



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:05 AM UTC

PDB ID : 5LA6 / pdb_00005la6
Title : Tubulin-pironetin complex
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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 types of validation reports are described at

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

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

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

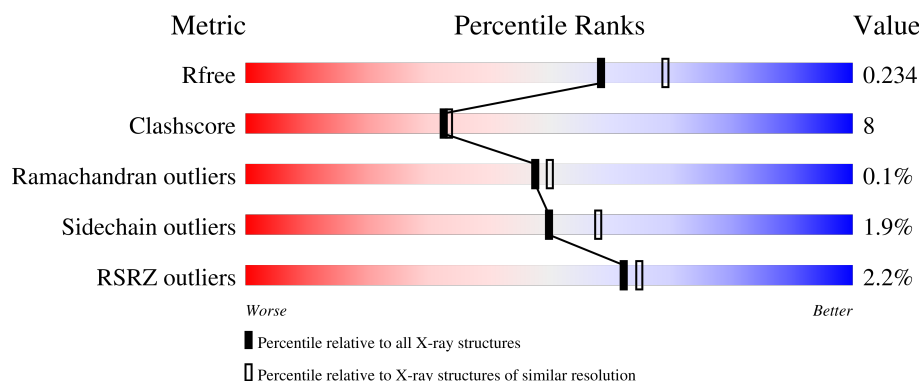
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	2% 77% 20% • •
1	C	451	2% 81% 15% •
2	B	445	0% 75% 19% 5%
2	D	445	2% 76% 18% • 5%
3	E	143	3% 70% 15% • 14%

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Mol	Chain	Length	Quality of chain
4	F	384	4% 71% 20% 9%

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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

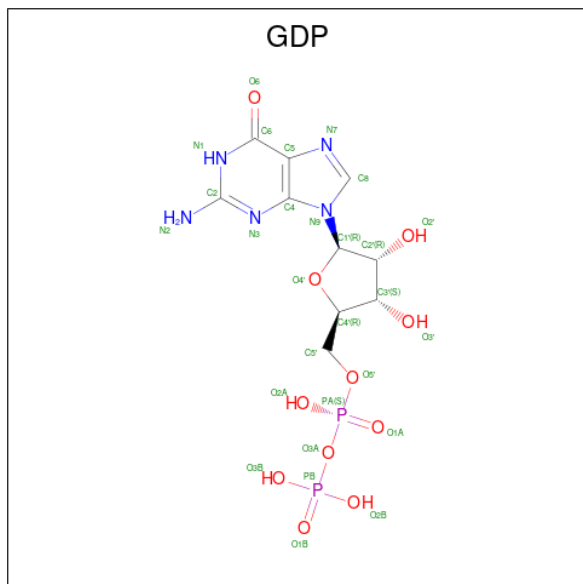
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

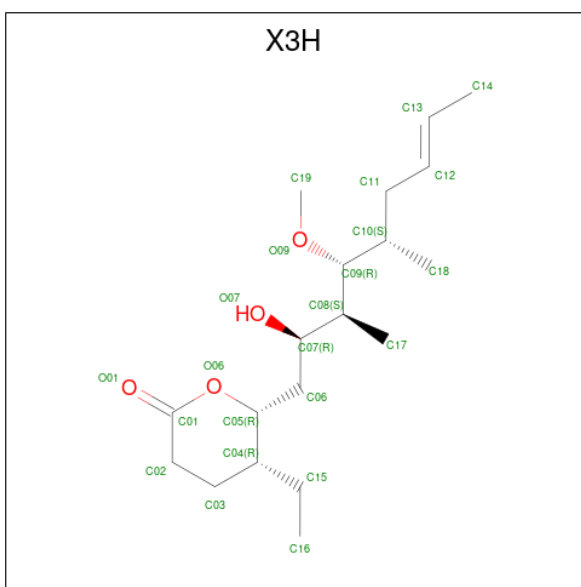
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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

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

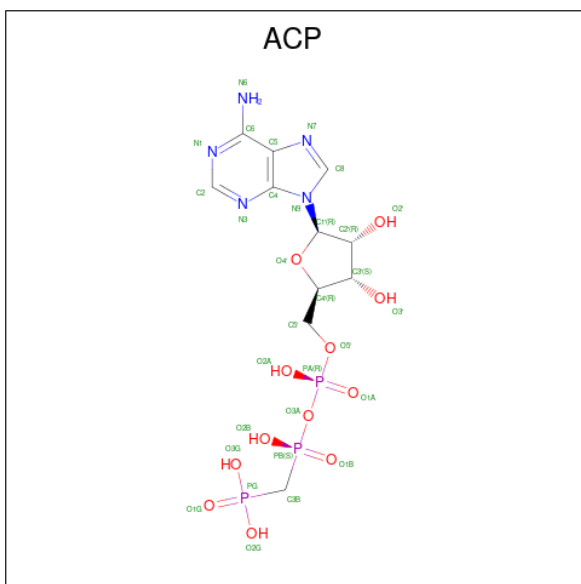
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





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 (CCD ID: 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		

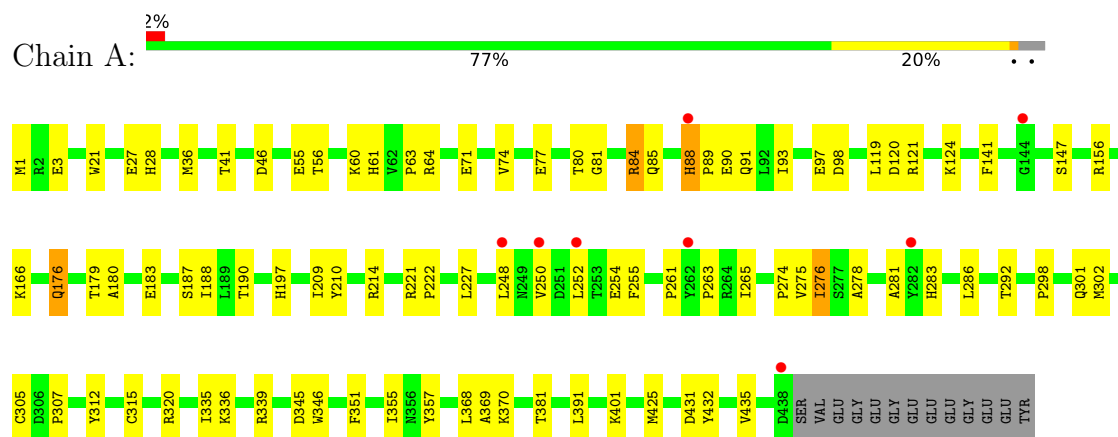
- Molecule 11 is water.

