



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:22 pm BST

PDB ID : 5LYJ
Title : Tubulin-Combretastatin A4 complex
Authors : Gaspari, R.; Prota, A.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2016-09-28
Resolution : 2.40 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

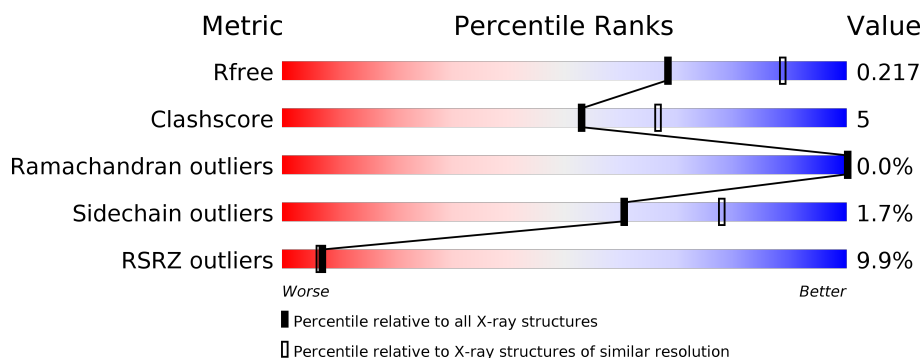
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	451	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div></div> </div> <div></div> </div>
2	B	445	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div></div> </div> <div></div> </div>
2	D	445	<div> <div>9%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div></div> </div> <div></div> </div>
3	E	143	<div> <div>10%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>14%</div> </div> <div></div> </div>
4	F	384	<div> <div>29%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>14%</div> </div> <div></div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17669 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	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	1	0
			3440	2177	584	656	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	1	0
			3351	2106	573	646	26			
2	D	427	Total	C	N	O	S	0	0	0
			3349	2101	572	650	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	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-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	1	0
			2714	1740	464	495	15			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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		

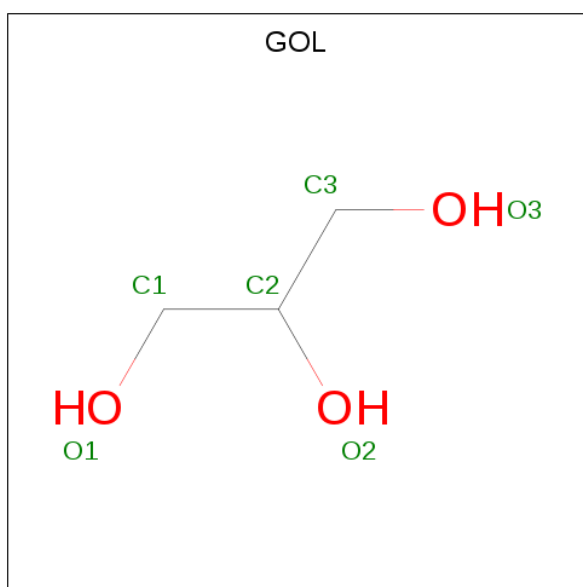
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		
6	C	1	Total	Mg	0	0
			1	1		

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

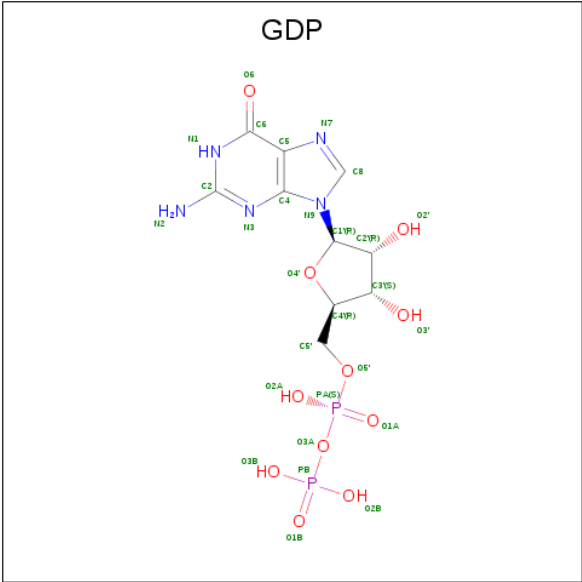
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Ca 2	0	0
7	A	1	Total 1	Ca 1	0	0
7	C	1	Total 1	Ca 1	0	0
7	E	1	Total 1	Ca 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



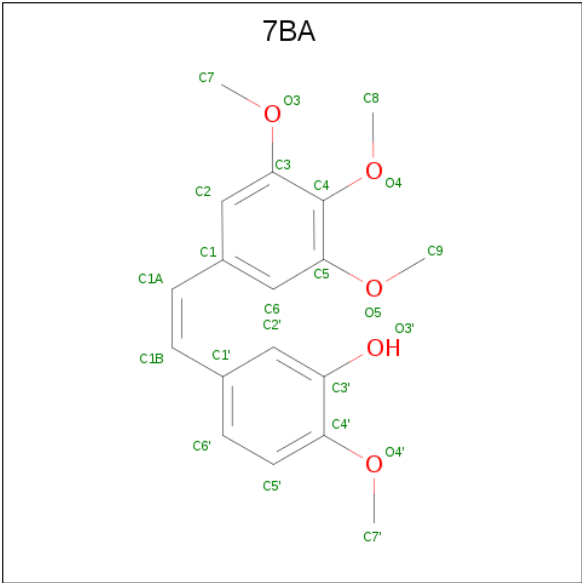
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 6	C 3	O 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



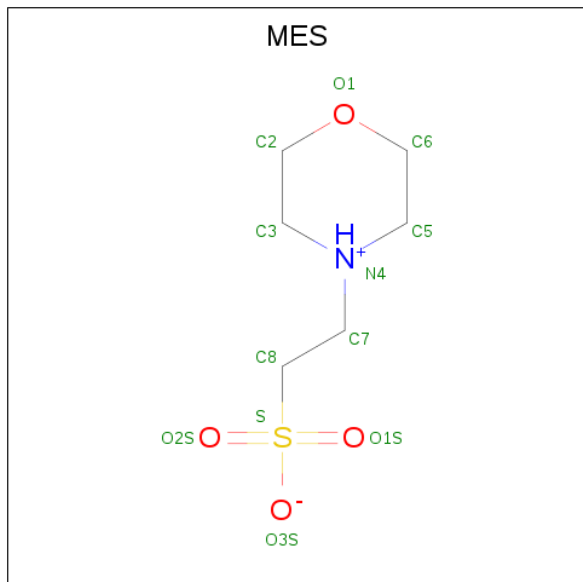
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is Combretastatin A4 (three-letter code: 7BA) (formula: C₁₈H₂₀O₅).



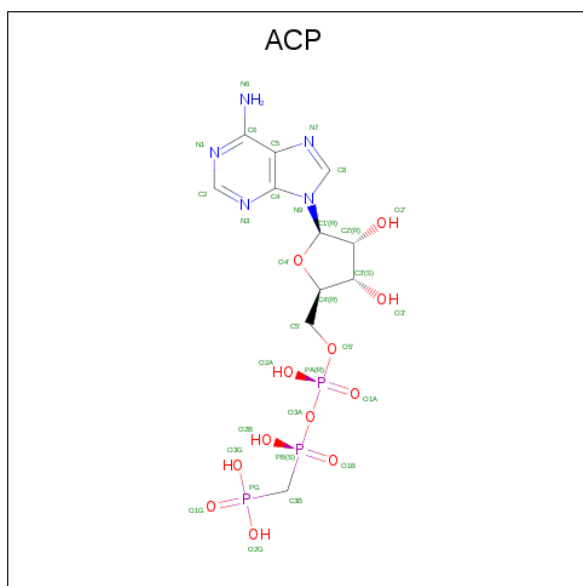
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			23	18	5		
10	D	1	Total	C	O	0	0
			23	18	5		

- 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		

- Molecule 12 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
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

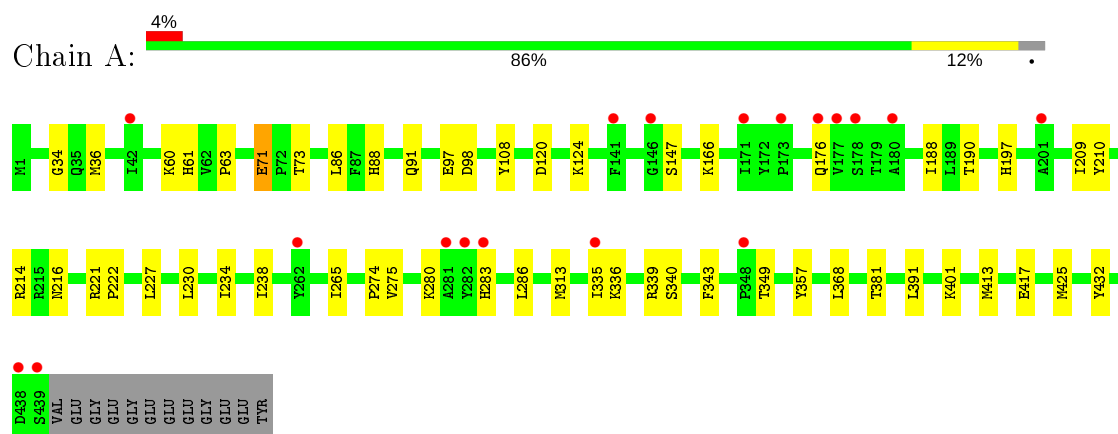
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	30	Total 30	O 30	0	0
13	B	29	Total 29	O 29	0	0
13	C	75	Total 75	O 75	0	0
13	D	6	Total 6	O 6	0	0
13	E	3	Total 3	O 3	0	0
13	F	4	Total 4	O 4	0	0

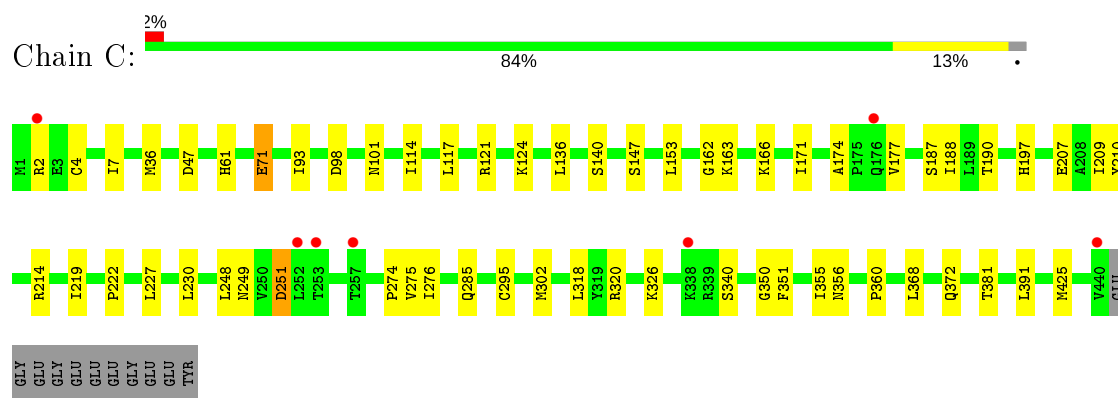
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

