



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2020 – 01:50 PM BST

PDB ID : 5LA6
Title : Tubulin-pironetin complex
Authors : Prota, A.E.; Setter, J.; Waight, A.B.; Bargsten, K.; Murga, J.; Diaz, J.F.; Steinmetz, M.O.
Deposited on : 2016-06-13
Resolution : 2.10 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 : 2.14.3.dev2
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) : 2.14.3.dev2

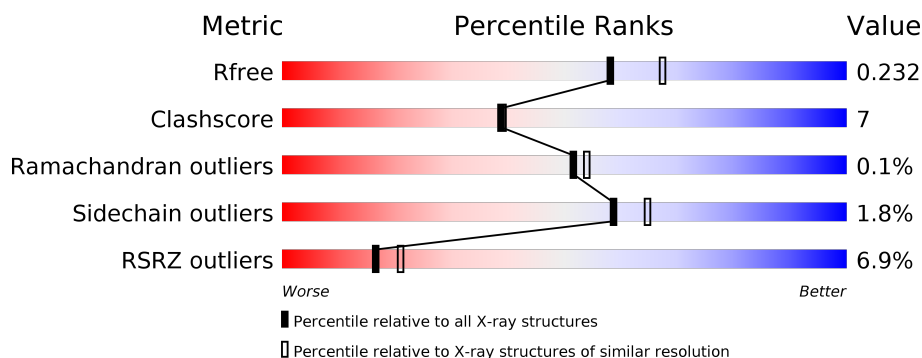
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
2	D	445	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>5%</div> </div> </div>
3	E	143	<div> <div>9%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>• 14%</div> </div> </div>
4	F	384	<div> <div>20%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17925 atoms, of which 32 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	432	Total	C	N	O	S	0	1	0
			3385	2143	575	644	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	2	0
			3329	2096	566	641	26			
2	D	421	Total	C	N	O	S	0	0	0
			3308	2079	562	641	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	350	Total	C	N	O	S	0	0	0
			2858	1831	490	523	14			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

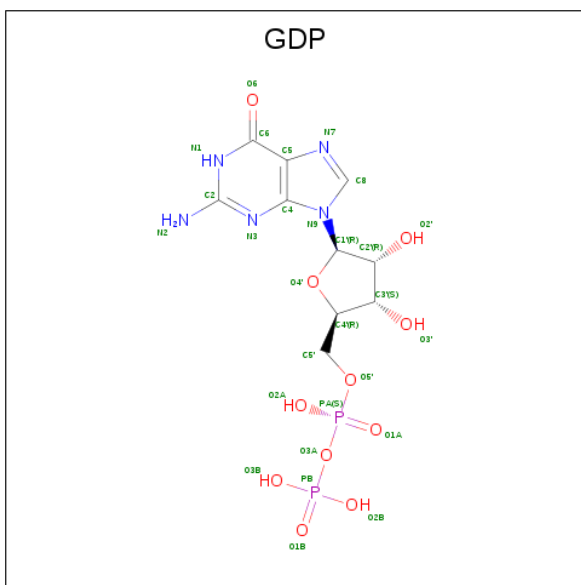
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	C	1	Total	Mg	0	0
			1	1		

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

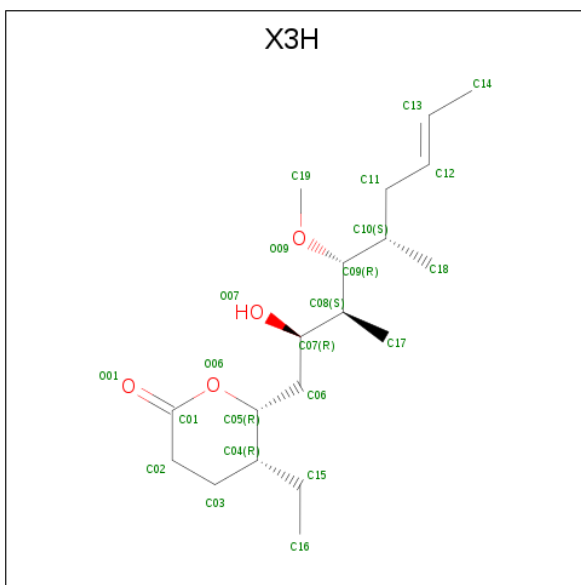
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



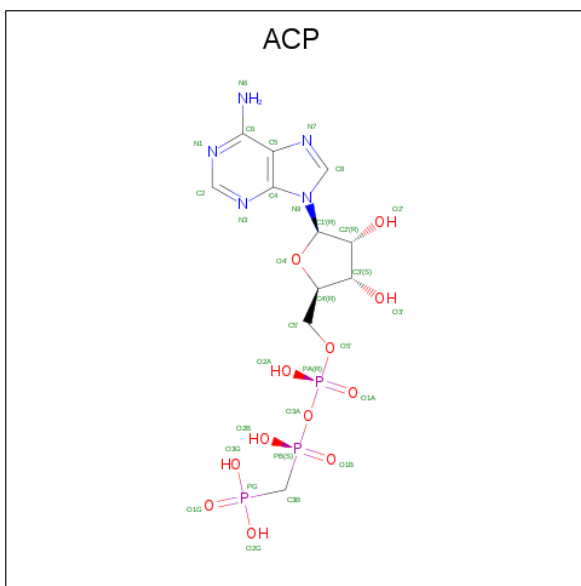
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is PIRONETIN (three-letter code: X3H) (formula: $C_{19}H_{34}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			55	19	32	4		

- Molecule 10 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
10	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

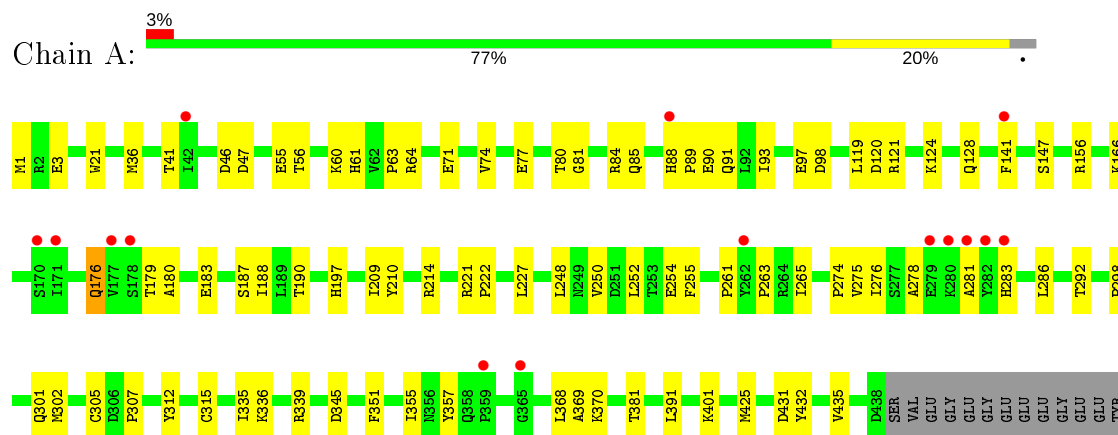
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	73	Total 73	O 73	0	0
11	B	67	Total 67	O 67	0	0
11	C	159	Total 159	O 159	0	0
11	D	51	Total 51	O 51	0	0
11	E	8	Total 8	O 8	0	0
11	F	30	Total 30	O 30	0	0

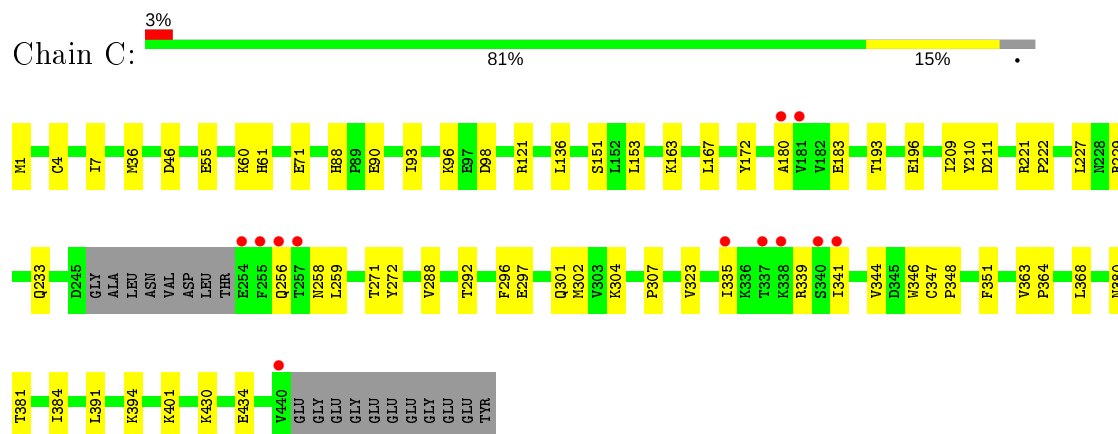
3 Residue-property plots [i](#)

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.

