



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:11 PM JST

PDB ID : 7DBC
Title : PRA in complex with tubulin
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2020-10-19
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 : 2.23.2
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) : 2.23.2

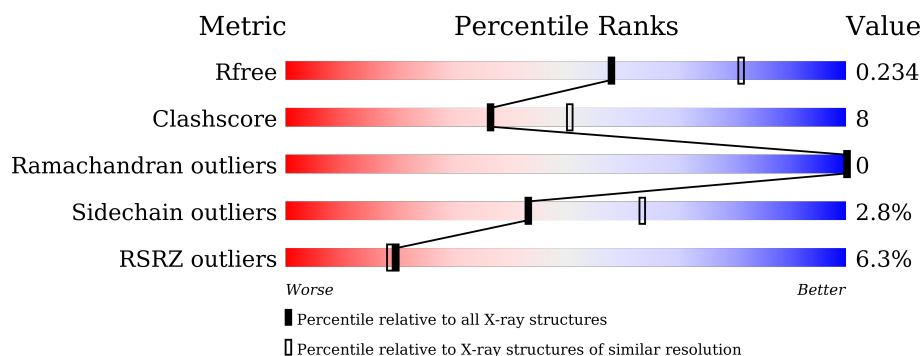
1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>••</div> </div> </div>
2	B	445	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>••</div> </div> </div>
2	D	445	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• 5%</div> </div> </div>
3	E	143	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>• 14%</div> </div> </div>
4	F	384	<div> <div>15%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>• 12%</div> </div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17950 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	438	Total	C	N	O	S	0	2	0
			3430	2171	582	653	24			
1	C	441	Total	C	N	O	S	0	5	0
			3462	2190	586	663	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3353	2106	574	647	26			
2	D	421	Total	C	N	O	S	0	2	0
			3313	2082	562	642	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	1	0
			1019	628	184	202	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP P63042
E	2	ALA	-	expression tag	UNP P63042

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	338	Total	C	N	O	S	0	0	0
			2750	1764	469	503	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 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	D	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: 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...

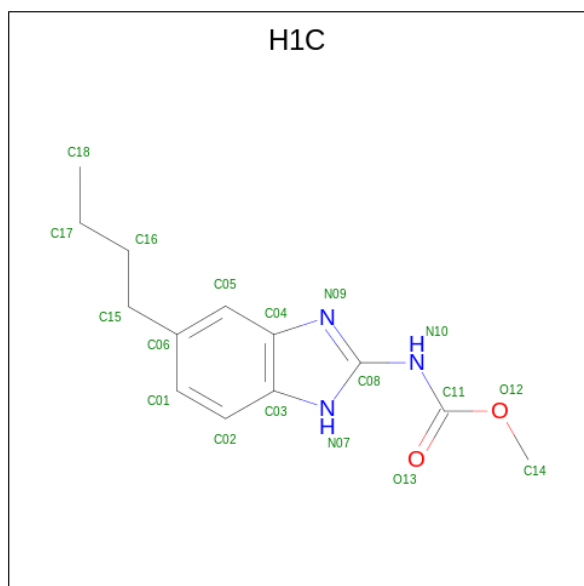
Continued from previous page...

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

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

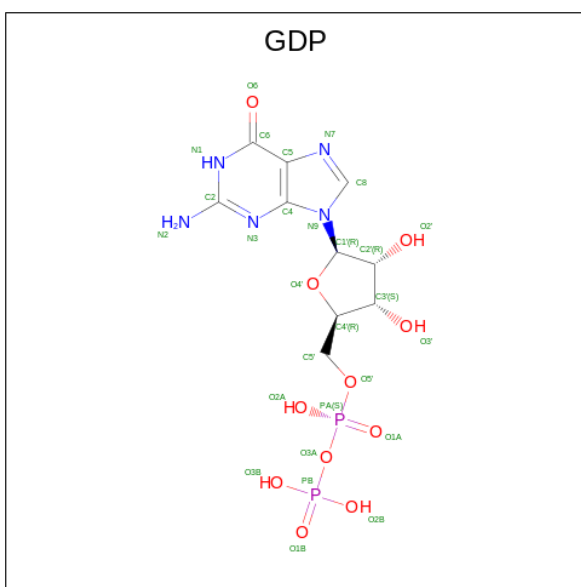
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is methyl {N}-(5-butyl-1 {H}-benzimidazol-2-yl)carbamate (three-letter code: H1C) (formula: C₁₃H₁₇N₃O₂) (labeled as "Ligand of Interest" by depositor).



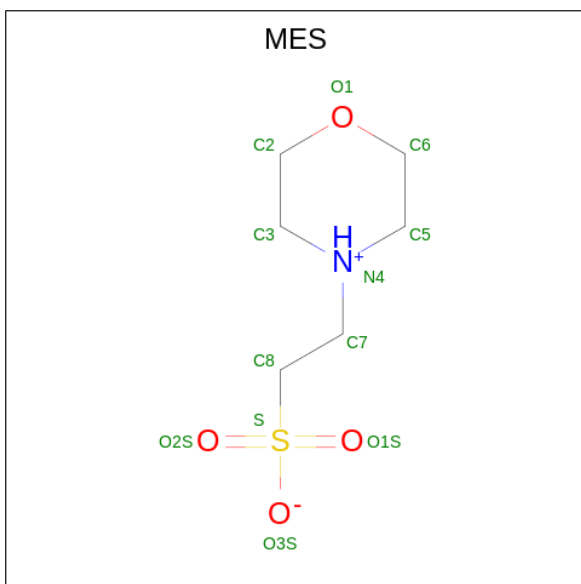
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			18	13	3	2		

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



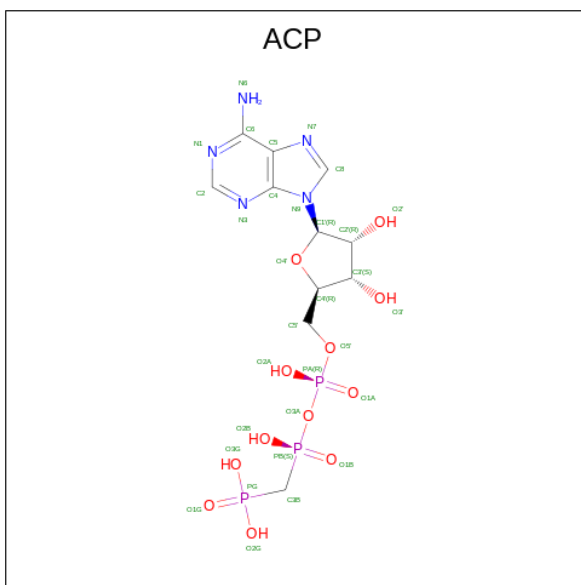
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

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

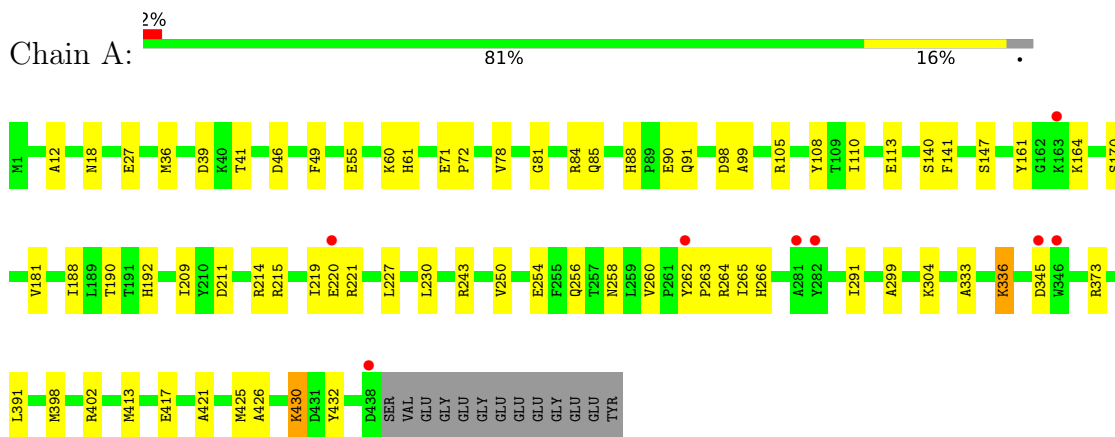
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	111	Total O 111 111	0	0
12	B	78	Total O 78 78	0	0
12	C	151	Total O 151 151	0	0
12	D	43	Total O 43 43	0	0
12	E	14	Total O 14 14	0	0
12	F	34	Total O 34 34	0	0

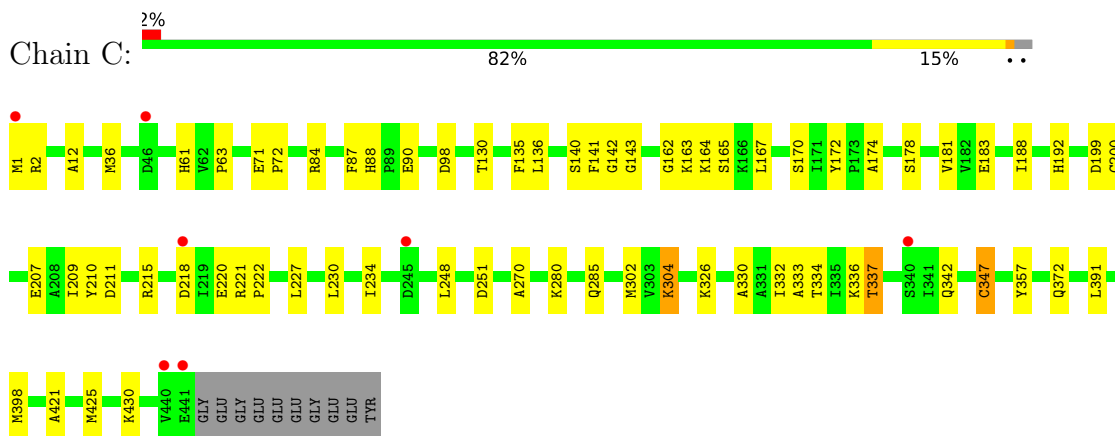
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

