



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:15 pm BST

PDB ID : 6EG5
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

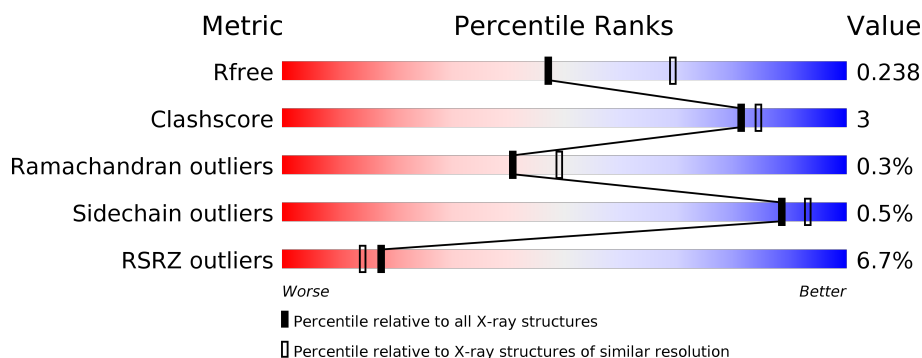
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	<div> <div>2%</div> <div>94%</div> <div>• •</div> </div>
1	C	450	<div> <div>%</div> <div>93%</div> <div>• •</div> </div>
2	B	445	<div> <div>3%</div> <div>89%</div> <div>7% •</div> </div>
2	D	445	<div> <div>7%</div> <div>88%</div> <div>6% 6%</div> </div>
3	E	143	<div> <div>9%</div> <div>84%</div> <div>• 12%</div> </div>
4	F	384	<div> <div>21%</div> <div>85%</div> <div>7% 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GOL	A	506	-	-	-	X

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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	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	C	1	Total	Mg	0	0
			1	1		
6	F	2	Total	Mg	0	0
			2	2		

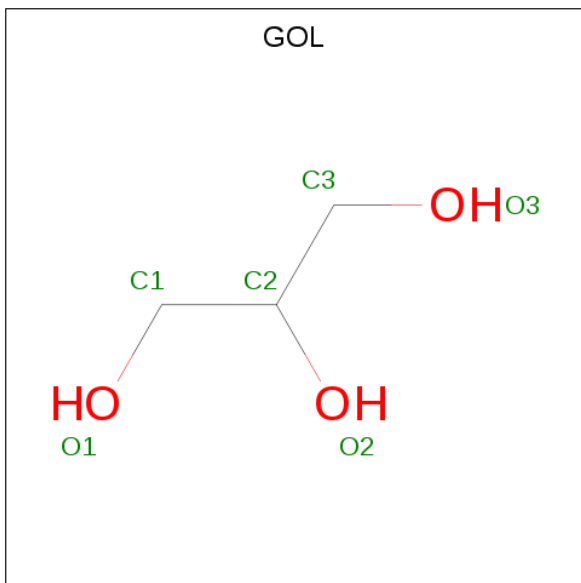
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

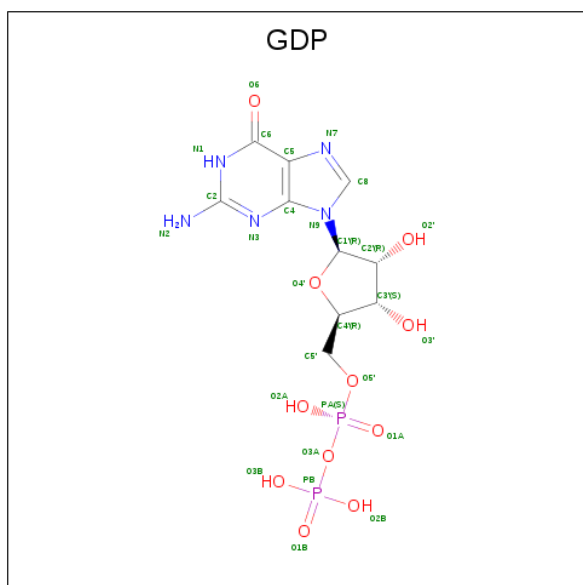
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: 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 (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



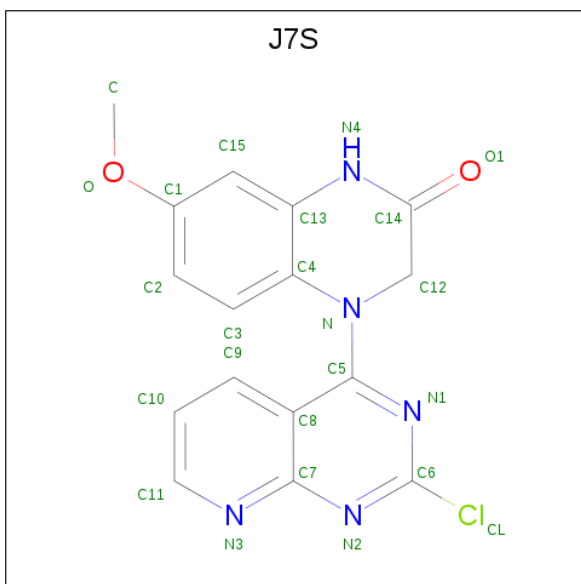
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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 (three-letter code: J7S) (formula: C₁₆H₁₂ClN₅O₂).



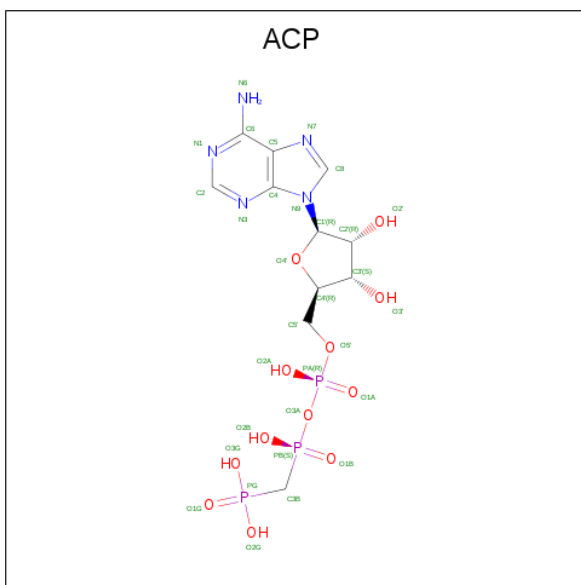
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Cl	N	O	0	0
			24	16	1	5	2		

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

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

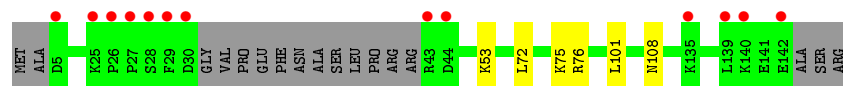
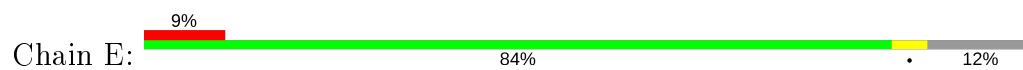


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	F	1	Total	C	N	O	P	
			31	11	5	12	3	
							0	0

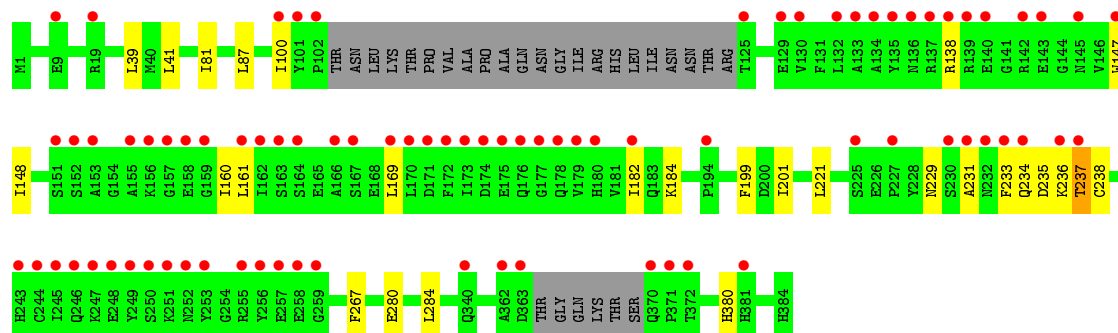
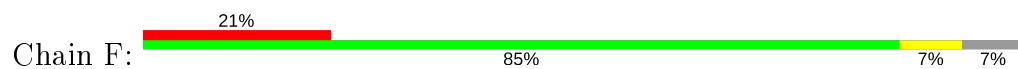
- Molecule 14 is water.