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

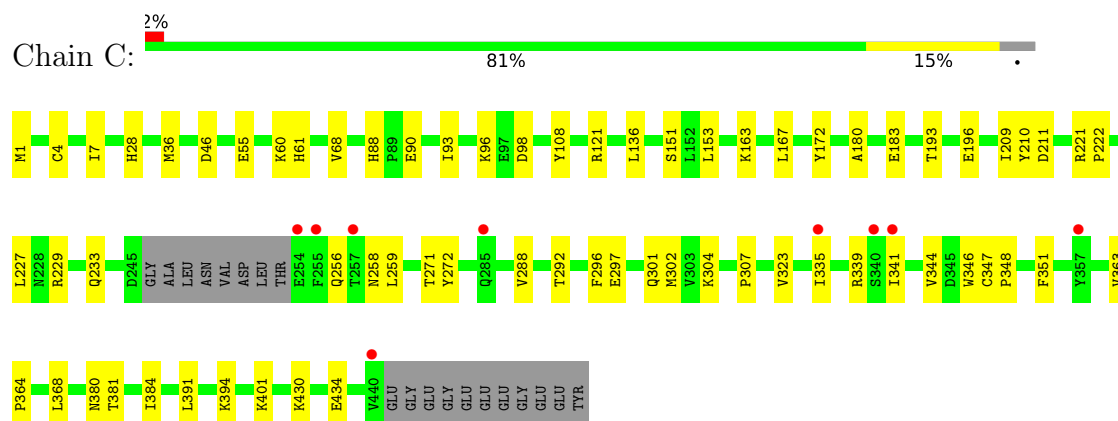
3 Residue-property plots

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.

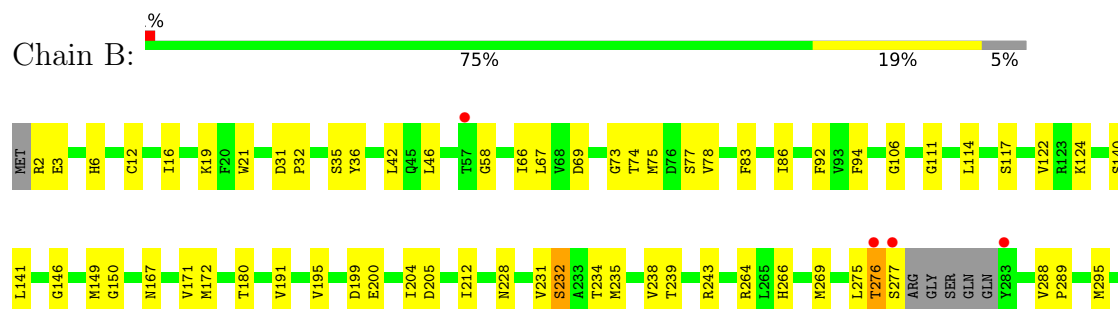
• Molecule 1: Tubulin alpha-1B chain

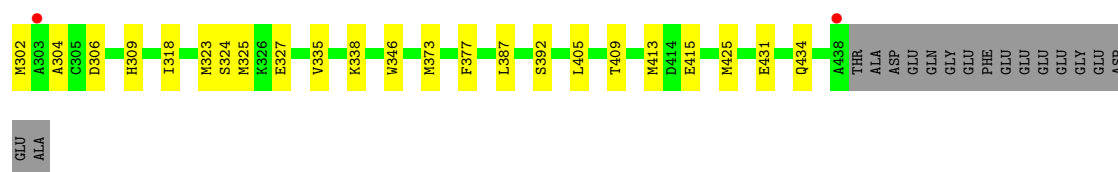


• Molecule 1: Tubulin alpha-1B chain

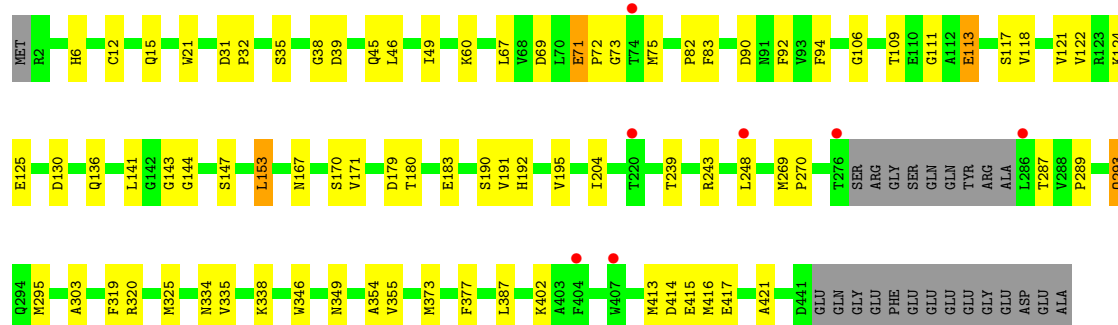
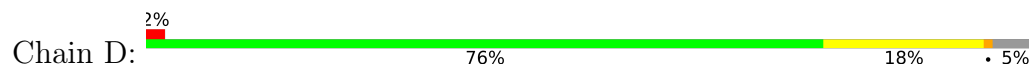


• Molecule 2: Tubulin beta-2B chain

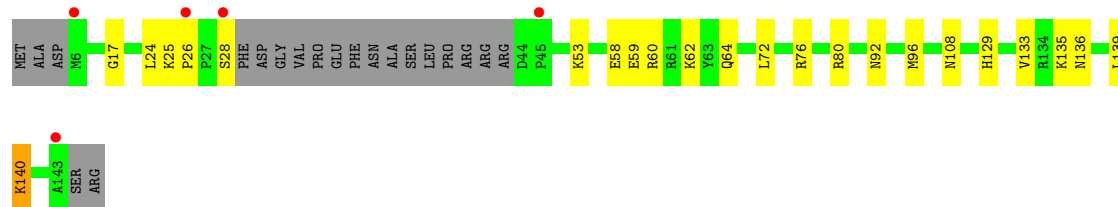




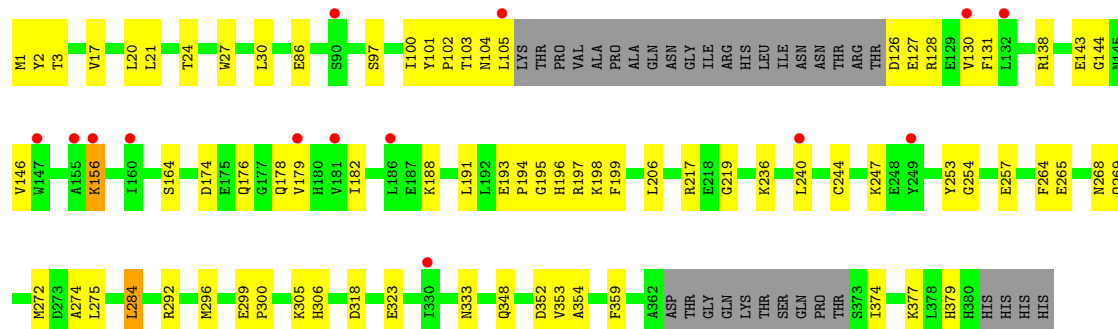
• Molecule 2: Tubulin beta-2B chain



• 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) 99.9 (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 0.191 , 0.234	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 , 50.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, ACP, GDP, CA, 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	0.44	0/3514	0.79	2/4770 (0.0%)
1	C	0.54	0/3465	0.78	0/4701
2	B	0.48	0/3409	0.76	1/4618 (0.0%)
2	D	0.41	0/3381	0.78	2/4581 (0.0%)
3	E	0.42	0/1022	0.70	0/1356
4	F	0.34	0/2923	0.72	1/3948 (0.0%)
All	All	0.45	0/17714	0.76	6/23974 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	71	GLU	CA-C-N	8.64	128.64	119.05
2	D	71	GLU	C-N-CA	8.64	128.64	119.05
2	B	58	GLY	N-CA-C	-5.76	107.70	115.36
4	F	156	LYS	CB-CA-C	-5.15	110.22	117.23
1	A	88	HIS	CA-C-N	5.07	126.18	119.84
1	A	88	HIS	C-N-CA	5.07	126.18	119.84