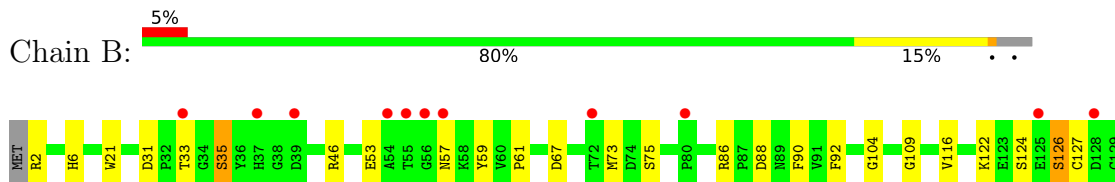
- Molecule 1: Tubulin alpha-1B chain

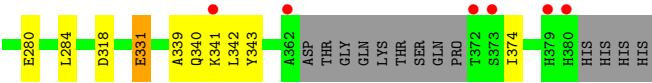


- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.42Å 158.27Å 180.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.40 19.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-2.40) 100.0 (19.92-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.41Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.198 , 0.234 0.198 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17950	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, ACP, CA, H1C, GTP, 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	0.46	0/3514	0.61	1/4770 (0.0%)
1	C	0.53	0/3552	0.65	1/4822 (0.0%)
2	B	0.48	1/3427 (0.0%)	0.59	0/4641
2	D	0.41	0/3391	0.57	1/4593 (0.0%)
3	E	0.50	0/1030	0.58	0/1367
4	F	0.39	0/2811	0.58	0/3799
All	All	0.46	1/17725 (0.0%)	0.60	3/23992 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	239	CYS	CB-SG	-5.25	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	330	MET	CA-CB-CG	-5.62	103.75	113.30
1	C	347	CYS	CB-CA-C	-5.19	100.02	110.40
1	A	391	LEU	CB-CG-CD2	-5.15	102.25	111.00