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

- 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 49.88 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.45) 97.6 (49.88-2.45)	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	5580 reflections (5.11%)	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 , 41.8	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/3520	0.68	0/4778
1	C	0.49	0/3540	0.70	0/4805
2	B	0.48	0/3444	0.66	0/4664
2	D	0.45	0/3374	0.65	0/4571
3	E	0.47	0/1064	0.63	0/1411
4	F	0.45	0/2983	0.65	0/4031
All	All	0.47	0/17925	0.67	0/24260

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	3436	0	3350	14	0
1	C	3456	0	3366	18	0
2	B	3369	0	3250	24	0
2	D	3301	0	3177	24	0
3	E	1052	0	1063	4	0
4	F	2913	0	2863	12	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
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	92	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 (92) 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:359:ARG:NH1	2:D:359:ARG:HB3	1.89	0.86
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.22	0.80
2:D:359:ARG:CZ	2:D:359:ARG:HB3	2.24	0.68
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.75	0.68
1:C:204:VAL:HG22	1:C:302[B]:MET:HE1	1.75	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:204:VAL:CG2	1:C:302[B]:MET:HE1	2.37	0.54
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: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:HH11	2:D:359:ARG:HB3	1.73	0.47
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.96	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.97	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
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
2:B:109:GLY:HA2	2:B:147:MET:HE2	2.00	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: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:399:TYR:O	1:A:402:ARG:NH1	2.52	0.41
1:A:179:THR:O	12:B:506:J7S:N4	2.54	0.41
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
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	19	22
4	F	350/384 (91%)	329 (94%)	15 (4%)	6 (2%)	9	7
All	All	2195/2317 (95%)	2131 (97%)	57 (3%)	7 (0%)	41	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	234	GLN
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%)	369 (99%)	3 (1%)	81	88
1	C	374/378 (99%)	373 (100%)	1 (0%)	92	95
2	B	370/383 (97%)	368 (100%)	2 (0%)	88	93
2	D	363/383 (95%)	361 (99%)	2 (1%)	86	91
3	E	115/127 (91%)	115 (100%)	0	100	100
4	F	318/342 (93%)	316 (99%)	2 (1%)	86	91
All	All	1912/1991 (96%)	1902 (100%)	10 (0%)	88	93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	251	ASP
1	A	381	THR
2	B	19	LYS
2	B	278	SER
1	C	221	ARG
2	D	35	SER
2	D	359	ARG
4	F	237	THR
4	F	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
2	B	137	HIS
2	B	190	HIS
2	D	99	ASN
3	E	18	GLN
3	E	108	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 carbohydrates 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$
11	MES	B	504	-	12,12,12	2.25	1 (8%)	14,16,16	1.91	4 (28%)
9	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.74	0
12	J7S	D	603	-	27,27,27	2.89	8 (29%)	34,39,39	2.63	9 (26%)
9	GOL	A	506	-	5,5,5	0.37	0	5,5,5	0.53	0
11	MES	B	505	-	12,12,12	2.13	1 (8%)	14,16,16	1.32	2 (14%)
5	GTP	A	501	6	26,34,34	1.09	2 (7%)	33,54,54	1.90	7 (21%)
10	GDP	B	501	6	24,30,30	1.18	3 (12%)	31,47,47	1.93	7 (22%)
5	GTP	C	501	6	26,34,34	1.02	2 (7%)	33,54,54	1.92	6 (18%)
12	J7S	B	506	-	27,27,27	2.89	8 (29%)	34,39,39	2.57	15 (44%)
13	ACP	F	703	6	27,33,33	2.12	9 (33%)	32,52,52	1.47	3 (9%)
5	GTP	D	601	6	26,34,34	1.25	2 (7%)	33,54,54	2.02	10 (30%)