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	3345	64	0
1	C	3385	0	3295	47	0
2	B	3329	0	3213	59	0
2	D	3308	0	3184	51	0
3	E	1014	0	1029	18	0
4	F	2858	0	2826	51	0
5	A	32	0	12	1	0
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	273	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 (273) 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
3:E:92:ASN:HD21	3:E:96:MET:HE2	1.48	0.78
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
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.32	0.69
2:B:323:MET:HE2	2:B:373:MET:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:MET:HE2	2:D:377:PHE:HB2	1.76	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
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
2:B:323:MET:HB3	2:B:373:MET:HE1	1.78	0.64
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: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
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.64	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: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:H	2:B:42:LEU:HD12	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:B:338:LYS:HE3	4:F:1:MET:HB3	1.83	0.59
2:D:147:SER:HB2	2:D:190:SER:OG	2.03	0.59
3:E:92:ASN:ND2	3:E:96:MET:HE2	2.18	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:LYS:HD3	2:B:124:LYS:C	2.29	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
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.86	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
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.40	0.56
2:B:141:LEU:HD12	2:B:172:MET:SD	2.45	0.56
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.71	0.56
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.36	0.56
1:A:28:HIS:O	1:A:36:MET:HE3	2.06	0.56
1:A:77:GLU:HA	1:A:80:THR:HG22	1.89	0.55
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.89	0.55
1:C:46:ASP:OD1	1:C:46:ASP:N	2.39	0.55
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.36	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:298:PRO:HA	1:A:301:GLN:CD	2.31	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
4:F:274:ALA:C	4:F:275:LEU:HD23	2.32	0.55
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.71	0.54
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:B:392:SER:HB2	2:B:425:MET:HE3	1.90	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:B:75:MET:HE3	2:B:92:PHE:CD2	2.43	0.53
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:60:LYS:NZ	1:A:85:GLN:O	2.42	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
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.50
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.11	0.49
1:A:141:PHE:O	1:A:147:SER:HB3	2.12	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
4:F:104:ASN:C	4:F:105:LEU:HD12	2.37	0.49
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.33	0.49
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.95	0.49
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:C:96:LYS:NZ	2:D:130:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:75:MET:HE2	2:D:94:PHE:CD2	2.45	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:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.48
2:D:144:GLY:HA3	8:D:501:GDP:O3B	2.14	0.48
1:C:28:HIS:O	1:C:36:MET:HE3	2.13	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:31:ASP:OD2	2:B:35:SER:HB2	2.14	0.47
2:B:67:LEU:N	2:B:67:LEU:HD12	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
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
4:F:269:GLN:HA	4:F:272:MET:HE2	1.96	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
1:A:346:TRP:CD1	1:A:346:TRP:H	2.33	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
2:D:325:MET:HE2	2:D:325:MET:HB2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.52	0.45
2:B:269:MET:HE2	2:B:269:MET:HB3	1.68	0.45
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.98	0.45
4:F:348:GLN:HE21	4:F:352:ASP:CG	2.25	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:HD12	4:F:284:LEU:HA	1.81	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.44
2:B:191:VAL:O	2:B:195:VAL:HG23	2.17	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:B:114:LEU:HD23	2:B:149:MET:HE1	1.99	0.44
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.98	0.44
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.26	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
4:F:20:LEU:O	4:F:24:THR:HG23	2.18	0.44
4:F:236:LYS:HB3	4:F:240:LEU:HD12	1.99	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:HE21	2:D:293:GLN:HB2	1.68	0.43
2:D:413:MET:HE3	2:D:417:GLU:CD	2.43	0.43
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.19	0.43
1:C:271:THR:HG22	1:C:272:TYR:N	2.34	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: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:83:PHE:O	2:B:86:ILE:HG22	2.19	0.43
2:B:234:THR:O	2:B:238:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:TYR:CZ	4:F:359:PHE:HB3	2.54	0.42
4:F:193:GLU:HA	4:F:194:PRO:C	2.44	0.42
4:F:198:LYS:HG2	4:F:199:PHE:N	2.34	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:OE2	2:B:3:GLU:N	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:A:315[A]:CYS:HG	1:A:351:PHE:HE2	1.65	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
2:D:124:LYS:HZ3	2:D:125:GLU:CD	2.28	0.42
1:C:167:LEU:HD12	1:C:167:LEU:N	2.35	0.41
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
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
2:B:387:LEU:C	2:B:387:LEU:HD23	2.46	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
1:C:108:TYR:CD1	3:E:108:ASN:CG	2.99	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:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.03	0.41
4:F:296:MET:HE1	4:F:299:GLU:OE1	2.21	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
4:F:103:THR:C	4:F:105:LEU:H	2.30	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
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%)	43	44
1	C	429/451 (95%)	415 (97%)	14 (3%)	0	100	100
2	B	420/445 (94%)	409 (97%)	10 (2%)	1 (0%)	43	44
2	D	417/445 (94%)	409 (98%)	7 (2%)	1 (0%)	43	44
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%)	48	50

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 [i](#)

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%)	45	53
1	C	366/379 (97%)	362 (99%)	4 (1%)	65	74
2	B	366/383 (96%)	359 (98%)	7 (2%)	50	58
2	D	364/383 (95%)	355 (98%)	9 (2%)	42	48
3	E	110/127 (87%)	107 (97%)	3 (3%)	39	45
4	F	312/342 (91%)	307 (98%)	5 (2%)	55	64
All	All	1889/1993 (95%)	1853 (98%)	36 (2%)	50	58

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	84	ARG
1	A	120	ASP
1	A	176	GLN
1	A	179	THR
1	A	248	LEU
1	A	276	ILE
1	A	381	THR
2	B	19	LYS
2	B	77	SER
2	B	117	SER
2	B	232	SER
2	B	276	THR
2	B	302	MET