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	3430	0	3345	48	0
1	C	3462	0	3373	50	0
2	B	3353	0	3231	48	0
2	D	3313	0	3191	72	0
3	E	1019	0	1035	14	0
4	F	2750	0	2701	60	0
5	A	32	0	12	0	0
5	C	32	0	12	2	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	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	18	0	0	0	0
9	B	28	0	12	1	0
10	B	12	0	12	0	0
11	F	31	0	14	1	0
12	A	111	0	0	2	0
12	B	78	0	0	2	0
12	C	151	0	0	3	0
12	D	43	0	0	2	0
12	E	14	0	0	0	0
12	F	34	0	0	2	0
All	All	17950	0	16950	271	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 8.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLU:HG2	2:D:324:LYS:HD2	1.54	0.89
4:F:74:LYS:HE3	4:F:331:GLU:OE2	1.72	0.89
4:F:165:GLU:HB2	4:F:168:GLU:HB2	1.55	0.88
1:C:430:LYS:HE2	12:C:637:HOH:O	1.77	0.85
4:F:95:PRO:HB2	4:F:183:GLN:NE2	1.90	0.84
2:D:107:THR:HG21	2:D:401:GLU:HG2	1.64	0.77
4:F:169:LEU:HD11	4:F:182:ILE:HD12	1.68	0.76
4:F:234:GLN:HA	4:F:236:LYS:HD3	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.69	0.74
2:D:50:TYR:OH	2:D:134:GLN:NE2	2.21	0.72
4:F:228:TYR:HA	4:F:238:CYS:SG	2.29	0.72
2:B:170:MET:HG2	2:B:377:LEU:HD21	1.71	0.71
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.73	0.71
1:A:88:HIS:N	1:A:91:GLN:OE1	2.22	0.71
3:E:23:LYS:HD3	3:E:24:PRO:O	1.90	0.70
1:C:333:ALA:O	1:C:337:THR:HG23	1.90	0.70
1:A:81:GLY:O	1:A:84:ARG:HG3	1.92	0.69
4:F:74:LYS:CE	4:F:331:GLU:OE2	2.39	0.69
4:F:99:VAL:N	4:F:127:GLU:OE1	2.24	0.69
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.56	0.68
2:B:196:THR:HG21	2:B:199:THR:OG1	1.93	0.68
4:F:98:TYR:HB2	4:F:182:ILE:HG23	1.76	0.68
1:C:221:ARG:HD2	2:D:323:MET:HG2	1.76	0.68
1:C:430:LYS:CE	12:C:637:HOH:O	2.40	0.67
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.77	0.67
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.76	0.66
4:F:247:LYS:HD3	4:F:253:TYR:CZ	2.31	0.66
1:C:162:GLY:HA2	3:E:92:ILE:HD11	1.76	0.65
2:D:401:GLU:HG3	3:E:135:LYS:HE3	1.79	0.65
2:B:276:ARG:HG2	2:B:276:ARG:NH2	2.11	0.64
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.27	0.64
2:D:2:ARG:HB3	2:D:131:GLN:HG2	1.79	0.64
1:C:221:ARG:HG3	2:D:323:MET:HG3	1.79	0.64
2:D:329:GLN:NE2	12:D:601:HOH:O	2.30	0.64
4:F:160:ILE:O	4:F:161:LEU:HD22	1.99	0.63
1:C:163:LYS:NZ	12:C:603:HOH:O	2.31	0.63
1:C:221:ARG:HG3	2:D:323:MET:CG	2.29	0.63
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.35	0.62
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.32	0.62
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.35	0.61
2:D:192:LEU:O	2:D:196:THR:HG22	1.99	0.61
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.31	0.61
1:C:181:VAL:HG12	1:C:398:MET:HE3	1.83	0.60
2:D:350:LYS:NZ	12:D:603:HOH:O	2.34	0.60
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.36	0.60
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.83	0.59
4:F:36:ARG:NH1	12:F:503:HOH:O	2.35	0.59
2:B:385:PHE:CE1	2:B:412:GLU:HB2	2.38	0.59
1:C:221:ARG:CG	2:D:323:MET:HG2	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.37	0.59
1:C:221:ARG:CD	2:D:323:MET:HG2	2.33	0.59
4:F:228:TYR:HA	4:F:238:CYS:HG	1.68	0.58
4:F:95:PRO:HB2	4:F:183:GLN:HE21	1.67	0.58
1:A:264:ARG:NH1	12:A:602:HOH:O	2.32	0.58
2:B:86:ARG:HH11	2:B:88:ASP:HB2	1.69	0.58
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.39	0.58
4:F:162:ILE:HD11	4:F:240:LEU:HD21	1.84	0.57
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.87	0.57
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.40	0.56
4:F:263:PHE:HE2	4:F:341:LYS:HD3	1.70	0.56
2:B:390:ARG:HG3	2:B:390:ARG:HH11	1.70	0.56
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.87	0.56
1:A:426:ALA:O	1:A:430:LYS:HE2	2.06	0.55
4:F:16:GLU:O	4:F:20:LEU:HG	2.05	0.55
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.87	0.55
2:D:210:ILE:O	2:D:214:THR:HB	2.07	0.55
2:B:276:ARG:CG	2:B:276:ARG:HH21	2.20	0.55
1:C:207:GLU:HG2	1:C:304:LYS:HE3	1.89	0.55
1:C:330:ALA:O	1:C:334:THR:HG23	2.07	0.55
2:B:126:SER:O	2:B:126:SER:OG	2.22	0.55
2:D:100:ASN:HB3	2:D:103:LYS:HB2	1.88	0.55
2:D:178:THR:O	2:D:181:GLU:HG3	2.07	0.55
4:F:88:SER:OG	4:F:90:SER:O	2.23	0.55
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.07	0.55
4:F:244:CYS:SG	4:F:245:ILE:N	2.80	0.54
1:A:99:ALA:HA	1:A:105:ARG:HG2	1.89	0.54
2:B:386:THR:O	2:B:390:ARG:HG2	2.07	0.53
1:A:88:HIS:NE2	1:A:90:GLU:HB2	2.23	0.53
2:D:401:GLU:HA	3:E:135:LYS:HG3	1.89	0.53
1:A:220:GLU:HG2	2:B:324:LYS:HD2	1.91	0.53
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.91	0.53
2:B:262:ARG:NE	2:B:421:GLU:OE1	2.31	0.53
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.90	0.52
2:D:67:ASP:OD2	2:D:72:THR:HG21	2.09	0.52
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.90	0.52
2:B:46:ARG:NH2	2:B:243:PRO:HA	2.25	0.52
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.92	0.52
2:D:375:GLN:O	2:D:379:LYS:HG2	2.10	0.52
2:B:276:ARG:NH2	2:B:276:ARG:CG	2.72	0.52
2:D:36:TYR:CD1	2:D:44:LEU:HD21	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:339:ALA:HB3	4:F:342:LEU:HD12	1.90	0.52
2:B:165:ASN:ND2	2:B:250:LEU:HD22	2.25	0.52
2:B:335:ASN:HD22	4:F:36:ARG:HD3	1.74	0.52
2:B:382:SER:O	2:B:386:THR:HG23	2.10	0.51
1:C:143:GLY:N	5:C:501:GTP:H5'	2.25	0.51
2:D:26:ASP:OD2	2:D:359:ARG:HD3	2.09	0.51
1:A:345:ASP:HB3	3:E:26:SER:HB3	1.91	0.51
2:D:106:TYR:CD1	3:E:131:VAL:HG11	2.45	0.51
3:E:128:ALA:HA	3:E:131:VAL:HG12	1.91	0.51
4:F:253:TYR:OH	4:F:259:GLY:HA2	2.09	0.51
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.91	0.51
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.91	0.51
2:D:130:LEU:HB3	2:D:162:ARG:NH1	2.26	0.51
2:B:276:ARG:HG2	2:B:276:ARG:HH21	1.76	0.51
1:A:36:MET:HE1	1:A:49:PHE:CZ	2.46	0.51
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.93	0.51
4:F:169:LEU:CD1	4:F:182:ILE:HD12	2.39	0.51
3:E:70:LEU:O	3:E:74:ARG:HG2	2.11	0.50
1:A:60:LYS:NZ	1:A:85:GLN:O	2.28	0.50
1:A:262:TYR:HD1	1:A:263:PRO:HD2	1.76	0.50
1:C:1:MET:HB3	1:C:130:THR:OG1	2.11	0.50
1:A:398:MET:HE3	2:B:345:ILE:HG23	1.92	0.50
2:D:141:GLY:O	2:D:184:ASN:ND2	2.44	0.50
1:A:147:SER:HB2	1:A:190:THR:HB	1.94	0.50
4:F:165:GLU:CB	4:F:168:GLU:HB2	2.34	0.50
1:A:36:MET:HE3	1:A:39:ASP:HB2	1.93	0.49
2:B:67:ASP:O	2:B:92:PHE:HA	2.12	0.49
4:F:318:ASP:OD2	11:F:401:ACP:O3G	2.30	0.49
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.47	0.49
2:D:268:PRO:HG2	2:D:300:MET:HB2	1.95	0.49
1:C:234:ILE:HD13	1:C:302:MET:SD	2.53	0.49
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.95	0.49
1:C:270:ALA:HB3	1:C:302:MET:HG2	1.95	0.49
2:B:186:THR:HA	2:B:415:MET:HE1	1.95	0.48
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.47	0.48
4:F:133:ALA:O	4:F:137:ARG:HG2	2.13	0.48
2:B:333:VAL:O	2:B:337:ASN:ND2	2.43	0.48
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.48
2:B:320:ARG:HH21	2:B:320:ARG:HG3	1.77	0.48
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.44	0.48
3:E:69:HIS:HA	3:E:72:GLU:OE1	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.48
2:B:219:THR:HG21	1:C:326:LYS:HA	1.96	0.48
1:C:332:ILE:O	1:C:336:LYS:HG3	2.13	0.48
2:D:23:VAL:O	2:D:27:GLU:HG3	2.14	0.48
1:C:181:VAL:HG12	1:C:398:MET:CE	2.44	0.47
2:D:402:GLY:C	3:E:131:VAL:HG23	2.34	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.50	0.47
2:D:386:THR:O	2:D:390:ARG:HB2	2.15	0.47
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.50	0.47
1:C:211[A]:ASP:OD2	1:C:304:LYS:HE2	2.15	0.47
2:D:189:VAL:HG11	2:D:415:MET:HG3	1.95	0.47
1:A:110:ILE:O	1:A:113:GLU:HG2	2.15	0.47
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.96	0.47
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.95	0.47
2:D:210:ILE:O	2:D:215:LEU:HD23	2.15	0.47
3:E:73:LYS:O	3:E:77:GLU:HG3	2.15	0.47
4:F:43:GLU:OE2	12:F:501:HOH:O	2.20	0.47
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.50	0.47
2:B:301:ALA:O	2:B:303:CYS:N	2.45	0.47
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.23	0.47
2:B:130:LEU:HB3	2:B:162:ARG:HH11	1.80	0.47
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.51	0.47
2:D:209:ASP:O	2:D:213:ARG:HB2	2.14	0.47
4:F:40:MET:HE2	4:F:47:LEU:HG	1.97	0.47
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.97	0.46
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.50	0.46
2:D:44:LEU:HA	2:D:47:ILE:HB	1.96	0.46
2:B:104:GLY:O	2:B:109:GLY:HA3	2.16	0.46
2:D:293:MET:SD	2:D:365:ALA:HB1	2.55	0.46
4:F:167:SER:O	4:F:171:ASP:HB2	2.14	0.46
4:F:252:ASN:HB3	4:F:255:ARG:HD3	1.96	0.46
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.15	0.46
4:F:192:LEU:HD12	4:F:192:LEU:H	1.80	0.46
4:F:226:GLU:HG2	4:F:250:SER:OG	2.15	0.46
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.16	0.46
2:B:2:ARG:N	12:B:614:HOH:O	2.47	0.46
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.98	0.46
2:B:173:PRO:HA	2:B:176:SER:HB2	1.98	0.46
2:B:335:ASN:HD21	4:F:36:ARG:HE	1.62	0.46
3:E:136:GLU:O	3:E:139:GLU:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:THR:HG1	2:B:35:SER:H	1.64	0.46
1:C:220:GLU:HG2	2:D:324:LYS:CD	2.36	0.46
1:C:221:ARG:CG	2:D:323:MET:CG	2.93	0.46
4:F:14:TYR:HA	4:F:17:VAL:HB	1.97	0.46
4:F:128:ARG:NH1	4:F:170:LEU:HD22	2.31	0.45
4:F:234:GLN:HA	4:F:236:LYS:CD	2.44	0.45
2:D:169:VAL:HA	2:D:202:ILE:O	2.16	0.45
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.99	0.45
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.99	0.45
2:D:228:LEU:O	2:D:232:THR:HG23	2.16	0.45
2:D:284:LEU:HD12	2:D:285:THR:H	1.82	0.45
2:D:16:ILE:HD11	2:D:136:THR:HB	1.98	0.45
2:D:55:THR:OG1	2:D:56:GLY:N	2.50	0.45
2:D:196:THR:HG21	2:D:199:THR:OG1	2.17	0.45
2:D:70:PRO:HG3	2:D:93:GLY:O	2.17	0.45
2:D:392:LYS:HE3	2:D:405:GLU:OE1	2.17	0.45
4:F:262:MET:HE3	4:F:262:MET:HB3	1.61	0.45
1:C:192:HIS:CG	1:C:421:ALA:HA	2.52	0.45
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.51	0.45
2:D:238:THR:HG23	2:D:242:PHE:HD2	1.81	0.45
2:B:53:GLU:HG2	2:B:59:TYR:CE1	2.52	0.44
1:C:398:MET:HE3	2:D:345:ILE:HG23	1.99	0.44
2:D:1:MET:HG3	2:D:48:ASN:HD22	1.81	0.44
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.52	0.44
2:D:290:THR:HG22	2:D:333:VAL:HG21	2.00	0.44
1:A:398:MET:CE	2:B:345:ILE:HG23	2.48	0.44
2:D:208:TYR:CE2	2:D:220:PRO:HG2	2.53	0.44
3:E:46:GLU:O	3:E:50:LYS:HG2	2.18	0.44
4:F:220:VAL:HG23	4:F:263:PHE:CD1	2.52	0.44
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.98	0.44
4:F:32:LYS:HB3	4:F:32:LYS:HE2	1.52	0.44
2:D:165:ASN:ND2	2:D:198:GLU:HG3	2.33	0.44
2:D:293:MET:CG	2:D:367:PHE:HB2	2.48	0.44
4:F:151:SER:OG	4:F:180:HIS:ND1	2.50	0.44
2:B:124:SER:O	2:B:127:CYS:HB2	2.18	0.44
2:D:218:THR:O	2:D:220:PRO:HD3	2.18	0.44
1:A:214:ARG:HG2	1:A:219:ILE:O	2.18	0.43
2:D:332:ASN:ND2	2:D:336:LYS:HD3	2.34	0.43
2:B:350:LYS:HD3	2:B:350:LYS:HA	1.56	0.43
2:D:196:THR:HG22	2:D:264:HIS:NE2	2.34	0.43
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.43
2:D:284:LEU:HD12	2:D:285:THR:N	2.33	0.43
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.01	0.43
1:A:333:ALA:O	1:A:336:LYS:HE3	2.18	0.43
1:A:402:ARG:HG3	12:A:606:HOH:O	2.19	0.43
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.36	0.43
2:D:12:CYS:O	2:D:16:ILE:HG12	2.19	0.43
2:D:105:HIS:ND1	2:D:150:LEU:HB2	2.34	0.43
1:A:181:VAL:HG22	1:A:398:MET:HE3	2.01	0.43
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.18	0.43
1:C:174:ALA:O	1:C:178:SER:HB2	2.19	0.43
2:D:395:LEU:O	2:D:399:THR:HG22	2.19	0.43
2:B:134:GLN:HA	2:B:165:ASN:O	2.19	0.42
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.51	0.42
2:D:266:PHE:O	2:D:268:PRO:HD3	2.19	0.42
4:F:243:HIS:CE1	4:F:247:LYS:HG3	2.53	0.42
2:B:33:THR:OG1	2:B:35:SER:HB2	2.19	0.42
1:C:209:ILE:HD11	1:C:302:MET:SD	2.59	0.42
2:D:161:ASP:OD1	2:D:161:ASP:N	2.49	0.42
1:A:215:ARG:NH2	1:A:299:ALA:O	2.52	0.42
1:A:256:GLN:HG2	1:A:260:VAL:HB	2.01	0.42
2:B:122:LYS:HE3	2:B:122:LYS:HB3	1.65	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.42
2:D:130:LEU:HB3	2:D:162:ARG:HH11	1.83	0.42
4:F:146:VAL:HG22	4:F:164:SER:OG	2.19	0.42
4:F:40:MET:HG2	4:F:62:VAL:HG23	2.02	0.42
4:F:39:LEU:HD13	4:F:61:LEU:HD23	2.02	0.42
4:F:139:ARG:HH21	4:F:139:ARG:HG3	1.85	0.42
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.83	0.42
4:F:192:LEU:HD22	4:F:262:MET:HE1	2.00	0.42
1:C:135:PHE:O	1:C:136:LEU:HD23	2.19	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.42
4:F:5:VAL:HG23	4:F:37:PHE:HB3	2.02	0.42
1:A:221:ARG:HD3	2:B:323:MET:HB2	2.01	0.41
4:F:192:LEU:HD21	4:F:262:MET:HE1	2.02	0.41
1:C:1:MET:O	1:C:2:ARG:HB2	2.20	0.41
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.35	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.41
2:D:174:LYS:HB2	2:D:174:LYS:HE2	1.80	0.41
4:F:217:ARG:NH1	4:F:374:ILE:HG22	2.36	0.41
1:C:143:GLY:HA3	5:C:501:GTP:O3A	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:236:LYS:HE2	4:F:236:LYS:H	1.85	0.41
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.86	0.41
1:C:211[A]:ASP:O	1:C:215:ARG:HG3	2.20	0.41
2:D:117:LEU:HD11	2:D:154:LYS:HB3	2.02	0.41
2:B:170:MET:CG	2:B:377:LEU:HD21	2.47	0.41
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.56	0.41
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.56	0.41
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.02	0.41
2:D:172:SER:HB2	2:D:205:GLU:OE1	2.20	0.41
9:B:503:GDP:O3B	12:B:601:HOH:O	2.22	0.40
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.40
2:D:322:SER:HB3	2:D:325:GLU:HB2	2.04	0.40
3:E:98:LYS:NZ	3:E:98:LYS:HB3	2.35	0.40
4:F:217:ARG:HG2	4:F:374:ILE:O	2.21	0.40
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.22	0.40
1:A:263:PRO:O	1:A:266:HIS:HD2	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/451 (97%)	427 (98%)	11 (2%)	0	100	100
1	C	443/451 (98%)	430 (97%)	13 (3%)	0	100	100
2	B	422/445 (95%)	406 (96%)	16 (4%)	0	100	100
2	D	418/445 (94%)	403 (96%)	15 (4%)	0	100	100
3	E	120/143 (84%)	120 (100%)	0	0	100	100
4	F	328/384 (85%)	317 (97%)	11 (3%)	0	100	100
All	All	2169/2319 (94%)	2103 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	371/379 (98%)	367 (99%)	4 (1%)	73	87
1	C	376/379 (99%)	367 (98%)	9 (2%)	49	68
2	B	368/383 (96%)	359 (98%)	9 (2%)	49	68
2	D	365/383 (95%)	355 (97%)	10 (3%)	44	65
3	E	111/127 (87%)	109 (98%)	2 (2%)	59	76
4	F	300/342 (88%)	282 (94%)	18 (6%)	19	31
All	All	1891/1993 (95%)	1839 (97%)	52 (3%)	43	65