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
11	MES	B	504	-	-	3/6/14/14	0/1/1/1
9	GOL	A	505	-	-	2/4/4/4	-
12	J7S	D	603	-	-	4/6/18/18	0/4/4/4
9	GOL	A	506	-	-	1/4/4/4	-
11	MES	B	505	-	-	2/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
12	J7S	B	506	-	-	3/6/18/18	0/4/4/4
13	ACP	F	703	6	-	3/15/38/38	0/3/3/3
5	GTP	D	601	6	-	6/18/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	603	J7S	O1-C14	8.62	1.40	1.23
12	B	506	J7S	O1-C14	8.40	1.40	1.23
11	B	504	MES	C8-S	-7.43	1.66	1.77
11	B	505	MES	C8-S	-7.13	1.67	1.77
12	D	603	J7S	C14-N4	6.97	1.42	1.35
12	B	506	J7S	C14-N4	6.66	1.42	1.35
12	B	506	J7S	C12-N	-5.78	1.39	1.46
13	F	703	ACP	PG-O1G	5.42	1.61	1.50
12	B	506	J7S	C13-N4	5.33	1.49	1.39
12	D	603	J7S	C4-N	5.31	1.49	1.40
12	D	603	J7S	C13-N4	4.54	1.47	1.39
13	F	703	ACP	PB-O3A	4.49	1.63	1.58
13	F	703	ACP	PB-O1B	4.27	1.61	1.51
12	D	603	J7S	C12-N	-4.14	1.41	1.46
5	D	601	GTP	C6-C5	3.96	1.48	1.41
12	B	506	J7S	C4-N	3.51	1.46	1.40
5	A	501	GTP	C6-C5	3.50	1.47	1.41
13	F	703	ACP	PB-O2B	-3.37	1.48	1.56
5	C	501	GTP	C6-C5	3.17	1.46	1.41
10	B	501	GDP	C6-C5	3.04	1.46	1.41
13	F	703	ACP	PG-O3G	-2.92	1.48	1.54
13	F	703	ACP	PG-O2G	2.89	1.61	1.54
5	D	601	GTP	C5-C4	2.88	1.48	1.40
10	B	501	GDP	C2'-C1'	-2.83	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	603	J7S	C5-N	2.70	1.45	1.39
12	B	506	J7S	O-C	-2.63	1.34	1.42
13	F	703	ACP	C5-C4	2.57	1.47	1.40
12	D	603	J7S	C6-N2	2.46	1.32	1.30
12	D	603	J7S	C12-C14	2.38	1.54	1.51
12	B	506	J7S	C5-N	2.37	1.44	1.39
5	A	501	GTP	C5-C4	2.26	1.46	1.40
5	C	501	GTP	C5-C4	2.24	1.46	1.40
13	F	703	ACP	C2-N3	2.21	1.35	1.32
12	B	506	J7S	C12-C14	2.17	1.53	1.51
10	B	501	GDP	C5-C4	2.12	1.46	1.40
13	F	703	ACP	O4'-C1'	2.02	1.43	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	603	J7S	N2-C6-N1	-6.88	123.69	130.62
12	D	603	J7S	CL-C6-N2	6.34	121.11	115.70
12	B	506	J7S	C13-N4-C14	-5.85	117.25	124.49
12	B	506	J7S	N2-C6-N1	-5.77	124.80	130.62
12	D	603	J7S	C6-N2-C7	5.60	118.52	114.09
12	D	603	J7S	C13-N4-C14	-5.30	117.93	124.49
12	D	603	J7S	C12-C14-N4	5.12	122.50	116.13
12	B	506	J7S	C6-N2-C7	5.09	118.12	114.09
5	C	501	GTP	C5-C6-N1	-4.96	116.64	123.43
5	C	501	GTP	C6-N1-C2	4.93	123.77	115.93
10	B	501	GDP	C6-N1-C2	4.91	123.73	115.93
5	A	501	GTP	C6-C5-C4	-4.66	116.34	120.80
12	B	506	J7S	C12-C14-N4	4.65	121.92	116.13
5	D	601	GTP	C6-N1-C2	4.59	123.22	115.93
12	B	506	J7S	CL-C6-N2	4.59	119.62	115.70
10	B	501	GDP	C5-C6-N1	-4.45	117.35	123.43
5	A	501	GTP	C6-N1-C2	4.44	122.99	115.93
10	B	501	GDP	C6-C5-C4	-4.43	116.57	120.80
5	D	601	GTP	C6-C5-C4	-4.27	116.72	120.80
5	D	601	GTP	C2-N3-C4	4.18	120.13	115.36
5	A	501	GTP	C5-C6-N1	-4.16	117.74	123.43
5	D	601	GTP	C5-C6-N1	-3.98	117.98	123.43
5	A	501	GTP	C2-N3-C4	3.88	119.79	115.36
5	C	501	GTP	C6-C5-C4	-3.81	117.17	120.80
10	B	501	GDP	N3-C2-N1	-3.80	122.15	127.22
5	C	501	GTP	C2-N3-C4	3.78	119.67	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-3.73	122.25	127.22
11	B	504	MES	C2-C3-N4	3.71	115.73	110.10
10	B	501	GDP	C2-N3-C4	3.60	119.47	115.36
12	D	603	J7S	C11-N3-C7	3.59	121.03	116.60
5	D	601	GTP	N3-C2-N1	-3.57	122.46	127.22
13	F	703	ACP	N3-C2-N1	-3.51	123.20	128.68
12	D	603	J7S	C6-N1-C5	3.47	121.34	111.04
5	A	501	GTP	N3-C2-N1	-3.46	122.61	127.22
11	B	504	MES	C5-N4-C3	3.38	116.44	108.83
11	B	505	MES	O3S-S-C8	3.37	111.21	105.77
11	B	504	MES	O3S-S-C8	3.27	111.06	105.77
12	B	506	J7S	C3-C4-N	-3.25	117.51	121.77
12	B	506	J7S	C6-N1-C5	3.22	120.59	111.04
13	F	703	ACP	C3'-C2'-C1'	3.11	105.65	100.98
5	D	601	GTP	PB-O3B-PG	-2.91	122.83	132.83
12	B	506	J7S	C11-N3-C7	2.87	120.14	116.60
13	F	703	ACP	C4-C5-N7	-2.83	106.45	109.40
12	B	506	J7S	C12-N-C5	2.82	121.27	116.39
12	B	506	J7S	C10-C9-C8	-2.69	117.16	120.89
5	D	601	GTP	PA-O3A-PB	-2.57	124.01	132.83
5	A	501	GTP	O3G-PG-O3B	-2.52	96.20	104.64
12	B	506	J7S	O1-C14-C12	-2.49	113.90	119.92
12	D	603	J7S	C10-C9-C8	-2.46	117.48	120.89
5	A	501	GTP	O3G-PG-O1G	2.42	120.15	110.68
5	D	601	GTP	C4-C5-N7	-2.35	106.95	109.40
12	B	506	J7S	O-C1-C2	-2.34	108.62	119.82
10	B	501	GDP	C1'-N9-C4	-2.30	122.59	126.64
11	B	504	MES	C6-O1-C2	2.30	117.58	109.89
5	D	601	GTP	O2B-PB-O1B	2.20	123.13	112.24
12	B	506	J7S	O1-C14-N4	2.19	123.37	121.43
5	C	501	GTP	PA-O3A-PB	-2.17	125.39	132.83
12	B	506	J7S	C15-C13-N4	2.15	123.73	119.84
10	B	501	GDP	C4-C5-N7	-2.05	107.26	109.40
12	B	506	J7S	O-C1-C15	2.05	129.76	119.94
11	B	505	MES	O1S-S-C8	2.04	109.37	106.92
12	D	603	J7S	N1-C5-N	-2.02	114.13	116.26
5	D	601	GTP	O3B-PG-O1G	-2.02	100.00	111.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

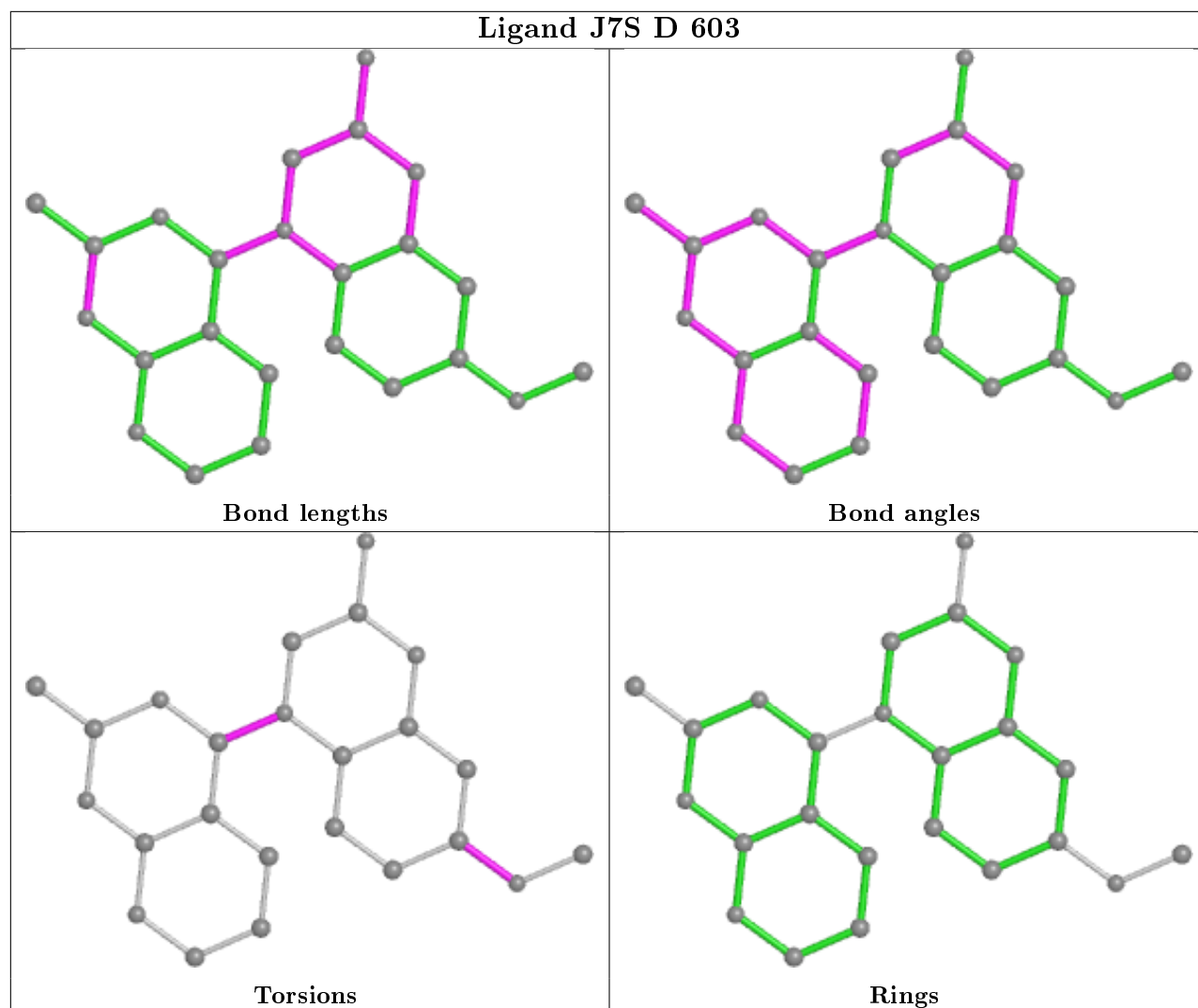
Mol	Chain	Res	Type	Atoms
9	A	505	GOL	C1-C2-C3-O3
12	B	506	J7S	C8-C5-N-C12
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	601	GTP	C5'-O5'-PA-O2A
5	D	601	GTP	O4'-C4'-C5'-O5'
12	D	603	J7S	C8-C5-N-C12
12	D	603	J7S	N1-C5-N-C12
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
5	D	601	GTP	C3'-C4'-C5'-O5'
12	B	506	J7S	N1-C5-N-C12
12	D	603	J7S	C15-C1-O-C
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
5	D	601	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	D	601	GTP	C5'-O5'-PA-O3A
9	A	506	GOL	O2-C2-C3-O3
5	D	601	GTP	C5'-O5'-PA-O1A
11	B	504	MES	C7-C8-S-O2S
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	C7-C8-S-O3S
13	F	703	ACP	PB-C3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
13	F	703	ACP	PB-O3A-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O3A
12	B	506	J7S	C15-C1-O-C
11	B	504	MES	C8-C7-N4-C3