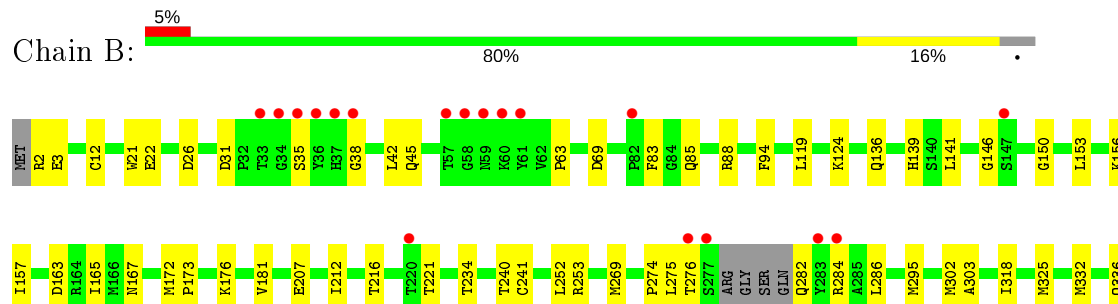
• Molecule 1: Tubulin alpha-1B chain



• Molecule 1: Tubulin alpha-1B chain

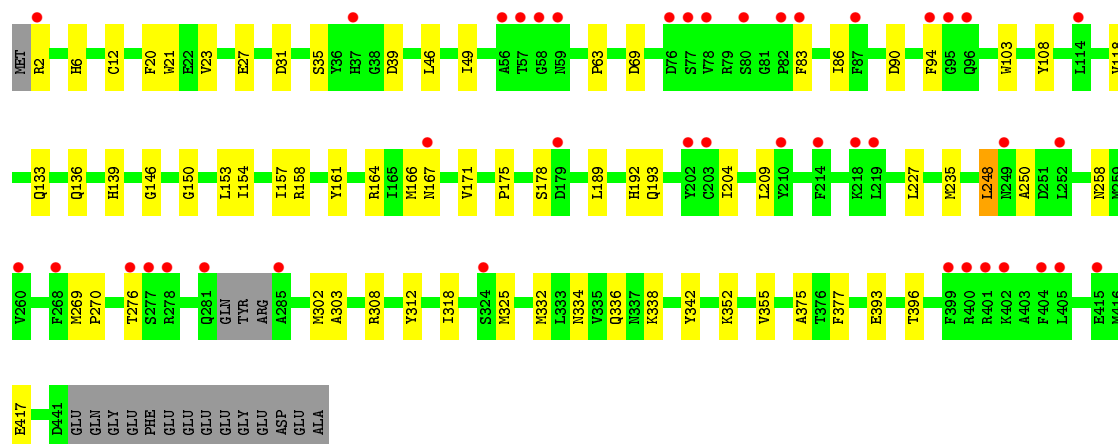
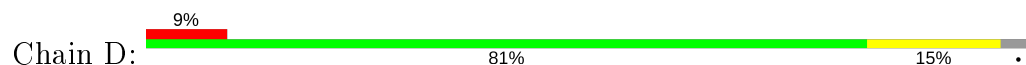


• Molecule 2: Tubulin beta-2B chain

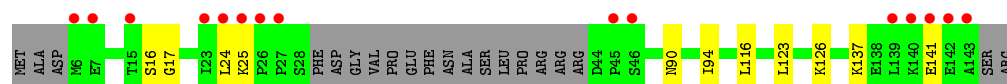
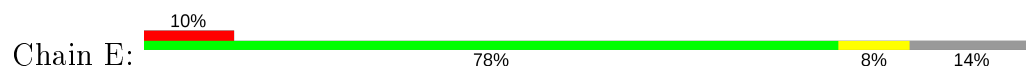




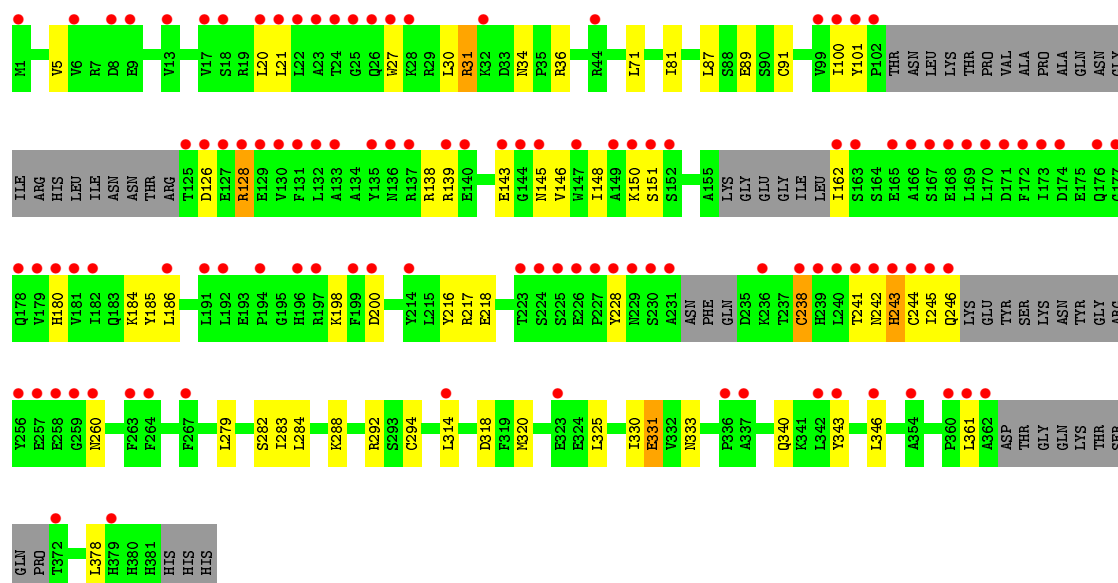
• Molecule 2: Tubulin beta-2B chain



• 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	104.59Å 157.17Å 180.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.40 49.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.43-2.40) 99.7 (49.43-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.191 , 0.217 0.191 , 0.217	Depositor DCC
R_{free} test set	5823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17669	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: GDP, GOL, MG, CA, GTP, ACP, MES, 7BA

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	0.33	0/3508	0.51	0/4762
1	C	0.38	1/3521 (0.0%)	0.54	0/4780
2	B	0.35	0/3428	0.55	0/4643
2	D	0.32	0/3422	0.50	0/4635
3	E	0.33	0/1022	0.43	0/1356
4	F	0.28	0/2777	0.45	0/3750
All	All	0.34	1/17678 (0.0%)	0.51	0/23926

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-5.16	1.73	1.81

There are no bond angle outliers.

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	3430	0	3339	39	0
1	C	3440	0	3353	35	0
2	B	3351	0	3233	43	0
2	D	3349	0	3223	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1014	0	1029	8	0
4	F	2714	0	2682	37	0
5	A	32	0	12	1	0
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
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	6	0	8	1	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	23	0	0	0	0
10	D	23	0	0	1	0
11	B	12	0	12	1	0
12	F	31	0	14	3	0
13	A	30	0	0	1	0
13	B	29	0	0	0	0
13	C	75	0	0	1	0
13	D	6	0	0	0	0
13	E	3	0	0	0	0
13	F	4	0	0	0	0
All	All	17669	0	16941	186	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 5.

