



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 PM UTC

PDB ID : 6EG5 / pdb_00006eg5
Title : The structure of SB-1-202-tubulin complex
Authors : Banerjee, A.K.; Wang, Y.; Chen, H.; Miller, D.; Li, W.
Deposited on : 2018-08-18
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

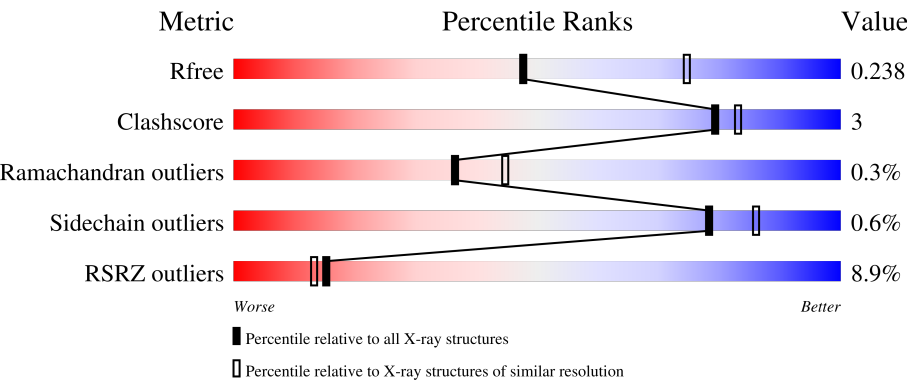
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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% 93%
1	C	450	2% 93% 5%
2	B	445	4% 88% 8%
2	D	445	10% 88% 6% 6%
3	E	143	11% 84% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	26% 85% 7% • 7%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18509 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	439	Total	C	N	O	S	0	2	0
			3436	2174	583	655	24			
1	C	441	Total	C	N	O	S	0	3	0
			3456	2187	585	661	23			

- Molecule 2 is a protein called Tubulin beta-2B 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	420	Total	C	N	O	S	0	1	0
			3301	2075	561	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	126	Total	C	N	O	S	0	1	0
			1052	649	189	208	6			

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	356	Total	C	N	O	S	0	0	0
			2913	1863	504	532	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total 1	Mg 1	0	0
6	F	2	Total 2	Mg 2	0	0

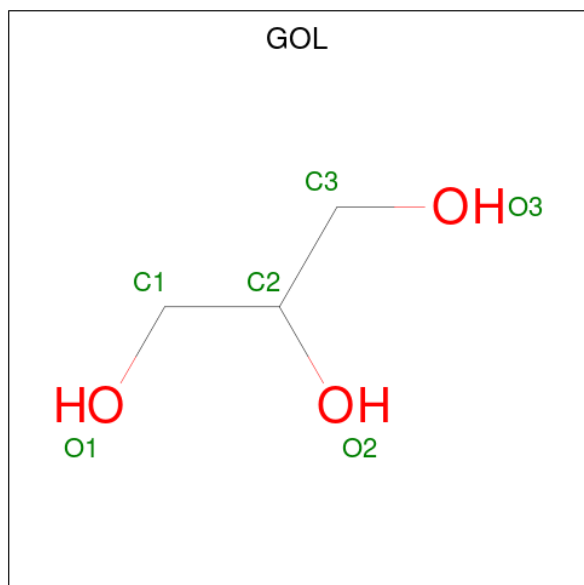
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

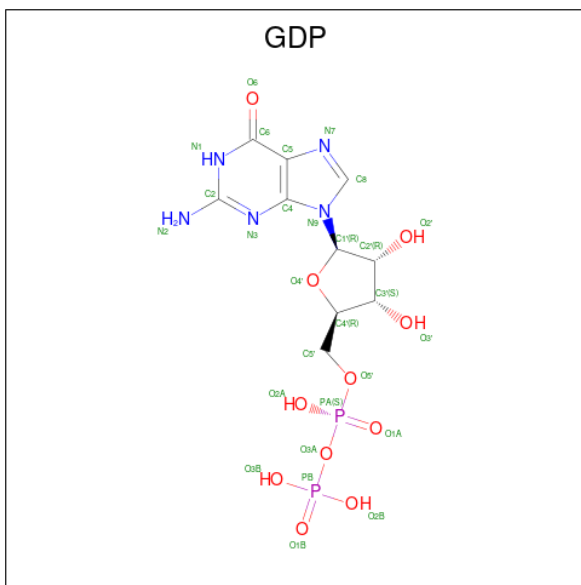
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Cl 1	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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



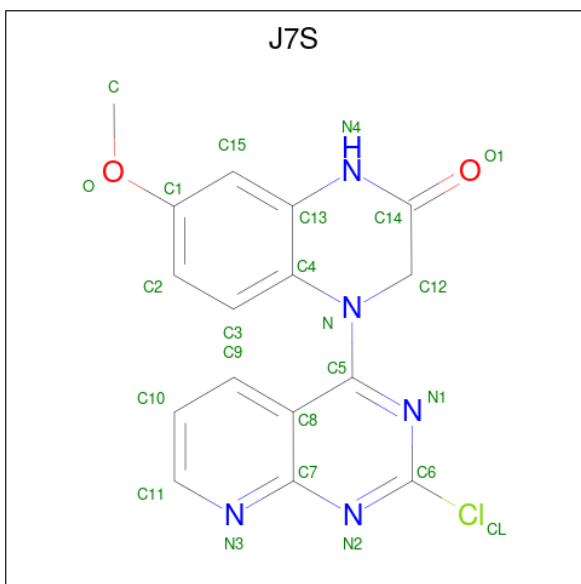
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

- Molecule 12 is 4-(2-chloropyrido[2,3-d]pyrimidin-4-yl)-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (CCD ID: J7S) (formula: C₁₆H₁₂ClN₅O₂).



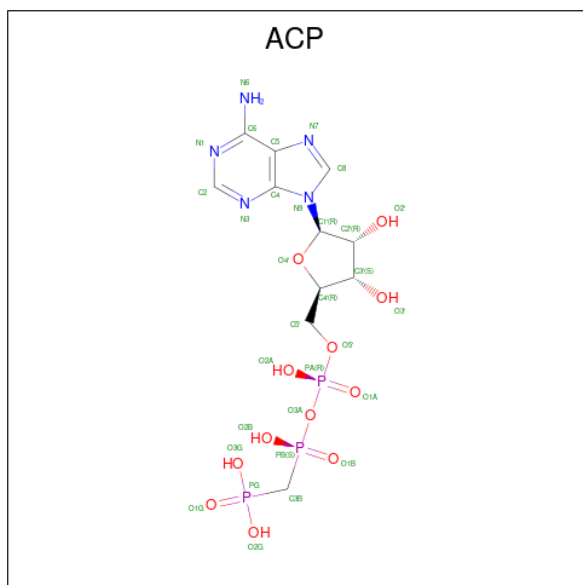
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Cl	N	O	0	0
			24	16	1	5	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	Cl	N	O	0	0
			24	16	1	5	2		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

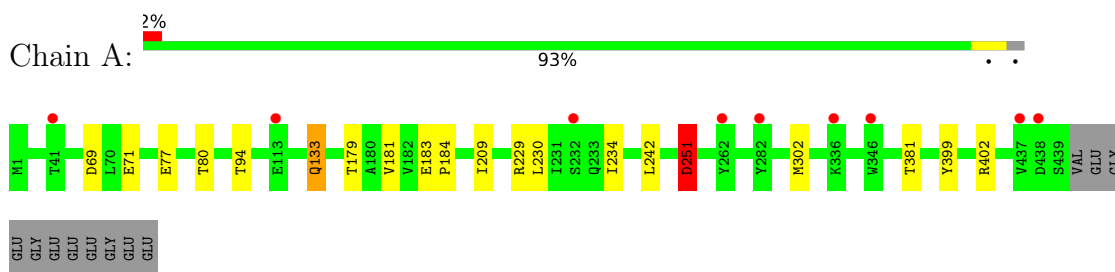
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	156	Total	O	0	0
			156	156		
14	B	144	Total	O	0	0
			144	144		
14	C	267	Total	O	0	0
			267	267		
14	D	65	Total	O	0	0
			65	65		
14	E	28	Total	O	0	0
			28	28		
14	F	72	Total	O	0	0
			72	72		

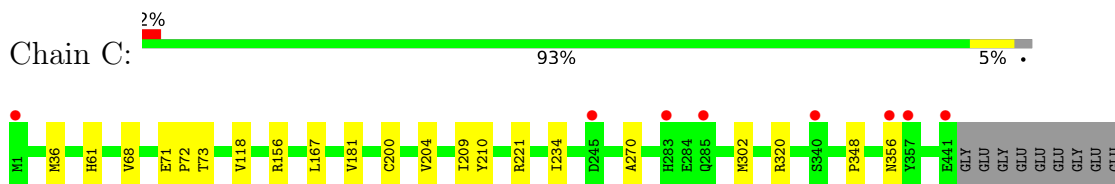
3 Residue-property plots

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.