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Mol	Chain	Res	Type
2	B	335	VAL
1	C	68	VAL
1	C	256	GLN
1	C	381	THR
1	C	384	ILE
2	D	15	GLN
2	D	39	ASP
2	D	90	ASP
2	D	113	GLU
2	D	153	LEU
2	D	179	ASP
2	D	293	GLN
2	D	335	VAL
2	D	387	LEU
3	E	53	LYS
3	E	59	GLU
3	E	140	LYS
4	F	86	GLU
4	F	97	SER
4	F	130	VAL
4	F	284	LEU
4	F	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	309	HIS
2	B	101	ASN
2	B	167	ASN
2	B	193	GLN
2	B	229	HIS
2	B	294	GLN
2	B	300	ASN
2	B	331	GLN
2	B	349	ASN
1	C	15	GLN
2	D	167	ASN
2	D	293	GLN
2	D	300	ASN
2	D	349	ASN
3	E	84	GLN

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Mol	Chain	Res	Type
3	E	92	ASN
4	F	178	GLN
4	F	242	ASN
4	F	269	GLN
4	F	348	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	31,33,33	1.97	6 (19%)	47,52,52	2.24	14 (29%)
8	GDP	B	501	6	29,30,30	1.07	2 (6%)	45,47,47	1.79	8 (17%)
5	GTP	C	501	6	33,34,34	0.94	2 (6%)	50,54,54	1.54	8 (16%)
9	X3H	C	504	1	23,23,23	0.88	1 (4%)	25,30,30	1.24	3 (12%)
8	GDP	D	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.70	7 (15%)
5	GTP	A	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.57	11 (22%)

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	-	-	2/19/38/38	0/3/3/3
8	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
9	X3H	C	504	1	-	0/24/37/37	0/1/1/1
8	GDP	D	501	-	-	6/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	501	ACP	PG-O1G	5.62	1.61	1.50
10	F	501	ACP	C6-N6	5.28	1.47	1.34
8	D	501	GDP	C5-C4	3.25	1.47	1.38
10	F	501	ACP	C2'-C3'	-3.21	1.44	1.53
9	C	504	X3H	O06-C05	-3.16	1.42	1.46
8	B	501	GDP	C5-C4	2.91	1.46	1.38
8	D	501	GDP	C6-N1	-2.46	1.34	1.38
10	F	501	ACP	PG-O3G	2.42	1.60	1.55
8	D	501	GDP	C5-N7	-2.36	1.34	1.39
5	A	501	GTP	PA-O3A	2.35	1.62	1.59
8	B	501	GDP	C6-N1	-2.29	1.34	1.38
10	F	501	ACP	O3'-C3'	-2.29	1.37	1.43
10	F	501	ACP	O5'-C5'	-2.29	1.35	1.44
5	C	501	GTP	PA-O3A	2.25	1.61	1.59
5	C	501	GTP	C2-N3	2.06	1.38	1.33
5	A	501	GTP	C2-N3	2.02	1.38	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	501	ACP	O4'-C1'-N9	-7.14	94.38	108.09
8	D	501	GDP	C5-C4-N3	-6.00	118.84	128.39
8	B	501	GDP	C5-C4-N3	-5.60	119.48	128.39
8	B	501	GDP	C2-N3-C4	5.20	121.26	112.30
10	F	501	ACP	C2'-C1'-N9	4.82	125.27	113.30
10	F	501	ACP	C5-C4-N3	-4.81	120.09	126.72
10	F	501	ACP	N3-C2-N1	-4.79	121.34	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	N9-C4-N3	4.65	135.26	125.95
8	D	501	GDP	C2-N3-C4	4.53	120.11	112.30
5	A	501	GTP	C2-N3-C4	4.41	119.89	112.30
5	A	501	GTP	C5-C4-N3	-4.40	121.39	128.39
5	C	501	GTP	C2-N3-C4	4.33	119.75	112.30
5	C	501	GTP	C5-C4-N3	-4.23	121.65	128.39
8	B	501	GDP	N9-C4-N3	4.16	134.27	125.95
10	F	501	ACP	N3-C4-N9	3.92	133.84	127.17
8	B	501	GDP	C6-C5-N7	3.81	137.22	130.29
10	F	501	ACP	C2-N3-C4	3.41	120.16	111.83
10	F	501	ACP	N9-C8-N7	-3.39	109.13	113.94
10	F	501	ACP	O5'-C5'-C4'	3.36	120.44	108.99
5	C	501	GTP	N9-C8-N7	-3.35	107.18	113.40
10	F	501	ACP	C4-N9-C8	3.30	109.21	105.74
5	A	501	GTP	C2-N1-C6	-3.07	119.54	125.11
5	C	501	GTP	O2B-PB-O3A	3.01	115.40	107.27
5	A	501	GTP	N9-C8-N7	-3.00	107.84	113.40
5	C	501	GTP	C8-N7-C5	2.90	109.43	104.26
8	B	501	GDP	O2B-PB-O3A	2.85	114.18	104.64
8	D	501	GDP	C6-C5-N7	2.83	135.44	130.29
5	A	501	GTP	C8-N7-C5	2.69	109.05	104.26
5	A	501	GTP	N9-C4-N3	2.62	131.20	125.95
5	C	501	GTP	N9-C4-N3	2.62	131.20	125.95
8	B	501	GDP	C4-C5-N7	-2.55	106.63	110.67
5	A	501	GTP	O6-C6-C5	-2.53	119.86	126.53
10	F	501	ACP	O2G-PG-C3B	2.45	112.34	106.40
9	C	504	X3H	O06-C01-O01	2.44	120.59	117.86
8	D	501	GDP	C4-C5-N7	-2.43	106.83	110.67
5	A	501	GTP	C5-C6-N1	2.37	119.29	113.25
10	F	501	ACP	C5-N7-C8	2.36	107.15	103.45
9	C	504	X3H	C10-C11-C12	-2.30	110.51	114.11
10	F	501	ACP	C3'-C2'-C1'	2.30	105.82	101.46
10	F	501	ACP	PB-O3A-PA	-2.26	124.99	132.37
5	A	501	GTP	O2A-PA-O3A	2.26	113.39	107.27
8	B	501	GDP	O6-C6-C5	-2.19	120.75	126.53
5	A	501	GTP	O2B-PB-O3A	2.17	113.14	107.27
8	D	501	GDP	O6-C6-C5	-2.09	121.00	126.53
5	C	501	GTP	C5-C6-N1	2.09	118.56	113.25
8	D	501	GDP	O2A-PA-O3A	2.05	112.83	107.27
5	C	501	GTP	N1-C2-N3	-2.04	119.59	123.32
5	A	501	GTP	N2-C2-N1	2.04	121.06	116.76
9	C	504	X3H	C17-C08-C09	-2.04	107.82	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	501	ACP	O1G-PG-C3B	-2.03	106.95	111.37
8	B	501	GDP	C5-C6-N1	2.01	118.38	113.25

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 7 short contacts:

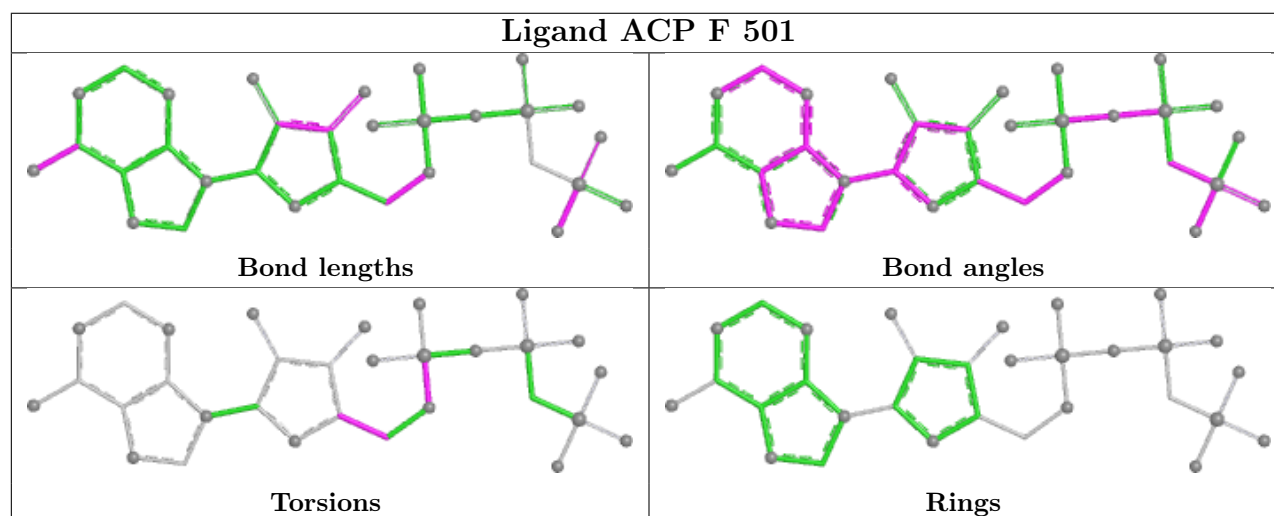
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	501	ACP	2	0
5	C	501	GTP	1	0