All (186) 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:270:PRO:HG2	2:D:302:MET:HB2	1.68	0.73
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.72	0.70
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.73	0.70
2:B:253[A]:ARG:NH1	11:B:504:MES:O2S	2.20	0.69
1:C:101:ASN:HD22	2:D:258:ASN:HD21	1.43	0.67
2:B:173:PRO:O	2:B:390:ARG:NH2	2.28	0.66
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.29	0.65
2:B:2:ARG:NH1	2:B:3:GLU:OE1	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:184:LYS:NZ	4:F:185:TYR:O	2.27	0.65
1:C:47:ASP:OD2	13:C:601:HOH:O	2.13	0.65
1:A:221:ARG:HD2	2:B:325:MET:HB3	1.79	0.63
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.35	0.61
2:B:345:GLU:OE1	2:B:345:GLU:N	2.30	0.61
2:B:439:THR:HG21	4:F:31:ARG:HH21	1.65	0.60
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.82	0.60
2:D:175:PRO:HA	2:D:178:SER:HB2	1.82	0.60
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.37	0.60
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.34	0.60
1:C:163:LYS:HE2	3:E:90:ASN:HA	1.83	0.59
1:A:97:GLU:OE2	2:B:253[B]:ARG:NH1	2.31	0.59
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.84	0.59
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.85	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.22	0.58
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.39	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.85	0.57
4:F:139:ARG:HG2	4:F:145:ASN:HD22	1.71	0.56
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.88	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.87	0.56
2:B:241:CYS:SG	2:B:318:ILE:HD12	2.47	0.55
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.89	0.55
2:B:240:THR:HB	2:B:318:ILE:HD13	1.90	0.54
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.89	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.09	0.54
2:B:146:GLY:O	2:B:150:GLY:HA3	2.08	0.53
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.41	0.53
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.90	0.53
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.29	0.53
4:F:150:LYS:HZ3	12:F:401:ACP:H8	1.74	0.53
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.50	0.52
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.92	0.52
1:A:88:HIS:N	1:A:91:GLN:OE1	2.39	0.52
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.92	0.52
2:D:393:GLU:O	2:D:396:THR:HG22	2.10	0.52
4:F:284:LEU:O	4:F:288:LYS:HG3	2.10	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.92	0.51
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.91	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.28	0.51
2:D:248:LEU:HD23	2:D:250:ALA:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:137:LYS:O	3:E:141:GLU:HG2	2.10	0.51
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.93	0.51
2:B:69:ASP:O	2:B:94:PHE:HA	2.11	0.51
1:A:280:LYS:O	1:A:283:HIS:NE2	2.44	0.50
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.45	0.50
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.50
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.46	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.49
4:F:331:GLU:OE2	12:F:401:ACP:O3G	2.29	0.49
2:B:337:ASN:OD1	4:F:36:ARG:NH1	2.46	0.49
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.93	0.49
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.48	0.49
4:F:138:ARG:HG3	4:F:143:GLU:HB3	1.93	0.49
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.94	0.49
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.48	0.48
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.13	0.48
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.96	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.54	0.48
1:C:147:SER:HB2	1:C:190:THR:HB	1.95	0.48
1:A:176:GLN:HG2	1:A:210:TYR:CE2	2.48	0.48
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.49	0.48
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.94	0.48
1:A:147:SER:HB2	1:A:190:THR:HB	1.95	0.47
4:F:148:ILE:HD12	4:F:162:ILE:HG12	1.95	0.47
2:D:325:MET:SD	2:D:355:VAL:HG11	2.54	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.55	0.47
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.29	0.47
2:D:153:LEU:O	2:D:157:ILE:HG13	2.14	0.47
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.96	0.47
4:F:139:ARG:HG2	4:F:145:ASN:ND2	2.29	0.47
2:B:234:THR:OG1	2:B:302:MET:SD	2.71	0.47
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.49	0.47
2:B:276:THR:HG21	2:B:371:LEU:HD21	1.97	0.46
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.97	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.46
1:A:176:GLN:HG2	1:A:210:TYR:CD2	2.50	0.46
1:C:2:ARG:NH2	1:C:251:ASP:OD2	2.47	0.46
2:B:181:VAL:HG21	2:B:404:PHE:CZ	2.51	0.46
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.97	0.46
1:A:216:ASN:ND2	8:A:504:GOL:H2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.98	0.46
4:F:242:ASN:O	4:F:243:HIS:HB3	2.15	0.46
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.97	0.46
4:F:292:ARG:HG3	4:F:378:LEU:HD23	1.97	0.46
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.97	0.45
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.16	0.45
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.97	0.45
2:D:189:LEU:O	2:D:192:HIS:HB3	2.16	0.45
4:F:228:TYR:HA	4:F:238:CYS:SG	2.57	0.45
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.99	0.45
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.45	0.45
1:A:176:GLN:HB2	13:A:621:HOH:O	2.17	0.45
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.44
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.52	0.44
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.89	0.44
2:D:146:GLY:O	2:D:150:GLY:HA3	2.17	0.44
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.52	0.44
1:C:274:PRO:HB2	1:C:276:ILE:HG12	2.00	0.44
4:F:284:LEU:HA	4:F:284:LEU:HD12	1.75	0.44
2:B:153:LEU:O	2:B:157:ILE:HG13	2.18	0.44
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.16	0.44
2:D:318:ILE:HG12	10:D:503:7BA:C8	2.48	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.99	0.44
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.99	0.44
1:C:368:LEU:HA	1:C:368:LEU:HD23	1.68	0.44
2:D:136:GLN:HA	2:D:167:ASN:O	2.17	0.44
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.53	0.44
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.99	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.53	0.43
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.36	0.43
2:D:2:ARG:HB3	2:D:133:GLN:HE21	1.83	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.43
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.43
2:B:269:MET:HG2	2:B:303:ALA:HB3	2.01	0.43
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.17	0.43
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.43
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.01	0.43
1:A:120:ASP:OD2	1:A:124:LYS:HE2	2.18	0.43
2:B:163:ASP:OD1	2:B:163:ASP:N	2.49	0.43
2:D:23:VAL:O	2:D:27:GLU:HG3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:O	1:A:238:ILE:HG13	2.18	0.43
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.82	0.43
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.44	0.43
2:D:318:ILE:O	2:D:375:ALA:HA	2.19	0.42
2:B:221:THR:HG21	1:C:326:LYS:HA	2.01	0.42
1:A:280:LYS:HE3	1:A:280:LYS:HB2	1.79	0.42
2:D:161:TYR:HB3	2:D:164:ARG:HG2	2.01	0.42
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.54	0.42
2:B:389:LYS:HB2	2:B:389:LYS:HE3	1.87	0.42
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.00	0.42
2:D:31:ASP:OD2	2:D:35:SER:HB2	2.19	0.42
2:D:46:LEU:HA	2:D:49:ILE:HB	2.00	0.42
1:A:221:ARG:CD	2:B:325:MET:HB3	2.47	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
2:D:332:MET:O	2:D:336:GLN:HG3	2.20	0.42
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.55	0.42
1:C:124:LYS:HE3	1:C:124:LYS:HB3	1.84	0.42
1:C:350:GLY:C	1:C:351:PHE:HD1	2.23	0.42
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.28	0.42
2:B:332:MET:O	2:B:336:GLN:HG3	2.20	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.42
2:D:39:ASP:N	2:D:39:ASP:OD1	2.46	0.42
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.55	0.41
2:B:282:GLN:HG3	2:B:284:ARG:H	1.85	0.41
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.84	0.41
1:A:313:MET:HB2	1:A:313:MET:HE3	1.91	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.41
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.41
4:F:89:GLU:OE1	4:F:89:GLU:N	2.34	0.41
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.55	0.41
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.02	0.41
2:B:88:ARG:HH21	2:B:124:LYS:NZ	2.19	0.41
1:A:280:LYS:HB3	1:A:283:HIS:NE2	2.35	0.41
2:B:216:THR:HG21	2:B:275:LEU:HD12	2.02	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.41
2:D:69:ASP:O	2:D:94:PHE:HA	2.20	0.41
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.02	0.41
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.03	0.41
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.56	0.41
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.56	0.41
2:D:83:PHE:O	2:D:86:ILE:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:101:TYR:N	4:F:126:ASP:OD1	2.47	0.41
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.31	0.41
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.01	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.03	0.41
4:F:216:TYR:CD2	4:F:346:LEU:HD13	2.56	0.41
4:F:27:TRP:HE1	4:F:361:LEU:HD21	1.86	0.41
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.20	0.41
4:F:30:LEU:HD13	4:F:34:ASN:ND2	2.35	0.41
4:F:21:LEU:O	4:F:27:TRP:HB2	2.20	0.41
3:E:116:LEU:HD23	3:E:116:LEU:HA	1.86	0.40
2:B:295:MET:CE	2:B:375:ALA:HB1	2.52	0.40
4:F:330:ILE:HA	4:F:330:ILE:HD13	1.92	0.40
4:F:146:VAL:O	4:F:184:LYS:NZ	2.39	0.40
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	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	437/451 (97%)	423 (97%)	14 (3%)	0	100	100
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
2	D	423/445 (95%)	415 (98%)	8 (2%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	321/384 (84%)	306 (95%)	14 (4%)	1 (0%)	41	55
All	All	2161/2319 (93%)	2102 (97%)	58 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	243	HIS

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	370/379 (98%)	367 (99%)	3 (1%)	81	91
1	C	372/379 (98%)	366 (98%)	6 (2%)	62	79
2	B	368/383 (96%)	364 (99%)	4 (1%)	73	87
2	D	368/383 (96%)	363 (99%)	5 (1%)	67	82
3	E	110/127 (87%)	108 (98%)	2 (2%)	59	76
4	F	298/342 (87%)	286 (96%)	12 (4%)	31	49
All	All	1886/1993 (95%)	1854 (98%)	32 (2%)	60	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	340	SER
1	A	381	THR
2	B	42	LEU
2	B	85	GLN
2	B	139	HIS
2	B	430	SER
1	C	71	GLU
1	C	177	VAL
1	C	251	ASP
1	C	318	LEU
1	C	340	SER
1	C	381	THR
2	D	90	ASP
2	D	139	HIS
2	D	248	LEU
2	D	276	THR
2	D	352	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	16	SER
3	E	25	LYS
4	F	20	LEU
4	F	31	ARG
4	F	91	CYS
4	F	128	ARG
4	F	200	ASP
4	F	238	CYS
4	F	241	THR
4	F	244	CYS
4	F	245	ILE
4	F	314	LEU
4	F	331	GLU
4	F	333	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 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
8	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.34	0
12	ACP	F	401	-	27,33,33	1.68	6 (22%)	32,52,52	1.29	4 (12%)
10	7BA	B	503	-	24,24,24	0.94	2 (8%)	32,32,32	2.21	10 (31%)
5	GTP	A	501	6	26,34,34	1.08	2 (7%)	33,54,54	1.85	8 (24%)
5	GTP	C	501	6	26,34,34	1.11	2 (7%)	33,54,54	1.76	7 (21%)
9	GDP	B	501	6	24,30,30	1.13	2 (8%)	31,47,47	1.78	7 (22%)
9	GDP	D	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.88	7 (22%)
10	7BA	D	503	-	24,24,24	0.98	2 (8%)	32,32,32	2.93	10 (31%)
11	MES	B	504	-	12,12,12	2.17	1 (8%)	14,16,16	1.92	2 (14%)

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
8	GOL	A	504	-	-	3/4/4/4	-
12	ACP	F	401	-	-	9/15/38/38	0/3/3/3
10	7BA	B	503	-	-	9/13/13/13	0/2/2/2
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
9	GDP	D	501	6	-	4/12/32/32	0/3/3/3
10	7BA	D	503	-	-	12/13/13/13	0/2/2/2
11	MES	B	504	-	-	1/6/14/14	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	MES	C8-S	-7.24	1.67	1.77
12	F	401	ACP	PB-O1B	4.15	1.61	1.51
9	D	501	GDP	C6-C5	3.96	1.48	1.41
9	B	501	GDP	C6-C5	3.87	1.48	1.41
12	F	401	ACP	PB-O2B	-3.46	1.48	1.56
5	C	501	GTP	C6-N1	3.27	1.38	1.33
12	F	401	ACP	PB-O3A	3.24	1.62	1.58
5	A	501	GTP	C6-N1	3.03	1.38	1.33
12	F	401	ACP	PG-O2G	2.84	1.61	1.54
12	F	401	ACP	PG-O3G	2.80	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	7BA	C1'-C1B	-2.48	1.40	1.47
12	F	401	ACP	C5-C4	2.46	1.47	1.40
9	D	501	GDP	C5-C4	2.37	1.47	1.40
10	D	503	7BA	C1'-C1B	-2.27	1.40	1.47
10	D	503	7BA	C1-C1A	-2.20	1.41	1.47
10	B	503	7BA	C1-C1A	-2.17	1.41	1.47
5	C	501	GTP	C2'-C1'	-2.10	1.50	1.53
9	B	501	GDP	C5-C4	2.10	1.46	1.40
5	A	501	GTP	C2-N1	2.08	1.39	1.35