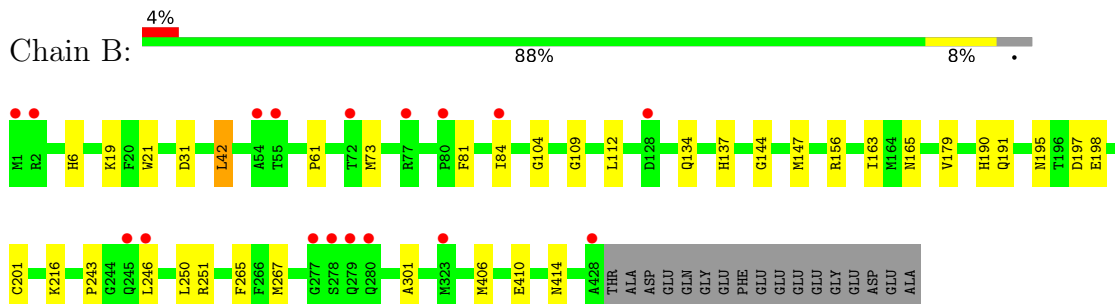
- Molecule 1: Tubulin alpha-1B chain



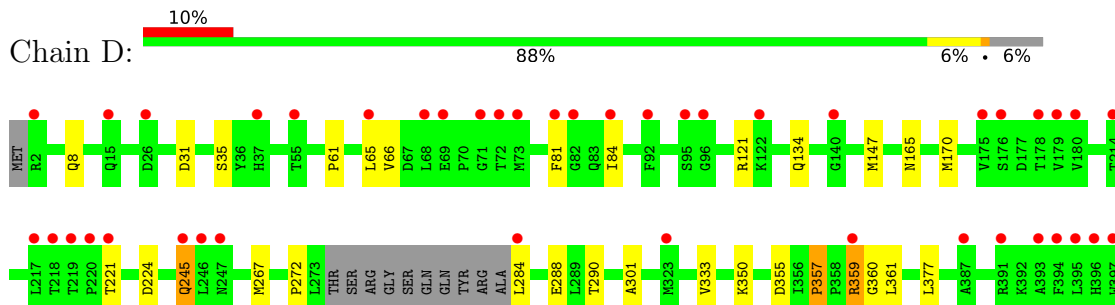
- Molecule 1: Tubulin alpha-1B chain

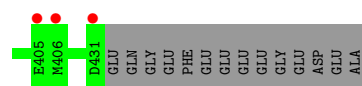


- Molecule 2: Tubulin beta-2B chain

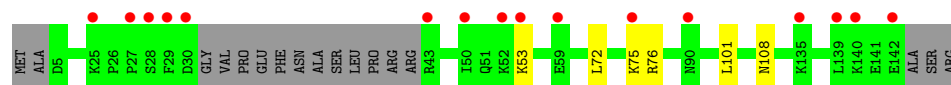
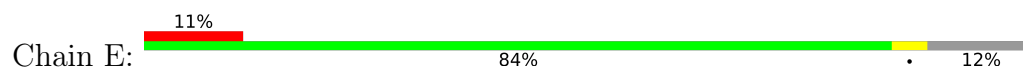


- Molecule 2: Tubulin beta-2B chain

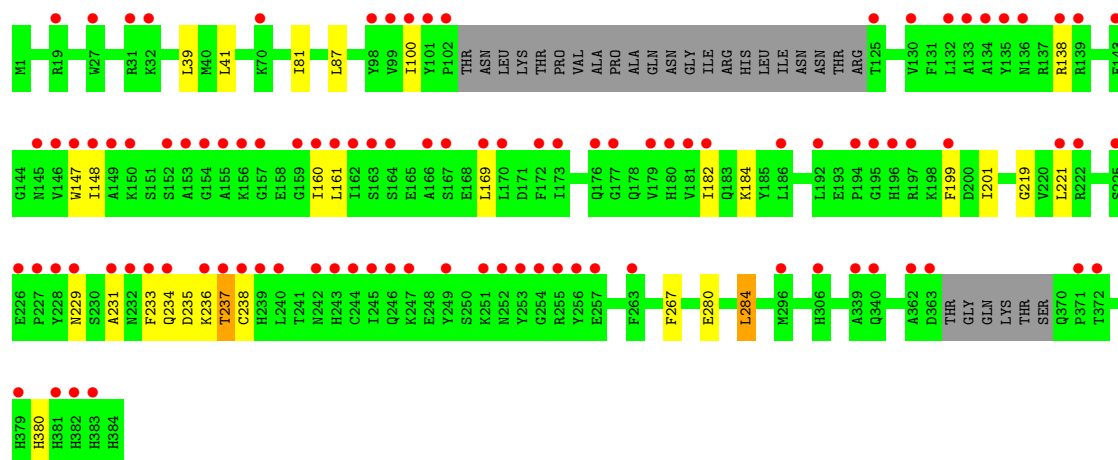
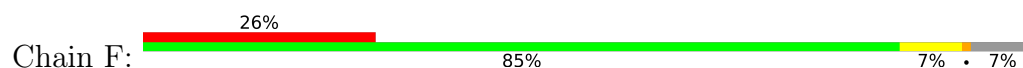




• Molecule 3: Stathmin-4



• 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	105.54Å 158.03Å 181.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 50.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.45) 97.5 (50.00-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.196 , 0.236 0.200 , 0.238	Depositor DCC
R_{free} test set	5583 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	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	18509	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CA, MG, GDP, GOL, CL, ACP, MES, J7S

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	0.67	1/3520 (0.0%)	0.86	1/4778 (0.0%)
1	C	0.68	0/3540	0.86	0/4805
2	B	0.66	0/3444	0.83	1/4664 (0.0%)
2	D	0.64	0/3374	0.87	3/4571 (0.1%)
3	E	0.66	0/1064	0.87	0/1411
4	F	0.63	0/2983	0.82	2/4031 (0.0%)
All	All	0.66	1/17925 (0.0%)	0.85	7/24260 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	LEU	C-O	-5.23	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	357	PRO	CA-C-N	-6.33	114.20	120.98
2	D	357	PRO	C-N-CA	-6.33	114.20	120.98
4	F	284	LEU	N-CA-C	5.43	117.19	111.28
1	A	251	ASP	CB-CA-C	5.19	119.96	109.68
2	D	245	GLN	N-CA-C	-5.03	103.03	110.48
4	F	219	GLY	N-CA-C	-5.03	105.87	112.81
2	B	195	ASN	N-CA-C	5.02	119.36	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3436	0	3350	14	0
1	C	3456	0	3366	18	0
2	B	3369	0	3250	26	0
2	D	3301	0	3177	25	0
3	E	1052	0	1063	4	0
4	F	2913	0	2863	12	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
6	D	1	0	0	0	0
6	F	2	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
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	12	0	16	0	0
10	B	28	0	12	0	0
11	B	24	0	26	4	0
12	B	24	0	0	3	0
12	D	24	0	0	2	0
13	F	31	0	14	0	0
14	A	156	0	0	1	0
14	B	144	0	0	2	0
14	C	267	0	0	0	0
14	D	65	0	0	3	0
14	E	28	0	0	1	0
14	F	72	0	0	1	0
All	All	18509	0	17173	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (95) 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:170:MET:HE2	2:D:377:LEU:HD21	1.56	0.87
2:D:359:ARG:HB3	2:D:359:ARG:NH1	1.89	0.86
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.22	0.80
2:D:359:ARG:HB3	2:D:359:ARG:CZ	2.24	0.68
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.75	0.68
2:D:245:GLN:NE2	14:D:701:HOH:O	2.25	0.66
1:A:181:VAL:HG13	12:B:506:J7S:C	2.25	0.66
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.78	0.66
1:A:133:GLN:HE22	1:A:251:ASP:HB2	1.61	0.65
1:C:204:VAL:HG13	1:C:302[B]:MET:HE2	1.79	0.63
2:B:109:GLY:HA2	2:B:147:MET:HE2	1.81	0.62
2:D:121:ARG:NH2	14:D:702:HOH:O	2.33	0.60
1:C:210:TYR:OH	1:C:221:ARG:HD3	2.01	0.60
3:E:108:ASN:ND2	14:E:301:HOH:O	2.35	0.59
1:A:209:ILE:HD11	1:A:302:MET:SD	2.42	0.59
2:B:190:HIS:CD2	2:B:414:ASN:HD22	2.21	0.59
4:F:201:ILE:HG12	4:F:221:LEU:HD22	1.84	0.58
2:B:42:LEU:HD22	2:B:243:PRO:CG	2.34	0.57
2:B:191:GLN:OE1	3:E:75:LYS:NZ	2.37	0.57
1:C:181:VAL:HB	12:D:603:J7S:C	2.35	0.57
2:B:251:ARG:NH1	11:B:504:MES:O2S	2.33	0.56
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.89	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.53
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.89	0.53
2:B:134:GLN:HA	2:B:165:ASN:O	2.10	0.52
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.91	0.52
1:A:181:VAL:CG1	12:B:506:J7S:C	2.87	0.52
1:A:229:ARG:NH1	14:A:601:HOH:O	2.34	0.52
2:D:165:ASN:ND2	14:D:703:HOH:O	2.43	0.51
2:D:66:VAL:HG12	2:D:147:MET:HE1	1.94	0.50
2:D:221:THR:HG22	2:D:224:ASP:OD2	2.12	0.50
2:B:197:ASP:OD1	11:B:504:MES:H32	2.11	0.50
1:A:234:ILE:HD13	1:A:302:MET:SD	2.51	0.50
2:D:360:GLY:O	2:D:361:LEU:HG	2.12	0.49
4:F:233:PHE:O	4:F:235:ASP:N	2.45	0.49
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.42	0.48
1:C:234:ILE:CD1	1:C:302[A]:MET:SD	2.99	0.48
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.95	0.48
1:C:156:ARG:HD3	3:E:101:LEU:HD21	1.96	0.47
2:D:359:ARG:HB3	2:D:359:ARG:HH11	1.73	0.47
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.96	0.47
2:B:406:MET:HE3	2:B:410:GLU:HG3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:ARG:CZ	11:B:504:MES:H21	2.45	0.47
4:F:184:LYS:HD2	14:F:860:HOH:O	2.15	0.47
1:A:179:THR:HG21	2:B:246:LEU:HD13	1.96	0.47
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.96	0.47
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.97	0.46
1:C:209:ILE:HD11	1:C:302[A]:MET:SD	2.56	0.46
2:D:355:ASP:O	2:D:357:PRO:HD3	2.15	0.45
2:B:81:PHE:HD2	2:B:84:ILE:HD12	1.81	0.45
2:B:61:PRO:HD2	2:B:84:ILE:HG22	1.99	0.45
4:F:81:ILE:O	4:F:87:LEU:O	2.35	0.45
2:D:134:GLN:HA	2:D:165:ASN:O	2.17	0.45
2:D:350:LYS:HG3	12:D:603:J7S:C15	2.47	0.44
2:B:216:LYS:NZ	14:B:614:HOH:O	2.50	0.44
1:C:68:VAL:HG21	1:C:118:VAL:HG21	2.00	0.44
2:D:61:PRO:CD	2:D:84:ILE:CG2	2.95	0.44
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.58	0.44
4:F:148:ILE:HD11	4:F:160:ILE:HG23	1.99	0.44
2:D:359:ARG:NH1	2:D:359:ARG:CB	2.73	0.44
2:B:112:LEU:HD23	2:B:147:MET:HE1	2.00	0.43
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.98	0.43
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.99	0.43
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
2:B:137:HIS:HD2	2:B:144:GLY:O	2.02	0.43
4:F:199:PHE:CD2	4:F:221:LEU:HD13	2.54	0.43
1:C:234:ILE:HD13	1:C:302[B]:MET:HE3	2.00	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.42
2:D:31:ASP:O	2:D:84:ILE:HD11	2.19	0.42
2:B:197:ASP:OD2	11:B:504:MES:H52	2.19	0.42
4:F:161:LEU:HD23	4:F:169:LEU:HD23	2.01	0.42
2:D:272:PRO:HB3	2:D:284:LEU:HD11	2.01	0.42
1:A:77:GLU:HA	1:A:80:THR:HG22	2.02	0.42
2:B:31:ASP:O	2:B:84:ILE:HD11	2.19	0.42
2:D:284:LEU:HD22	2:D:288:GLU:HG3	2.00	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
2:D:61:PRO:HD2	2:D:84:ILE:HG22	2.01	0.41
2:B:61:PRO:CD	2:B:84:ILE:HG22	2.51	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.38	0.41
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.61	0.41
1:A:179:THR:O	12:B:506:J7S:N4	2.54	0.41
1:A:399:TYR:O	1:A:402:ARG:NH1	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:HE22	1:A:251:ASP:CB	2.31	0.41
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.61	0.41
2:D:359:ARG:HH11	2:D:359:ARG:CB	2.33	0.41
2:B:104:GLY:O	2:B:109:GLY:HA3	2.21	0.41
1:C:71:GLU:OE2	1:C:73:THR:CB	2.69	0.41
4:F:100:ILE:HD12	4:F:182:ILE:HD12	2.03	0.41
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.56	0.41
2:B:73:MET:N	14:B:613:HOH:O	2.50	0.41
2:D:8:GLN:CG	2:D:65:LEU:HD23	2.51	0.40
1:C:320:ARG:HA	1:C:356:ASN:O	2.21	0.40
4:F:138:ARG:CZ	4:F:147:TRP:CZ2	3.05	0.40
2:D:81:PHE:HD2	2:D:84:ILE:HD12	1.85	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	439/450 (98%)	429 (98%)	10 (2%)	0	100	100
1	C	441/450 (98%)	431 (98%)	10 (2%)	0	100	100
2	B	426/445 (96%)	415 (97%)	11 (3%)	0	100	100
2	D	416/445 (94%)	407 (98%)	9 (2%)	0	100	100
3	E	123/143 (86%)	120 (98%)	2 (2%)	1 (1%)	16	20
4	F	350/384 (91%)	329 (94%)	15 (4%)	6 (2%)	7	6
All	All	2195/2317 (95%)	2131 (97%)	57 (3%)	7 (0%)	36	45