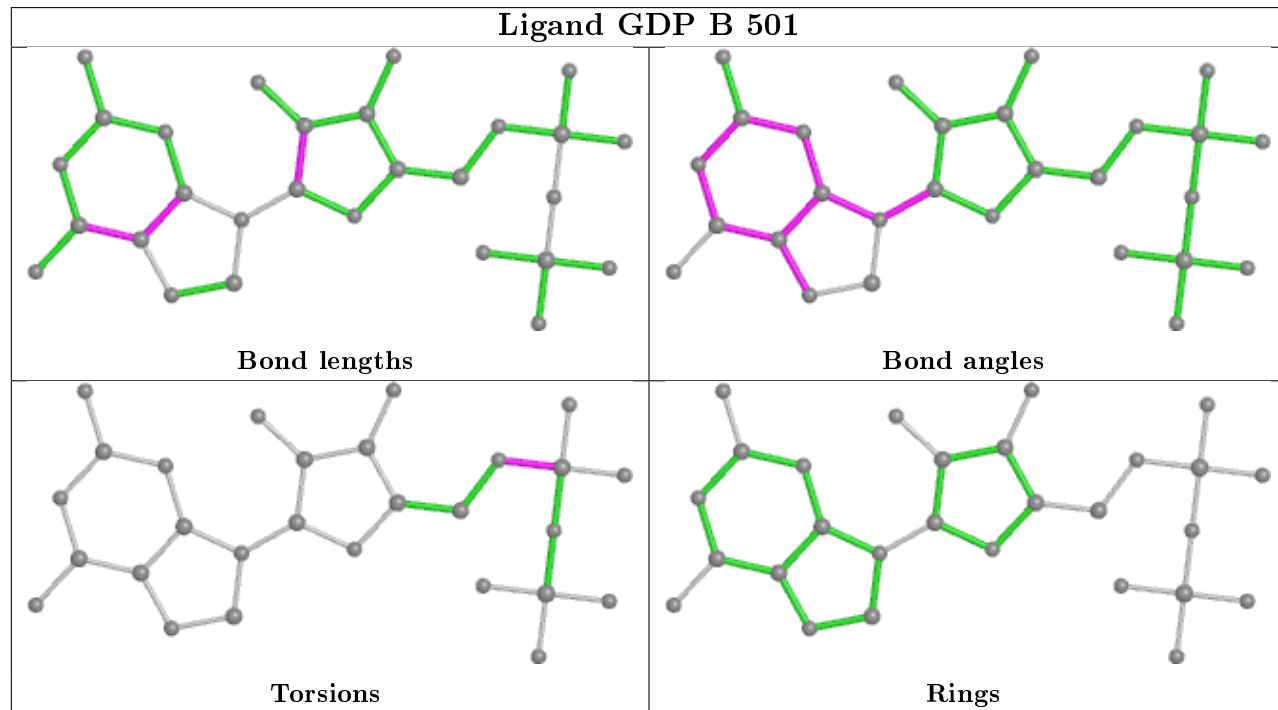
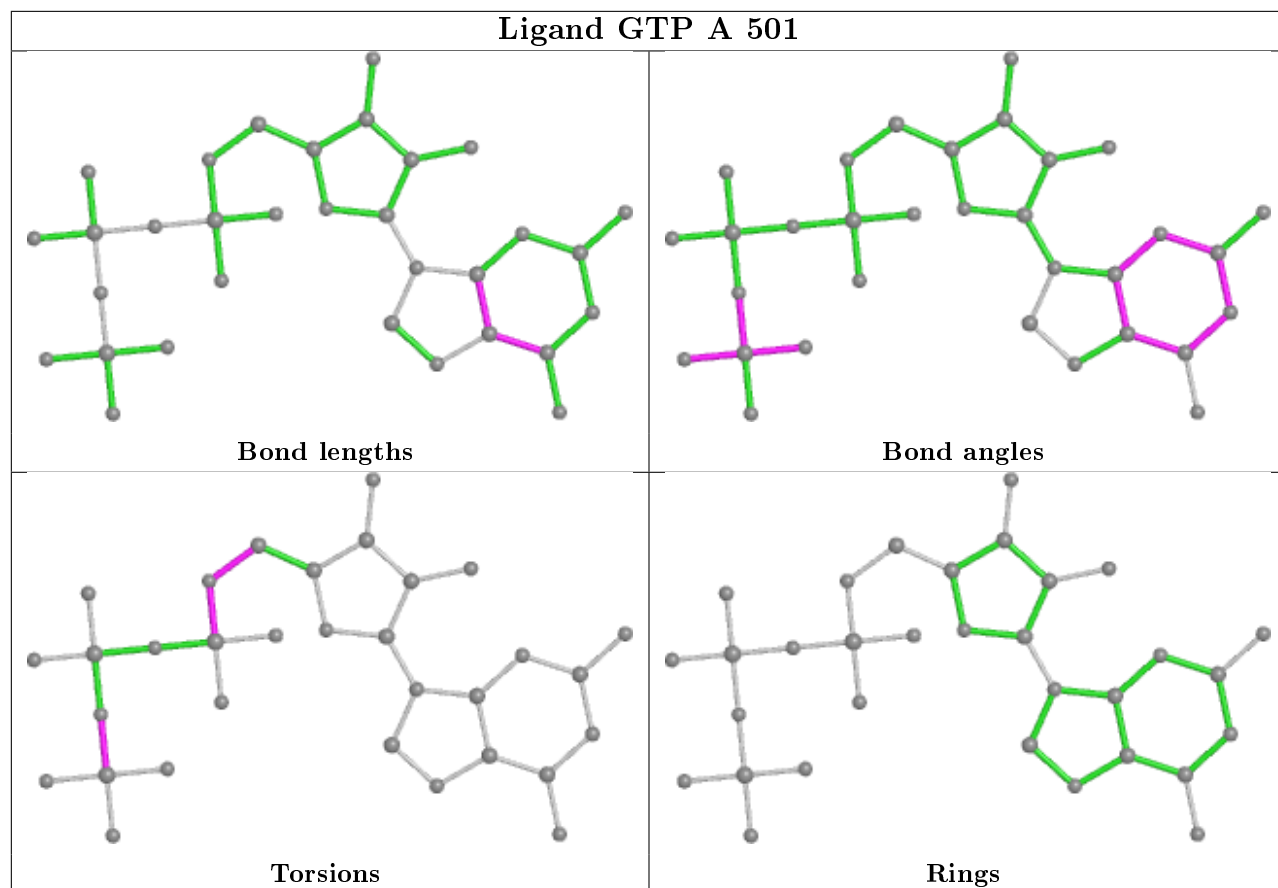
There are no ring outliers.