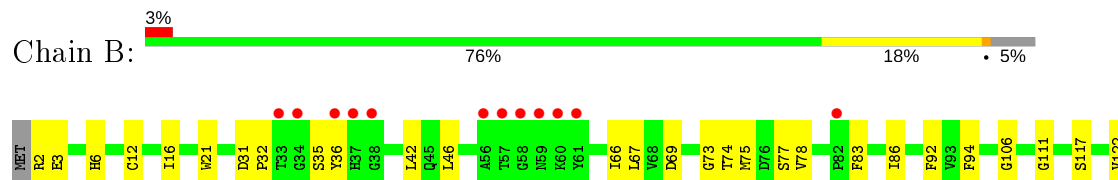
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

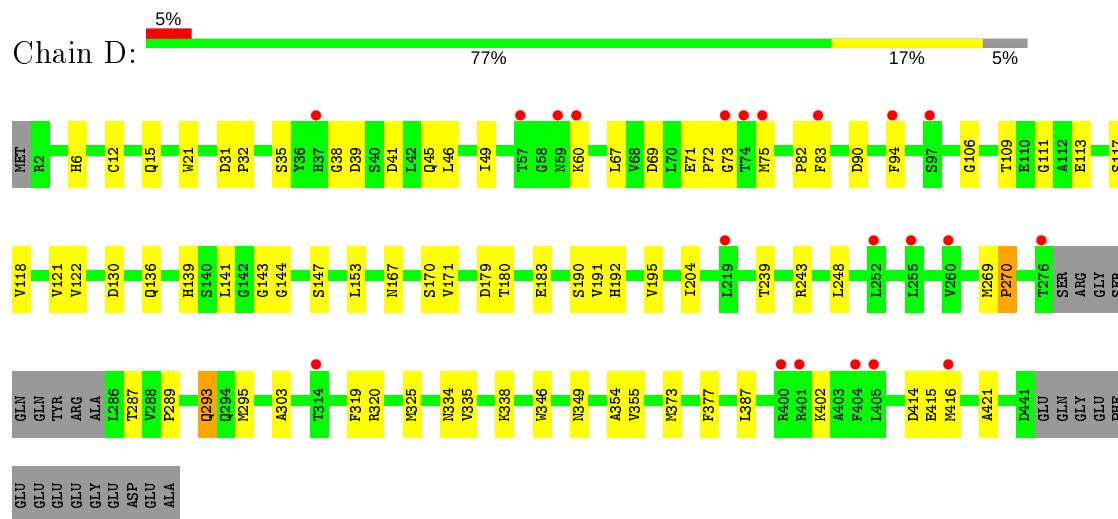


- Molecule 2: Tubulin beta-2B chain

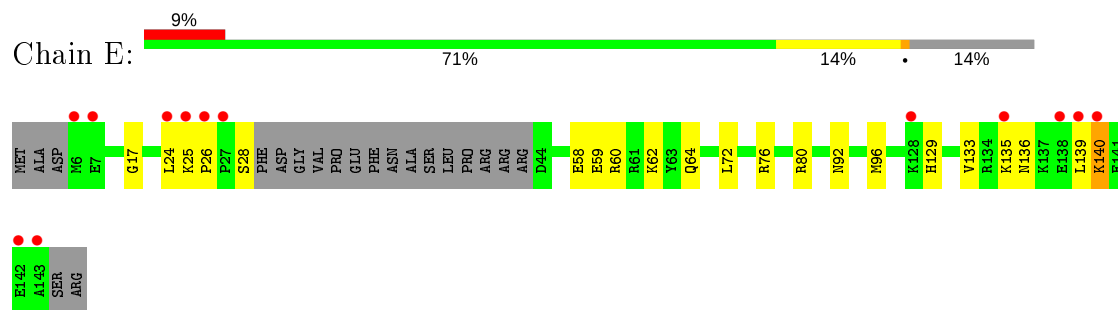




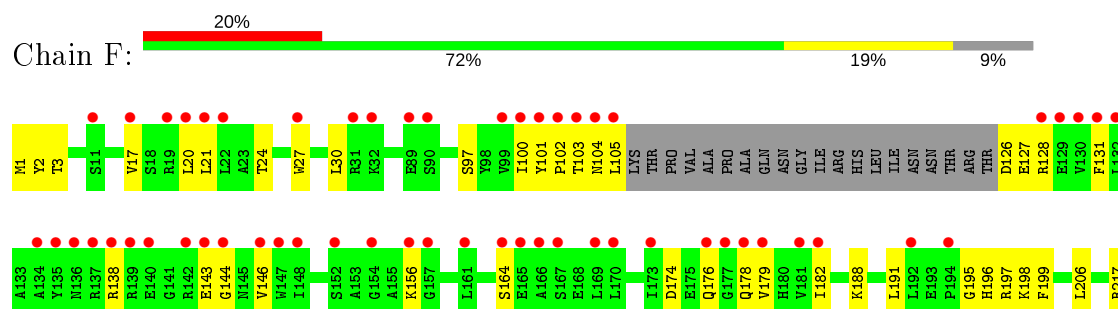
- Molecule 2: Tubulin beta-2B chain

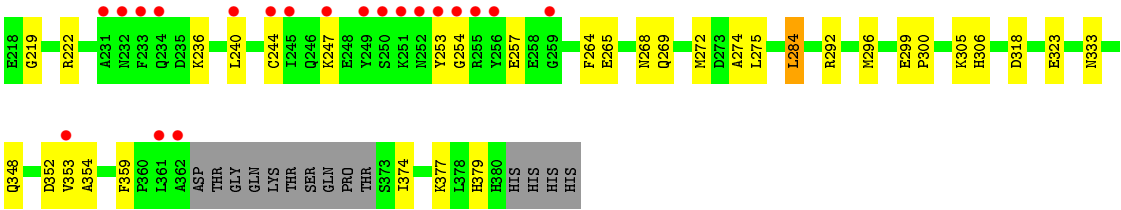


- Molecule 3: Stathmin-4



- Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.68Å 157.20Å 180.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 – 2.10 48.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.27-2.10) 100.0 (48.27-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.184 , 0.231 0.188 , 0.232	Depositor DCC
R_{free} test set	8728 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17925	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CA, GTP, ACP, X3H

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	0.35	0/3514	0.49	0/4770
1	C	0.43	0/3465	0.54	0/4701
2	B	0.37	0/3409	0.50	0/4618
2	D	0.32	0/3381	0.48	0/4581
3	E	0.32	0/1022	0.42	0/1356
4	F	0.28	0/2923	0.45	0/3948
All	All	0.36	0/17714	0.49	0/23974