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	46	ASP
1	A	336	LYS
1	A	430	LYS
2	B	35	SER
2	B	57	ASN
2	B	75	SER
2	B	126	SER
2	B	137	HIS
2	B	276	ARG
2	B	281	TYR
2	B	323	MET
2	B	339	SER
1	C	84	ARG
1	C	164	LYS
1	C	218	ASP
1	C	251	ASP
1	C	280	LYS
1	C	304	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	337	THR
1	C	342	GLN
1	C	347	CYS
2	D	1	MET
2	D	41	ASP
2	D	58	LYS
2	D	126	SER
2	D	137	HIS
2	D	177	ASP
2	D	215	LEU
2	D	219	THR
2	D	320	ARG
2	D	330	MET
3	E	50	LYS
3	E	59	ARG
4	F	11	SER
4	F	32	LYS
4	F	131	PHE
4	F	168	GLU
4	F	171	ASP
4	F	172	PHE
4	F	183	GLN
4	F	211	TYR
4	F	217	ARG
4	F	222	ARG
4	F	236	LYS
4	F	238	CYS
4	F	242	ASN
4	F	244	CYS
4	F	247	LYS
4	F	250	SER
4	F	262	MET
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	335	ASN
2	B	414	ASN
2	D	48	ASN
2	D	99	ASN
2	D	134	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	245	GLN
2	D	332	ASN
2	D	396	HIS
4	F	183	GLN
4	F	252	ASN
4	F	380	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	501	6	26,34,34	1.25	3 (11%)	33,54,54	1.97	5 (15%)
5	GTP	C	501	6	26,34,34	0.99	2 (7%)	33,54,54	1.85	10 (30%)
9	GDP	B	503	6	24,30,30	1.27	4 (16%)	31,47,47	1.88	7 (22%)
8	H1C	B	501	-	19,19,19	1.97	4 (21%)	18,25,25	1.81	5 (27%)
10	MES	B	504	-	12,12,12	2.11	1 (8%)	14,16,16	2.26	5 (35%)
11	ACP	F	401	6	27,33,33	1.46	4 (14%)	32,52,52	1.56	6 (18%)
5	GTP	A	501	6	26,34,34	1.10	1 (3%)	33,54,54	1.87	8 (24%)

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	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	503	6	-	3/12/32/32	0/3/3/3
8	H1C	B	501	-	-	2/8/10/10	0/2/2/2
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
11	ACP	F	401	6	-	3/15/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-6.88	1.67	1.77
8	B	501	H1C	C08-N10	5.02	1.45	1.38
8	B	501	H1C	C11-N10	4.15	1.44	1.36
8	B	501	H1C	O12-C11	3.82	1.41	1.34
5	D	501	GTP	C6-N1	3.66	1.39	1.33
9	B	503	GDP	C6-C5	3.58	1.47	1.41
5	A	501	GTP	C6-N1	3.49	1.39	1.33
11	F	401	ACP	C2'-C1'	-3.33	1.48	1.53
11	F	401	ACP	PB-O1B	-3.26	1.43	1.51
5	C	501	GTP	C6-N1	2.98	1.38	1.33
9	B	503	GDP	C5-C4	2.54	1.47	1.40
9	B	503	GDP	C2'-C1'	-2.54	1.49	1.53
8	B	501	H1C	O12-C14	-2.42	1.39	1.45
11	F	401	ACP	C4-N3	-2.37	1.32	1.35
11	F	401	ACP	C5-N7	-2.22	1.31	1.39
9	B	503	GDP	O4'-C1'	2.21	1.44	1.41
5	D	501	GTP	PB-O2B	-2.17	1.45	1.55
5	C	501	GTP	C2-N1	2.14	1.39	1.35
5	D	501	GTP	C8-N7	-2.09	1.31	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	C5-C6-N1	-8.49	111.83	123.43
5	A	501	GTP	N3-C2-N1	-5.39	120.03	127.22
10	B	504	MES	C5-N4-C3	5.34	120.84	108.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	H1C	O12-C11-N10	5.22	116.55	109.25
5	D	501	GTP	C6-N1-C2	5.10	124.03	115.93
5	A	501	GTP	C2-N3-C4	5.04	121.11	115.36
9	B	503	GDP	C2-N3-C4	4.81	120.85	115.36
5	C	501	GTP	N3-C2-N1	-4.72	120.93	127.22
9	B	503	GDP	C5-C6-N1	-4.17	117.73	123.43
9	B	503	GDP	C6-N1-C2	4.16	122.54	115.93
10	B	504	MES	O3S-S-C8	3.78	111.89	105.77
11	F	401	ACP	C3'-C2'-C1'	3.74	106.60	100.98
5	C	501	GTP	C5-C6-N1	-3.71	118.36	123.43
9	B	503	GDP	N3-C2-N1	-3.62	122.40	127.22
5	C	501	GTP	PA-O3A-PB	-3.48	120.88	132.83
9	B	503	GDP	C6-C5-C4	-3.42	117.53	120.80
5	C	501	GTP	C2-N3-C4	3.06	118.85	115.36
5	A	501	GTP	C5-C6-N1	-3.02	119.30	123.43
5	C	501	GTP	C6-N1-C2	2.94	120.61	115.93
11	F	401	ACP	C4-C5-N7	-2.93	106.34	109.40
5	A	501	GTP	PB-O3B-PG	-2.93	122.77	132.83
8	B	501	H1C	C06-C05-C04	-2.92	118.52	121.08
11	F	401	ACP	N3-C2-N1	-2.87	124.19	128.68
5	A	501	GTP	N2-C2-N1	2.81	121.62	117.25
11	F	401	ACP	O2'-C2'-C1'	-2.80	100.52	110.85
11	F	401	ACP	O2G-PG-C3B	2.72	113.01	106.40
5	C	501	GTP	PB-O3B-PG	-2.67	123.68	132.83
8	B	501	H1C	O13-C11-N10	-2.62	120.41	126.11
5	A	501	GTP	C4-C5-N7	-2.59	106.70	109.40
10	B	504	MES	O3S-S-O1S	-2.57	105.01	111.27
5	D	501	GTP	C2-N3-C4	-2.53	112.47	115.36
9	B	503	GDP	C4-C5-N7	-2.47	106.83	109.40
8	B	501	H1C	C08-N10-C11	-2.38	124.15	127.67
9	B	503	GDP	PA-O3A-PB	-2.38	124.68	132.83
11	F	401	ACP	PA-O3A-PB	-2.32	125.22	132.56
5	C	501	GTP	O5'-PA-O1A	2.27	117.94	109.07
5	A	501	GTP	PA-O3A-PB	-2.25	125.12	132.83
5	A	501	GTP	C6-N1-C2	2.24	119.49	115.93
5	D	501	GTP	O4'-C1'-C2'	-2.24	103.65	106.93
10	B	504	MES	O1S-S-C8	2.18	109.55	106.92
5	C	501	GTP	O3'-C3'-C4'	-2.17	104.78	111.05
10	B	504	MES	C7-N4-C3	2.16	116.75	111.23
5	D	501	GTP	N3-C2-N1	-2.11	124.41	127.22
5	C	501	GTP	C4-C5-N7	-2.10	107.21	109.40
5	C	501	GTP	O3G-PG-O1G	2.07	118.79	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	H1C	C01-C02-C03	-2.00	118.32	120.84