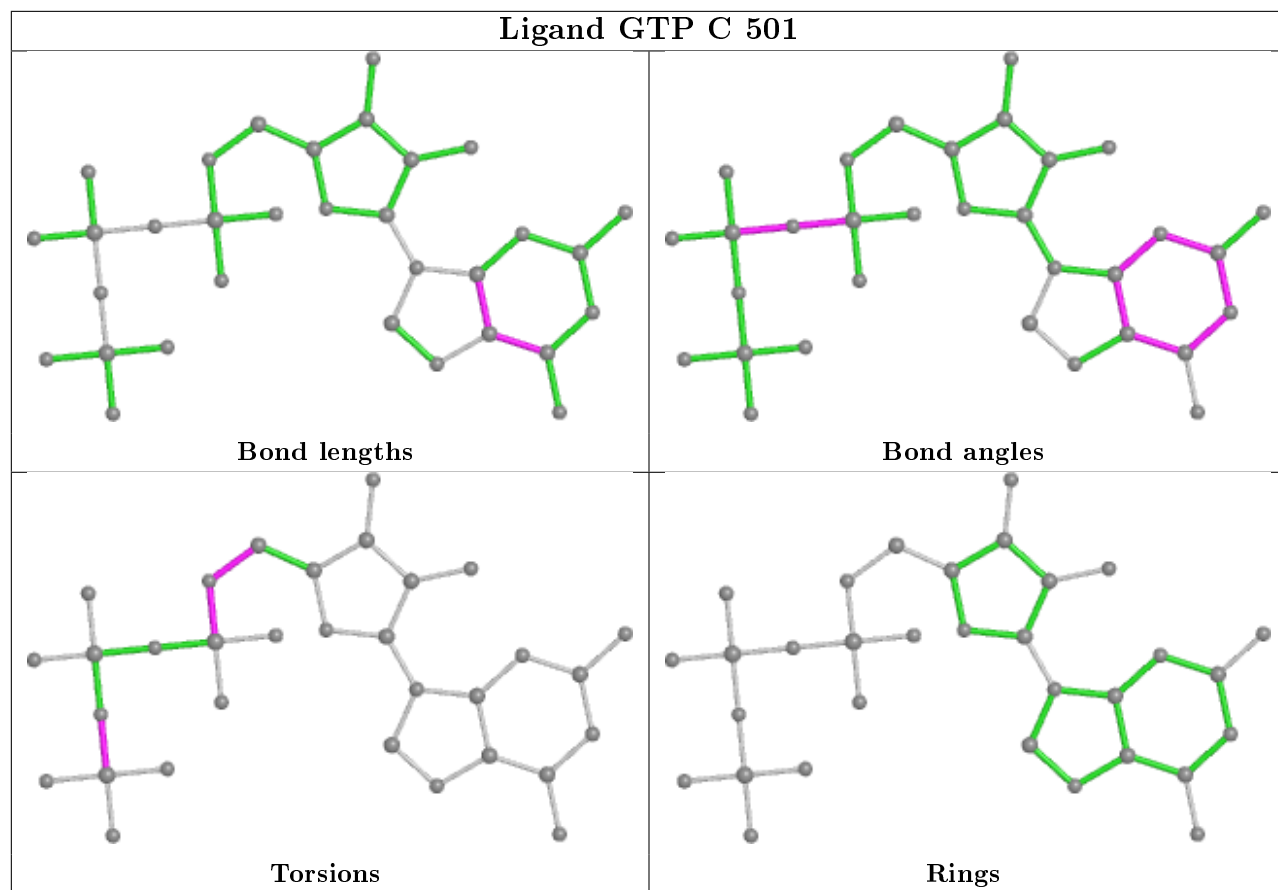
3 monomers are involved in 9 short contacts:

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

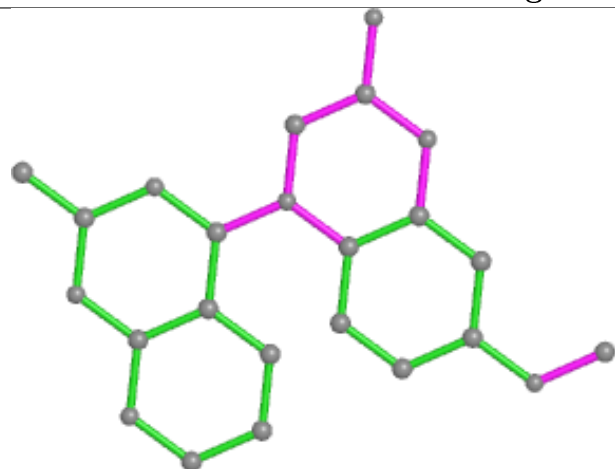
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