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	7BA	O4'-C4'-C3'	9.11	127.77	114.57
10	D	503	7BA	C7'-O4'-C4'	7.02	128.12	117.53
10	D	503	7BA	C7-O3-C3	6.24	126.95	117.53
5	C	501	GTP	N3-C2-N1	-5.53	119.85	127.22
10	D	503	7BA	O4'-C4'-C5'	-5.47	114.99	124.37
5	A	501	GTP	N3-C2-N1	-5.46	119.93	127.22
10	B	503	7BA	O4'-C4'-C3'	5.23	122.15	114.57
11	B	504	MES	C5-N4-C3	5.04	120.18	108.83
10	B	503	7BA	C7'-O4'-C4'	5.03	125.12	117.53
10	D	503	7BA	O5-C5-C4	4.61	123.26	115.16
9	B	501	GDP	C2-N3-C4	4.51	120.51	115.36
9	D	501	GDP	C2-N3-C4	4.49	120.49	115.36
10	B	503	7BA	C8-O4-C4	4.25	126.42	114.78
9	D	501	GDP	C5-C6-N1	-4.17	117.72	123.43
10	B	503	7BA	C7-O3-C3	4.11	123.73	117.53
5	C	501	GTP	C2-N3-C4	4.02	119.95	115.36
5	A	501	GTP	C2-N3-C4	3.96	119.88	115.36
9	B	501	GDP	C6-C5-C4	-3.95	117.02	120.80
9	D	501	GDP	C6-N1-C2	3.95	122.20	115.93
10	B	503	7BA	O5-C5-C4	3.80	121.84	115.16
9	B	501	GDP	C6-N1-C2	3.77	121.92	115.93
9	D	501	GDP	C6-C5-C4	-3.76	117.21	120.80
9	B	501	GDP	C5-C6-N1	-3.63	118.47	123.43
11	B	504	MES	O1S-S-C8	3.60	111.25	106.92
10	D	503	7BA	O5-C5-C6	-3.40	118.27	124.12
5	A	501	GTP	C5-C6-N1	-3.25	118.98	123.43
9	B	501	GDP	N3-C2-N1	-3.24	122.90	127.22
12	F	401	ACP	N3-C2-N1	-3.20	123.67	128.68
12	F	401	ACP	C3'-C2'-C1'	3.17	105.75	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	7BA	O4'-C4'-C5'	-3.10	119.06	124.37
5	C	501	GTP	C5-C6-N1	-3.00	119.33	123.43
9	D	501	GDP	N3-C2-N1	-2.95	123.29	127.22
10	D	503	7BA	O3-C3-C2	-2.91	119.12	124.12
5	A	501	GTP	C6-N1-C2	2.86	120.47	115.93
10	B	503	7BA	O3-C3-C2	-2.85	119.22	124.12
9	D	501	GDP	PA-O3A-PB	-2.83	123.10	132.83
5	C	501	GTP	PB-O3B-PG	-2.83	123.11	132.83
5	A	501	GTP	O3'-C3'-C4'	-2.79	102.97	111.05
10	B	503	7BA	O5-C5-C6	-2.79	119.31	124.12
10	D	503	7BA	O3-C3-C4	2.79	120.07	115.16
5	A	501	GTP	PA-O3A-PB	-2.79	123.26	132.83
10	B	503	7BA	O4-C4-C5	2.73	124.06	120.12
5	C	501	GTP	C6-N1-C2	2.72	120.25	115.93
9	D	501	GDP	C4-C5-N7	-2.70	106.58	109.40
5	A	501	GTP	N2-C2-N1	2.63	121.34	117.25
5	C	501	GTP	O3'-C3'-C4'	-2.59	103.56	111.05
9	B	501	GDP	C4-C5-N7	-2.59	106.70	109.40
10	B	503	7BA	O3-C3-C4	2.55	119.64	115.16
5	A	501	GTP	O2G-PG-O3B	2.45	112.84	104.64
5	C	501	GTP	N2-C2-N1	2.43	121.03	117.25
12	F	401	ACP	PA-O3A-PB	-2.42	124.88	132.56
12	F	401	ACP	C4-C5-N7	-2.39	106.91	109.40
10	D	503	7BA	C9-O5-C5	2.27	120.95	117.53
10	D	503	7BA	C5'-C4'-C3'	-2.12	117.22	119.86
9	B	501	GDP	O3'-C3'-C4'	-2.09	105.01	111.05

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	504	GOL	O1-C1-C2-C3
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A
10	D	503	7BA	C5'-C4'-O4'-C7'
10	D	503	7BA	C3'-C4'-O4'-C7'
12	F	401	ACP	O4'-C4'-C5'-O5'
10	D	503	7BA	C6-C5-O5-C9
10	D	503	7BA	C2-C3-O3-C7
12	F	401	ACP	C3'-C4'-C5'-O5'
10	B	503	7BA	C5'-C4'-O4'-C7'
10	D	503	7BA	C4-C3-O3-C7
10	D	503	7BA	C4-C5-O5-C9
10	B	503	7BA	C3'-C4'-O4'-C7'
8	A	504	GOL	O1-C1-C2-O2
10	B	503	7BA	C2-C1-C1A-C1B
10	B	503	7BA	C3-C4-O4-C8
10	D	503	7BA	C6'-C1'-C1B-C1A
10	B	503	7BA	C6-C1-C1A-C1B
10	D	503	7BA	C3-C4-O4-C8
10	D	503	7BA	C2'-C1'-C1B-C1A
10	D	503	7BA	C2-C1-C1A-C1B
10	B	503	7BA	C6'-C1'-C1B-C1A
10	D	503	7BA	C6-C1-C1A-C1B
11	B	504	MES	C8-C7-N4-C3
10	B	503	7BA	C2'-C1'-C1B-C1A
10	D	503	7BA	C5-C4-O4-C8
9	D	501	GDP	C5'-O5'-PA-O3A
10	B	503	7BA	C5-C4-O4-C8
12	F	401	ACP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
12	F	401	ACP	PB-O3A-PA-O1A
5	C	501	GTP	C4'-C5'-O5'-PA
9	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

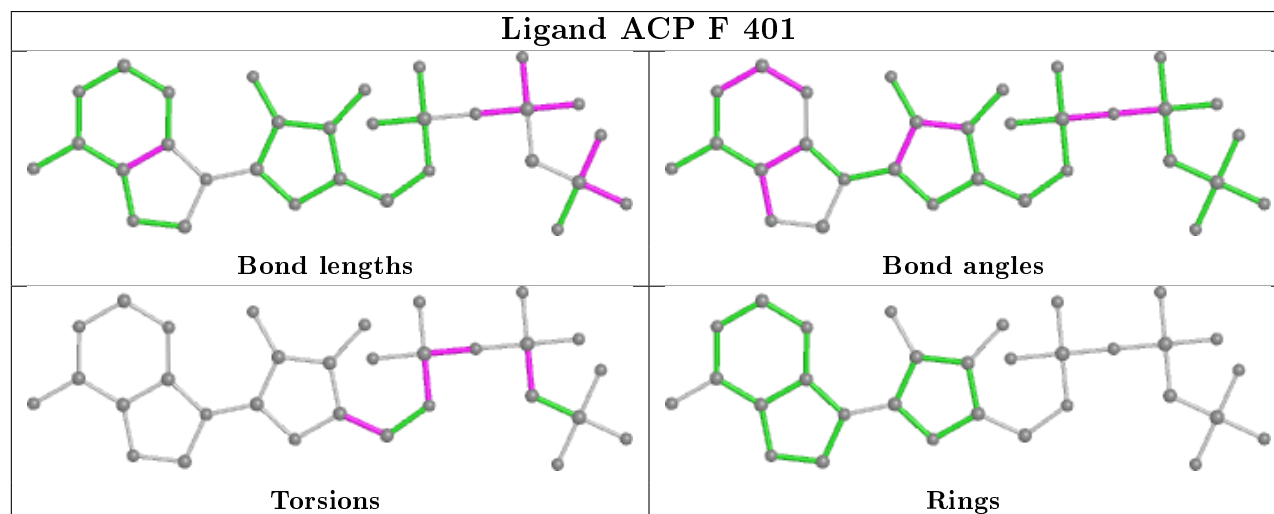
Mol	Chain	Res	Type	Atoms
9	B	501	GDP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O2A
8	A	504	GOL	C1-C2-C3-O3
10	B	503	7BA	C1-C1A-C1B-C1'

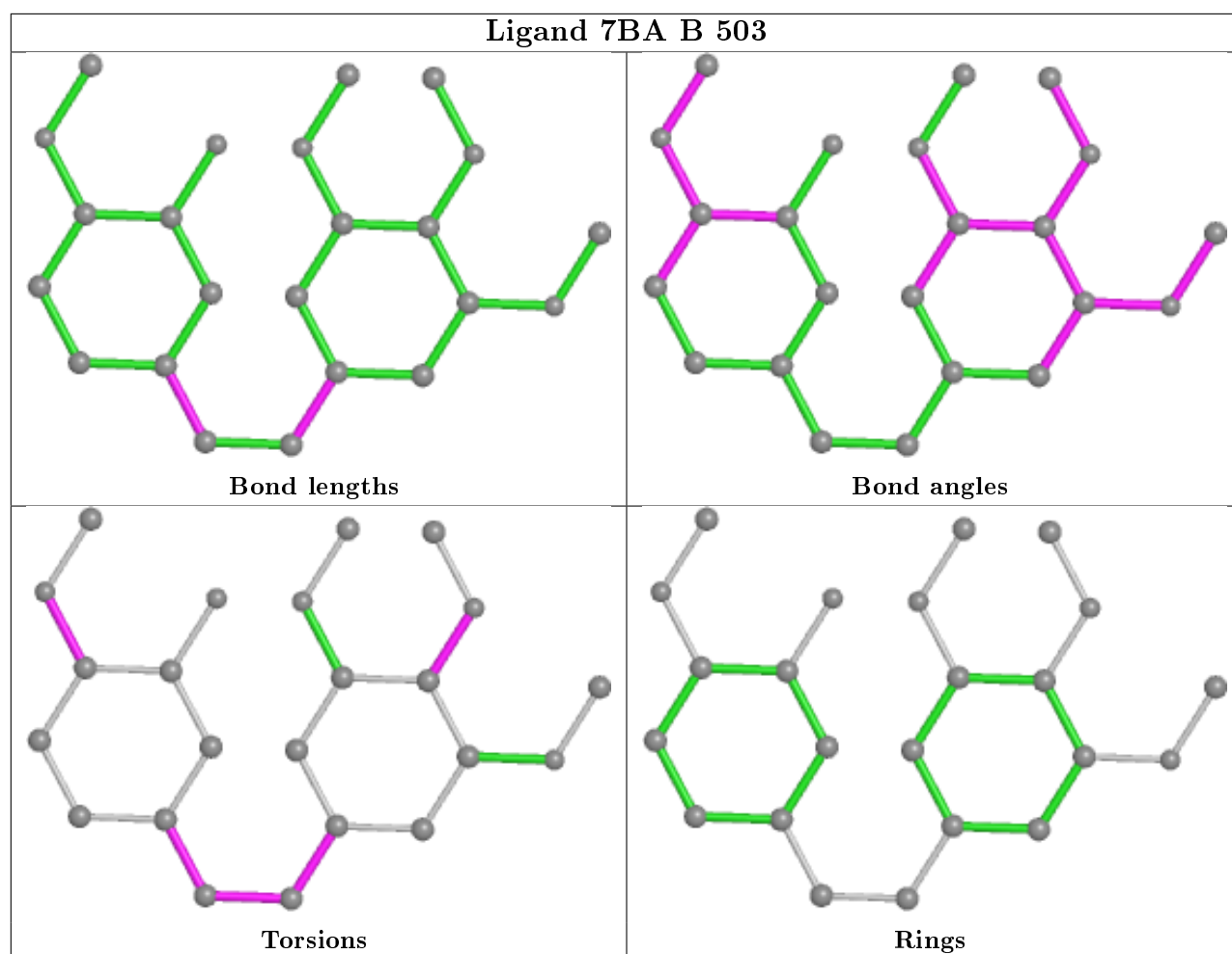
There are no ring outliers.