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3345	62	0
1	C	3385	0	3295	45	0
2	B	3329	0	3213	57	0
2	D	3308	0	3184	46	0
3	E	1014	0	1029	15	0
4	F	2858	0	2826	48	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	3	0
9	C	23	32	0	0	0
10	F	31	0	14	2	0
11	A	73	0	0	3	0
11	B	67	0	0	1	0
11	C	159	0	0	4	0
11	D	51	0	0	1	0
11	E	8	0	0	1	0
11	F	30	0	0	2	0
All	All	17893	32	16954	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (257) 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:A:221:ARG:HG2	2:B:325:MET:HG2	1.55	0.89
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.55	0.89
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.65	0.79
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.48	0.77
4:F:101:TYR:HB3	4:F:105:LEU:HD22	1.67	0.76
1:C:221:ARG:HG3	2:D:325:MET:HG3	1.66	0.76
3:E:80:ARG:NH2	11:E:201:HOH:O	2.20	0.73
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.71	0.73
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.32	0.69
1:A:221:ARG:HG2	2:B:325:MET:CG	2.22	0.69
1:A:370:LYS:NZ	11:A:601:HOH:O	2.25	0.68
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.09	0.67
1:C:221:ARG:HG3	2:D:325:MET:CG	2.25	0.67
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.78	0.66
1:C:1:MET:O	11:C:601:HOH:O	2.15	0.65
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:LEU:HD21	2:B:415:GLU:HG2	1.78	0.65
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.31	0.65
1:C:151:SER:HB3	1:C:193:THR:HG21	1.79	0.65
1:C:196:GLU:OE1	11:C:602:HOH:O	2.15	0.65
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.30	0.64
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.32	0.64
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.62	0.64
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.63
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.14	0.63
2:D:191:VAL:O	2:D:195:VAL:HG23	1.97	0.63
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.63	0.63
1:A:209:ILE:HD11	1:A:302:MET:SD	2.38	0.62
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.34	0.62
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.80	0.62
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.80	0.61
8:D:501:GDP:O3B	11:D:601:HOH:O	2.16	0.61
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.82	0.61
2:B:239:THR:O	2:B:243:ARG:HG3	2.01	0.61
4:F:217:ARG:NH1	4:F:374:ILE:HG22	2.16	0.61
1:C:297:GLU:HG2	1:C:339:ARG:HH22	1.64	0.61
2:D:414:ASP:OD2	2:D:416:MET:HB3	2.01	0.60
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.82	0.60
2:B:75:MET:CE	2:B:92:PHE:HB3	2.31	0.60
2:B:42:LEU:HD12	2:B:42:LEU:H	1.67	0.60
1:C:209:ILE:HD11	1:C:302:MET:SD	2.42	0.60
1:A:166:LYS:HE2	1:A:197:HIS:O	2.01	0.59
2:D:106:GLY:O	2:D:111:GLY:HA3	2.01	0.59
1:C:430:LYS:HE2	1:C:434:GLU:OE1	2.02	0.59
2:D:147:SER:HB2	2:D:190:SER:OG	2.03	0.59
2:B:338:LYS:HE3	4:F:1:MET:HB3	1.83	0.59
4:F:265:GLU:O	11:F:601:HOH:O	2.17	0.58
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.30	0.58
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.85	0.58
4:F:333:ASN:ND2	10:F:501:ACP:O1G	2.32	0.58
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.39	0.57
1:C:163:LYS:HE3	11:C:619:HOH:O	2.05	0.57
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.34	0.57
1:A:305:CYS:O	1:A:307:PRO:HD3	2.05	0.56
2:D:180:THR:O	2:D:183:GLU:HG3	2.05	0.56
2:B:141:LEU:HD12	2:B:172:MET:SD	2.45	0.56
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.36	0.56
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.89	0.55
1:A:77:GLU:HA	1:A:80:THR:HG22	1.89	0.55
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.36	0.55
1:C:46:ASP:OD1	1:C:46:ASP:N	2.39	0.55
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.36	0.55
1:A:345:ASP:O	3:E:28:SER:N	2.34	0.55
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.42	0.55
4:F:188:LYS:HD3	4:F:323:GLU:OE1	2.05	0.55
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.88	0.54
1:A:431:ASP:O	1:A:435:VAL:HG23	2.07	0.54
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.89	0.54
2:D:319:PHE:HB2	2:D:355:VAL:HG22	1.89	0.54
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.38	0.54
2:D:136:GLN:HA	2:D:167:ASN:O	2.07	0.53
3:E:92:ASN:O	3:E:96:MET:HG2	2.08	0.53
2:B:124:LYS:C	2:B:124:LYS:HD3	2.29	0.53
2:B:231:VAL:O	2:B:235:MET:HG3	2.09	0.53
1:C:296:PHE:HZ	1:C:351:PHE:HE2	1.57	0.53
3:E:136:ASN:O	3:E:140:LYS:HD2	2.09	0.52
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.43	0.52
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.37	0.52
2:B:171:VAL:HA	2:B:204:ILE:O	2.09	0.52
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.44	0.52
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.91	0.52
1:A:180:ALA:O	1:A:183:GLU:HG3	2.10	0.52
1:A:56:THR:CG2	1:A:60:LYS:HB3	2.39	0.52
2:B:146:GLY:O	2:B:150:GLY:HA3	2.10	0.52
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.45	0.52
2:D:109:THR:O	2:D:113:GLU:HG2	2.09	0.51
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.35	0.51
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.46	0.51
2:D:118:VAL:CG1	2:D:153:LEU:HD21	2.40	0.51
1:A:298:PRO:HA	1:A:301:GLN:CD	2.31	0.51
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.92	0.51
4:F:102:PRO:O	4:F:105:LEU:HD13	2.11	0.51
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.92	0.51
1:A:1:MET:HB3	1:A:46:ASP:HB2	1.93	0.51
2:D:239:THR:O	2:D:243:ARG:HG3	2.11	0.51
4:F:126:ASP:OD1	4:F:127:GLU:N	2.43	0.51
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.94	0.50
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.50
4:F:217:ARG:HB2	4:F:374:ILE:O	2.11	0.50
1:A:97:GLU:OE2	2:B:2:ARG:NH2	2.45	0.50
2:D:118:VAL:O	2:D:122:VAL:HG23	2.12	0.50
2:D:118:VAL:HG11	2:D:153:LEU:HD21	1.94	0.50
4:F:274:ALA:C	4:F:275:LEU:HD23	2.32	0.50
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.50
1:A:141:PHE:O	1:A:147:SER:HB3	2.12	0.49
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.11	0.49
2:B:405:LEU:CD2	2:B:415:GLU:HG2	2.41	0.49
3:E:72:LEU:O	3:E:76:ARG:HG2	2.12	0.49
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.47	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.49
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.42	0.49
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.40	0.49
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.47	0.49
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
1:A:210:TYR:OH	1:A:221:ARG:HD2	2.13	0.49
4:F:3:THR:HB	4:F:30:LEU:HD11	1.95	0.49
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.33	0.49
1:A:60:LYS:NZ	1:A:85:GLN:O	2.42	0.49
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.95	0.49
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.32	0.48
2:B:74:THR:HB	11:B:628:HOH:O	2.12	0.48
1:C:180:ALA:O	1:C:183:GLU:HG3	2.12	0.48
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.95	0.48
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.96	0.48
3:E:129:HIS:O	3:E:133:VAL:HG23	2.13	0.48
1:C:347:CYS:HB2	1:C:348:PRO:HD2	1.95	0.48
1:A:276:ILE:HD12	1:A:283:HIS:CE1	2.48	0.48
2:D:144:GLY:HA3	8:D:501:GDP:O3B	2.14	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.48
1:C:335:ILE:HG22	1:C:341:ILE:HD12	1.96	0.47
4:F:217:ARG:HH12	4:F:374:ILE:HG22	1.79	0.47
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.49	0.47
2:B:302:MET:HA	2:B:302:MET:HE2	1.97	0.47
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.14	0.47
2:B:67:LEU:HD12	2:B:67:LEU:N	2.30	0.47
2:D:35:SER:OG	2:D:60:LYS:HE2	2.15	0.47
2:D:46:LEU:HA	2:D:49:ILE:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
2:B:276:THR:OG1	2:B:277:SER:N	2.48	0.47
1:A:1:MET:CB	1:A:46:ASP:HB2	2.45	0.46
4:F:292:ARG:O	4:F:296:MET:HG2	2.15	0.46
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.15	0.46
1:C:151:SER:HB3	1:C:193:THR:CG2	2.45	0.46
1:C:301:GLN:OE1	1:C:307:PRO:HG2	2.15	0.46
1:A:176:GLN:HB2	11:A:648:HOH:O	2.14	0.46
2:B:180:THR:HG22	1:C:258:ASN:HD21	1.80	0.46
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.46
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.50	0.46
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.97	0.46
2:B:318:ILE:N	2:B:318:ILE:HD12	2.31	0.46
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.46
2:B:409:THR:HA	2:B:413:MET:O	2.16	0.46
1:A:90:GLU:HG2	1:A:124:LYS:NZ	2.31	0.46
4:F:268:ASN:HB3	11:F:601:HOH:O	2.15	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.45
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.31	0.45
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.52	0.45
2:B:324:SER:HB3	2:B:327:GLU:HB3	1.99	0.45
2:D:402:LYS:HE2	2:D:415:GLU:OE2	2.17	0.45
4:F:104:ASN:C	4:F:105:LEU:HD12	2.37	0.45
4:F:269:GLN:HA	4:F:272:MET:HE2	1.98	0.45
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.52	0.45
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.98	0.45
4:F:2:TYR:HB3	4:F:27:TRP:CZ3	2.52	0.45
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.17	0.45
1:C:394:LYS:NZ	2:D:349:ASN:HD21	2.15	0.45
1:C:288:VAL:HG22	1:C:323:VAL:HG22	1.99	0.45
1:A:210:TYR:CD2	1:A:214:ARG:HD2	2.52	0.45
4:F:176:GLN:HB3	4:F:178:GLN:HE21	1.81	0.45
4:F:284:LEU:HA	4:F:284:LEU:HD12	1.81	0.45
2:B:191:VAL:O	2:B:195:VAL:HG23	2.17	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.44
4:F:318:ASP:OD2	10:F:501:ACP:O3G	2.34	0.44
1:A:81:GLY:O	1:A:84:ARG:HB3	2.18	0.44
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.98	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.52	0.44
2:D:192:HIS:CG	2:D:421:ALA:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:236:LYS:HB3	4:F:240:LEU:HD12	1.99	0.44
4:F:20:LEU:O	4:F:24:THR:HG23	2.18	0.44
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.98	0.44
4:F:138:ARG:NH1	4:F:143:GLU:HB3	2.33	0.44
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.83	0.43
1:C:259:LEU:O	1:C:380:ASN:ND2	2.44	0.43
1:C:292:THR:HG22	1:C:335:ILE:HD11	2.00	0.43
2:D:293:GLN:HB2	2:D:293:GLN:HE21	1.68	0.43
2:B:75:MET:HE1	2:B:92:PHE:HB3	2.00	0.43
1:C:271:THR:HG22	1:C:272:TYR:N	2.34	0.43
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.19	0.43
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.53	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.43
1:C:229:ARG:HD2	11:C:605:HOH:O	2.19	0.43
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.52	0.43
2:B:269:MET:HE2	2:B:301:MET:SD	2.58	0.43
2:B:431:GLU:O	2:B:434:GLN:HB3	2.19	0.43
4:F:17:VAL:O	4:F:21:LEU:HG	2.18	0.43
2:B:234:THR:O	2:B:238:VAL:HG13	2.19	0.43
2:B:323:MET:HB3	2:B:373:MET:HE1	1.99	0.43
2:B:83:PHE:O	2:B:86:ILE:HG22	2.19	0.43
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.99	0.43
2:B:12:CYS:HB3	2:B:140:SER:HB3	2.01	0.42
2:B:212:ILE:HG23	2:B:275:LEU:HD13	2.00	0.42
2:B:323:MET:HB3	2:B:373:MET:CE	2.48	0.42
4:F:198:LYS:HG2	4:F:199:PHE:N	2.34	0.42
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.54	0.42
1:A:252:LEU:O	1:A:255:PHE:HB2	2.19	0.42
2:D:143:GLY:HA3	2:D:144:GLY:HA3	1.79	0.42
2:B:3:GLU:N	2:B:3:GLU:OE2	2.49	0.42
1:A:55:GLU:HA	1:A:60:LYS:O	2.19	0.42
4:F:156:LYS:HB3	4:F:244:CYS:SG	2.60	0.42
1:A:56:THR:HG23	1:A:60:LYS:HB3	2.01	0.42
2:D:320:ARG:O	2:D:373:MET:HA	2.19	0.42
3:E:60:ARG:O	3:E:64:GLN:HG3	2.19	0.42
1:C:163:LYS:HD2	1:C:163:LYS:HA	1.91	0.42
4:F:247:LYS:HA	4:F:253:TYR:CD1	2.55	0.42
4:F:377:LYS:HE2	4:F:379:HIS:HD2	1.85	0.42
1:A:315[A]:CYS:HG	1:A:351:PHE:HE2	1.65	0.41
1:C:167:LEU:HD12	1:C:167:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:HG13	1:C:364:PRO:HD2	2.02	0.41
4:F:305:LYS:HE2	4:F:306:HIS:NE2	2.35	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.55	0.41
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.20	0.41
1:A:261:PRO:O	1:A:263:PRO:HD3	2.20	0.41
2:D:75:MET:CE	2:D:94:PHE:HD2	2.33	0.41
3:E:25:LYS:HA	3:E:26:PRO:HD3	1.79	0.41
4:F:138:ARG:NH1	4:F:144:GLY:O	2.53	0.41
2:B:288:VAL:N	2:B:289:PRO:CD	2.84	0.41
1:C:55:GLU:HA	1:C:60:LYS:O	2.20	0.41
2:D:71:GLU:HA	2:D:72:PRO:HD3	1.75	0.41
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.80	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.55	0.41
1:C:335:ILE:HG22	1:C:341:ILE:CD1	2.49	0.41
2:B:306:ASP:HB3	2:B:309:HIS:CG	2.55	0.41
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.21	0.41
4:F:254:GLY:HA2	4:F:257:GLU:O	2.21	0.41
2:B:74:THR:O	2:B:78:VAL:HG23	2.21	0.41
2:B:42:LEU:HD12	2:B:42:LEU:N	2.36	0.41
2:B:228:ASN:O	2:B:232:SER:HB2	2.21	0.41
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.41
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.03	0.41
1:A:74:VAL:HB	11:A:636:HOH:O	2.20	0.41
1:A:355:ILE:O	3:E:17:GLY:HA3	2.21	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.40
2:D:117:SER:O	2:D:121:VAL:HG23	2.21	0.40
2:D:270:PRO:HA	2:D:377:PHE:O	2.21	0.40
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.04	0.40
1:A:312:TYR:CD2	1:A:315[B]:CYS:SG	3.15	0.40
1:A:84:ARG:HG2	1:A:85:GLN:N	2.36	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.40
3:E:135:LYS:O	3:E:139:LEU:HG	2.22	0.40
4:F:348:GLN:HE21	4:F:352:ASP:CG	2.25	0.40
2:B:199:ASP:O	2:B:266:HIS:HB2	2.21	0.40
4:F:131:PHE:CZ	4:F:182:ILE:HG21	2.57	0.40
4:F:195:GLY:HA3	4:F:197:ARG:HD3	2.03	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%)	426 (97%)	11 (2%)	1 (0%)	47	49
1	C	429/451 (95%)	415 (97%)	14 (3%)	0	100	100
2	B	420/445 (94%)	409 (97%)	10 (2%)	1 (0%)	47	49
2	D	417/445 (94%)	409 (98%)	7 (2%)	1 (0%)	47	49
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	328 (95%)	16 (5%)	0	100	100
All	All	2167/2319 (93%)	2104 (97%)	60 (3%)	3 (0%)	51	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	73	GLY
1	A	281	ALA
2	B	73	GLY