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	234	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	380	HIS
3	E	53	LYS
4	F	231	ALA
4	F	237	THR
4	F	229	ASN
4	F	236	LYS

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%)	368 (99%)	4 (1%)	65	76
1	C	374/378 (99%)	374 (100%)	0	100	100
2	B	370/383 (97%)	367 (99%)	3 (1%)	73	83
2	D	363/383 (95%)	361 (99%)	2 (1%)	78	86
3	E	115/127 (91%)	115 (100%)	0	100	100
4	F	318/342 (93%)	316 (99%)	2 (1%)	78	86
All	All	1912/1991 (96%)	1901 (99%)	11 (1%)	78	86

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	133	GLN
1	A	251	ASP
1	A	381	THR
2	B	19	LYS
2	B	42	LEU
2	B	198	GLU
2	D	35	SER
2	D	359	ARG
4	F	237	THR
4	F	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	102	ASN
1	A	133	GLN
1	A	372	GLN
2	B	57	ASN
2	B	137	HIS
2	B	190	HIS
2	B	329	GLN
2	B	337	ASN
2	B	347	ASN
1	C	15	GLN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	15	GLN
2	D	165	ASN
2	D	195	ASN
2	D	329	GLN
2	D	347	ASN
3	E	18	GLN
3	E	92	ASN
3	E	108	ASN
4	F	180	HIS
4	F	333	ASN

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 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 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	D	601	6	33,34,34	1.34	3 (9%)	50,54,54	1.71	9 (18%)
10	GDP	B	501	6	29,30,30	1.33	4 (13%)	45,47,47	1.61	7 (15%)
5	GTP	A	501	6	33,34,34	1.30	5 (15%)	50,54,54	1.64	8 (16%)
9	GOL	A	505	-	5,5,5	0.35	0	5,5,5	0.79	0
9	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.55	0
12	J7S	B	506	-	27,27,27	2.78	8 (29%)	35,39,39	2.56	15 (42%)
12	J7S	D	603	-	27,27,27	2.82	9 (33%)	35,39,39	2.70	11 (31%)
5	GTP	C	501	6	33,34,34	1.28	5 (15%)	50,54,54	1.56	7 (14%)
11	MES	B	504	-	12,12,12	2.30	1 (8%)	15,16,16	1.77	4 (26%)
13	ACP	F	703	6	31,33,33	2.33	12 (38%)	47,52,52	1.95	8 (17%)
11	MES	B	505	-	12,12,12	2.17	1 (8%)	15,16,16	1.12	1 (6%)

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	D	601	6	-	6/22/38/38	0/3/3/3
10	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
9	GOL	A	505	-	-	2/4/4/4	-
9	GOL	A	506	-	-	1/4/4/4	-
12	J7S	B	506	-	-	3/6/18/18	0/4/4/4
12	J7S	D	603	-	-	4/6/18/18	0/4/4/4
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
11	MES	B	504	-	-	2/6/14/14	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ACP	F	703	6	-	4/19/38/38	0/3/3/3
11	MES	B	505	-	-	2/6/14/14	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	603	J7S	O1-C14	8.84	1.40	1.23
12	B	506	J7S	O1-C14	8.61	1.40	1.23
11	B	504	MES	C8-S	-7.59	1.66	1.77
11	B	505	MES	C8-S	-7.28	1.67	1.77
12	D	603	J7S	C14-N4	6.72	1.42	1.35
12	B	506	J7S	C14-N4	6.43	1.42	1.35
13	F	703	ACP	PG-O1G	5.60	1.61	1.50
12	B	506	J7S	C13-N4	5.36	1.49	1.39
12	D	603	J7S	C4-N	5.07	1.49	1.40
13	F	703	ACP	C5-C4	4.84	1.47	1.39
12	D	603	J7S	C13-N4	4.56	1.47	1.39
13	F	703	ACP	PB-O3A	4.47	1.63	1.58
13	F	703	ACP	PB-O1B	4.36	1.61	1.51
12	B	506	J7S	C12-N	-3.84	1.39	1.46
5	D	601	GTP	C5-C4	3.56	1.48	1.38
13	F	703	ACP	PA-O3A	3.46	1.63	1.59
12	B	506	J7S	C4-N	3.37	1.46	1.40
5	D	601	GTP	PB-O3A	3.36	1.63	1.59
10	B	501	GDP	PA-O3A	3.35	1.63	1.59
5	C	501	GTP	PA-O3A	3.29	1.63	1.59
13	F	703	ACP	PB-O2B	-3.25	1.48	1.56
5	A	501	GTP	PB-O3B	3.14	1.62	1.59
13	F	703	ACP	PG-O3G	-3.01	1.48	1.55
5	A	501	GTP	C5-C4	2.98	1.46	1.38
5	C	501	GTP	C5-C4	2.95	1.46	1.38
13	F	703	ACP	PG-O2G	2.93	1.61	1.55
13	F	703	ACP	C5-N7	-2.88	1.33	1.39
12	B	506	J7S	O-C	-2.86	1.34	1.42
10	B	501	GDP	C5-C4	2.84	1.46	1.38
13	F	703	ACP	C5-C6	2.76	1.48	1.41
12	D	603	J7S	C12-N	-2.72	1.41	1.46
12	D	603	J7S	C5-N	2.70	1.45	1.39
5	A	501	GTP	PA-O3A	2.58	1.62	1.59
12	D	603	J7S	C6-N2	2.48	1.32	1.30
5	D	601	GTP	C5-N7	-2.47	1.34	1.39
5	A	501	GTP	C4-N9	-2.44	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C5-N7	-2.41	1.34	1.39
12	B	506	J7S	C5-N	2.37	1.44	1.39
10	B	501	GDP	C6-N1	-2.36	1.34	1.38
12	D	603	J7S	C12-C14	2.29	1.54	1.51
5	A	501	GTP	C5-N7	-2.29	1.34	1.39
10	B	501	GDP	C5-N7	-2.25	1.34	1.39
13	F	703	ACP	C8-N7	2.19	1.35	1.31
5	C	501	GTP	PB-O3B	2.15	1.61	1.59
5	C	501	GTP	C4-N9	-2.12	1.32	1.38
13	F	703	ACP	C8-N9	-2.09	1.34	1.37
12	B	506	J7S	C12-C14	2.08	1.53	1.51
12	D	603	J7S	O-C	-2.03	1.37	1.42