There are no chirality outliers.

All (27) torsion outliers are listed below:

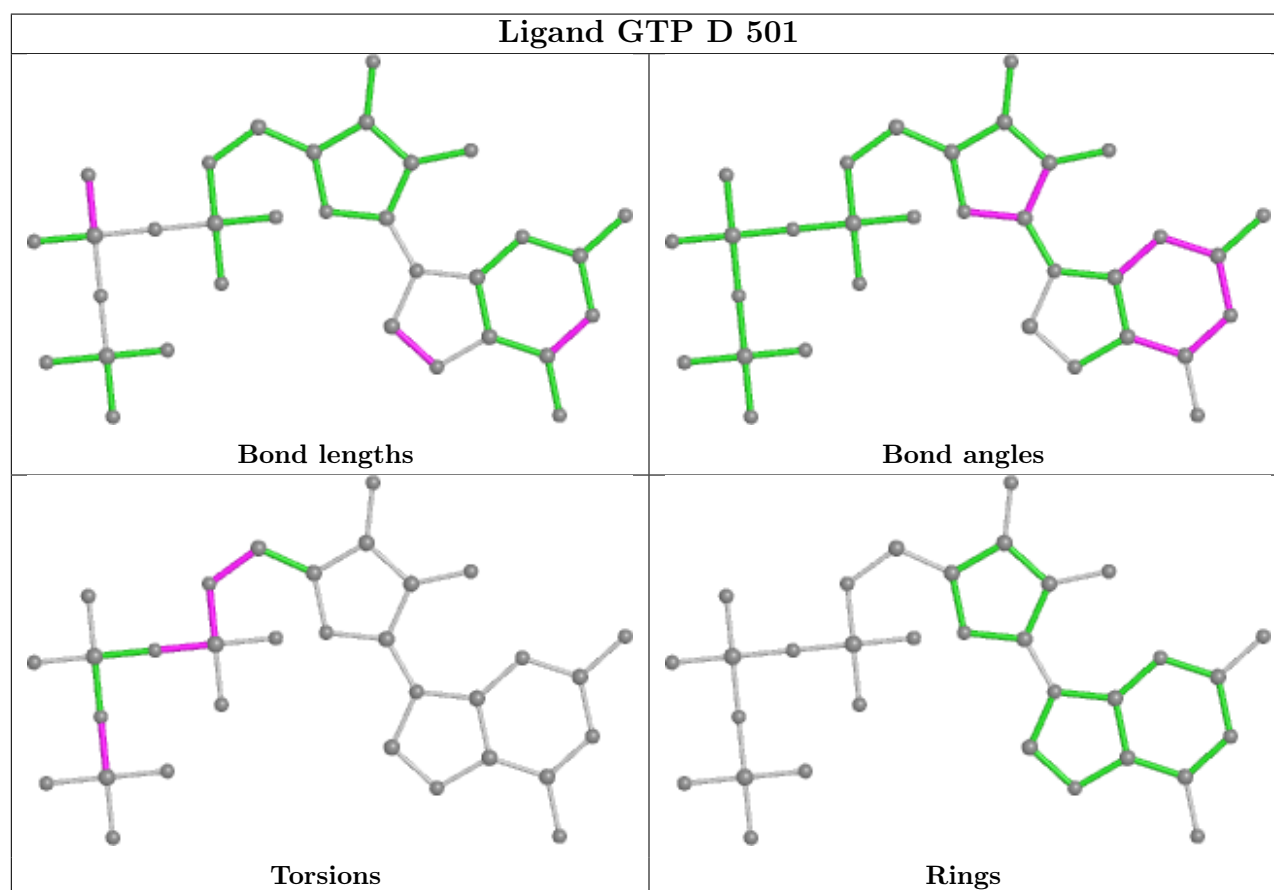
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	503	GDP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C3'-C4'-C5'-O5'
5	D	501	GTP	PB-O3B-PG-O1G
10	B	504	MES	C8-C7-N4-C5
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
9	B	503	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
9	B	503	GDP	C5'-O5'-PA-O3A
8	B	501	H1C	C01-C06-C15-C16
8	B	501	H1C	C05-C06-C15-C16
5	D	501	GTP	C4'-C5'-O5'-PA

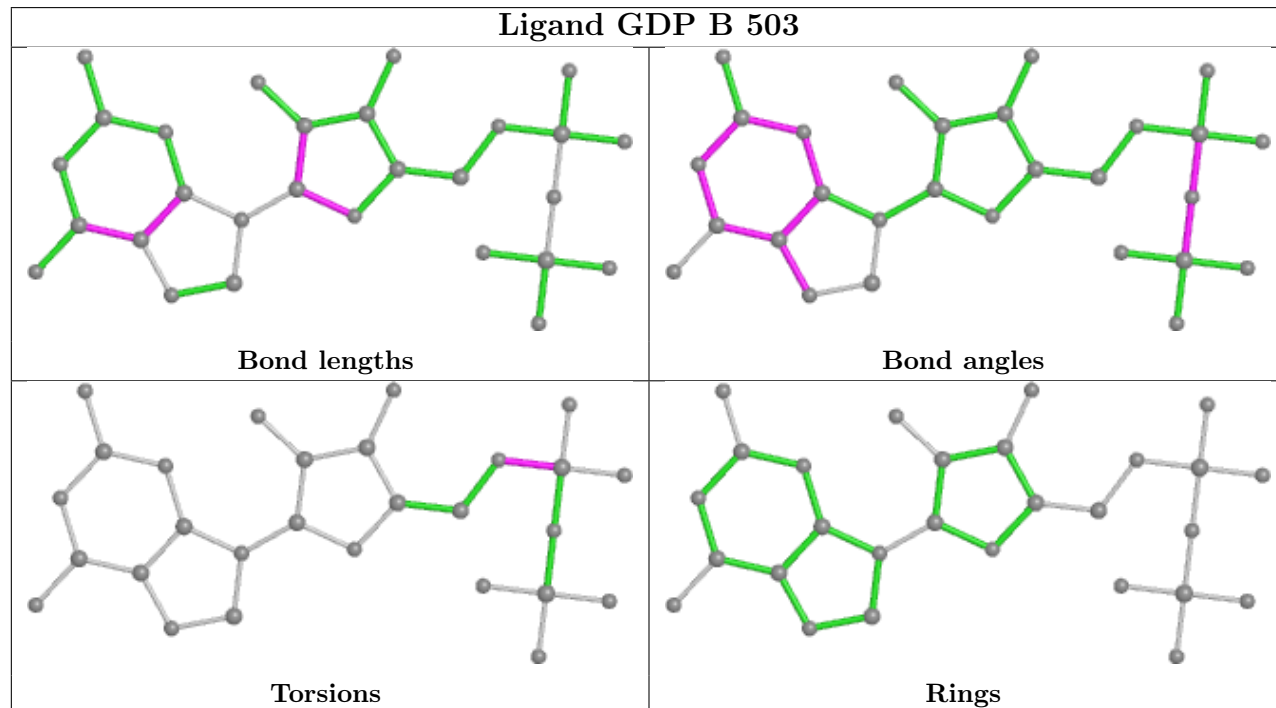
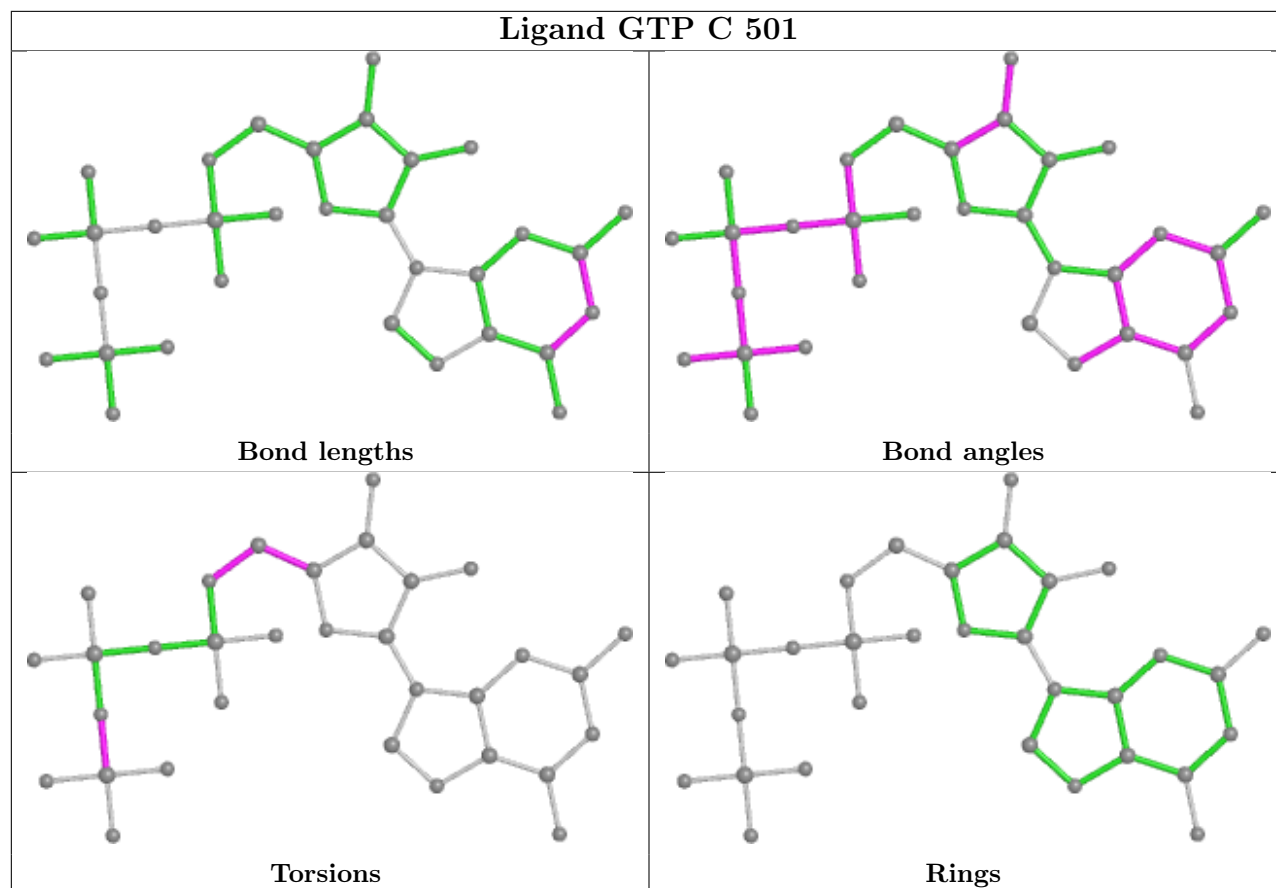
There are no ring outliers.