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%)	363 (98%)	8 (2%)	52	57
1	C	366/379 (97%)	362 (99%)	4 (1%)	73	79
2	B	366/383 (96%)	360 (98%)	6 (2%)	62	69
2	D	364/383 (95%)	354 (97%)	10 (3%)	44	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	110/127 (87%)	108 (98%)	2 (2%)	59	65
4	F	312/342 (91%)	308 (99%)	4 (1%)	69	75
All	All	1889/1993 (95%)	1855 (98%)	34 (2%)	59	65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	47	ASP
1	A	120	ASP
1	A	128	GLN
1	A	176	GLN
1	A	179	THR
1	A	248	LEU
1	A	381	THR
2	B	77	SER
2	B	117	SER
2	B	139	HIS
2	B	232	SER
2	B	276	THR
2	B	302	MET
1	C	71	GLU
1	C	256	GLN
1	C	381	THR
1	C	384	ILE
2	D	15	GLN
2	D	39	ASP
2	D	41	ASP
2	D	90	ASP
2	D	139	HIS
2	D	179	ASP
2	D	270	PRO
2	D	293	GLN
2	D	335	VAL
2	D	387	LEU
3	E	59	GLU
3	E	140	LYS
4	F	97	SER
4	F	222	ARG
4	F	284	LEU
4	F	353	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	176	GLN
2	B	101	ASN
2	B	136	GLN
2	B	167	ASN
2	B	229	HIS
2	D	293	GLN
2	D	349	ASN
3	E	92	ASN
4	F	178	GLN
4	F	269	GLN
4	F	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
10	ACP	F	501	-	27,33,33	2.00	7 (25%)	32,52,52	1.61	5 (15%)
9	X3H	C	504	1	23,23,23	0.87	1 (4%)	26,30,30	1.19	2 (7%)
8	GDP	D	501	-	24,30,30	1.18	2 (8%)	31,47,47	1.88	7 (22%)
5	GTP	A	501	6	26,34,34	1.07	1 (3%)	33,54,54	1.67	7 (21%)
5	GTP	C	501	6	26,34,34	1.03	1 (3%)	33,54,54	1.87	6 (18%)
8	GDP	B	501	6	24,30,30	1.18	3 (12%)	31,47,47	2.08	8 (25%)

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
10	ACP	F	501	-	-	3/15/38/38	0/3/3/3
9	X3H	C	504	1	-	0/24/37/37	0/1/1/1
8	GDP	D	501	-	-	5/12/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	501	ACP	PG-O1G	5.43	1.61	1.50
10	F	501	ACP	C2'-C1'	-4.21	1.47	1.53
8	B	501	GDP	C6-C5	3.95	1.48	1.41
10	F	501	ACP	C6-N6	3.74	1.47	1.34
8	D	501	GDP	C6-C5	3.70	1.47	1.41
5	A	501	GTP	C6-N1	3.54	1.39	1.33
5	C	501	GTP	C6-N1	3.45	1.39	1.33
10	F	501	ACP	C2'-C3'	-3.17	1.44	1.53
9	C	504	X3H	O06-C05	-3.14	1.42	1.46
8	D	501	GDP	C5-C4	2.55	1.47	1.40
10	F	501	ACP	O3'-C3'	-2.41	1.37	1.43
10	F	501	ACP	PG-O3G	2.39	1.60	1.54
10	F	501	ACP	O5'-C5'	-2.29	1.35	1.44
8	B	501	GDP	C5-C4	2.19	1.46	1.40
8	B	501	GDP	O4'-C1'	2.17	1.44	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.72	119.59	127.22
8	B	501	GDP	C2-N3-C4	5.17	121.26	115.36
5	A	501	GTP	N3-C2-N1	-5.05	120.49	127.22
8	B	501	GDP	C6-C5-C4	-4.87	116.15	120.80
10	F	501	ACP	N3-C2-N1	-4.70	121.34	128.68
8	D	501	GDP	C5-C6-N1	-4.43	117.37	123.43
8	D	501	GDP	C6-N1-C2	4.33	122.80	115.93
8	B	501	GDP	C6-N1-C2	4.23	122.66	115.93
8	D	501	GDP	C2-N3-C4	4.16	120.11	115.36
5	A	501	GTP	C2-N3-C4	3.97	119.89	115.36
8	B	501	GDP	N3-C2-N1	-3.86	122.07	127.22
5	C	501	GTP	C2-N3-C4	3.85	119.75	115.36
8	B	501	GDP	C5-C6-N1	-3.70	118.38	123.43
8	D	501	GDP	PA-O3A-PB	-3.57	120.59	132.83
5	C	501	GTP	C5-C6-N1	-3.56	118.56	123.43
5	C	501	GTP	C6-N1-C2	3.52	121.52	115.93
10	F	501	ACP	O5'-C5'-C4'	3.33	120.44	108.99
8	D	501	GDP	C6-C5-C4	-3.22	117.72	120.80
10	F	501	ACP	C3'-C2'-C1'	3.21	105.82	100.98
8	D	501	GDP	N3-C2-N1	-3.05	123.16	127.22
5	A	501	GTP	C5-C6-N1	-3.03	119.29	123.43
8	B	501	GDP	PA-O3A-PB	-2.86	123.01	132.83
8	B	501	GDP	O2B-PB-O3A	2.85	114.18	104.64
5	A	501	GTP	PA-O3A-PB	-2.71	123.54	132.83
8	B	501	GDP	C4-C5-N7	-2.66	106.63	109.40
5	C	501	GTP	PA-O3A-PB	-2.60	123.92	132.83
5	C	501	GTP	PB-O3B-PG	-2.55	124.08	132.83
9	C	504	X3H	O06-C01-O01	2.53	120.59	117.88
8	D	501	GDP	C4-C5-N7	-2.47	106.83	109.40
10	F	501	ACP	O2G-PG-C3B	2.45	112.34	106.40
5	A	501	GTP	N2-C2-N1	2.45	121.06	117.25
10	F	501	ACP	PA-O3A-PB	-2.39	124.99	132.56
5	A	501	GTP	C6-N1-C2	2.27	119.54	115.93
9	C	504	X3H	C10-C11-C12	-2.26	110.51	113.98
5	A	501	GTP	PB-O3B-PG	-2.09	125.66	132.83