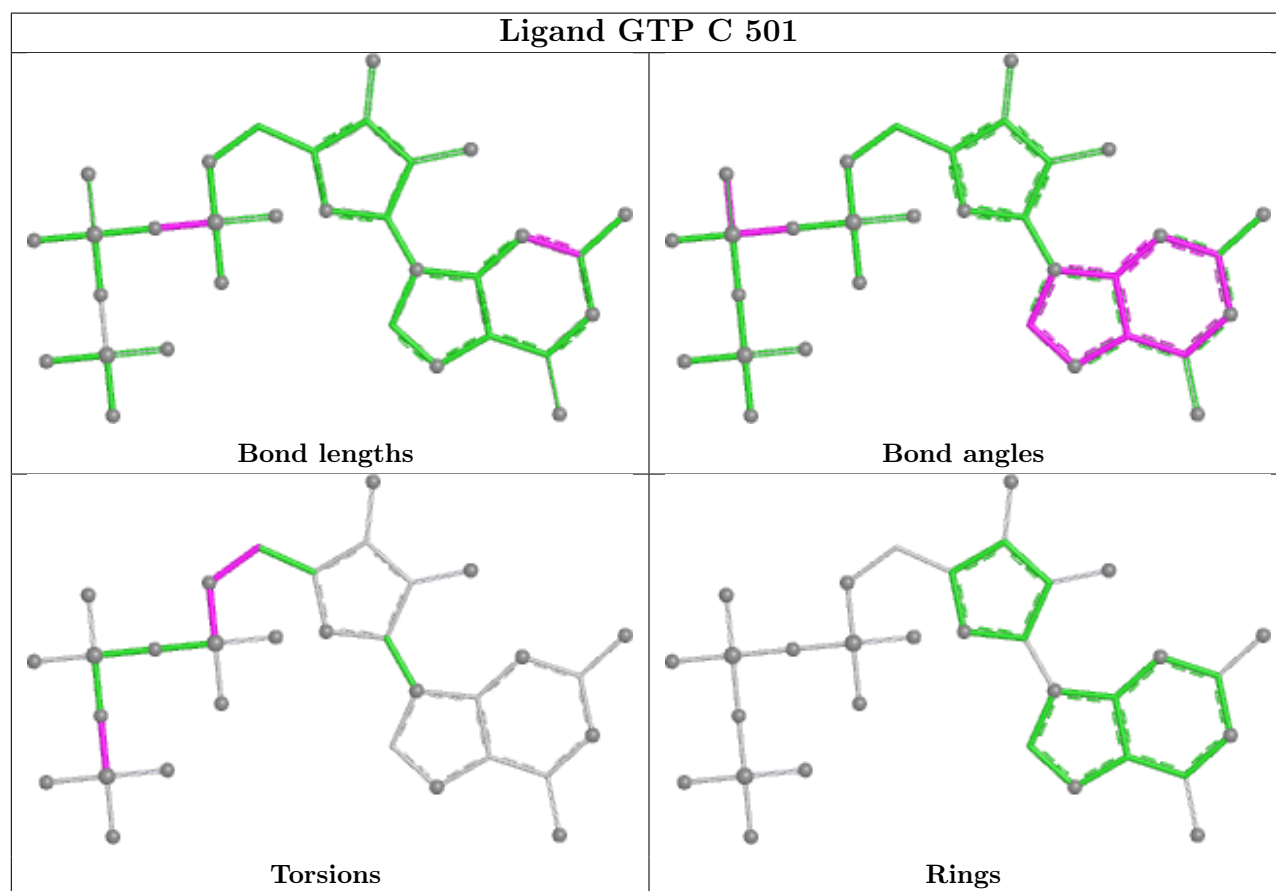
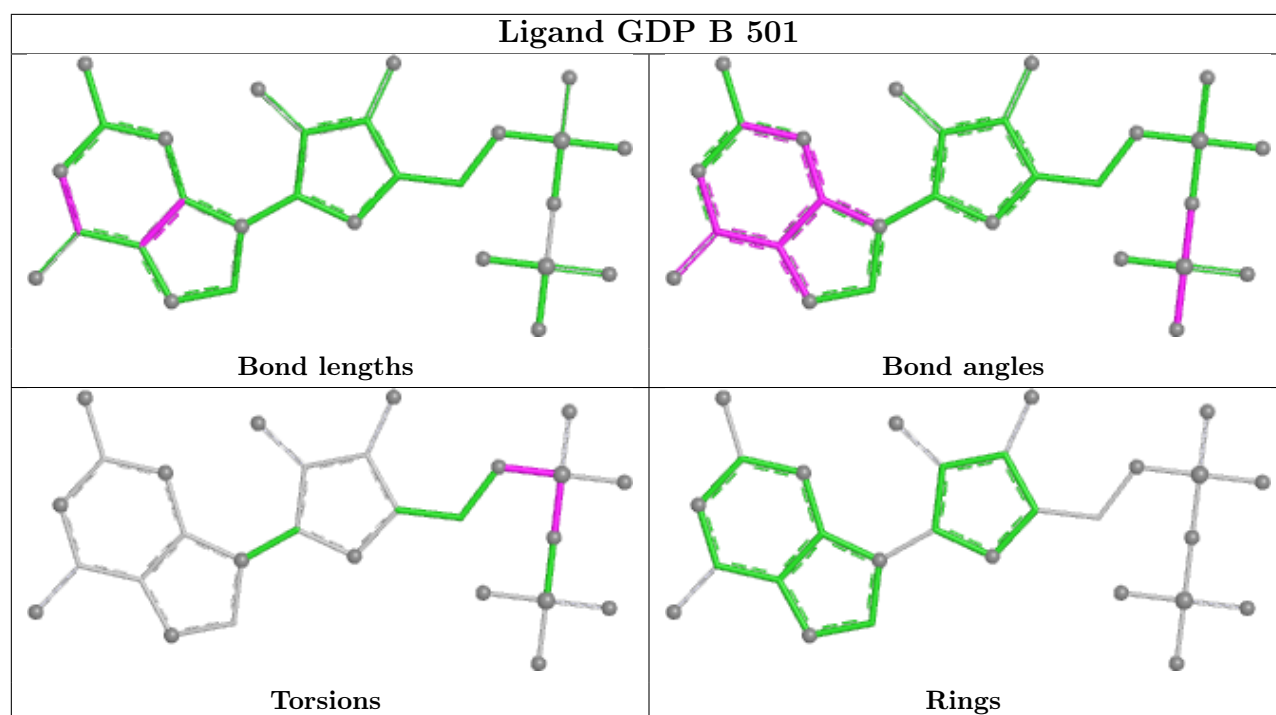
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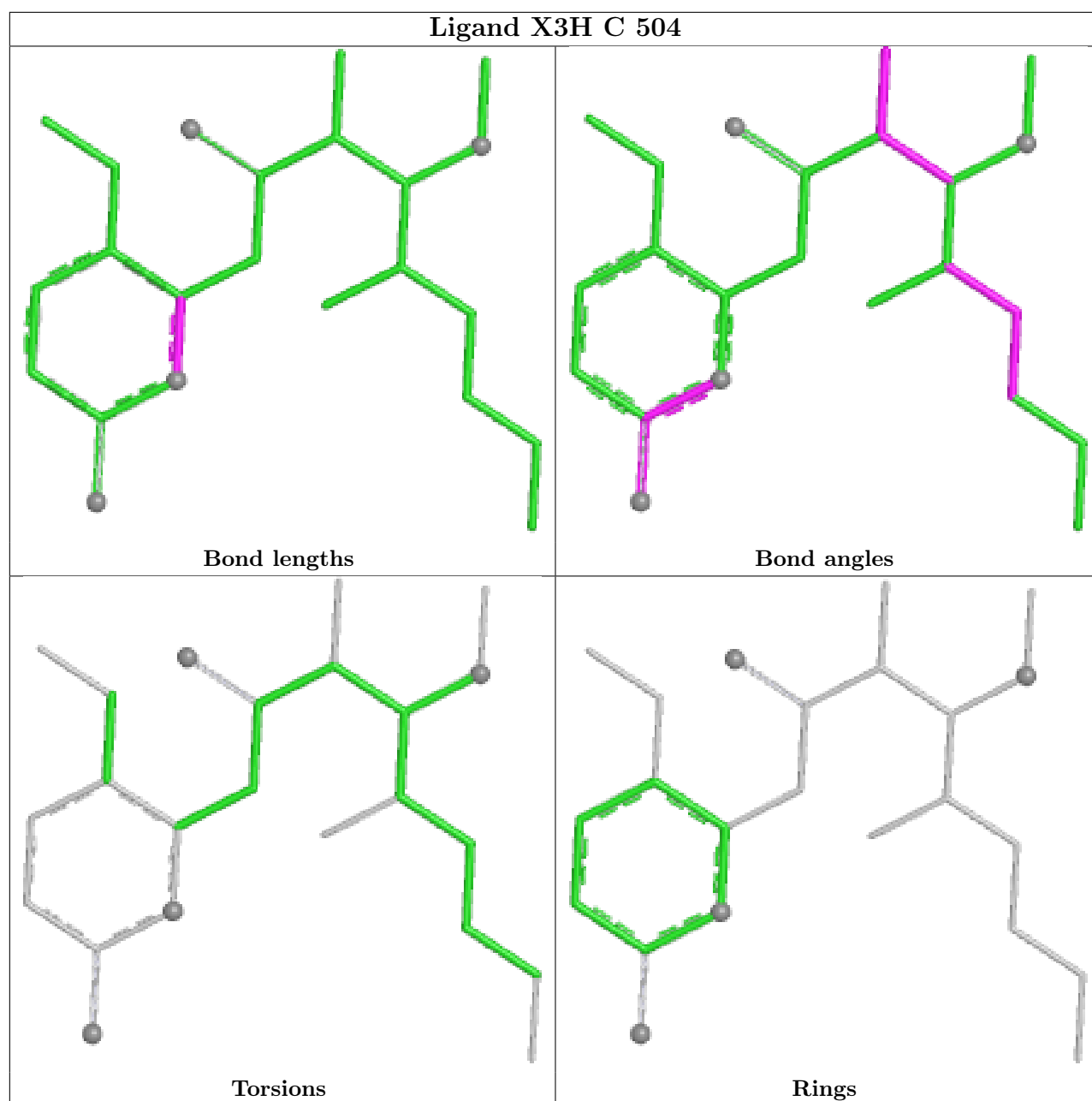
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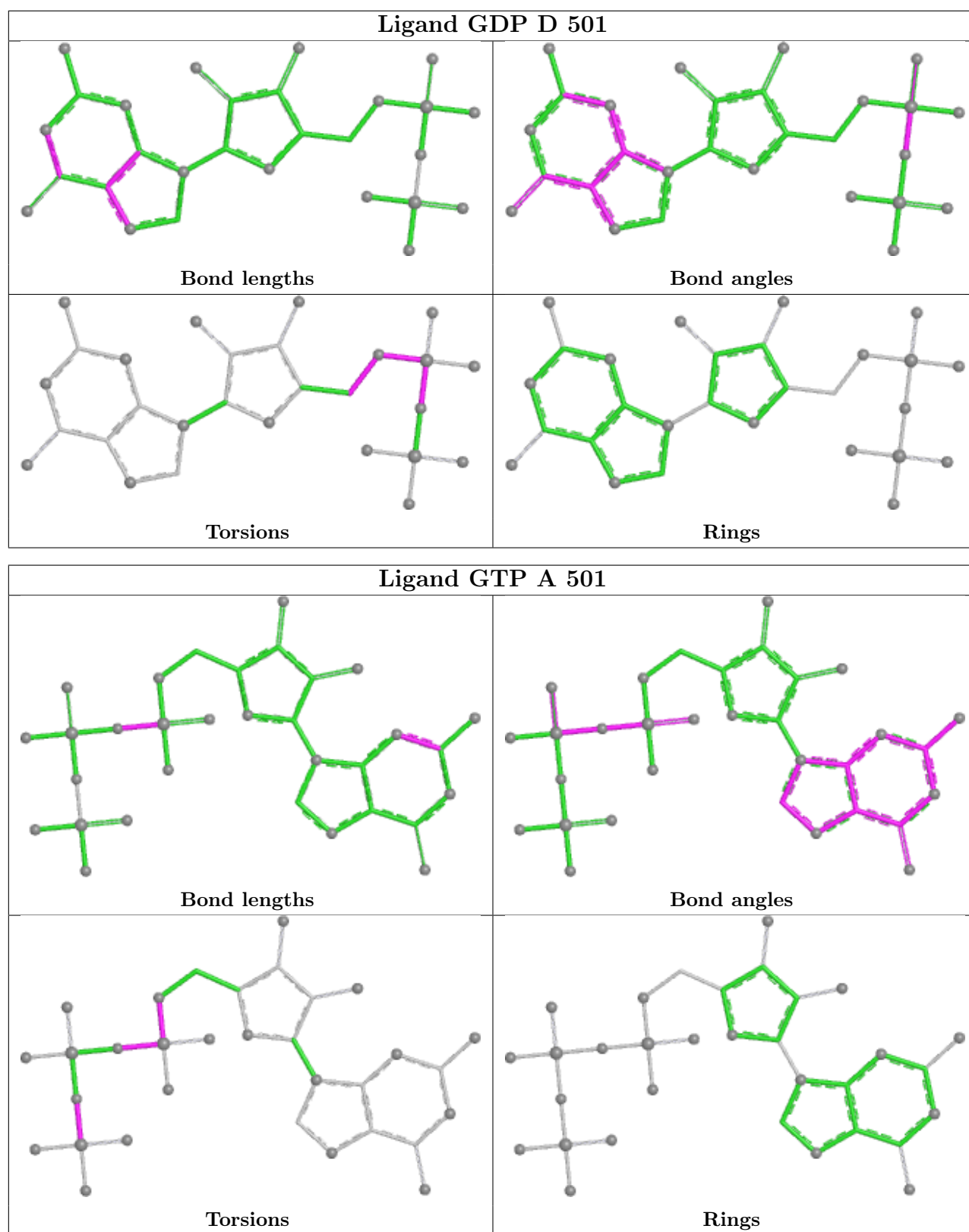
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	3	0
5	A	501	GTP	1	0

