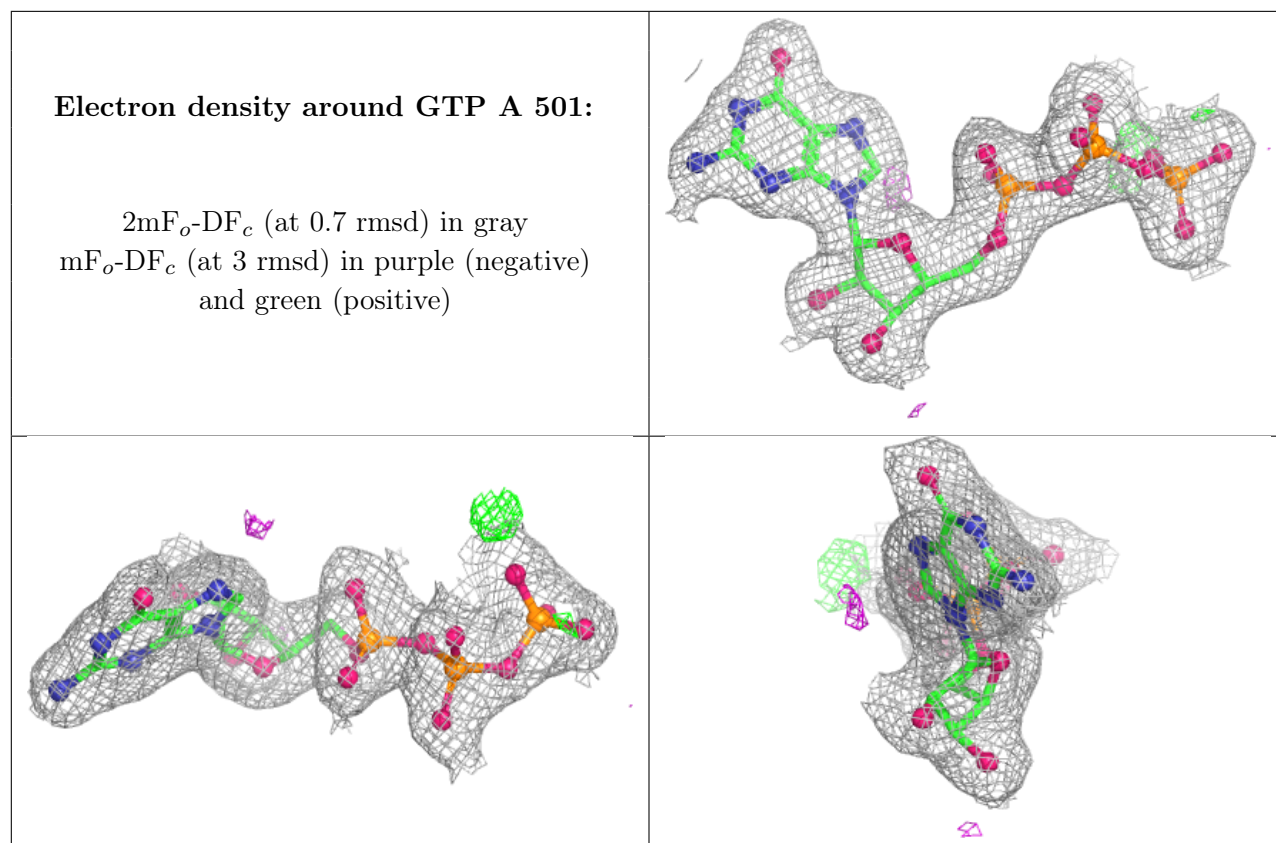
Electron density around NW6 B 504:

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

**Electron density around GTP 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 ⓘ

There are no such residues in this entry.