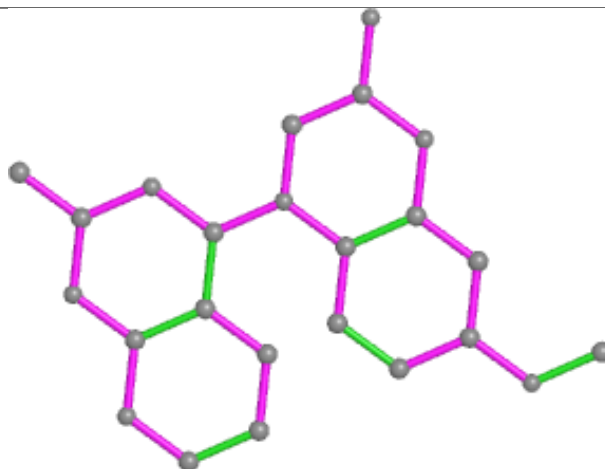




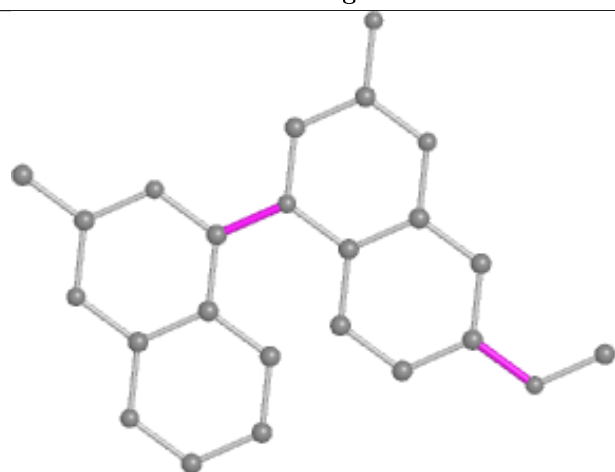
Ligand J7S B 506



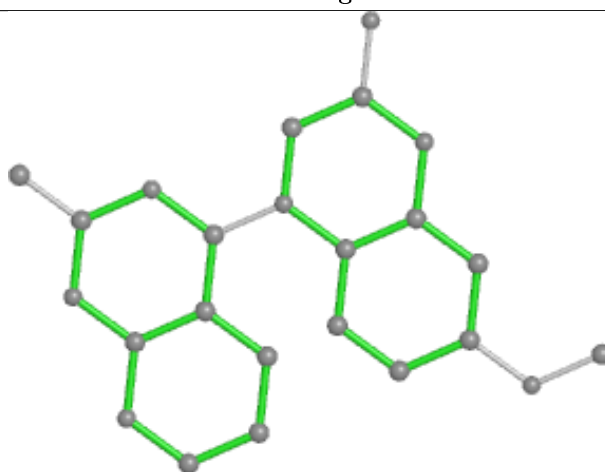
Bond lengths



Bond angles

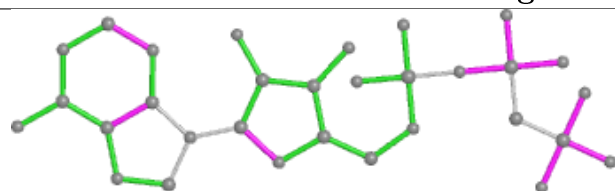


Torsions

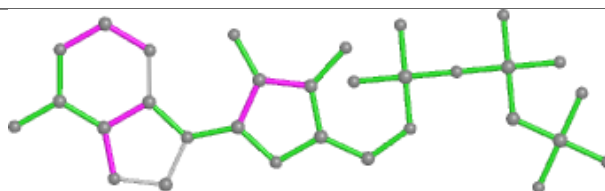


Rings

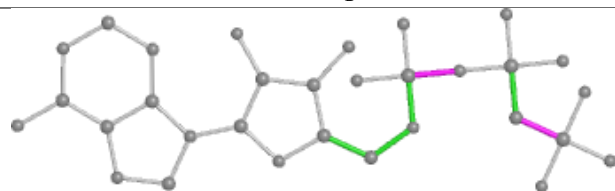
Ligand ACP F 703



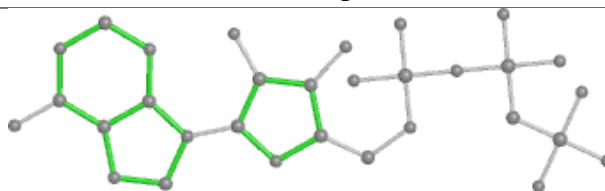
Bond lengths



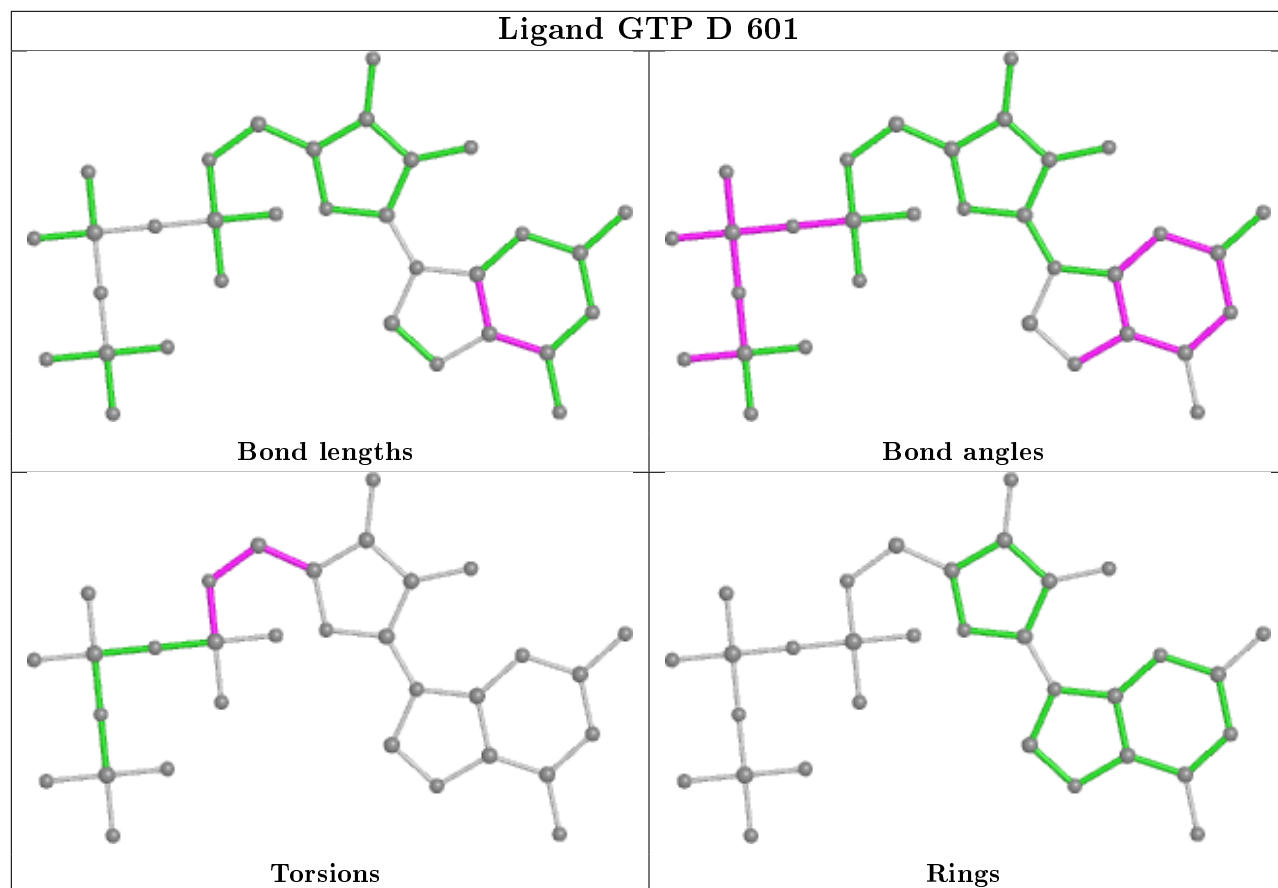
Bond angles



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	7 (1%) 72 69	19, 37, 64, 92	0
1	C	441/450 (98%)	-0.35	3 (0%) 87 88	14, 27, 49, 104	0
2	B	428/445 (96%)	-0.16	12 (2%) 53 49	17, 34, 74, 110	2 (0%)
2	D	420/445 (94%)	0.42	31 (7%) 14 11	25, 53, 89, 112	3 (0%)
3	E	126/143 (88%)	0.59	13 (10%) 6 4	29, 51, 100, 123	0
4	F	356/384 (92%)	0.93	81 (22%) 0 0	27, 62, 129, 155	0
All	All	2210/2317 (95%)	0.14	147 (6%) 17 14	14, 41, 97, 155	5 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	143	GLU	10.4
4	F	370	GLN	10.4
3	E	30	ASP	7.6
4	F	232	ASN	7.3
4	F	372	THR	6.7
4	F	371	PRO	6.6
4	F	142	ARG	6.6
4	F	249	TYR	6.1
4	F	155	ALA	6.0
3	E	29	PHE	6.0
4	F	136	ASN	5.8
4	F	152	SER	5.8
4	F	133	ALA	5.7
4	F	250	SER	5.5
4	F	177	GLY	5.5
4	F	173	ILE	5.4
4	F	244	CYS	5.4
2	D	37	HIS	5.3
4	F	101	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	5.0
4	F	362	ALA	4.9
4	F	251	LYS	4.9
4	F	138	ARG	4.8
4	F	130	VAL	4.8
4	F	125	THR	4.8
2	B	55	THR	4.8
2	B	279	GLN	4.7
4	F	170	LEU	4.7
4	F	157	GLY	4.6
3	E	140	LYS	4.6
4	F	137	ARG	4.6
3	E	28	SER	4.5
3	E	139	LEU	4.5
4	F	256	TYR	4.5
4	F	140	GLU	4.5
4	F	171	ASP	4.4
1	A	439	SER	4.3
2	D	55	THR	4.3
4	F	178	GLN	4.2
4	F	252	ASN	4.2
2	D	72	THR	4.1
4	F	246	GLN	4.1
4	F	161	LEU	4.1
3	E	43	ARG	4.1
4	F	230	SER	4.1
1	A	438	ASP	4.0
4	F	162	ILE	4.0
4	F	153	ALA	4.0
2	B	37	HIS	3.9
2	D	359	ARG	3.9
2	D	95	SER	3.9
4	F	255	ARG	3.9
4	F	139	ARG	3.8
3	E	142	GLU	3.8
4	F	100	ILE	3.8
4	F	236	LYS	3.8
4	F	176	GLN	3.8
4	F	159	GLY	3.7
2	D	71	GLY	3.6
2	D	96	GLY	3.6
1	C	441	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	391	ARG	3.5
4	F	225	SER	3.5
2	D	92	PHE	3.5
4	F	363	ASP	3.5
4	F	134	ALA	3.4
4	F	167	SER	3.4
1	A	262	TYR	3.4
4	F	253	TYR	3.4
2	D	57	ASN	3.4
4	F	245	ILE	3.3
4	F	145	ASN	3.3
4	F	166	ALA	3.3
4	F	129	GLU	3.3
2	D	56	GLY	3.3
4	F	248	GLU	3.3
4	F	175	GLU	3.2
4	F	237	THR	3.2
4	F	158	GLU	3.2
4	F	135	TYR	3.1
4	F	156	LYS	3.1
2	D	217	LEU	3.1
1	C	440	VAL	3.1
4	F	259	GLY	3.1
4	F	231	ALA	3.1
2	D	81	PHE	3.0
4	F	233	PHE	3.0
2	B	57	ASN	3.0
2	D	58	LYS	2.9
2	B	36	TYR	2.9
2	D	33	THR	2.9
4	F	151	SER	2.9
4	F	234	GLN	2.9
2	D	69	GLU	2.9
2	D	395	LEU	2.8
4	F	174	ASP	2.8
4	F	194	PRO	2.8
4	F	340	GLN	2.8
2	D	390	ARG	2.7
1	A	345	ASP	2.7
4	F	132	LEU	2.7
2	D	83	GLN	2.7
2	D	219	THR	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	247	LYS	2.7
3	E	5	ASP	2.7
4	F	257	GLU	2.6
4	F	381	HIS	2.6
2	D	177	ASP	2.6
3	E	135	LYS	2.6
3	E	26	PRO	2.6
4	F	179	VAL	2.6
4	F	227	PRO	2.5
4	F	180	HIS	2.5
4	F	243	HIS	2.5
3	E	27	PRO	2.5
2	D	406	MET	2.5
4	F	102	PRO	2.5
4	F	182	ILE	2.5
1	A	282	TYR	2.5
2	B	33	THR	2.5
2	D	405	GLU	2.4
2	D	175	VAL	2.4
3	E	25	LYS	2.4
4	F	172	PHE	2.4
4	F	9	GLU	2.4
1	C	245	ASP	2.4
1	A	163	LYS	2.4
4	F	258	GLU	2.4
2	B	39	ASP	2.3
3	E	44	ASP	2.3
4	F	164	SER	2.3
2	D	94	GLN	2.3
2	B	427	ASP	2.3
2	B	245	GLN	2.2
4	F	147	TRP	2.2
2	D	74	ASP	2.2
4	F	19	ARG	2.2
2	D	97	ALA	2.2
4	F	163	SER	2.1
2	B	38	GLY	2.1
1	A	281	ALA	2.1
2	D	394	PHE	2.1
2	D	98	GLY	2.1
2	B	54	ALA	2.0
2	B	29	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	246	LEU	2.0
2	D	73	MET	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 carbohydrates 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
9	GOL	A	506	6/6	0.68	0.41	78,80,84,90	0
6	MG	F	702	1/1	0.75	0.25	76,76,76,76	0
7	CA	B	503	1/1	0.79	0.09	76,76,76,76	0
6	MG	D	602	1/1	0.80	0.14	63,63,63,63	0
13	ACP	F	703	31/31	0.88	0.18	75,90,107,112	0
9	GOL	A	505	6/6	0.88	0.18	53,59,61,65	0
7	CA	E	201	1/1	0.91	0.08	73,73,73,73	0
5	GTP	D	601	32/32	0.91	0.17	39,46,72,79	0
11	MES	B	504	12/12	0.92	0.16	40,45,58,63	0
8	CL	A	504	1/1	0.92	0.20	74,74,74,74	0
6	MG	F	701	1/1	0.92	0.22	72,72,72,72	0
6	MG	B	502	1/1	0.94	0.13	27,27,27,27	0
11	MES	B	505	12/12	0.94	0.18	60,66,68,68	0
6	MG	A	502	1/1	0.96	0.08	28,28,28,28	0
12	J7S	B	506	24/24	0.96	0.15	25,28,32,39	0
7	CA	A	503	1/1	0.96	0.05	52,52,52,52	0
12	J7S	D	603	24/24	0.97	0.17	26,33,44,48	0
6	MG	C	502	1/1	0.98	0.07	25,25,25,25	0
7	CA	C	503	1/1	0.99	0.04	35,35,35,35	0
5	GTP	A	501	32/32	0.99	0.14	19,21,22,23	0
10	GDP	B	501	28/28	0.99	0.14	18,21,23,24	0