7 monomers are involved in 9 short contacts:

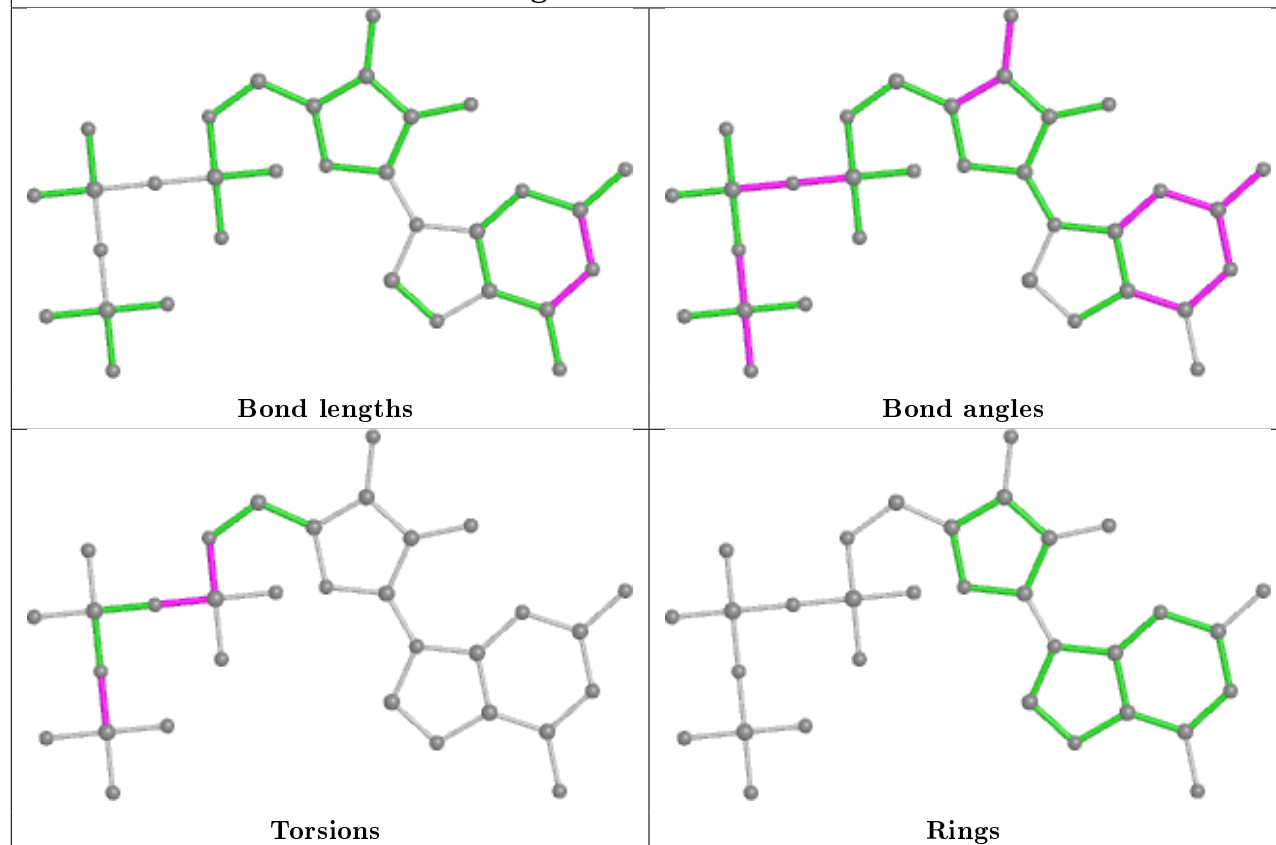
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	504	GOL	1	0
12	F	401	ACP	3	0
5	A	501	GTP	1	0
9	B	501	GDP	1	0
9	D	501	GDP	1	0
10	D	503	7BA	1	0
11	B	504	MES	1	0

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.