3 monomers are involved in 4 short contacts:

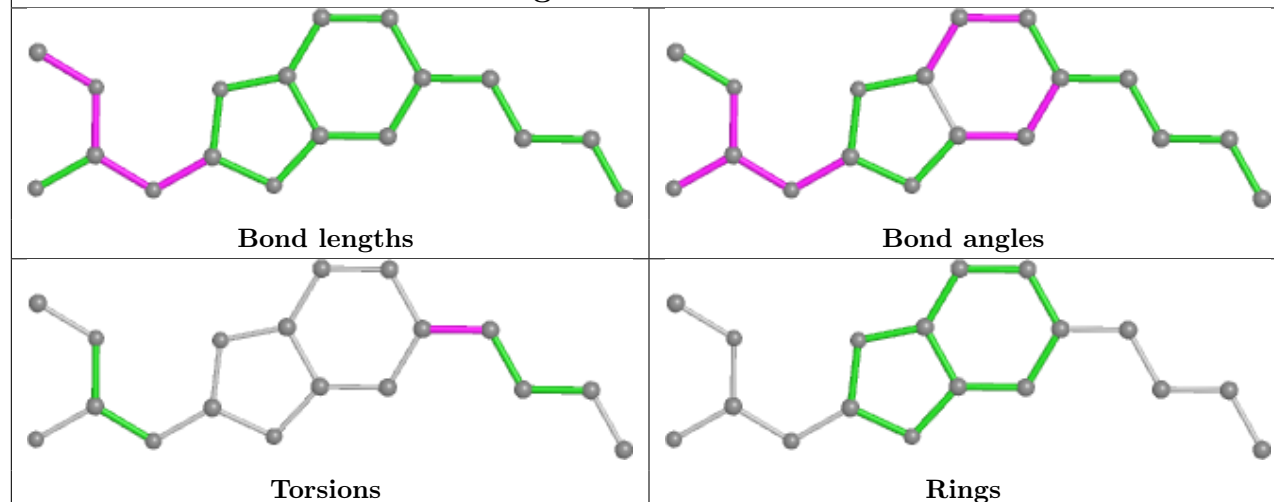
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	2	0
9	B	503	GDP	1	0
11	F	401	ACP	1	0

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.