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O3G
10	F	501	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
10	F	501	ACP	C5'-O5'-PA-O1A
10	F	501	ACP	C3'-C4'-C5'-O5'
8	D	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA

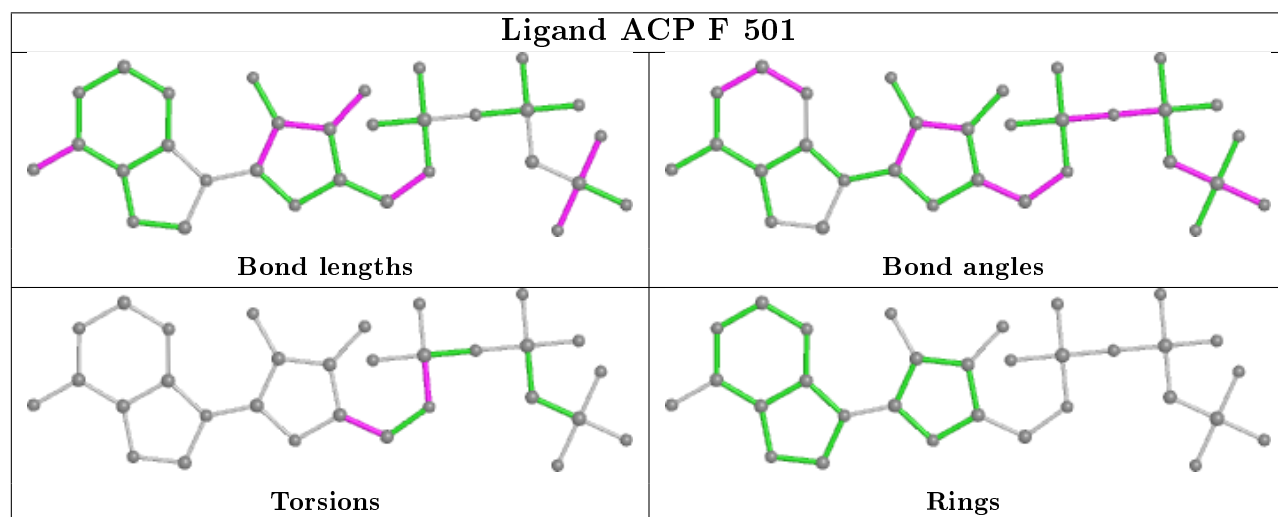
There are no ring outliers.

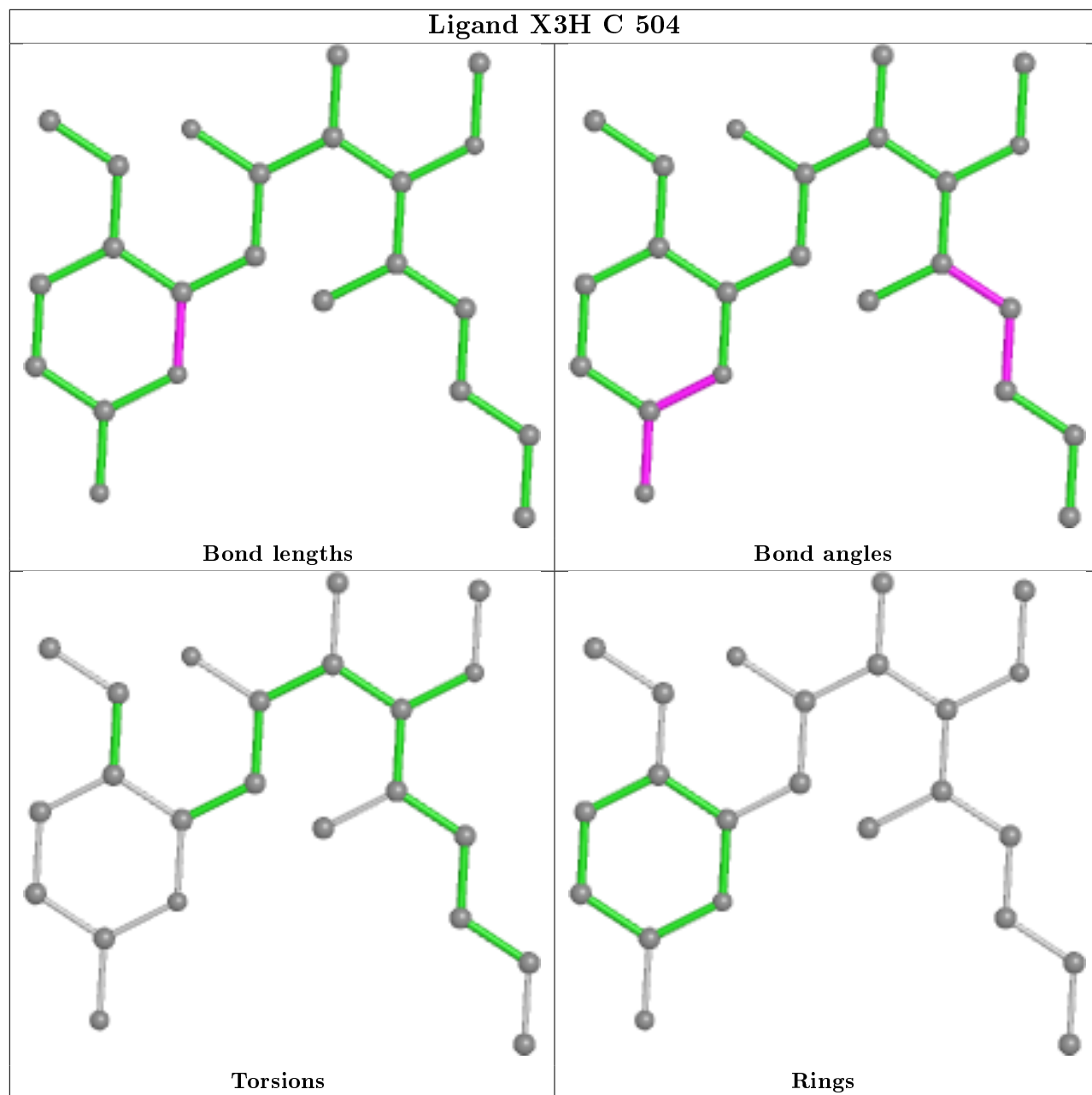
4 monomers are involved in 7 short contacts:

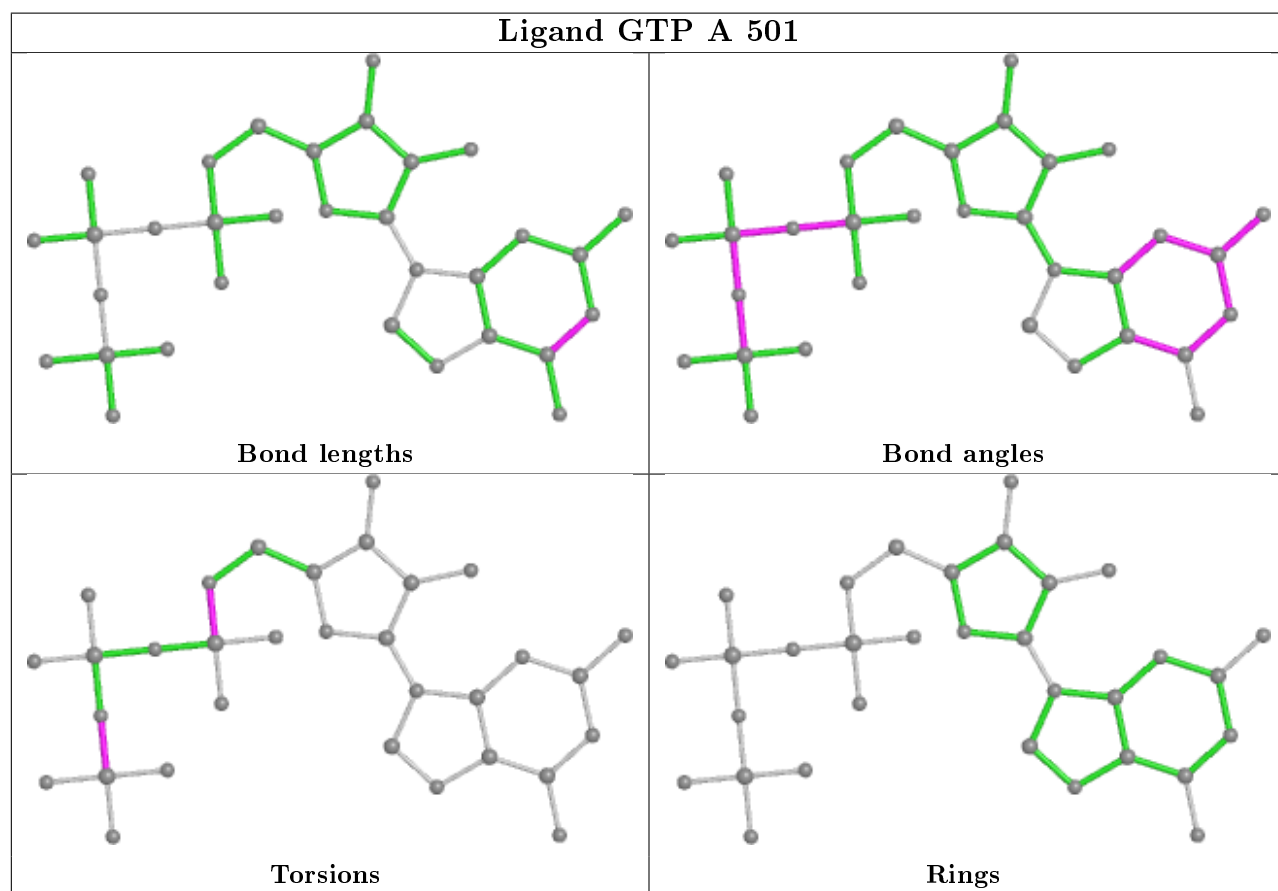
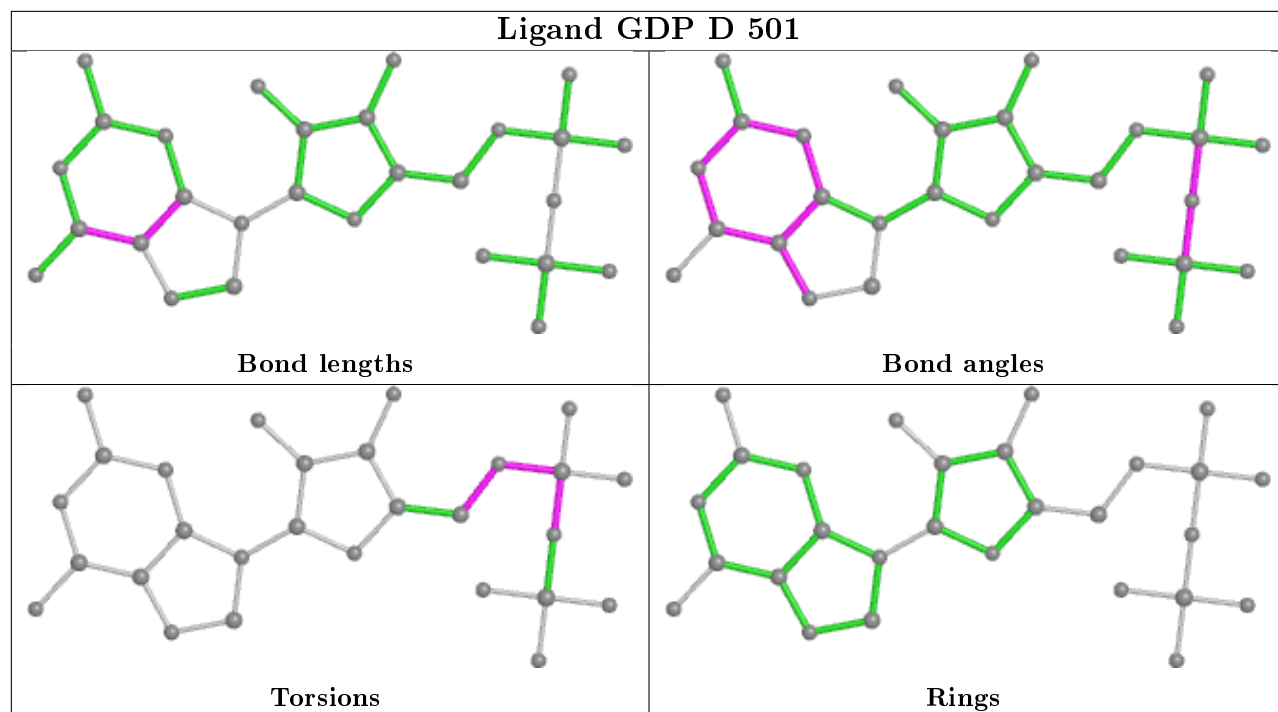
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	501	ACP	2	0
8	D	501	GDP	3	0
5	A	501	GTP	1	0
5	C	501	GTP	1	0