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	603	J7S	N2-C6-N1	-6.95	123.69	130.58
13	F	703	ACP	C5-C4-N3	-6.61	117.61	126.72
12	D	603	J7S	CL-C6-N2	6.52	121.11	115.72
12	B	506	J7S	C13-N4-C14	-6.01	117.25	124.45
12	B	506	J7S	N2-C6-N1	-5.82	124.80	130.58
5	D	601	GTP	C5-C4-N3	-5.60	119.47	128.39
12	D	603	J7S	C13-N4-C14	-5.44	117.93	124.45
12	D	603	J7S	C6-N2-C7	5.32	118.52	114.18
13	F	703	ACP	N3-C4-N9	5.17	135.96	127.17
12	D	603	J7S	C12-C14-N4	5.12	122.50	116.13
5	C	501	GTP	C5-C4-N3	-4.97	120.48	128.39
5	A	501	GTP	C5-C4-N3	-4.94	120.53	128.39
12	B	506	J7S	C6-N2-C7	4.82	118.12	114.18
10	B	501	GDP	C5-C4-N3	-4.81	120.73	128.39
12	B	506	J7S	CL-C6-N2	4.71	119.62	115.72
12	B	506	J7S	C12-C14-N4	4.65	121.92	116.13
5	D	601	GTP	C2-N3-C4	4.55	120.13	112.30
5	D	601	GTP	N9-C4-N3	4.40	134.74	125.95
5	A	501	GTP	N9-C4-N3	4.37	134.70	125.95
5	A	501	GTP	C2-N3-C4	4.35	119.79	112.30
5	C	501	GTP	C2-N3-C4	4.28	119.67	112.30
10	B	501	GDP	C2-N3-C4	4.16	119.47	112.30
13	F	703	ACP	C2-N3-C4	4.05	121.73	111.83
5	C	501	GTP	N9-C4-N3	4.05	134.06	125.95
10	B	501	GDP	N9-C4-N3	3.97	133.90	125.95
11	B	504	MES	C2-C3-N4	3.69	115.73	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	603	J7S	C11-N3-C7	3.68	121.03	116.64
13	F	703	ACP	C4-C5-N7	-3.62	106.45	110.58
12	D	603	J7S	C12-N-C4	3.58	118.63	114.97
13	F	703	ACP	N3-C2-N1	-3.56	123.20	128.58
11	B	504	MES	C5-N4-C3	3.53	116.44	108.84
12	D	603	J7S	C6-N1-C5	3.49	121.34	111.13
5	D	601	GTP	C6-C5-N7	3.32	136.32	130.29
10	B	501	GDP	C6-C5-N7	3.23	136.17	130.29
12	B	506	J7S	C6-N1-C5	3.23	120.59	111.13
12	B	506	J7S	C3-C4-N	-3.12	117.51	121.76
5	A	501	GTP	C6-C5-N7	3.11	135.94	130.29
12	B	506	J7S	C11-N3-C7	2.94	120.14	116.64
12	B	506	J7S	C10-C9-C8	-2.78	117.16	120.91
5	C	501	GTP	C6-C5-N7	2.78	135.35	130.29
5	A	501	GTP	O6-C6-C5	-2.74	119.29	126.53
11	B	505	MES	O3S-S-C8	2.66	111.21	106.00
12	D	603	J7S	C13-C4-N	2.65	120.94	118.05
11	B	504	MES	O3S-S-C8	2.58	111.06	106.00
12	D	603	J7S	C10-C9-C8	-2.54	117.48	120.91
12	B	506	J7S	C12-N-C4	2.52	117.55	114.97
5	A	501	GTP	O3G-PG-O3B	-2.52	96.20	104.64
5	C	501	GTP	O2A-PA-O3A	2.52	114.07	107.27
13	F	703	ACP	C5-N7-C8	2.51	107.40	103.45
10	B	501	GDP	O6-C6-C5	-2.46	120.03	126.53
12	B	506	J7S	C13-C4-N	2.46	120.74	118.05
5	D	601	GTP	O3B-PB-O1B	-2.44	103.36	110.70
5	A	501	GTP	O3G-PG-O1G	2.39	120.15	110.83
11	B	504	MES	C6-O1-C2	2.38	117.58	109.88
12	B	506	J7S	O-C1-C2	-2.36	108.62	119.82
5	D	601	GTP	C4-C5-N7	-2.35	106.95	110.67
5	C	501	GTP	O6-C6-C5	-2.30	120.45	126.53
5	D	601	GTP	O2B-PB-O1B	2.30	123.13	112.44
12	B	506	J7S	C15-C13-N4	2.29	123.73	119.76
5	A	501	GTP	C8-N9-C4	2.24	110.22	106.03
13	F	703	ACP	C3'-C2'-C1'	2.22	105.65	101.46
10	B	501	GDP	C4-C5-N7	-2.15	107.26	110.67
12	B	506	J7S	O1-C14-C12	-2.12	113.90	119.47
5	D	601	GTP	O6-C6-C5	-2.11	120.96	126.53
5	D	601	GTP	O3B-PG-O1G	-2.10	100.00	111.04
10	B	501	GDP	O4'-C1'-N9	-2.07	103.68	108.36
12	B	506	J7S	O-C1-C15	2.05	129.76	120.00
13	F	703	ACP	C4-N9-C8	2.04	107.88	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	603	J7S	N3-C7-N2	2.03	117.98	115.77
5	C	501	GTP	C4-C5-N7	-2.01	107.48	110.67

There are no chirality outliers.

All (40) 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	601	GTP	C5'-O5'-PA-O2A
5	D	601	GTP	O4'-C4'-C5'-O5'
9	A	505	GOL	C1-C2-C3-O3
10	B	501	GDP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
12	D	603	J7S	N1-C5-N-C12
12	B	506	J7S	N1-C5-N-C12
12	D	603	J7S	C15-C1-O-C
5	D	601	GTP	C3'-C4'-C5'-O5'
12	D	603	J7S	C2-C1-O-C
9	A	505	GOL	O2-C2-C3-O3
11	B	505	MES	C8-C7-N4-C3
11	B	505	MES	C8-C7-N4-C5
13	F	703	ACP	PB-O3A-PA-O1A
9	A	506	GOL	O2-C2-C3-O3
11	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	D	601	GTP	C4'-C5'-O5'-PA
5	D	601	GTP	C5'-O5'-PA-O3A
5	D	601	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
11	B	504	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
13	F	703	ACP	PB-C3B-PG-O1G

Continued on next page...

Continued from previous page...

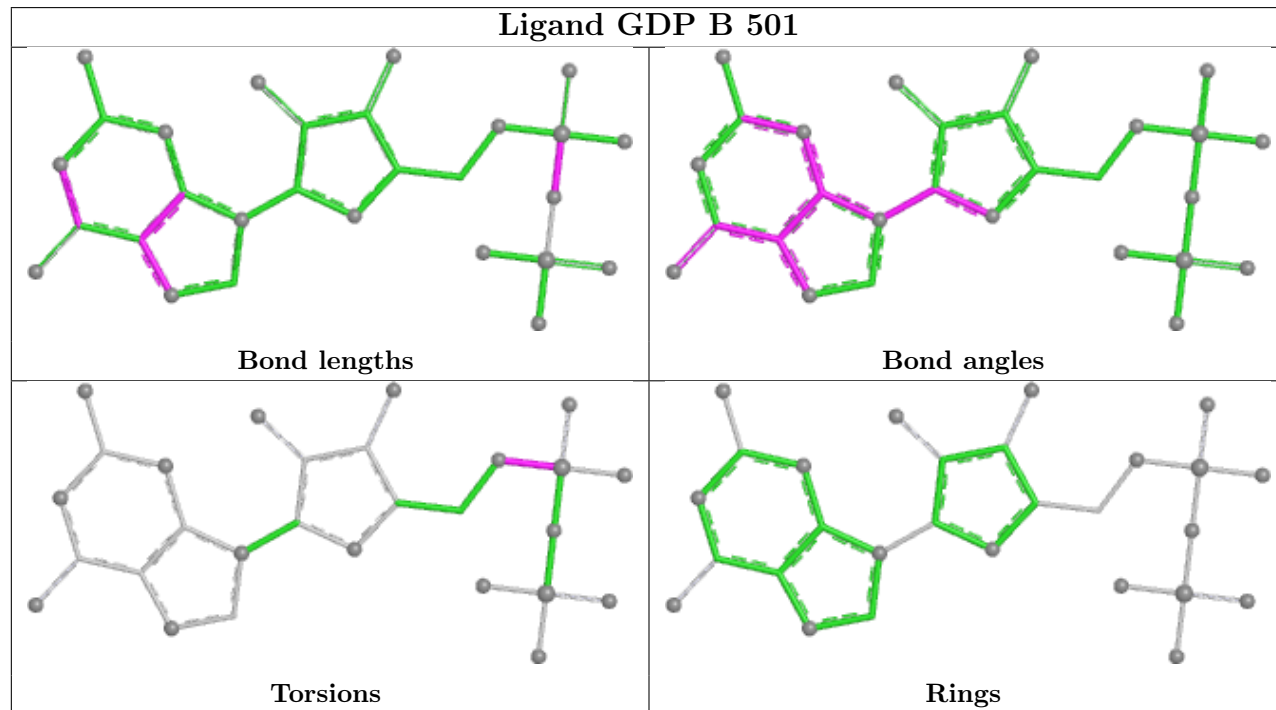
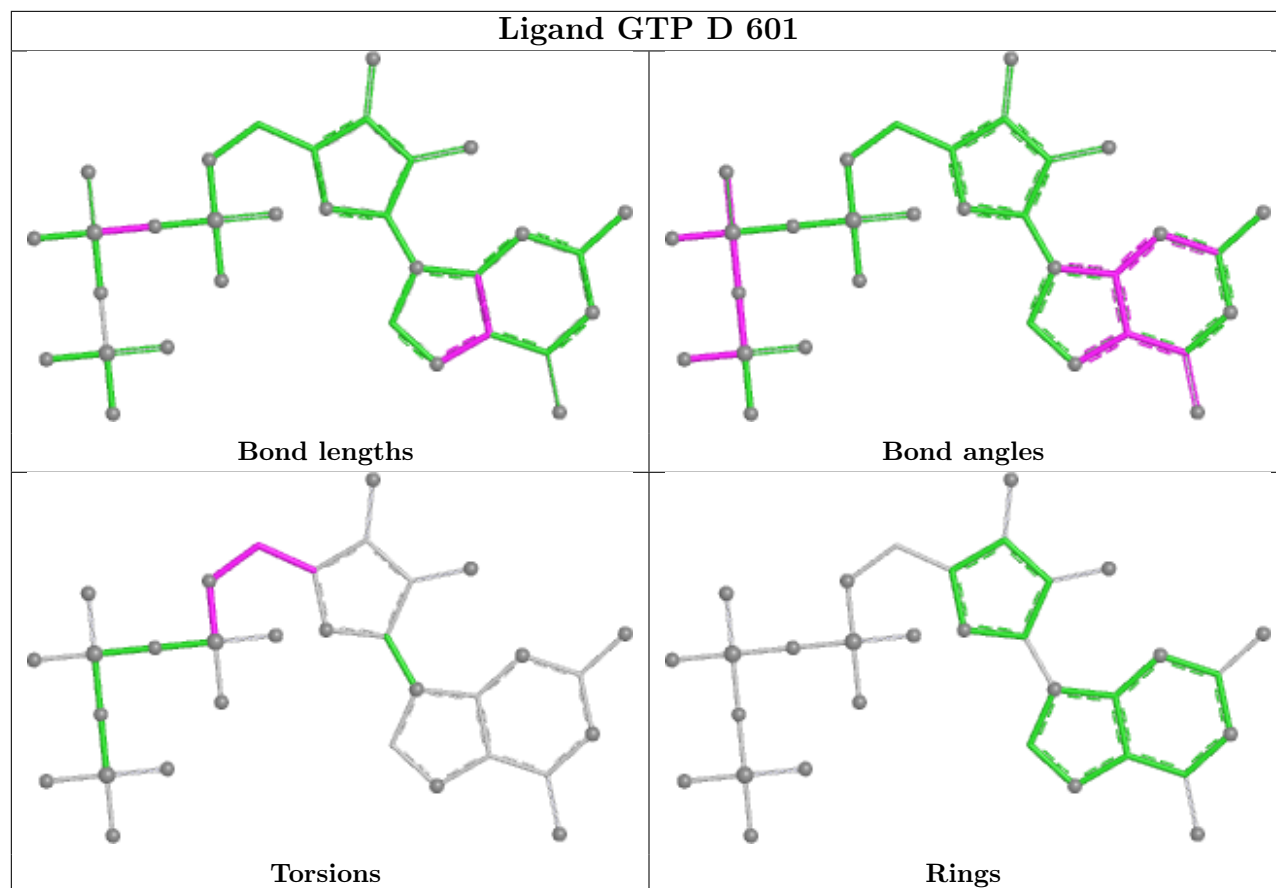
Mol	Chain	Res	Type	Atoms
13	F	703	ACP	PB-O3A-PA-O2A
12	B	506	J7S	C15-C1-O-C
12	B	506	J7S	C8-C5-N-C12
12	D	603	J7S	C8-C5-N-C12
13	F	703	ACP	O4'-C4'-C5'-O5'