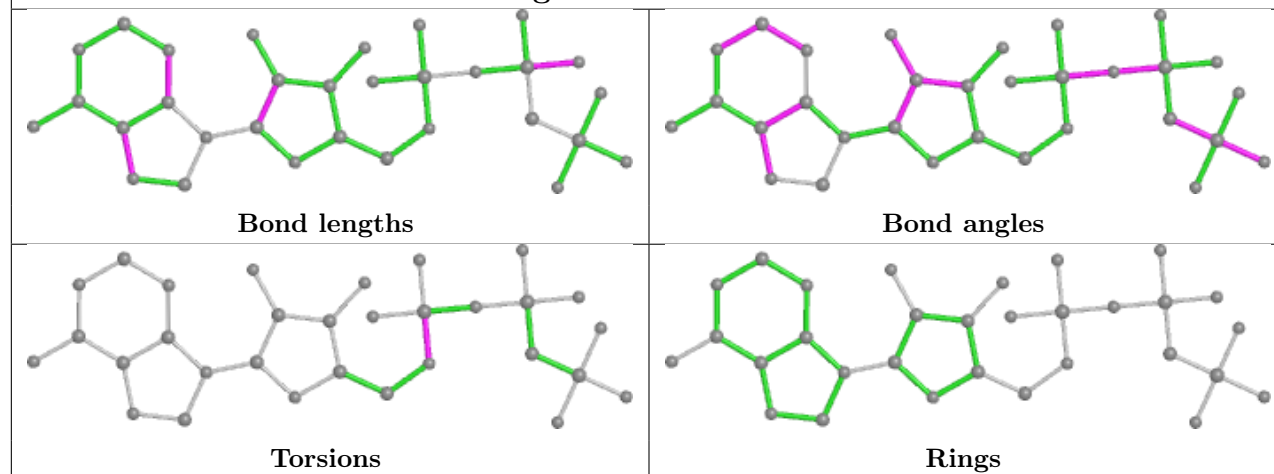


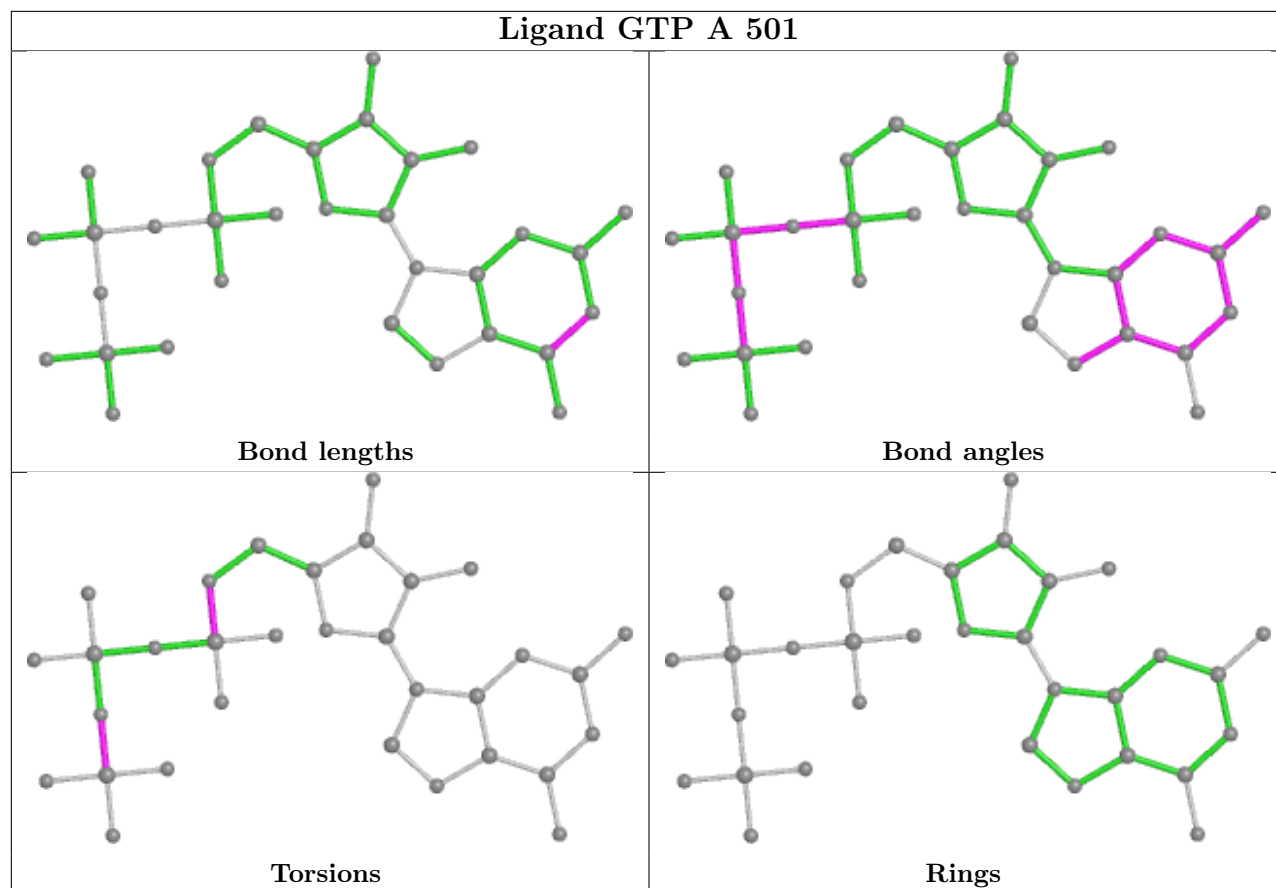


Ligand H1C B 501



Ligand ACP F 401





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	438/451 (97%)	-0.16	8 (1%) 68 66	31, 46, 69, 91	0
1	C	441/451 (97%)	-0.32	7 (1%) 72 70	26, 38, 58, 96	0
2	B	426/445 (95%)	0.03	23 (5%) 25 24	28, 46, 79, 106	0
2	D	421/445 (94%)	0.27	24 (5%) 23 22	36, 64, 103, 123	2 (0%)
3	E	123/143 (86%)	0.59	16 (13%) 3 3	36, 61, 103, 128	0
4	F	338/384 (88%)	0.74	59 (17%) 1 1	39, 72, 128, 140	0
All	All	2187/2319 (94%)	0.11	137 (6%) 20 18	26, 50, 103, 140	2 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	55	THR	7.1
4	F	169	LEU	6.2
4	F	248	GLU	6.2
4	F	142	ARG	6.2
4	F	141	GLY	6.2
4	F	372	THR	5.5
2	B	428	ALA	5.1
4	F	140	GLU	4.8
4	F	234	GLN	4.6
2	B	429	THR	4.5
1	A	282	TYR	4.5
3	E	140	GLU	4.4
2	D	37	HIS	4.3
4	F	137	ARG	4.3
3	E	25	PRO	4.2
4	F	253	TYR	4.2
2	D	1	MET	4.2
4	F	173	ILE	4.1
4	F	232	ASN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	4.1
2	D	390	ARG	4.1
2	D	431	ASP	4.0
4	F	148	ILE	4.0
3	E	139	GLU	4.0
4	F	231	ALA	4.0
3	E	46	GLU	3.8
4	F	165	GLU	3.8
2	D	95	SER	3.7
4	F	10	ASN	3.7
4	F	143	GLU	3.7
4	F	379	HIS	3.7
1	A	438	ASP	3.6
2	B	244	GLY	3.6
2	B	247	ASN	3.6
4	F	45	ASN	3.6
4	F	233	PHE	3.6
1	C	441	GLU	3.6
1	A	281	ALA	3.5
1	C	1	MET	3.4
3	E	141	ALA	3.4
4	F	255	ARG	3.4
1	C	245	ASP	3.4
4	F	224	SER	3.4
1	A	163	LYS	3.3
4	F	90	SER	3.3
4	F	244	CYS	3.3
4	F	147	TRP	3.2
4	F	199	PHE	3.2
2	D	125	GLU	3.2
2	D	284	LEU	3.2
2	D	73	MET	3.2
4	F	25	GLY	3.2
3	E	44	SER	3.1
2	B	276	ARG	3.1
4	F	250	SER	3.1
2	B	80	PRO	3.0
4	F	158	GLU	3.0
2	D	83	GLN	3.0
4	F	101	TYR	3.0
2	B	427	ASP	3.0
4	F	159	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	168	GLU	2.9
2	B	56	GLY	2.9
4	F	249	TYR	2.9
2	D	55	THR	2.9
3	E	138	LYS	2.9
4	F	182	ILE	2.9
4	F	24	THR	2.9
1	C	440	VAL	2.8
2	D	219	THR	2.8
4	F	180	HIS	2.8
4	F	89	GLU	2.8
4	F	162	ILE	2.7
3	E	26	SER	2.7
2	B	57	ASN	2.7
1	A	346	TRP	2.7
4	F	380	HIS	2.7
4	F	198	LYS	2.7
2	B	275	SER	2.7
3	E	42	ASP	2.7
2	B	33	THR	2.6
3	E	43	PRO	2.6
4	F	225	SER	2.6
2	D	92	PHE	2.6
4	F	362	ALA	2.6
2	D	397	TRP	2.6
4	F	9	GLU	2.6
4	F	139	ARG	2.6
2	B	243	PRO	2.5
4	F	100	ILE	2.5
4	F	252	ASN	2.5
1	A	262	TYR	2.5
4	F	130	VAL	2.5
1	C	340	SER	2.5
4	F	251	LYS	2.5
3	E	4	MET	2.5
4	F	171	ASP	2.5
2	B	72	THR	2.5
4	F	172	PHE	2.4
2	B	39	ASP	2.4
4	F	247	LYS	2.4
2	B	37	HIS	2.4
2	D	102	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	137	LEU	2.3
3	E	126	LYS	2.3
2	B	274	THR	2.3
2	B	277	GLY	2.3
2	D	429	THR	2.3
1	A	345	ASP	2.3
2	D	65	LEU	2.3
3	E	24	PRO	2.3
4	F	149	ALA	2.3
4	F	136	ASN	2.2
2	D	216	LYS	2.2
3	E	120	ARG	2.2
2	D	183	TYR	2.2
1	C	218	ASP	2.2
4	F	167	SER	2.2
1	C	46	ASP	2.2
2	B	320	ARG	2.2
4	F	373	SER	2.2
2	D	126	SER	2.2
2	B	54	ALA	2.1
2	D	57	ASN	2.1
4	F	39	LEU	2.1
4	F	181	VAL	2.1
1	A	220	GLU	2.1
2	B	218	THR	2.1
2	D	64	ILE	2.1
3	E	5	GLU	2.1
4	F	235	ASP	2.0
2	D	214	THR	2.0
2	D	142	GLY	2.0
4	F	341	LYS	2.0
2	B	128	ASP	2.0
2	D	41	ASP	2.0
2	B	125	GLU	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

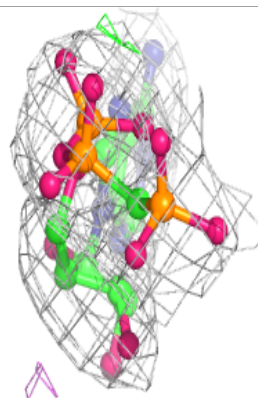
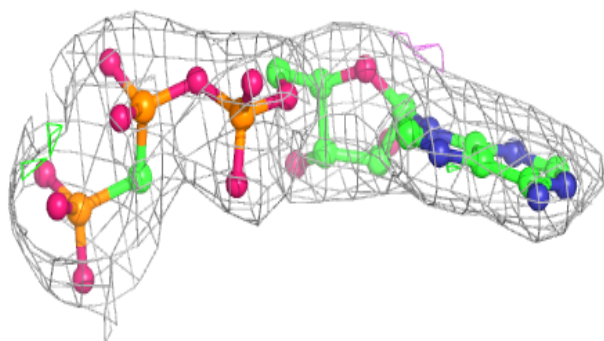
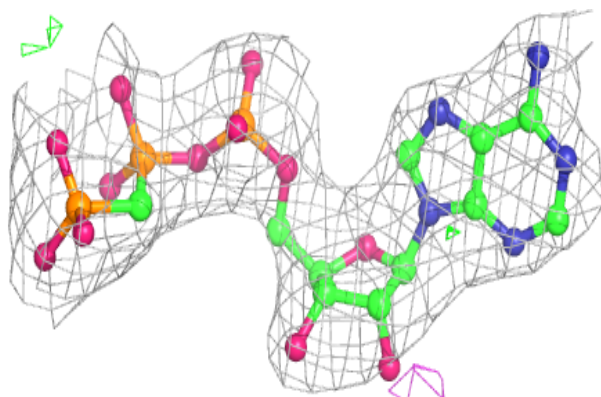
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	B	502	1/1	0.41	0.15	41,41,41,41	0
6	MG	D	502	1/1	0.75	0.29	85,85,85,85	0
6	MG	A	502	1/1	0.77	0.11	32,32,32,32	0
6	MG	F	402	1/1	0.83	0.08	97,97,97,97	0
11	ACP	F	401	31/31	0.87	0.16	74,89,102,103	0
8	H1C	B	501	18/18	0.88	0.17	43,52,56,57	0
5	GTP	D	501	32/32	0.88	0.21	65,74,109,144	0
7	CA	C	503	1/1	0.89	0.11	52,52,52,52	0
6	MG	C	502	1/1	0.94	0.07	28,28,28,28	0
10	MES	B	504	12/12	0.95	0.11	41,47,68,69	0
7	CA	A	503	1/1	0.95	0.13	67,67,67,67	0
9	GDP	B	503	28/28	0.98	0.10	28,36,39,45	0
5	GTP	C	501	32/32	0.98	0.11	25,30,34,36	0
5	GTP	A	501	32/32	0.98	0.09	28,34,38,39	0