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 ⓘ

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%)	0.17	8 (1%) 67 70	39, 67, 101, 130	2 (0%)
1	C	432/451 (95%)	-0.07	9 (2%) 63 66	33, 53, 83, 105	1 (0%)
2	B	422/445 (94%)	0.09	6 (1%) 73 75	28, 63, 97, 138	4 (0%)
2	D	421/445 (94%)	0.25	7 (1%) 69 71	47, 74, 111, 132	6 (1%)
3	E	123/143 (86%)	0.50	5 (4%) 41 43	53, 80, 110, 129	0
4	F	350/384 (91%)	0.43	14 (4%) 42 44	54, 89, 150, 178	0
All	All	2186/2319 (94%)	0.18	49 (2%) 62 65	28, 69, 116, 178	13 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	255	PHE	5.1
2	B	276	THR	3.1
2	D	407	TRP	3.0
3	E	143	ALA	2.9
2	D	276	THR	2.8
3	E	28	SER	2.8
2	D	404	PHE	2.8
2	B	283	TYR	2.8
2	D	220	THR	2.8
1	C	440	VAL	2.7
1	C	254	GLU	2.7
4	F	156	LYS	2.7
1	A	250	VAL	2.7
1	A	252	LEU	2.7
1	A	248	LEU	2.6
4	F	155	ALA	2.6
2	B	57	THR	2.5
4	F	181	VAL	2.4
1	A	262	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	2.4
1	A	144	GLY	2.4
3	E	26	PRO	2.4
2	B	303	ALA	2.3
1	A	282	TYR	2.3
3	E	6	MET	2.3
4	F	186	LEU	2.3
4	F	90	SER	2.3
4	F	160	ILE	2.3
3	E	45	PRO	2.3
4	F	130	VAL	2.2
4	F	132	LEU	2.2
1	A	88	HIS	2.2
1	C	257	THR	2.2
1	C	285	GLN	2.2
1	C	341	ILE	2.1
2	B	438	ALA	2.1
2	D	248	LEU	2.1
1	C	340	SER	2.1
2	B	277	SER	2.1
4	F	330	ILE	2.1
2	D	74	THR	2.1
1	C	335	ILE	2.1
4	F	179	VAL	2.1
4	F	147	TRP	2.1
4	F	240	LEU	2.0
4	F	249	TYR	2.0
2	D	286	LEU	2.0
1	A	438	ASP	2.0
1	C	357	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

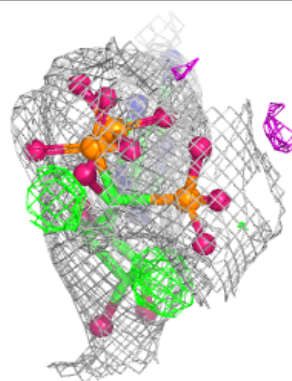
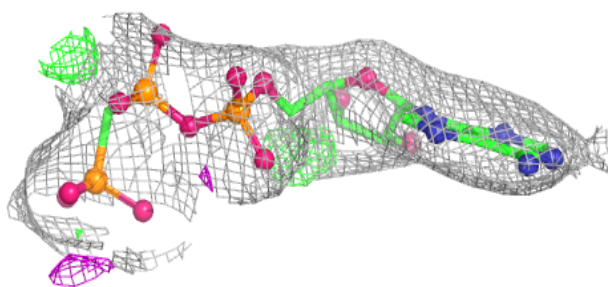
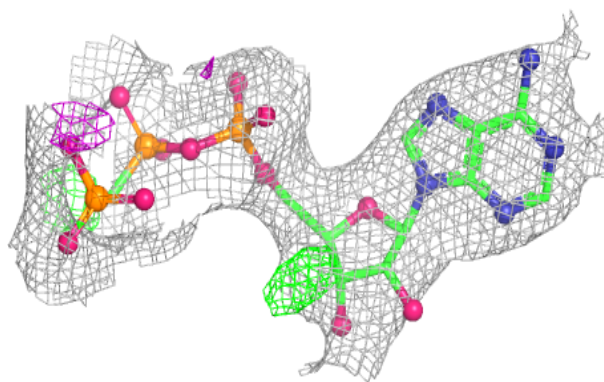
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	504	1/1	0.88	0.10	119,119,119,119	0
7	CA	B	503	1/1	0.90	0.07	111,111,111,111	0
6	MG	B	502	1/1	0.91	0.09	67,67,67,67	0
10	ACP	F	501	31/31	0.91	0.11	78,99,134,148	0
8	GDP	D	501	28/28	0.94	0.08	53,63,79,147	0
9	X3H	C	504	23/23	0.95	0.08	47,61,75,77	0
7	CA	A	503	1/1	0.96	0.07	88,88,88,88	0
8	GDP	B	501	28/28	0.98	0.05	43,49,56,59	0
5	GTP	A	501	32/32	0.98	0.06	39,47,53,66	0
6	MG	A	502	1/1	0.99	0.04	51,51,51,51	0
5	GTP	C	501	32/32	0.99	0.04	36,41,49,51	0
6	MG	C	502	1/1	0.99	0.09	58,58,58,58	0
7	CA	C	503	1/1	0.99	0.03	72,72,72,72	0