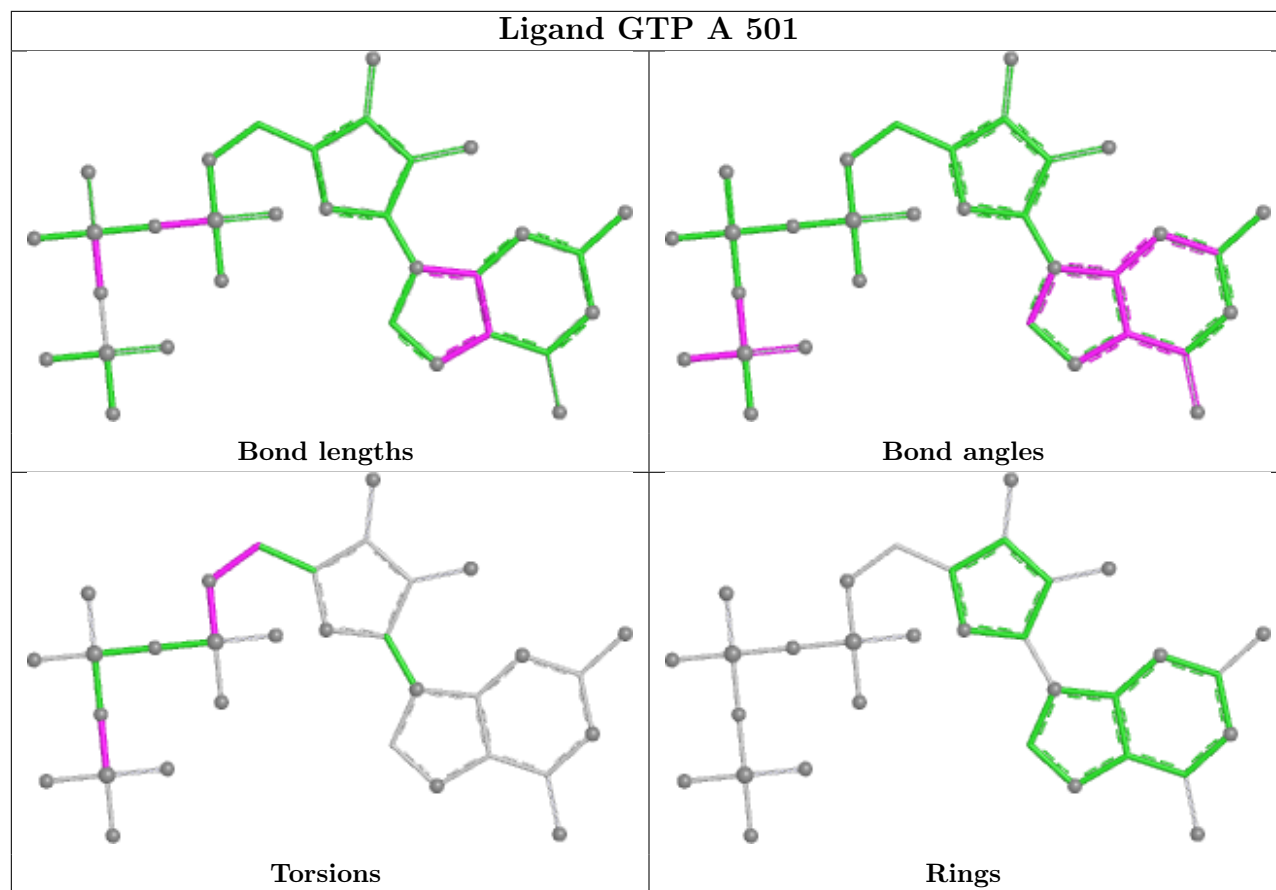
There are no ring outliers.

3 monomers are involved in 9 short contacts:

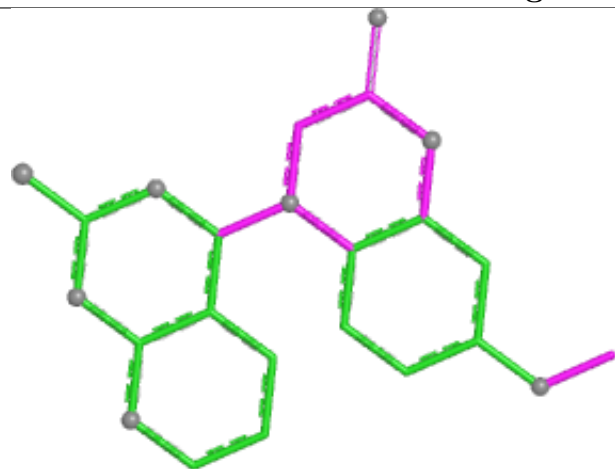
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	506	J7S	3	0
12	D	603	J7S	2	0
11	B	504	MES	4	0

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.