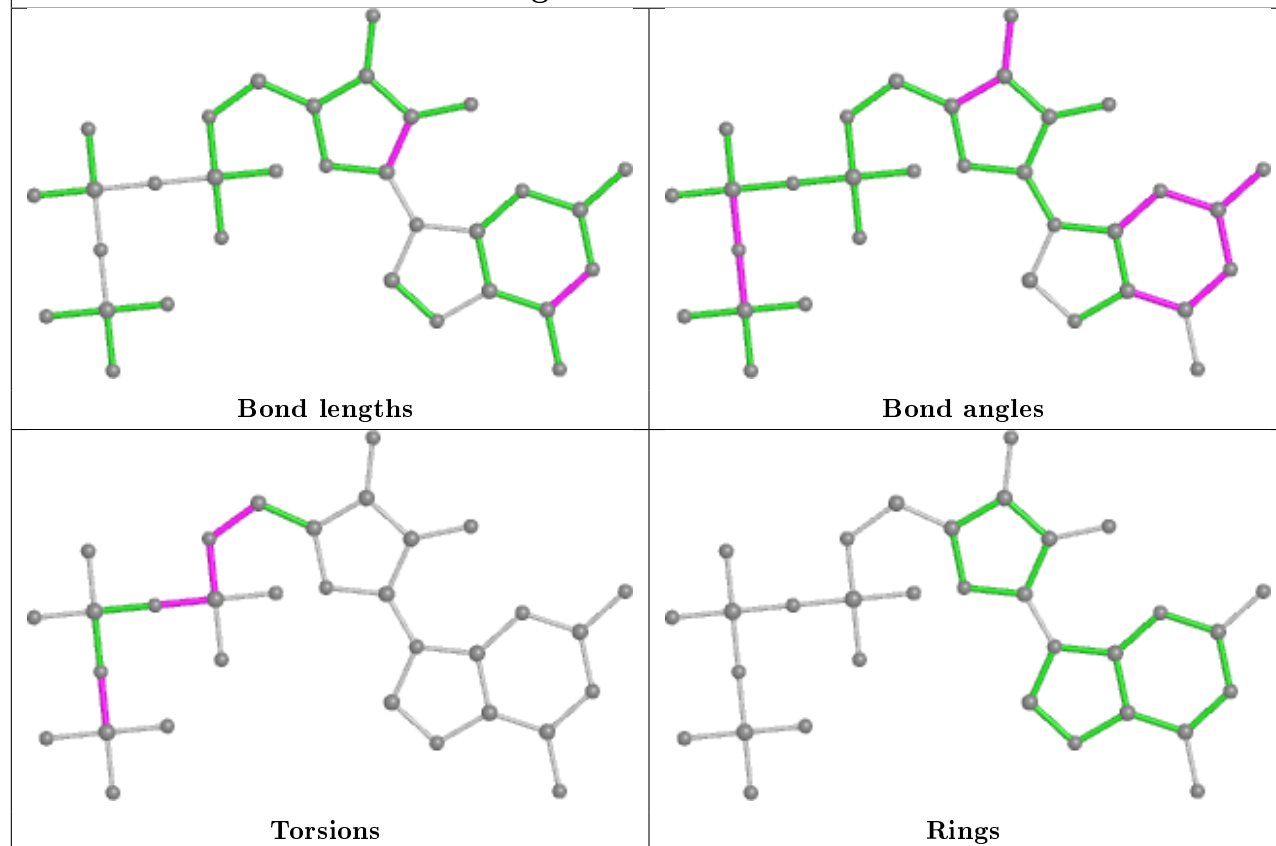


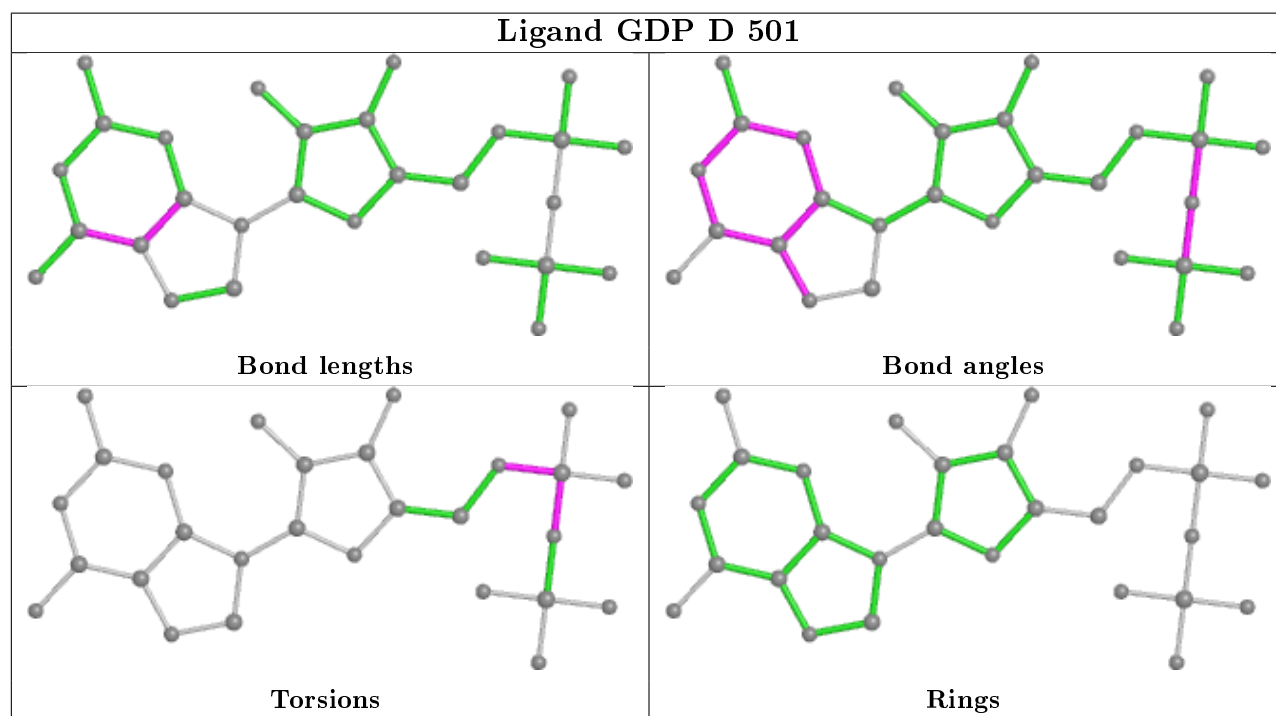
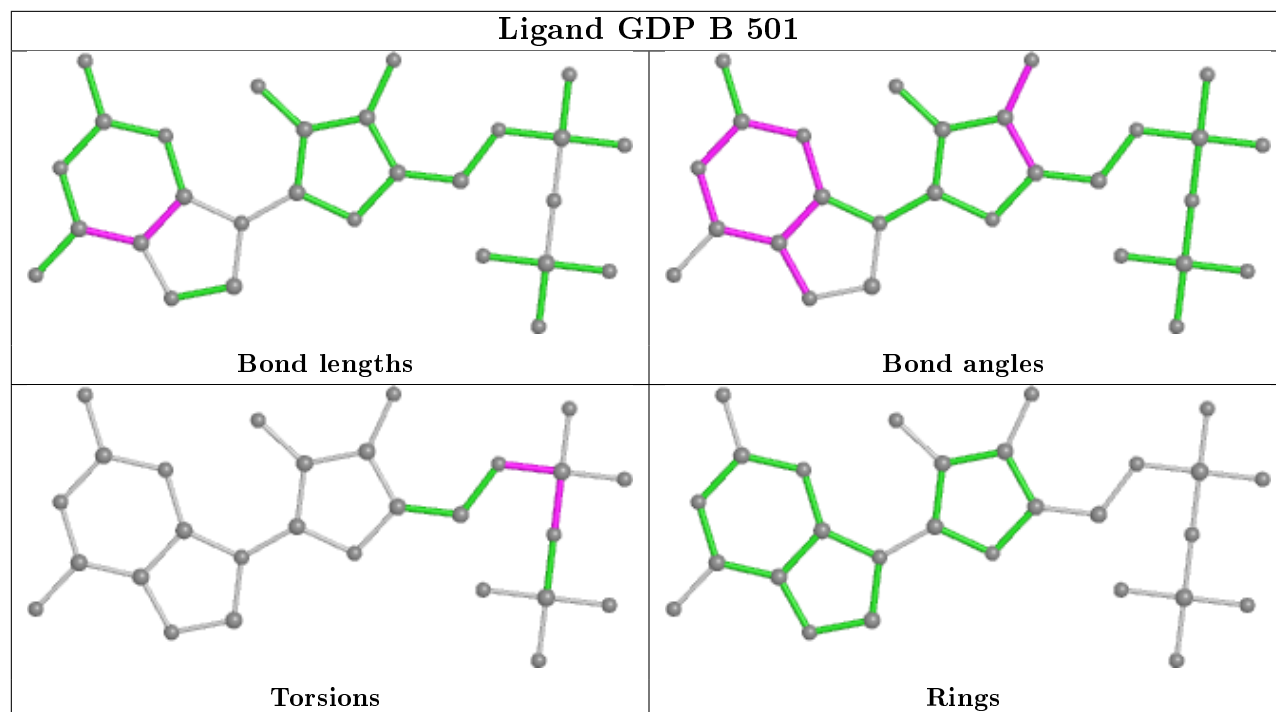