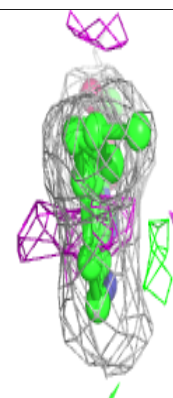
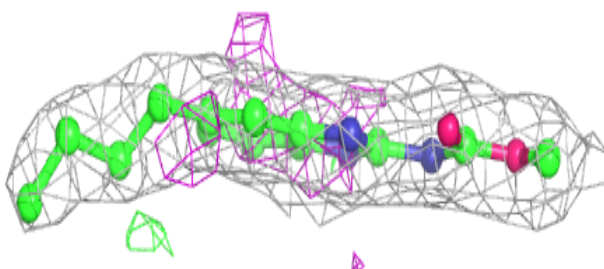
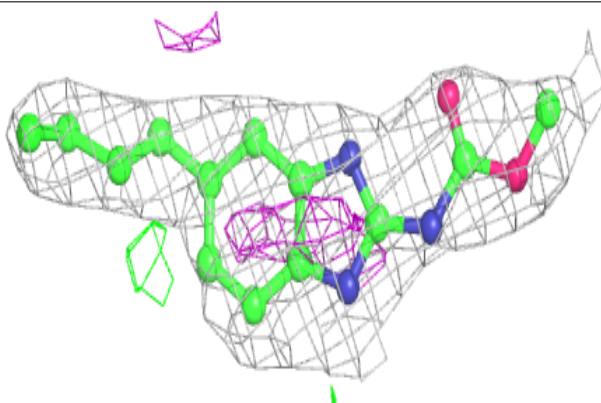
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

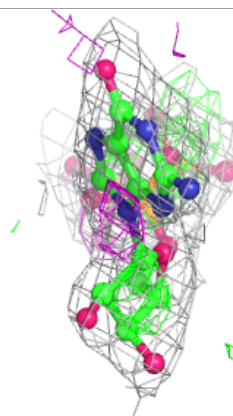
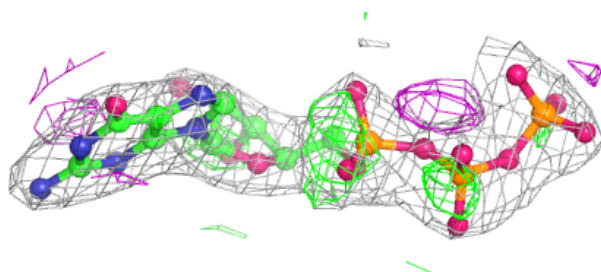
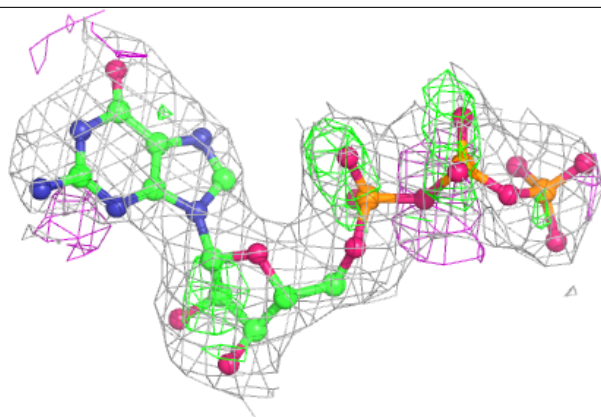
**Electron density around H1C B 501:**

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

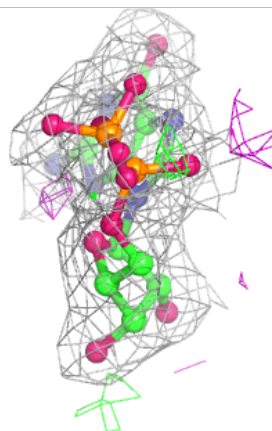
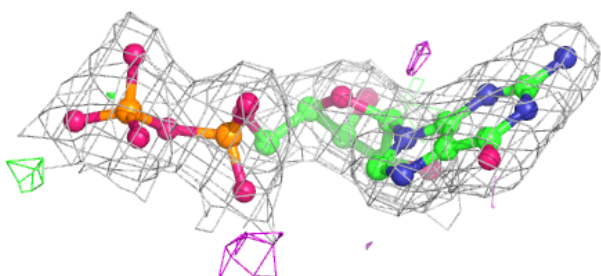
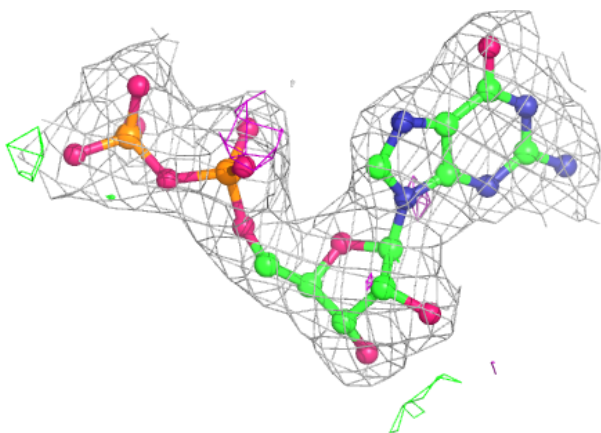


Electron density around GTP D 501:

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

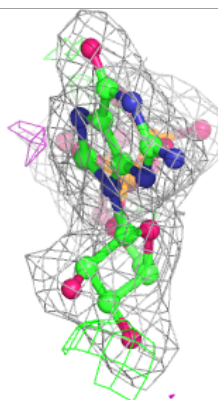
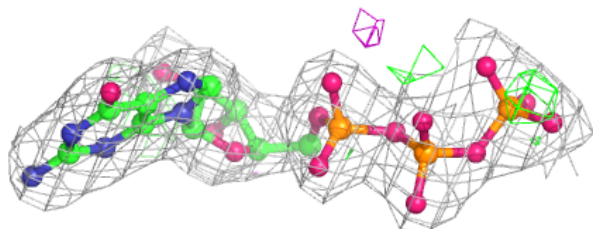
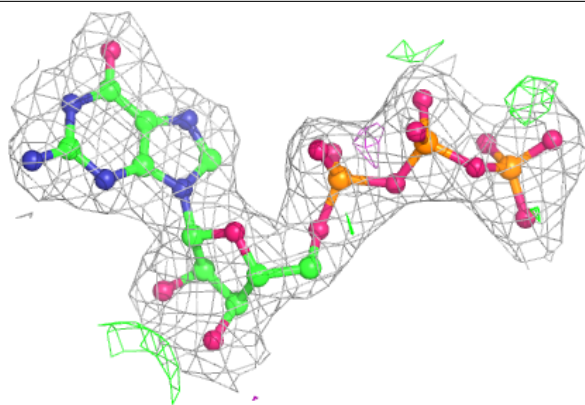
**Electron density around GDP B 503:**

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

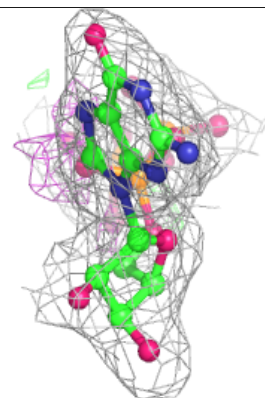
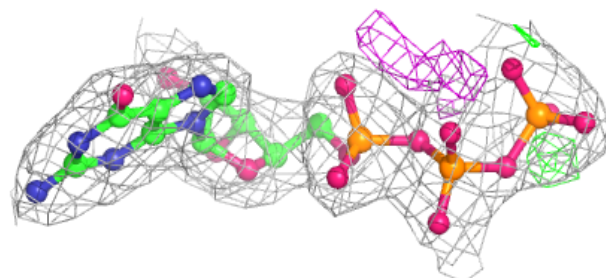
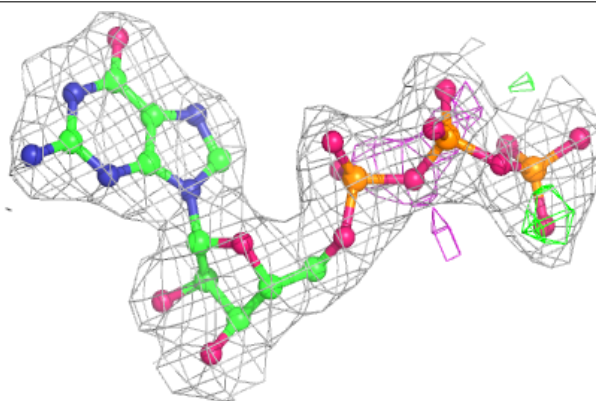


Electron density around GTP C 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.