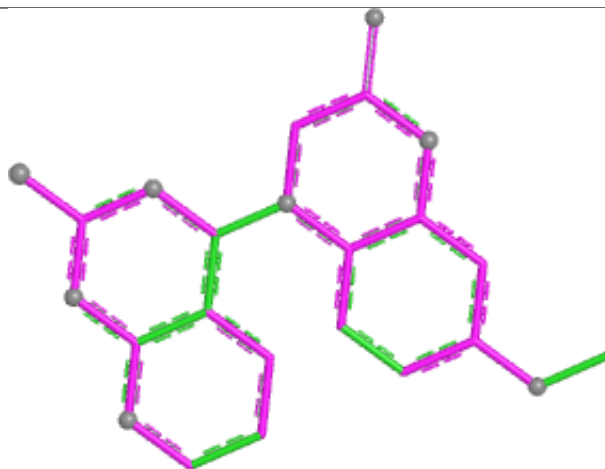




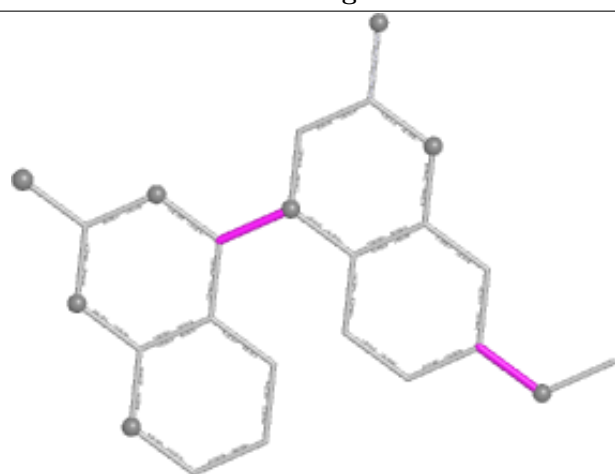
Ligand J7S B 506



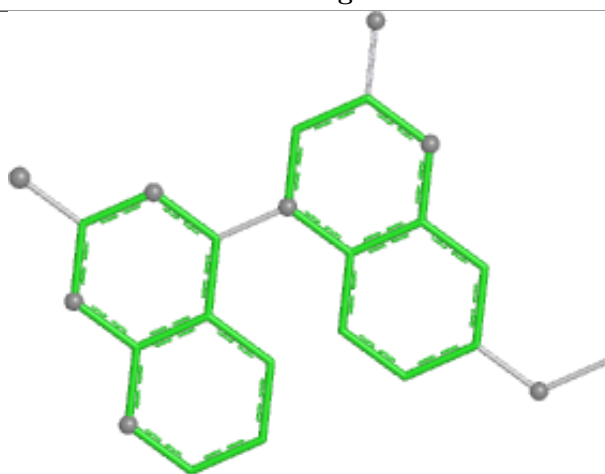
Bond lengths



Bond angles

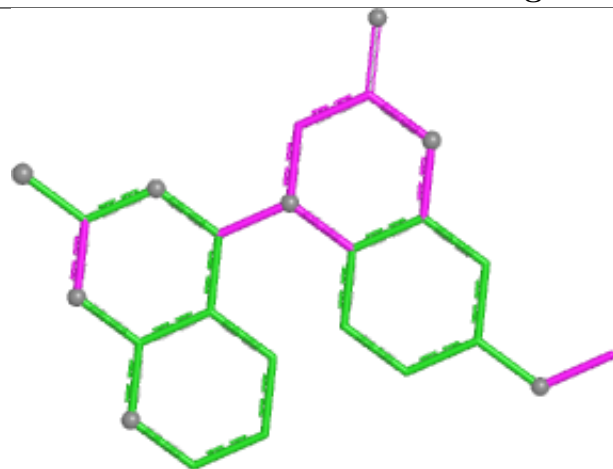


Torsions

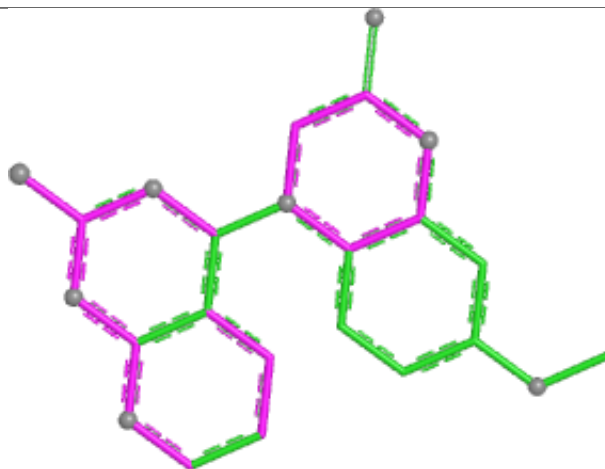


Rings

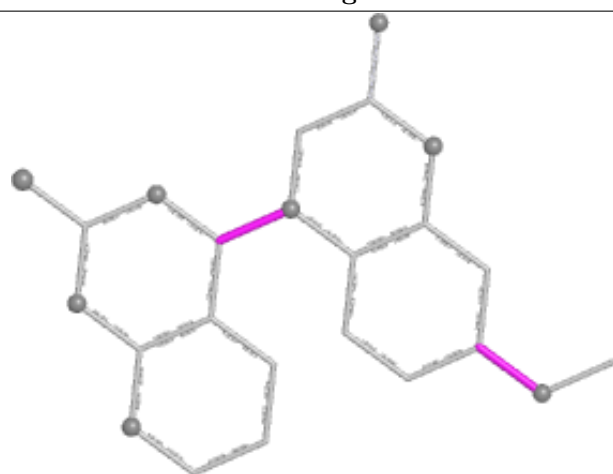
Ligand J7S D 603



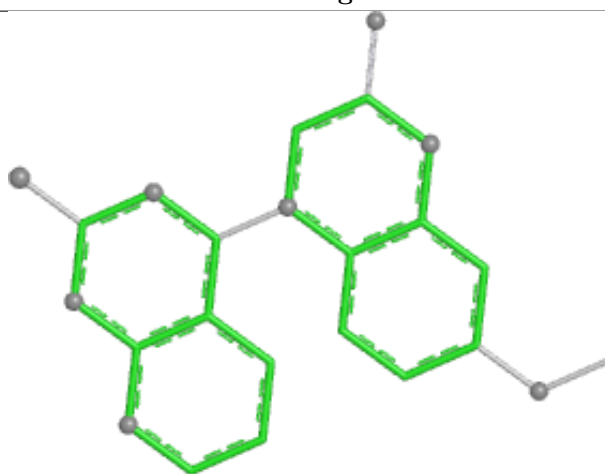
Bond lengths



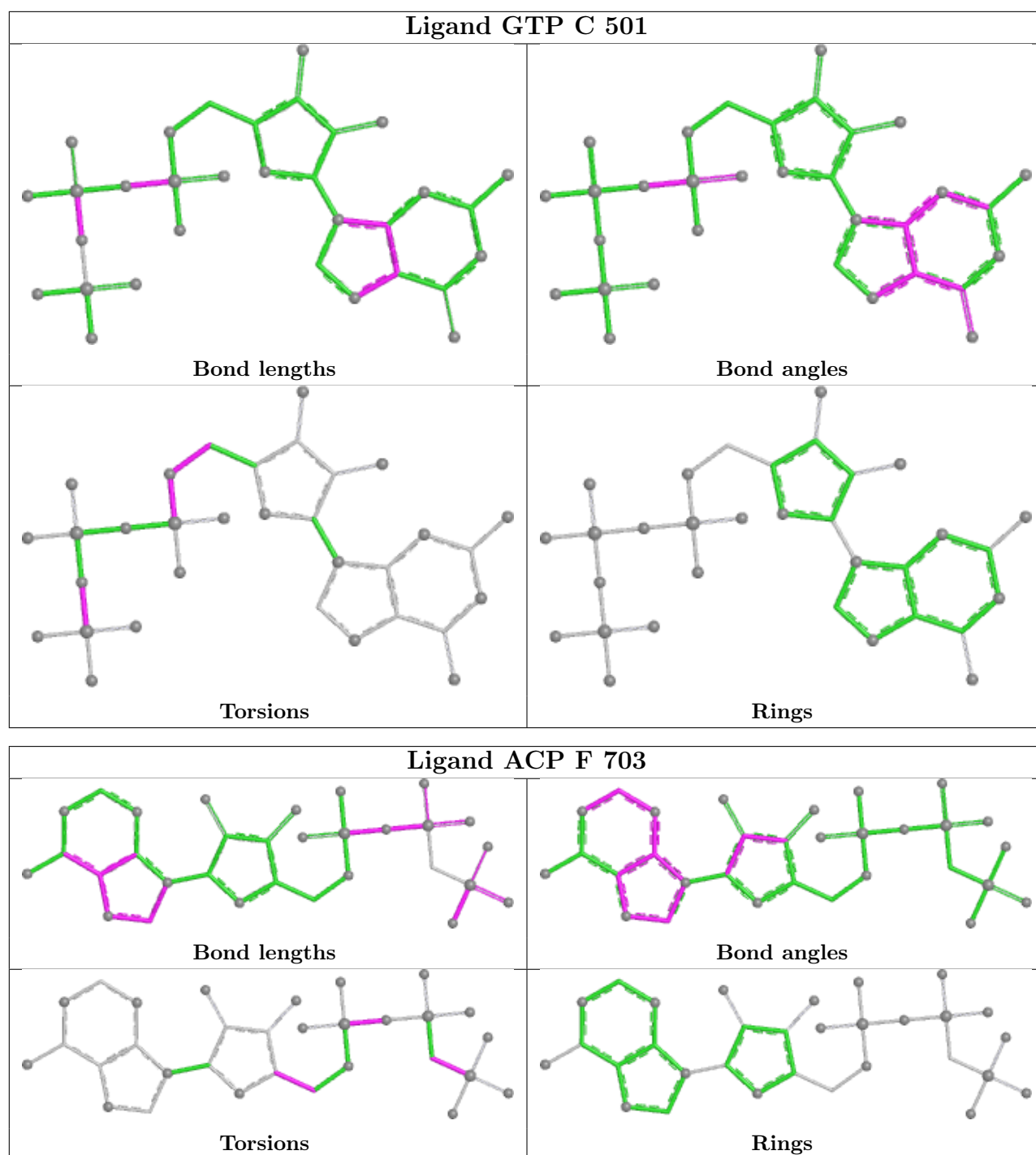
Bond angles



Torsions



Rings



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	439/450 (97%)	0.10	9 (2%) 63 65	19, 37, 64, 92	2 (0%)
1	C	441/450 (98%)	-0.28	8 (1%) 67 69	14, 27, 49, 104	2 (0%)
2	B	428/445 (96%)	0.04	17 (3%) 42 41	17, 34, 74, 110	2 (0%)
2	D	420/445 (94%)	0.83	46 (10%) 10 8	25, 53, 89, 112	2 (0%)
3	E	126/143 (88%)	0.91	16 (12%) 8 6	24, 51, 100, 123	1 (0%)
4	F	356/384 (92%)	1.16	100 (28%) 1 1	27, 62, 129, 155	0
All	All	2210/2317 (95%)	0.37	196 (8%) 15 13	14, 41, 97, 155	9 (0%)