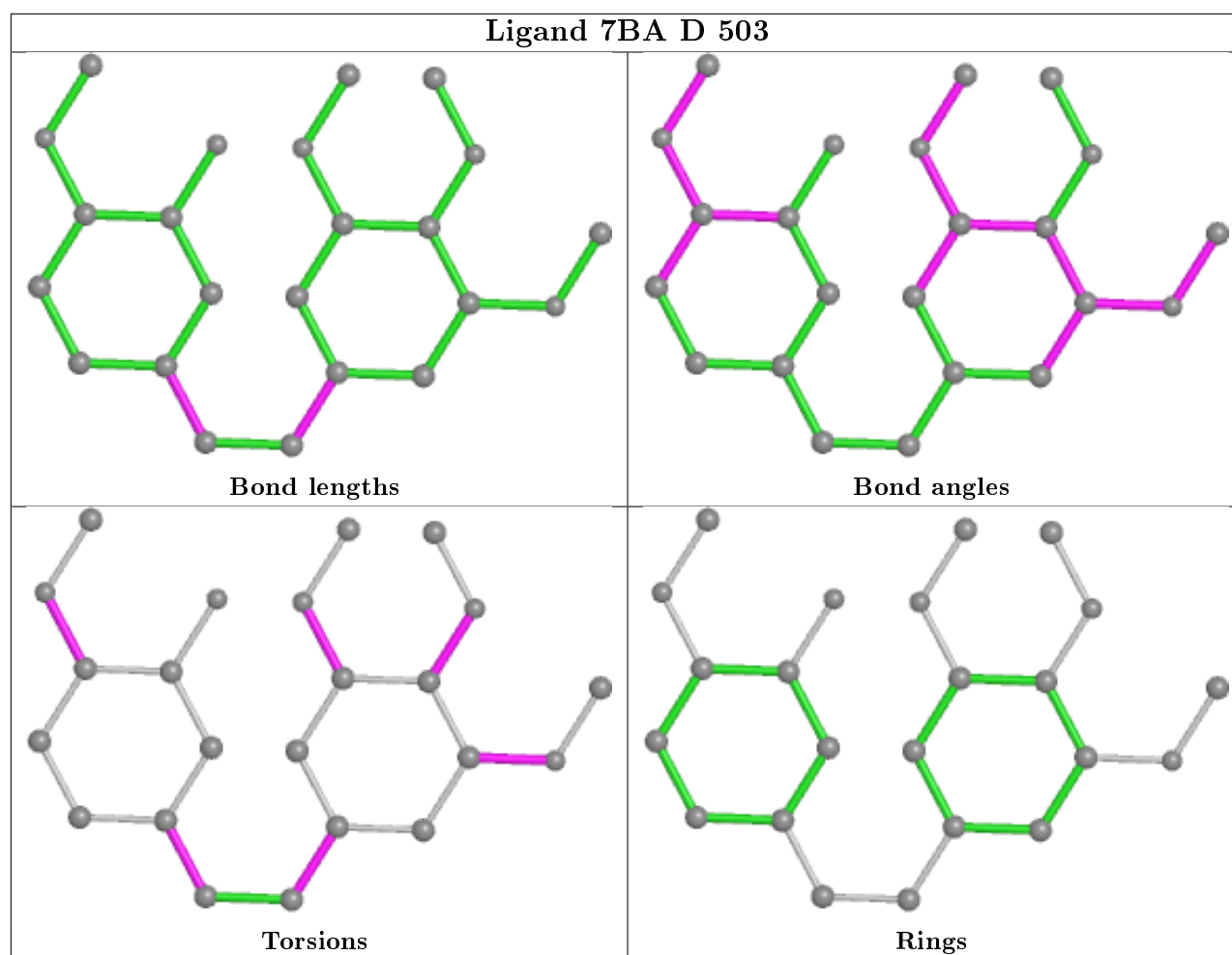
Ligand GTP A 501



Ligand GTP C 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	0.34	18 (4%) 37 36	48, 73, 105, 152	0
1	C	440/451 (97%)	0.08	7 (1%) 72 70	40, 56, 85, 100	0
2	B	425/445 (95%)	0.36	22 (5%) 27 26	41, 64, 103, 143	2 (0%)
2	D	427/445 (95%)	0.57	42 (9%) 7 7	49, 87, 122, 145	4 (0%)
3	E	123/143 (86%)	0.61	15 (12%) 4 3	54, 84, 135, 161	0
4	F	332/384 (86%)	1.50	112 (33%) 0 0	66, 108, 161, 181	0
All	All	2186/2319 (94%)	0.53	216 (9%) 7 6	40, 75, 131, 181	6 (0%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.1
1	A	282	TYR	9.1
4	F	170	LEU	7.7
4	F	131	PHE	7.1
4	F	132	LEU	6.7
4	F	240	LEU	6.6
4	F	182	ILE	6.5
3	E	27	PRO	6.5
3	E	24	LEU	6.5
4	F	169	LEU	6.5
4	F	177	GLY	6.4
4	F	100	ILE	6.3
2	B	438	ALA	6.3
4	F	133	ALA	6.0
4	F	130	VAL	5.7
4	F	225	SER	5.7
4	F	361	LEU	5.5
2	B	439	THR	5.4
4	F	244	CYS	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	59	ASN	5.2
4	F	199	PHE	5.2
4	F	259	GLY	5.2
4	F	21	LEU	5.1
4	F	245	ILE	5.0
4	F	224	SER	5.0
4	F	150	LYS	4.9
4	F	149	ALA	4.9
4	F	179	VAL	4.9
2	D	281	GLN	4.8
4	F	20	LEU	4.8
4	F	101	TYR	4.8
1	A	439	SER	4.7
3	E	143	ALA	4.7
2	B	58	GLY	4.5
2	D	57	THR	4.5
2	D	401	ARG	4.5
4	F	178	GLN	4.5
3	E	140	LYS	4.5
4	F	181	VAL	4.3
4	F	238	CYS	4.3
4	F	145	ASN	4.3
1	C	176	GLN	4.3
4	F	231	ALA	4.2
4	F	17	VAL	4.2
2	B	440	ALA	4.2
4	F	239	HIS	4.2
4	F	27	TRP	4.2
2	D	400	ARG	4.2
4	F	129	GLU	4.2
4	F	186	LEU	4.1
4	F	167	SER	4.1
4	F	176	GLN	4.1
4	F	236	LYS	4.1
1	A	281	ALA	4.1
4	F	227	PRO	4.1
4	F	256	TYR	4.0
4	F	172	PHE	4.0
4	F	163	SER	4.0
4	F	174	ASP	3.9
4	F	362	ALA	3.9
2	B	61	TYR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	405	LEU	3.9
3	E	141	GLU	3.8
2	D	58	GLY	3.8
2	B	37	HIS	3.8
2	B	277	SER	3.8
3	E	139	LEU	3.7
4	F	166	ALA	3.7
4	F	99	VAL	3.6
3	E	25	LYS	3.6
3	E	26	PRO	3.6
4	F	342	LEU	3.6
2	B	437	ASP	3.6
4	F	223	THR	3.6
3	E	7	GLU	3.5
2	B	57	THR	3.5
4	F	125	THR	3.5
4	F	9	GLU	3.5
3	E	6	MET	3.5
2	D	82	PRO	3.5
4	F	23	ALA	3.5
4	F	230	SER	3.5
1	A	348	PRO	3.4
4	F	162	ILE	3.4
4	F	25	GLY	3.3
4	F	260	ASN	3.3
4	F	180	HIS	3.3
4	F	24	THR	3.3
2	D	285	ALA	3.3
4	F	242	ASN	3.2
1	A	178	SER	3.2
4	F	192	LEU	3.2
4	F	135	TYR	3.2
4	F	139	ARG	3.2
1	C	253	THR	3.2
2	B	82	PRO	3.2
4	F	152	SER	3.2
1	A	42	ILE	3.1
4	F	28	LYS	3.1
3	E	142	GLU	3.1
4	F	26	GLN	3.1
4	F	228	TYR	3.1
4	F	137	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	102	PRO	3.1
4	F	140	GLU	3.1
4	F	6	VAL	3.1
1	A	283	HIS	3.1
4	F	128	ARG	3.1
2	D	37	HIS	3.0
2	D	179	ASP	3.0
4	F	22	LEU	3.0
4	F	168	GLU	3.0
2	D	202	TYR	3.0
4	F	241	THR	3.0
2	B	36	TYR	3.0
4	F	200	ASP	3.0
4	F	197	ARG	3.0
4	F	372	THR	2.9
2	D	96	GLN	2.9
4	F	246	GLN	2.9
4	F	143	GLU	2.9
4	F	258	GLU	2.9
2	D	80	SER	2.9
1	A	177	VAL	2.8
4	F	336	PRO	2.8
4	F	264	PHE	2.8
2	D	415	GLU	2.8
4	F	151	SER	2.8
4	F	136	ASN	2.7
4	F	229	ASN	2.7
1	A	171	ILE	2.7
2	D	404	PHE	2.7
2	B	284	ARG	2.7
4	F	194	PRO	2.7
1	A	262	TYR	2.7
2	B	33	THR	2.7
4	F	243	HIS	2.6
2	D	95	GLY	2.6
2	D	59	ASN	2.6
4	F	144	GLY	2.6
2	B	60	LYS	2.6
3	E	45	PRO	2.6
4	F	257	GLU	2.6
4	F	314	LEU	2.6
2	D	399	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	267	PHE	2.6
2	D	2	ARG	2.6
4	F	191	LEU	2.6
2	D	94	PHE	2.6
4	F	13	VAL	2.6
4	F	343	TYR	2.5
1	A	173	PRO	2.5
2	D	77	SER	2.5
2	D	210	TYR	2.5
1	C	2	ARG	2.5
4	F	196	HIS	2.5
2	D	278	ARG	2.4
3	E	46	SER	2.4
2	D	83	PHE	2.4
4	F	126	ASP	2.4
4	F	1	MET	2.4
4	F	147	TRP	2.4
4	F	165	GLU	2.4
2	B	276	THR	2.4
2	D	78	VAL	2.4
1	C	252	LEU	2.4
4	F	226	GLU	2.4
2	D	114	LEU	2.4
4	F	346	LEU	2.4
2	B	147	SER	2.4
2	D	402	LYS	2.3
2	B	34	GLY	2.3
2	D	218	LYS	2.3
3	E	15	THR	2.3
4	F	263	PHE	2.3
1	C	338	LYS	2.3
2	D	276	THR	2.3
4	F	323	GLU	2.3
4	F	171	ASP	2.3
1	A	176	GLN	2.3
4	F	8	ASP	2.2
4	F	360	PRO	2.2
1	A	335	ILE	2.2
2	B	220	THR	2.2
1	C	440	VAL	2.2
3	E	23	ILE	2.2
4	F	337	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	219	LEU	2.2
2	D	260	VAL	2.2
4	F	214	TYR	2.2
4	F	127	GLU	2.2
4	F	44	ARG	2.2
2	B	38	GLY	2.2
1	C	257	THR	2.1
2	D	268	PHE	2.1
2	D	76	ASP	2.1
4	F	32	LYS	2.1
2	D	252	LEU	2.1
2	D	203	CYS	2.1
2	D	56	ALA	2.1
2	D	214	PHE	2.1
1	A	146	GLY	2.1
2	D	277	SER	2.1
2	D	324	SER	2.1
4	F	354	ALA	2.1
1	A	141	PHE	2.1
2	D	249	ASN	2.1
1	A	438	ASP	2.1
2	B	35	SER	2.1
2	D	87	PHE	2.1
1	A	201	ALA	2.1
2	B	283	TYR	2.0
2	D	167	ASN	2.0
1	A	180	ALA	2.0
4	F	18	SER	2.0
4	F	379	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

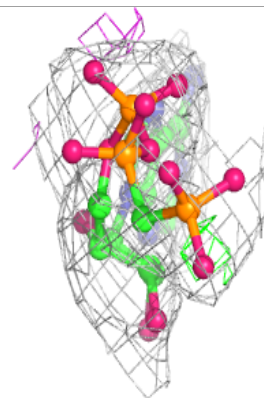
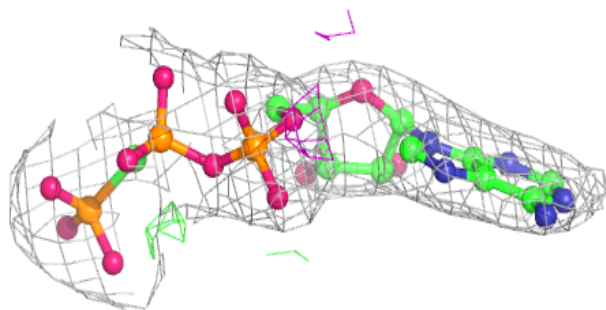
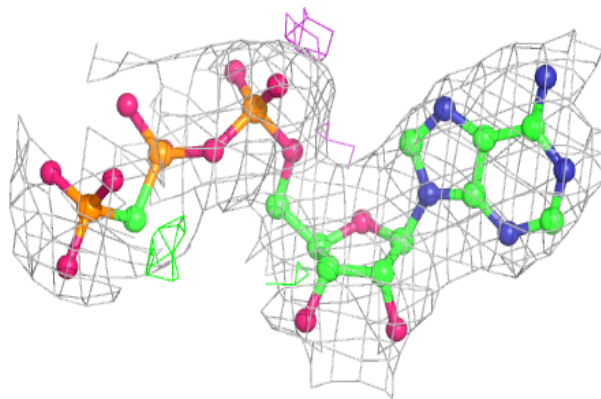
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	505	1/1	0.82	0.04	120,120,120,120	0
8	GOL	A	504	6/6	0.84	0.14	87,90,98,101	0
6	MG	D	502	1/1	0.86	0.06	99,99,99,99	0
7	CA	E	201	1/1	0.91	0.07	108,108,108,108	0
12	ACP	F	401	31/31	0.92	0.12	119,125,136,138	0
9	GDP	D	501	28/28	0.94	0.13	70,77,85,87	0
6	MG	C	502	1/1	0.94	0.25	53,53,53,53	0
7	CA	B	506	1/1	0.95	0.26	94,94,94,94	0
10	7BA	B	503	23/23	0.96	0.21	50,67,86,91	0
10	7BA	D	503	23/23	0.96	0.20	56,75,94,98	0
6	MG	A	502	1/1	0.97	0.27	69,69,69,69	0
7	CA	C	503	1/1	0.97	0.10	82,82,82,82	0
6	MG	B	502	1/1	0.97	0.29	47,47,47,47	0
9	GDP	B	501	28/28	0.98	0.22	38,47,53,58	0
5	GTP	C	501	32/32	0.98	0.17	41,46,51,52	0
11	MES	B	504	12/12	0.98	0.14	63,67,71,71	0
5	GTP	A	501	32/32	0.99	0.24	46,57,62,66	0
7	CA	A	503	1/1	0.99	0.03	91,91,91,91	0

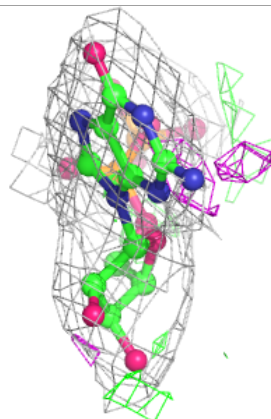
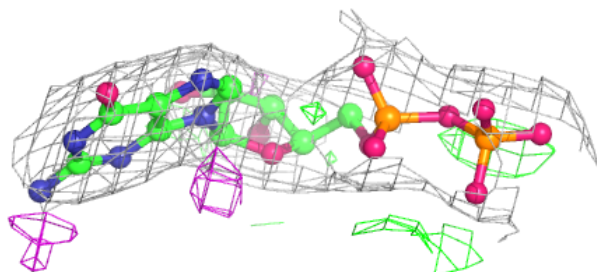
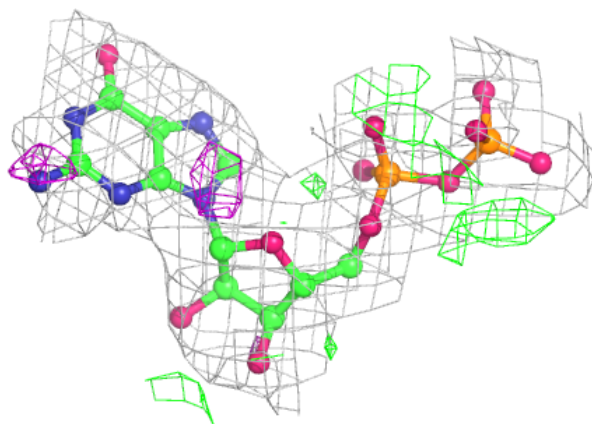
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