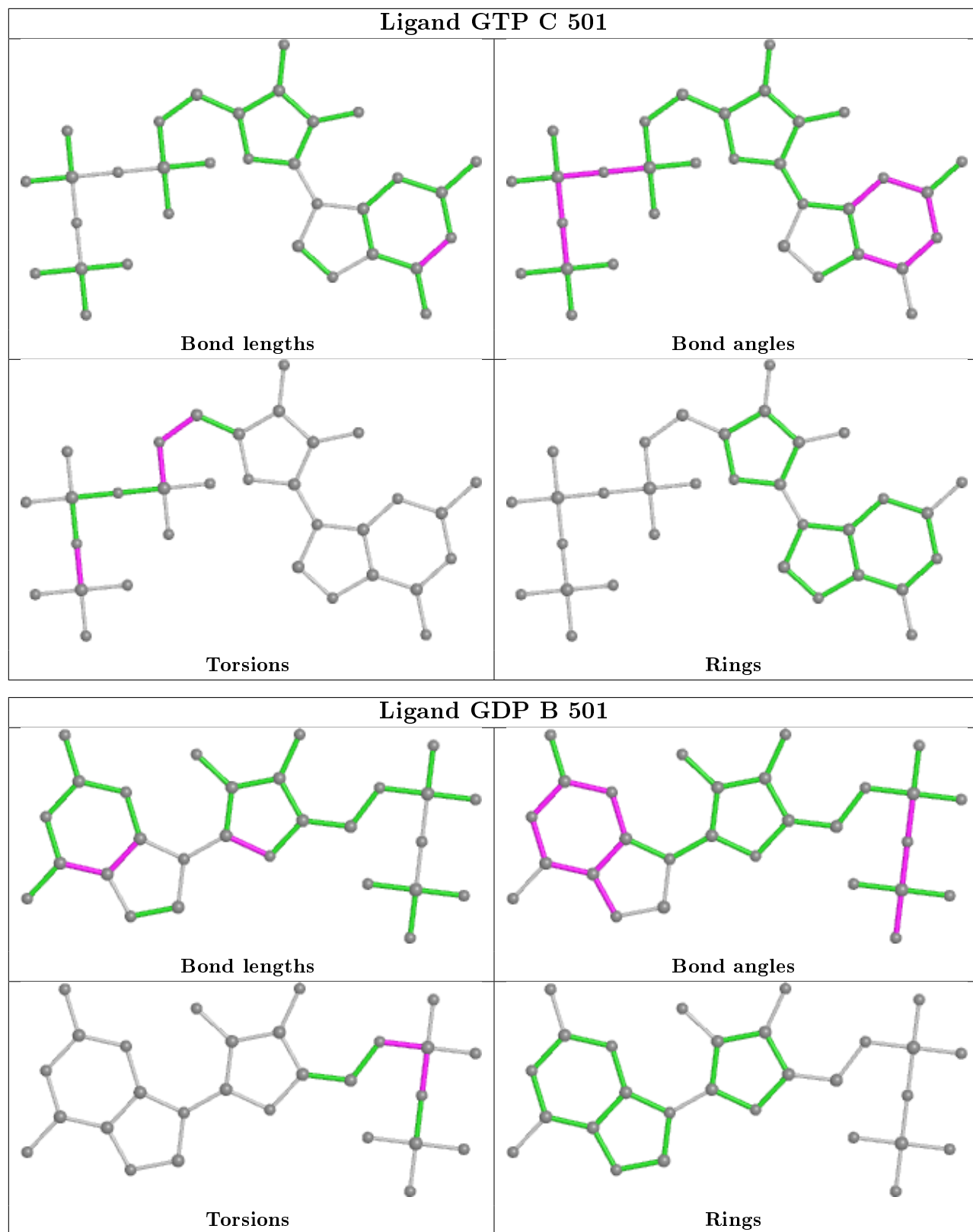
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.19	15 (3%)	45	51	41, 67, 101, 130	0
1	C	432/451 (95%)	-0.01	12 (2%)	53	59	38, 53, 83, 105	0
2	B	422/445 (94%)	0.04	14 (3%)	46	53	44, 63, 97, 138	2 (0%)
2	D	421/445 (94%)	0.21	21 (4%)	28	34	47, 74, 111, 132	6 (1%)
3	E	123/143 (86%)	0.24	13 (10%)	6	7	53, 80, 110, 129	0
4	F	350/384 (91%)	0.83	76 (21%)	0	0	54, 89, 150, 178	0
All	All	2186/2319 (94%)	0.23	151 (6%)	16	21	38, 69, 116, 178	8 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	8.9
4	F	177	GLY	7.4
4	F	249	TYR	6.3
2	D	276	THR	5.6
4	F	173	ILE	5.5
4	F	233	PHE	5.4
3	E	139	LEU	5.4
4	F	169	LEU	5.4
4	F	142	ARG	5.4
2	B	59	ASN	5.3
1	C	255	PHE	5.3
3	E	26	PRO	5.1
4	F	105	LEU	5.0
2	B	58	GLY	5.0
4	F	251	LYS	4.8
1	C	440	VAL	4.7
4	F	131	PHE	4.7
2	D	57	THR	4.6
1	A	365	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	4.5
2	B	57	THR	4.5
3	E	143	ALA	4.4
4	F	137	ARG	4.4
4	F	250	SER	4.3
4	F	89	GLU	4.3
4	F	132	LEU	4.2
4	F	256	TYR	4.1
4	F	245	ILE	4.1
4	F	103	THR	4.0
4	F	138	ARG	4.0
4	F	101	TYR	4.0
1	C	340	SER	3.9
4	F	104	ASN	3.9
4	F	361	LEU	3.9
2	B	56	ALA	3.8
4	F	20	LEU	3.8
4	F	17	VAL	3.8
4	F	135	TYR	3.7
4	F	90	SER	3.7
4	F	362	ALA	3.6
2	D	94	PHE	3.6
1	A	281	ALA	3.6
4	F	22	LEU	3.5
4	F	182	ILE	3.5
4	F	99	VAL	3.5
4	F	147	TRP	3.5
1	C	335	ILE	3.4
4	F	253	TYR	3.4
4	F	252	ASN	3.4
1	A	42	ILE	3.4
1	C	337	THR	3.4
4	F	194	PRO	3.3
1	A	280	LYS	3.2
4	F	31	ARG	3.2
2	B	61	TYR	3.2
3	E	25	LYS	3.2
2	D	97	SER	3.2
1	C	257	THR	3.2
1	C	254	GLU	3.1
2	B	37	HIS	3.1
1	A	177	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	140	LYS	3.0
4	F	244	CYS	3.0
4	F	234	GLN	3.0
4	F	143	GLU	3.0
4	F	178	GLN	3.0
4	F	255	ARG	3.0
1	A	283	HIS	2.9
2	D	74	THR	2.9
4	F	232	ASN	2.9
3	E	27	PRO	2.9
3	E	6	MET	2.8
2	D	73	GLY	2.8
2	D	59	ASN	2.8
4	F	231	ALA	2.8
4	F	21	LEU	2.8
2	D	400	ARG	2.7
3	E	24	LEU	2.7
4	F	166	ALA	2.7
4	F	161	LEU	2.7
4	F	170	LEU	2.7
3	E	142	GLU	2.7
4	F	179	VAL	2.7
4	F	102	PRO	2.7
4	F	164	SER	2.6
1	A	171	ILE	2.6
4	F	148	ILE	2.6
2	D	255	LEU	2.6
4	F	192	LEU	2.6
4	F	139	ARG	2.6
3	E	135	LYS	2.6
2	D	75	MET	2.6
1	A	262	TYR	2.6
2	B	36	TYR	2.6
2	B	82	PRO	2.5
4	F	165	GLU	2.5
1	A	170	SER	2.5
1	A	178	SER	2.5
4	F	157	GLY	2.5
2	B	33	THR	2.5
4	F	100	ILE	2.5
3	E	7	GLU	2.5
4	F	181	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	341	ILE	2.5
2	D	219	LEU	2.4
4	F	128	ARG	2.4
2	D	37	HIS	2.4
1	A	141	PHE	2.3
2	D	404	PHE	2.3
4	F	129	GLU	2.3
2	B	60	LYS	2.3
4	F	152	SER	2.3
2	B	34	GLY	2.3
4	F	240	LEU	2.3
4	F	247	LYS	2.3
4	F	144	GLY	2.3
2	D	401	ARG	2.3
4	F	259	GLY	2.3
2	D	60	LYS	2.2
2	D	314	THR	2.2
4	F	154	GLY	2.2
2	D	416	MET	2.2
4	F	146	VAL	2.2
1	A	359	PRO	2.2
4	F	11	SER	2.2
4	F	156	LYS	2.2
2	B	38	GLY	2.2
2	B	438	ALA	2.2
4	F	134	ALA	2.2
4	F	353	VAL	2.2
2	D	252	LEU	2.2
2	D	260	VAL	2.1
4	F	136	ASN	2.1
4	F	32	LYS	2.1
4	F	167	SER	2.1
3	E	138	GLU	2.1
2	D	405	LEU	2.1
4	F	27	TRP	2.1
4	F	254	GLY	2.1
1	A	88	HIS	2.1
1	C	181	VAL	2.1
2	D	83	PHE	2.1
4	F	176	GLN	2.1
1	A	279	GLU	2.1
4	F	19	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	140	GLU	2.0
1	C	338	LYS	2.0
1	C	256	GLN	2.0
1	C	180	ALA	2.0
2	B	255	LEU	2.0
3	E	128	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

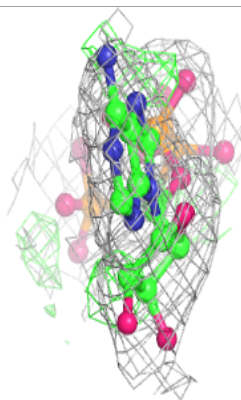
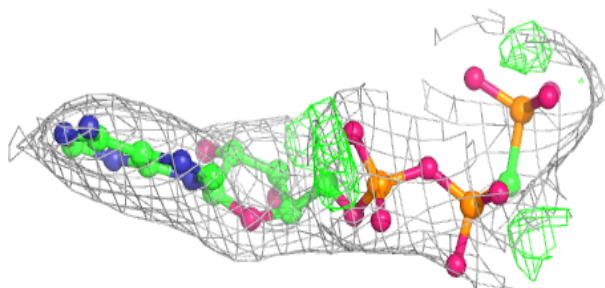
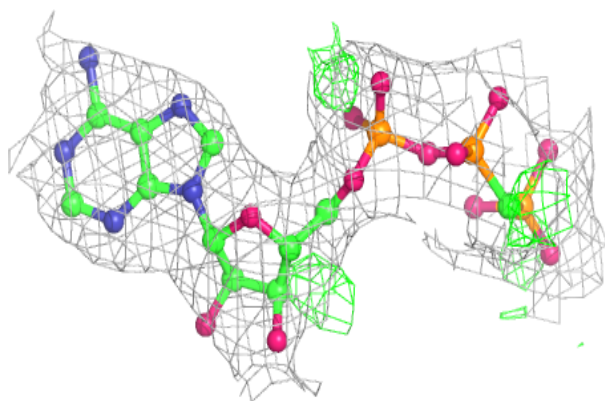
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	502	1/1	0.85	0.27	58,58,58,58	0
6	MG	B	502	1/1	0.88	0.28	67,67,67,67	0
7	CA	A	504	1/1	0.89	0.10	119,119,119,119	0
6	MG	A	502	1/1	0.90	0.19	51,51,51,51	0
10	ACP	F	501	31/31	0.91	0.12	78,99,134,148	0
9	X3H	C	504	23/23	0.95	0.11	47,61,75,77	0
7	CA	B	503	1/1	0.95	0.07	111,111,111,111	0
8	GDP	D	501	28/28	0.97	0.10	53,63,79,147	0
7	CA	A	503	1/1	0.97	0.04	88,88,88,88	0
5	GTP	A	501	32/32	0.98	0.18	39,47,53,66	0
8	GDP	B	501	28/28	0.98	0.14	43,49,56,59	0
7	CA	C	503	1/1	0.98	0.09	72,72,72,72	0
5	GTP	C	501	32/32	0.99	0.17	36,41,49,51	0

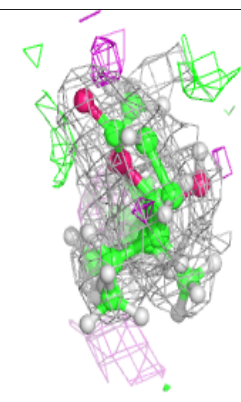
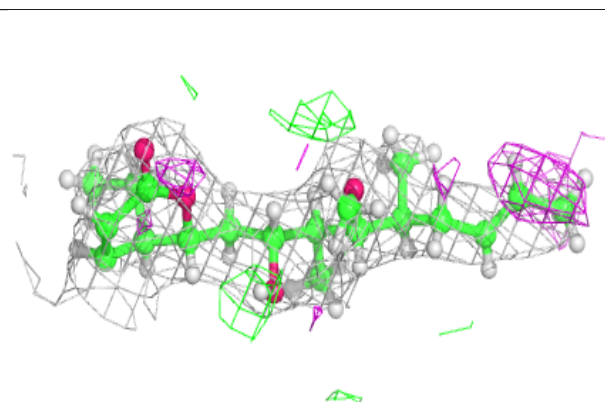
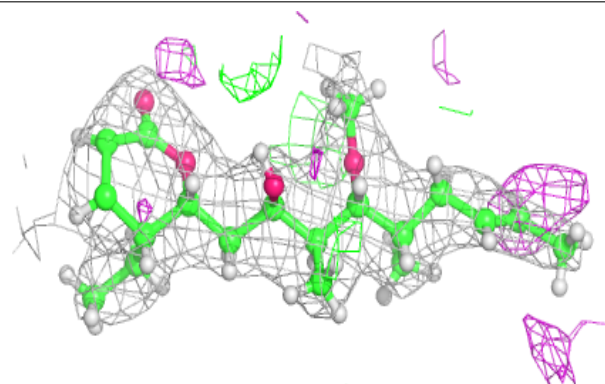
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 501:

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

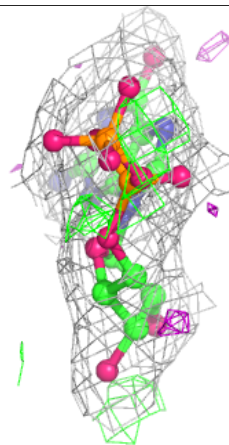
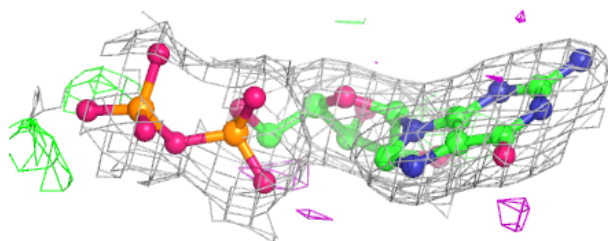
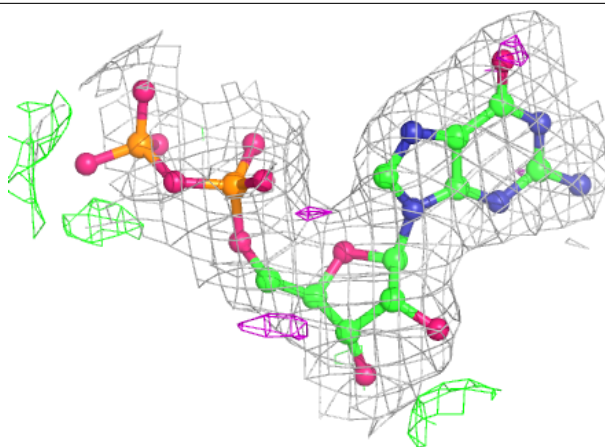
**Electron density around X3H C 504:**

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

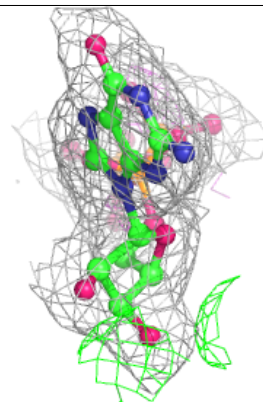
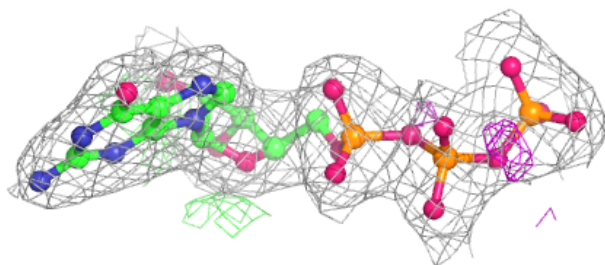
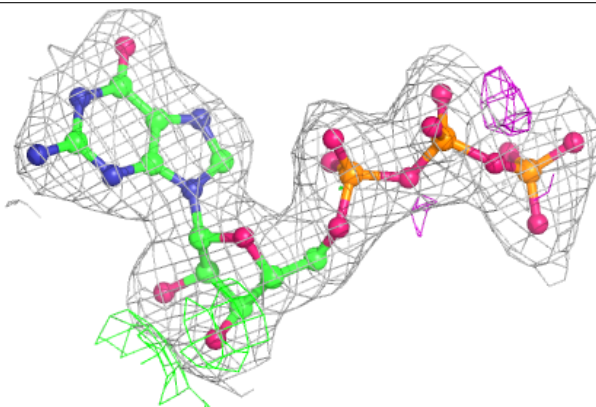


Electron density around GDP D 501:

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

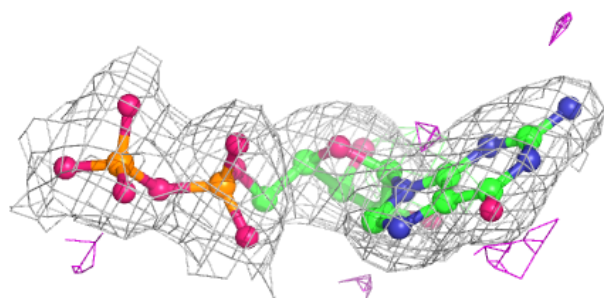
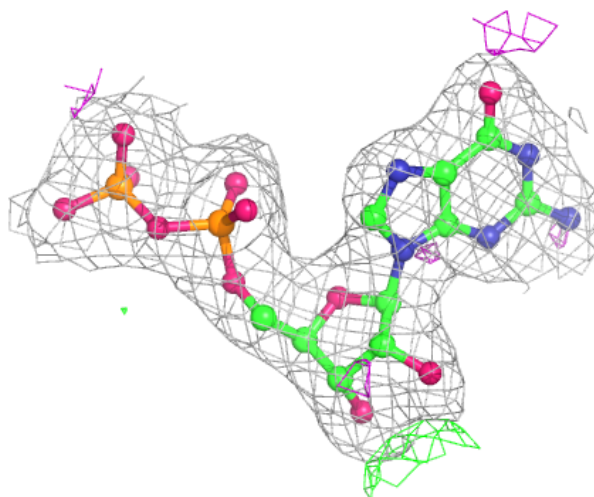
**Electron density around GTP A 501:**

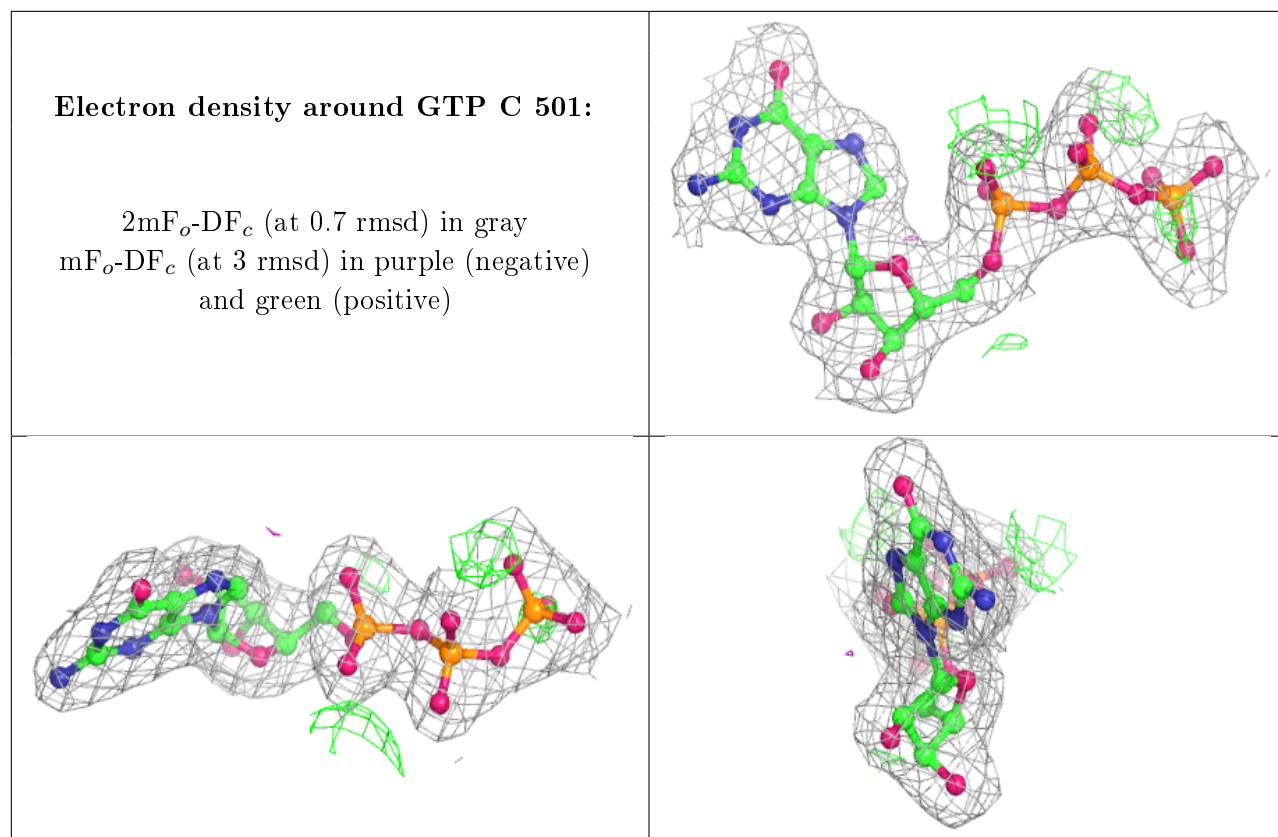
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.