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	217	LEU	5.3
4	F	125	THR	5.3
4	F	153	ALA	4.8
4	F	161	LEU	4.8
2	D	72	THR	4.7
4	F	152	SER	4.6
4	F	155	ALA	4.5
4	F	162	ILE	4.5
4	F	257	GLU	4.5
2	D	96	GLY	4.4
4	F	169	LEU	4.3
4	F	371	PRO	4.3
3	E	29	PHE	4.3
4	F	222	ARG	4.2
4	F	130	VAL	4.1
4	F	256	TYR	4.0
4	F	381	HIS	4.0
4	F	132	LEU	4.0
4	F	150	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	236	LYS	3.7
2	D	92	PHE	3.7
1	A	282	TYR	3.7
2	D	2	ARG	3.7
4	F	379	HIS	3.6
4	F	159	GLY	3.6
2	D	73	MET	3.6
4	F	254	GLY	3.6
4	F	362	ALA	3.5
3	E	27	PRO	3.5
4	F	135	TYR	3.5
4	F	133	ALA	3.5
4	F	163	SER	3.4
4	F	170	LEU	3.3
4	F	233	PHE	3.3
2	B	245	GLN	3.3
4	F	147	TRP	3.2
4	F	149	ALA	3.2
2	B	55	THR	3.2
2	D	71	GLY	3.2
2	D	219	THR	3.2
2	D	55	THR	3.1
4	F	166	ALA	3.1
1	C	1	MET	3.1
1	C	245	ASP	3.1
2	D	394	PHE	3.1
3	E	139	LEU	3.1
4	F	186	LEU	3.1
4	F	100	ILE	3.1
4	F	148	ILE	3.0
4	F	199	PHE	3.0
4	F	372	THR	3.0
4	F	253	TYR	3.0
2	D	26	ASP	3.0
3	E	52	LYS	2.9
4	F	246	GLN	2.9
4	F	181	VAL	2.9
2	D	359	ARG	2.9
4	F	228	TYR	2.9
2	D	245	GLN	2.9
4	F	232	ASN	2.9
1	C	441	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	397	TRP	2.9
4	F	249	TYR	2.9
2	D	95	SER	2.8
3	E	28	SER	2.8
2	B	2	ARG	2.8
2	D	178	THR	2.8
4	F	156	LYS	2.8
4	F	157	GLY	2.8
4	F	164	SER	2.8
4	F	238	CYS	2.8
4	F	251	LYS	2.8
4	F	160	ILE	2.8
4	F	136	ASN	2.8
2	D	284	LEU	2.8
4	F	138	ARG	2.8
1	C	283	HIS	2.8
4	F	382	HIS	2.8
4	F	263	PHE	2.8
4	F	225	SER	2.7
2	B	54	ALA	2.7
2	D	218	THR	2.7
2	B	84	ILE	2.7
4	F	240	LEU	2.7
2	B	428	ALA	2.7
4	F	154	GLY	2.7
1	A	262	TYR	2.7
2	D	214	THR	2.7
4	F	245	ILE	2.7
2	D	246	LEU	2.7
4	F	237	THR	2.7
3	E	135	LYS	2.6
4	F	102	PRO	2.6
4	F	244	CYS	2.6
4	F	296	MET	2.6
2	D	180	VAL	2.6
4	F	173	ILE	2.6
4	F	243	HIS	2.6
4	F	182	ILE	2.6
2	D	405	GLU	2.6
4	F	143	GLU	2.6
4	F	196	HIS	2.6
4	F	255	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	176	GLN	2.6
4	F	239	HIS	2.6
4	F	383	HIS	2.5
1	A	336	LYS	2.5
3	E	30	ASP	2.5
4	F	172	PHE	2.5
4	F	192	LEU	2.5
4	F	340	GLN	2.5
4	F	252	ASN	2.5
2	B	77	ARG	2.5
2	D	431	ASP	2.5
4	F	363	ASP	2.5
1	C	357	TYR	2.5
4	F	145	ASN	2.5
4	F	229	ASN	2.4
1	A	41	THR	2.4
4	F	70	LYS	2.4
3	E	142	GLU	2.4
2	D	81	PHE	2.4
2	D	247	ASN	2.4
4	F	27	TRP	2.4
4	F	134	ALA	2.4
3	E	53	LYS	2.4
2	B	246	LEU	2.4
1	C	356	ASN	2.4
4	F	242	ASN	2.4
2	D	69	GLU	2.4
4	F	194	PRO	2.3
4	F	234	GLN	2.3
2	B	323	MET	2.3
2	D	323	MET	2.3
4	F	146	VAL	2.3
2	D	176	SER	2.3
4	F	195	GLY	2.3
4	F	227	PRO	2.3
2	D	82	GLY	2.3
2	D	396	HIS	2.3
4	F	179	VAL	2.3
2	B	72	THR	2.3
2	D	221	THR	2.3
1	A	232	SER	2.3
4	F	32	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	2.2
2	B	277	GLY	2.2
2	D	68	LEU	2.2
4	F	306	HIS	2.2
1	C	340	SER	2.2
4	F	139	ARG	2.2
2	D	393	ALA	2.2
2	B	280	GLN	2.2
2	D	140	GLY	2.2
2	D	395	LEU	2.2
4	F	177	GLY	2.2
2	D	175	VAL	2.2
2	D	122	LYS	2.2
3	E	90	ASN	2.2
2	D	15	GLN	2.2
2	D	37	HIS	2.2
4	F	221	LEU	2.2
2	B	278	SER	2.2
4	F	167	SER	2.2
1	A	113	GLU	2.2
4	F	197	ARG	2.2
3	E	75	LYS	2.2
3	E	140	LYS	2.2
2	D	65	LEU	2.1
4	F	19	ARG	2.1
4	F	226	GLU	2.1
3	E	25	LYS	2.1
1	A	437	VAL	2.1
4	F	180	HIS	2.1
2	B	279	GLN	2.1
3	E	59	GLU	2.1
4	F	101	TYR	2.1
1	A	438	ASP	2.1
2	B	128	ASP	2.1
4	F	247	LYS	2.1
4	F	339	ALA	2.1
2	D	391	ARG	2.1
2	D	84	ILE	2.1
4	F	99	VAL	2.1
2	D	387	ALA	2.1
1	A	346	TRP	2.1
3	E	43	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	285	GLN	2.0
2	D	179	VAL	2.0
4	F	31	ARG	2.0
2	D	220	PRO	2.0
2	D	406	MET	2.0
3	E	50	ILE	2.0
2	B	1	MET	2.0
2	B	80	PRO	2.0
4	F	98	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	702	1/1	0.74	0.19	76,76,76,76	0
9	GOL	A	506	6/6	0.80	0.22	78,80,84,90	0
6	MG	D	602	1/1	0.82	0.12	63,63,63,63	0
13	ACP	F	703	31/31	0.84	0.15	75,90,107,112	0
5	GTP	D	601	32/32	0.87	0.12	39,46,72,79	0
9	GOL	A	505	6/6	0.87	0.16	53,59,61,65	0
7	CA	B	503	1/1	0.88	0.09	76,76,76,76	0
11	MES	B	504	12/12	0.88	0.14	40,45,58,63	0
6	MG	F	701	1/1	0.88	0.14	72,72,72,72	0
8	CL	A	504	1/1	0.90	0.11	74,74,74,74	0
11	MES	B	505	12/12	0.91	0.14	60,66,68,68	0
7	CA	E	201	1/1	0.91	0.08	73,73,73,73	0
12	J7S	D	603	24/24	0.95	0.08	26,33,44,48	0
12	J7S	B	506	24/24	0.95	0.08	25,28,32,39	0

Continued on next page...

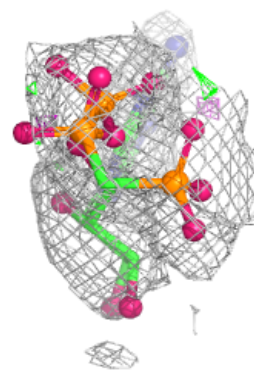
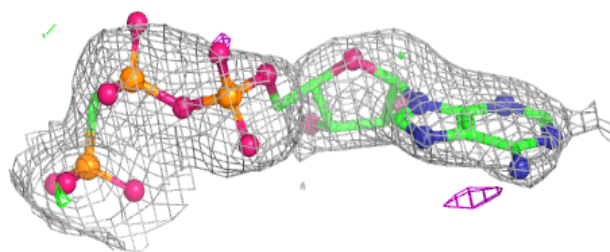
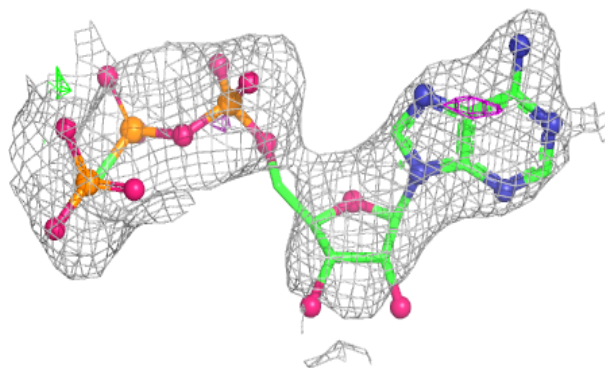
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	502	1/1	0.97	0.04	27,27,27,27	0
7	CA	A	503	1/1	0.97	0.04	52,52,52,52	0
6	MG	A	502	1/1	0.98	0.02	28,28,28,28	0
7	CA	C	503	1/1	0.99	0.03	35,35,35,35	0
5	GTP	A	501	32/32	0.99	0.04	19,21,22,23	0
10	GDP	B	501	28/28	0.99	0.05	18,21,23,24	0
5	GTP	C	501	32/32	0.99	0.04	18,19,20,21	0
6	MG	C	502	1/1	1.00	0.01	25,25,25,25	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.

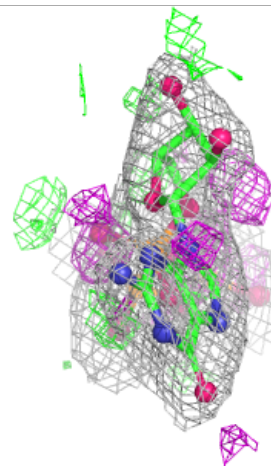
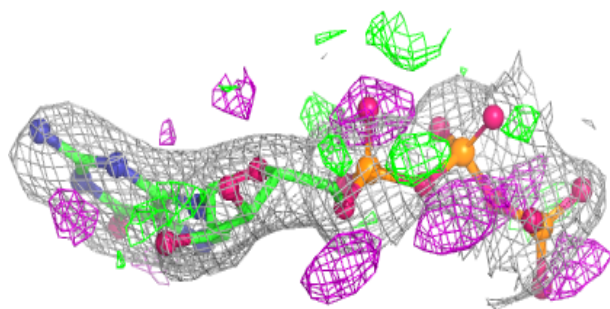
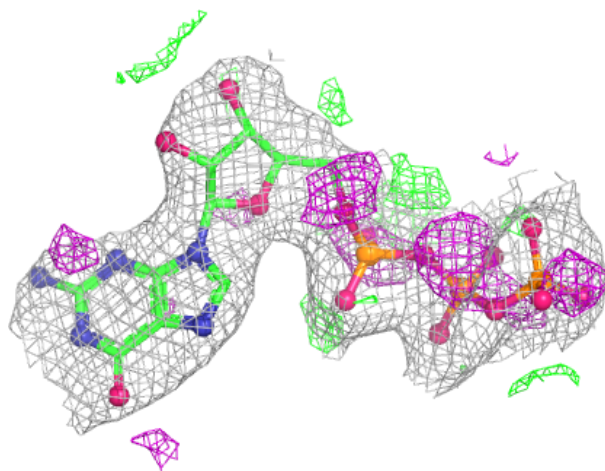
Electron density around ACP F 703:

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



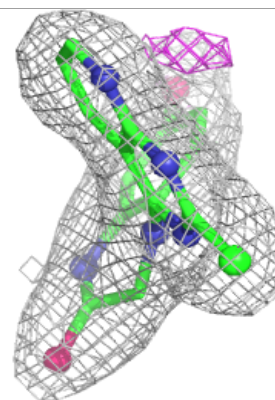
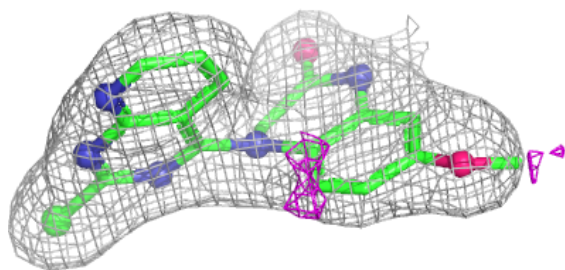
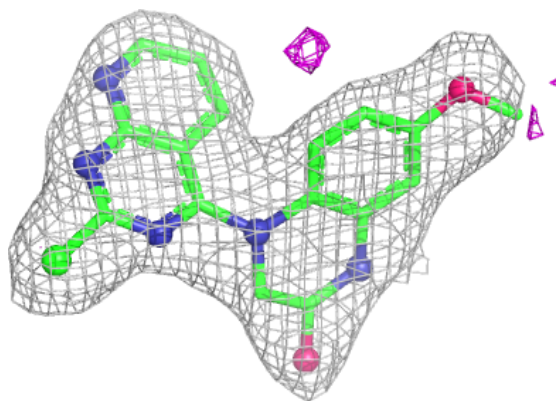
Electron density around GTP D 601:

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



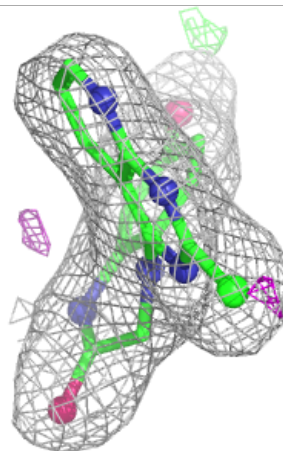
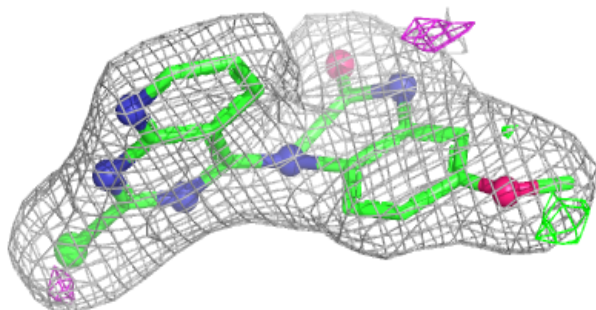
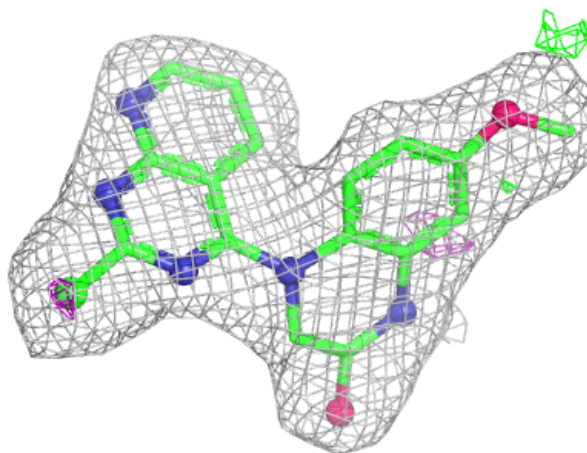
Electron density around J7S D 603:

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



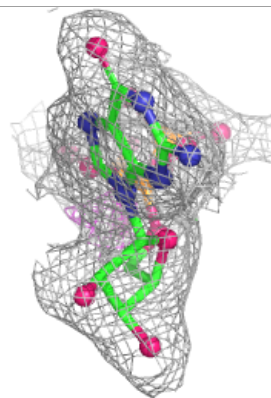
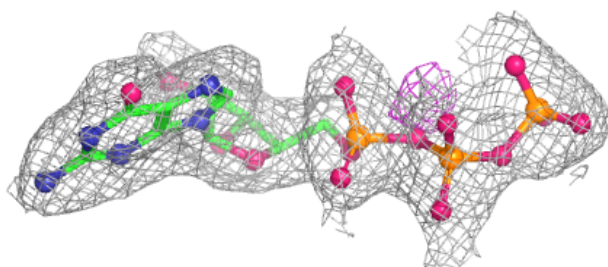
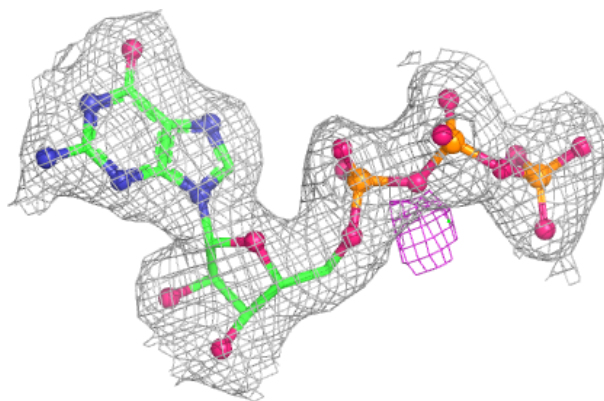
Electron density around J7S B 506:

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

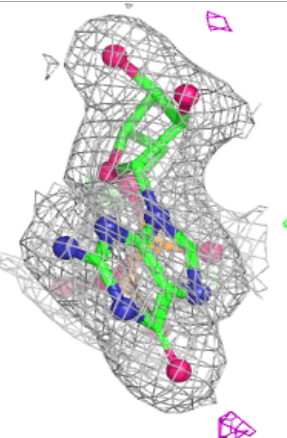
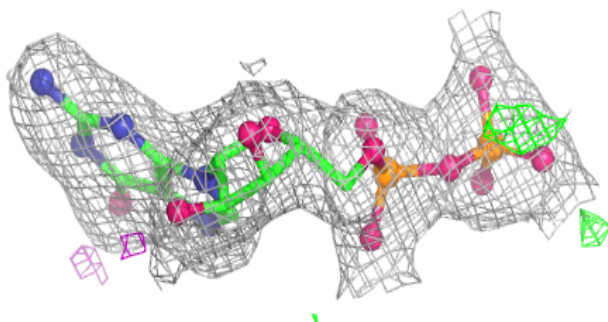
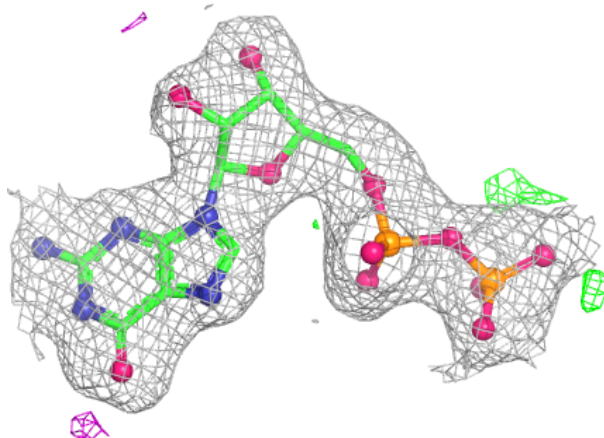


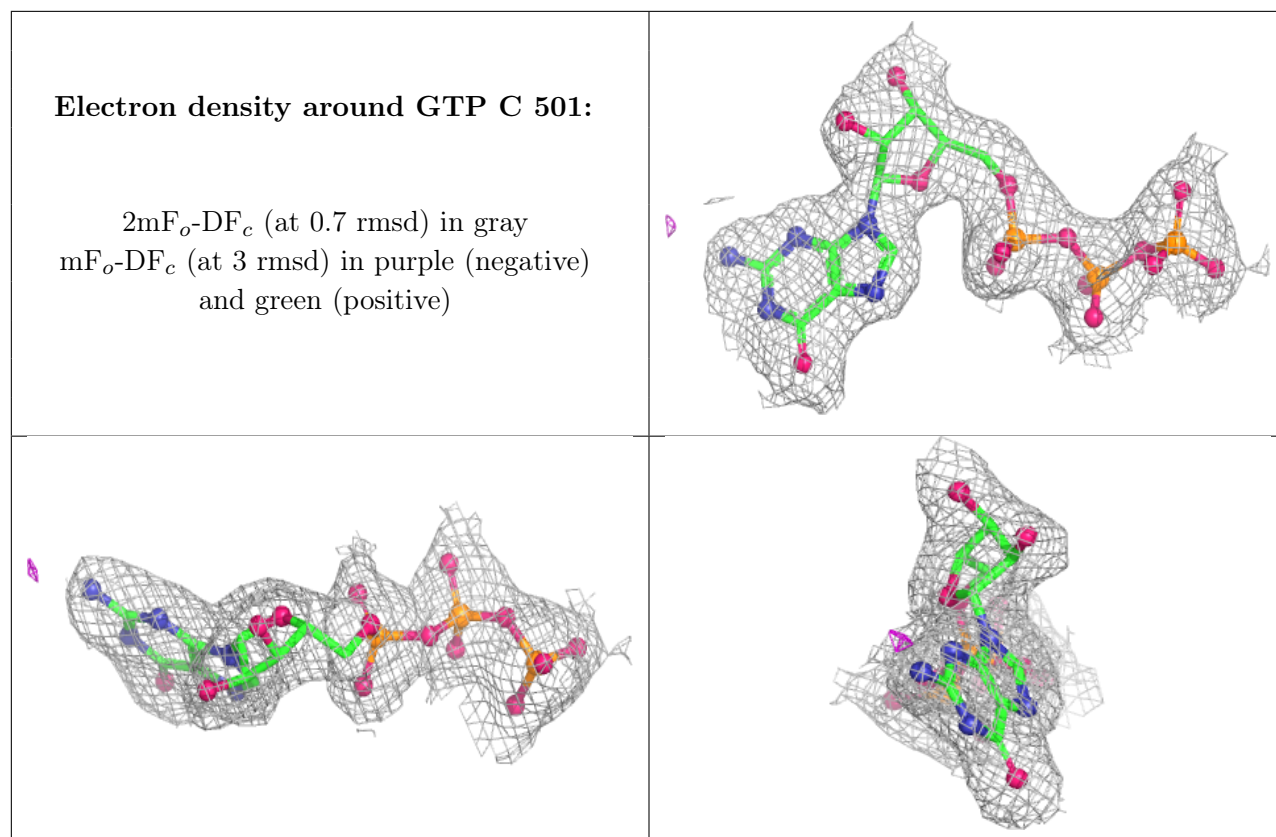
Electron density around GTP A 501:

$2mF_o-DF_c$ (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.