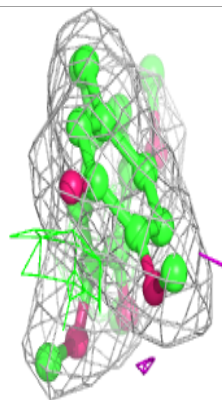
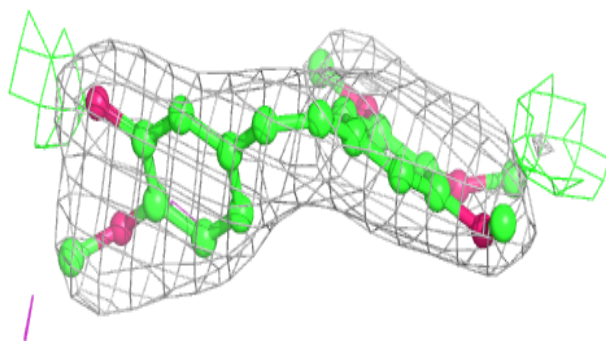
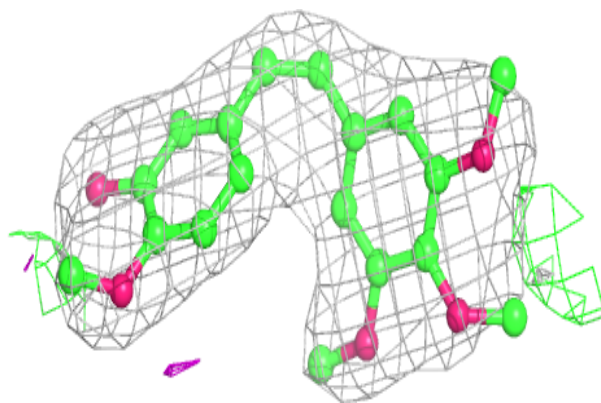
**Electron density around GDP D 501:**

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

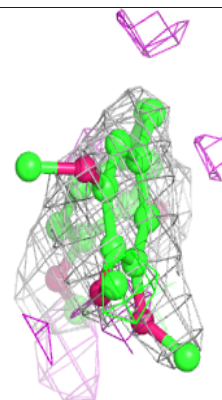
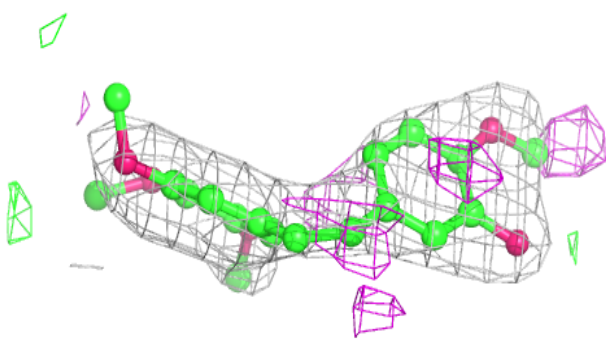
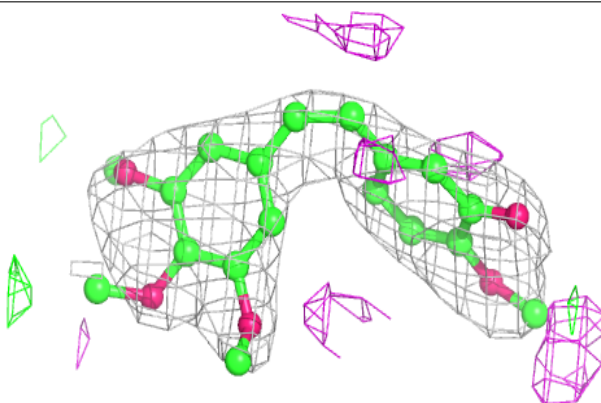


Electron density around 7BA B 503:

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

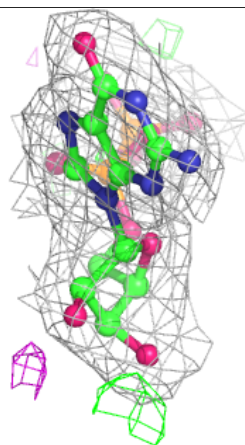
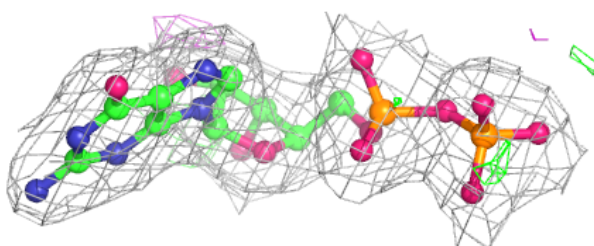
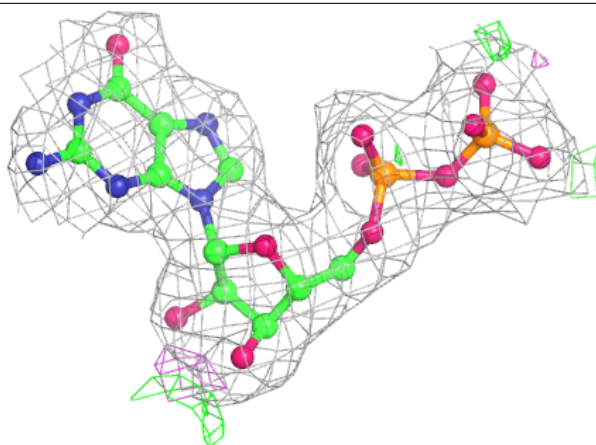
**Electron density around 7BA D 503:**

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

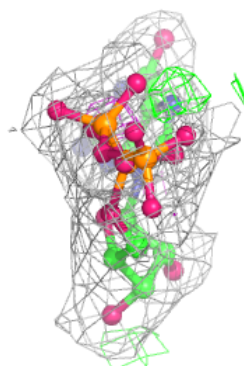
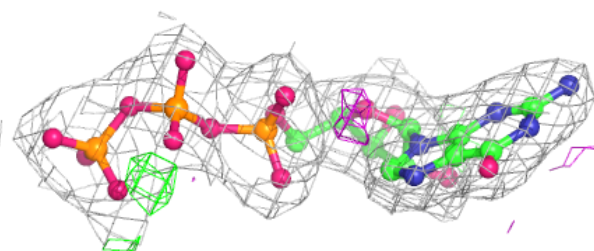
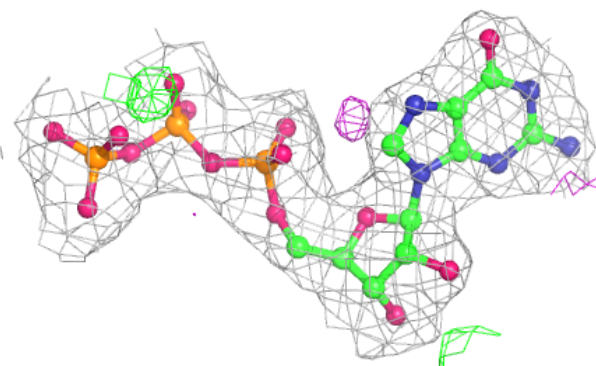


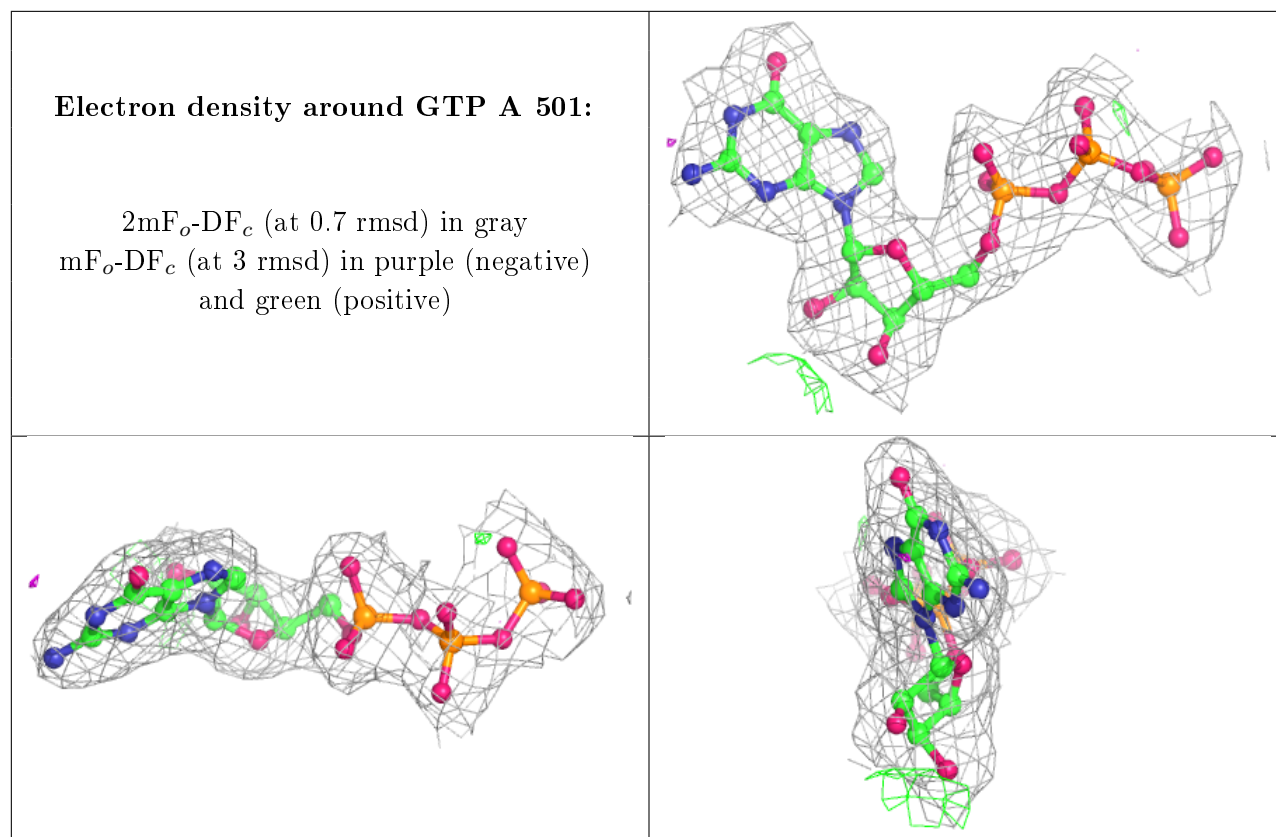
Electron density around GDP B 501:

$2mF_o-DF_c$ (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.