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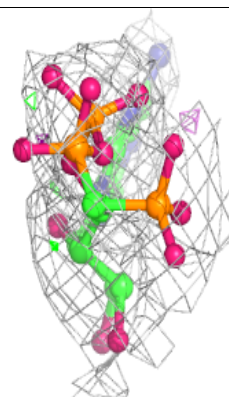
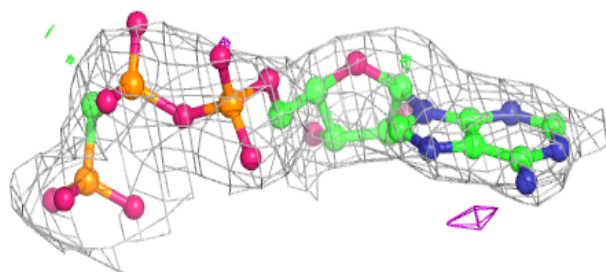
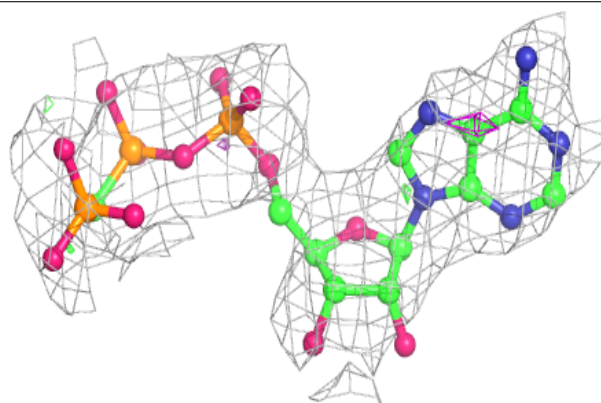
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	C	501	32/32	0.99	0.11	18,19,20,21	0

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.

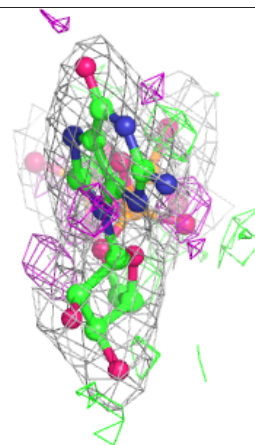
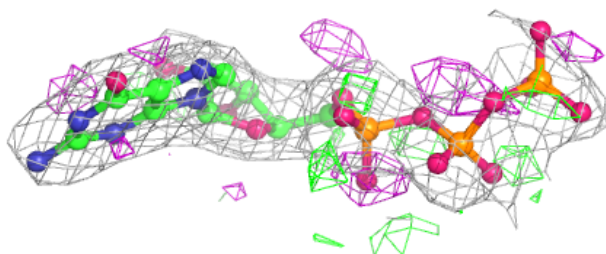
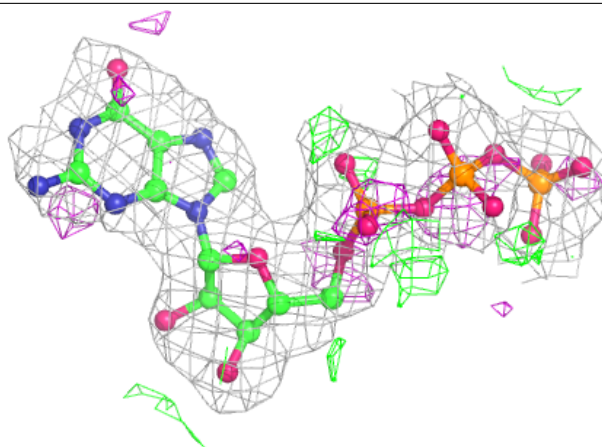
Electron density around ACP F 703:

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



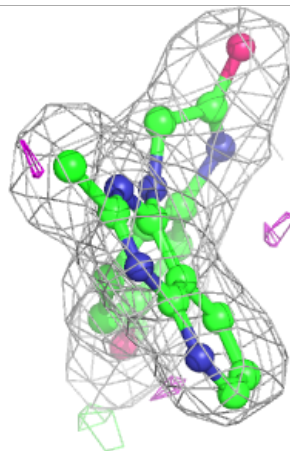
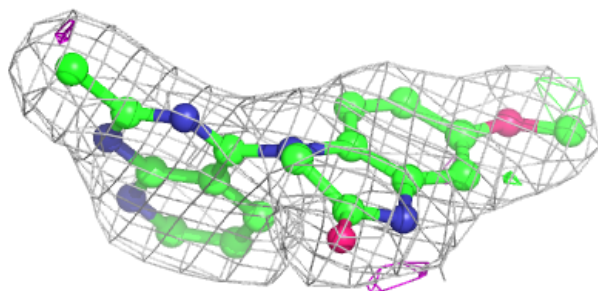
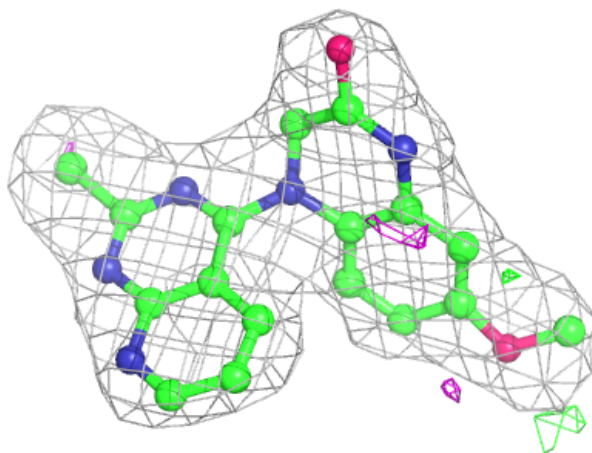
Electron density around GTP D 601:

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



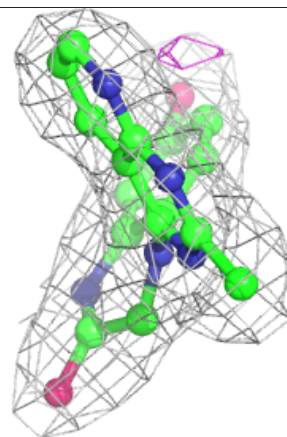
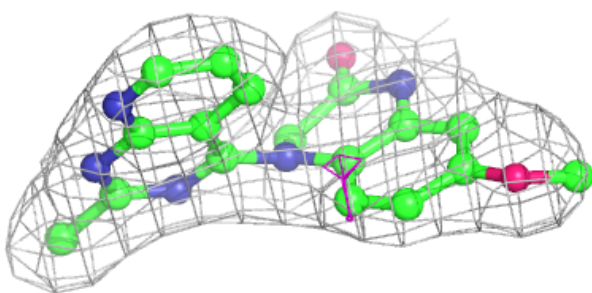
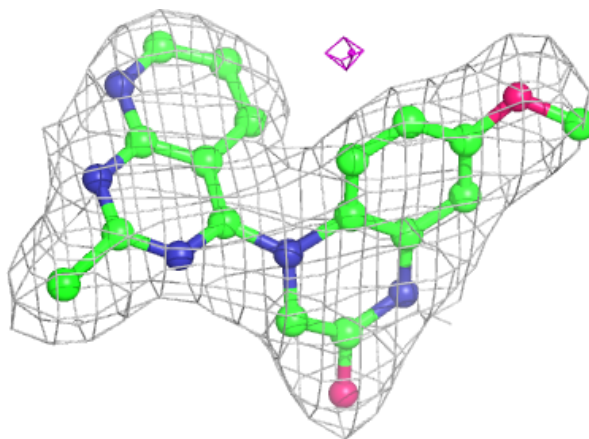
Electron density around J7S B 506:

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

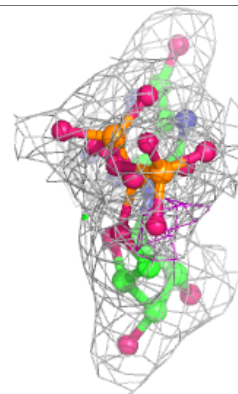
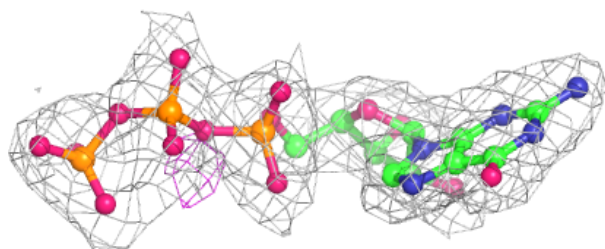
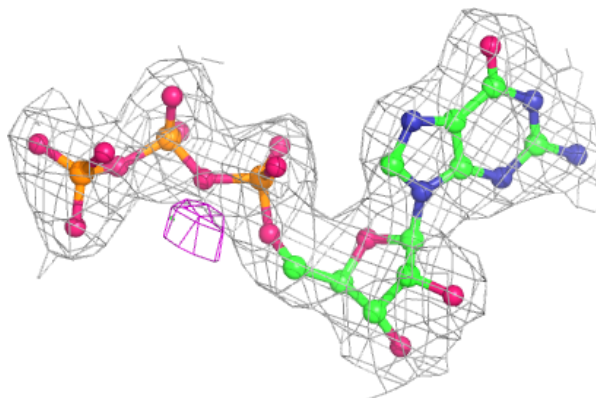


Electron density around J7S D 603:

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

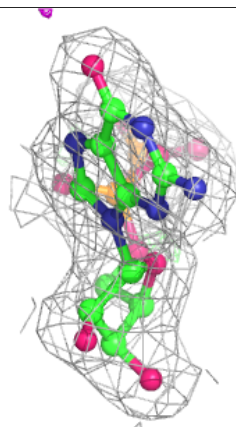
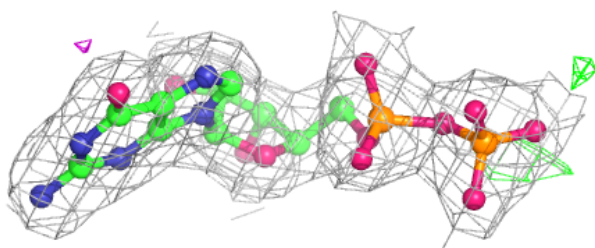
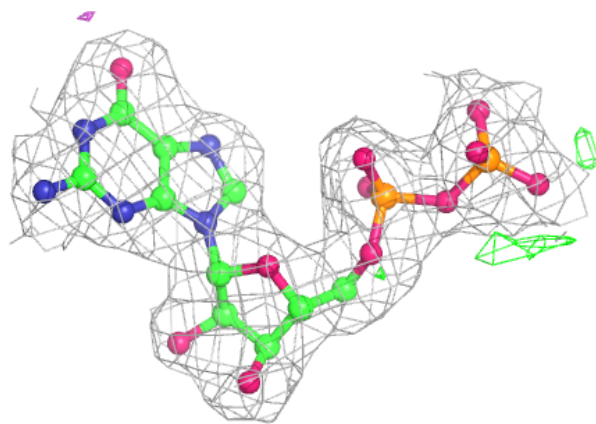
**Electron density around GTP A 501:**

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

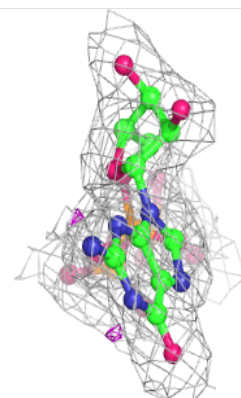
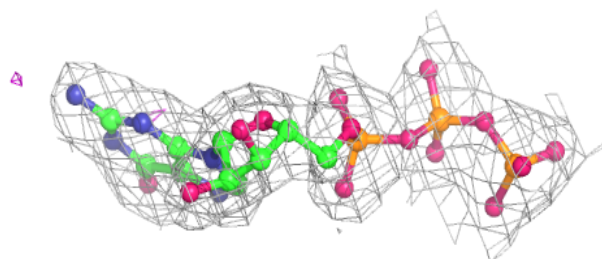
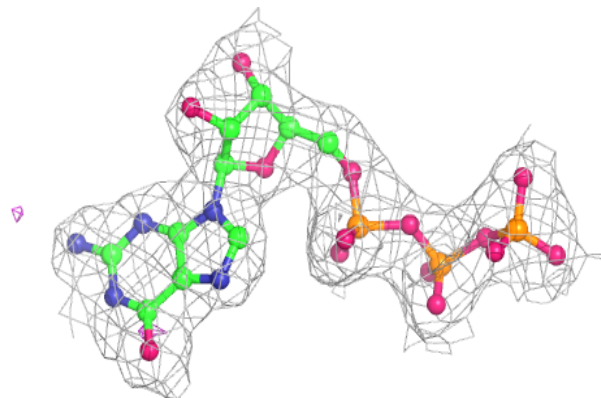


Electron density around GDP B 501:

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

**Electron density around GTP C 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.