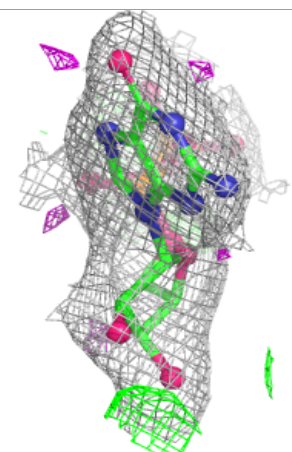
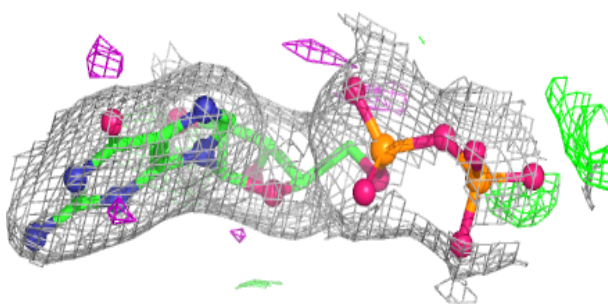
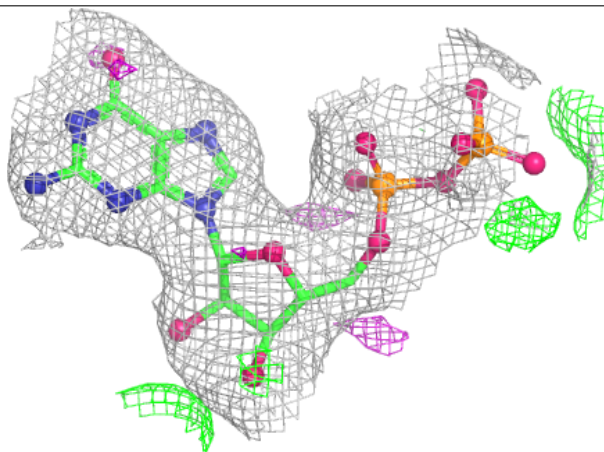
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

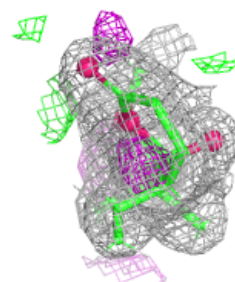
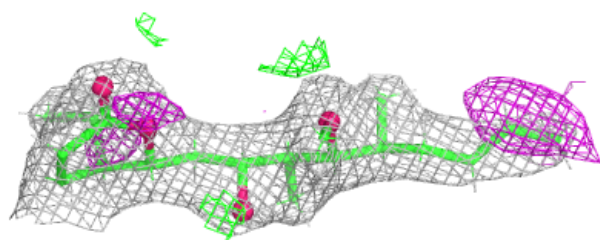
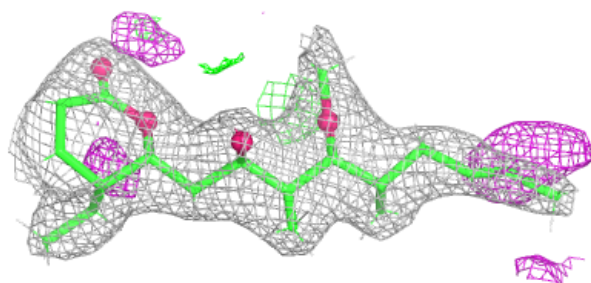
**Electron density around GDP D 501:**

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



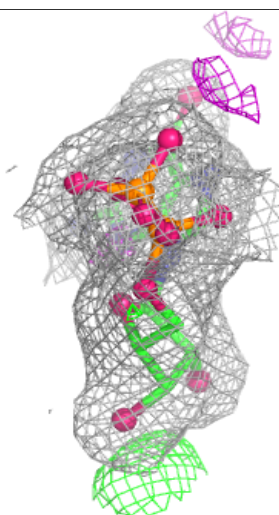
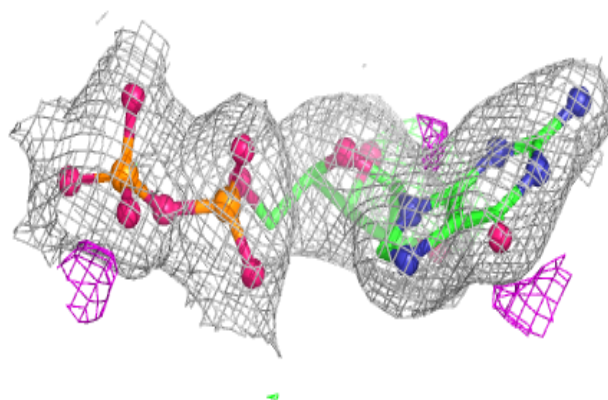
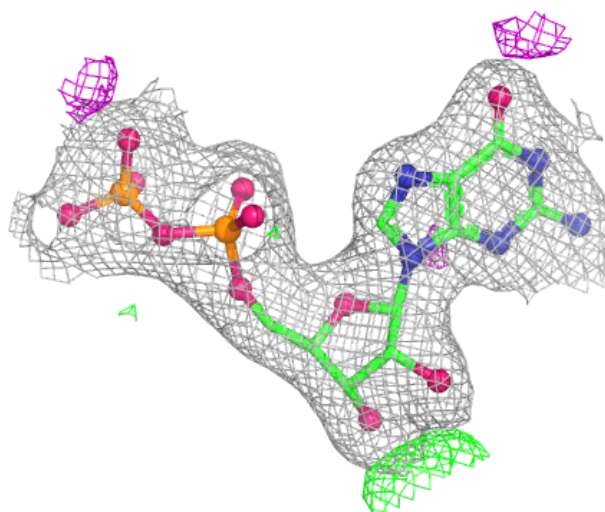
Electron density around X3H C 504:

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



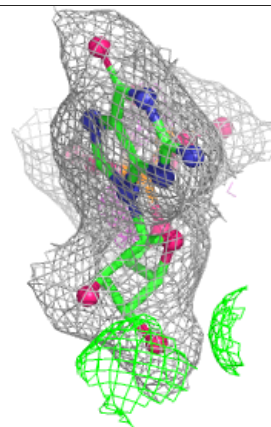
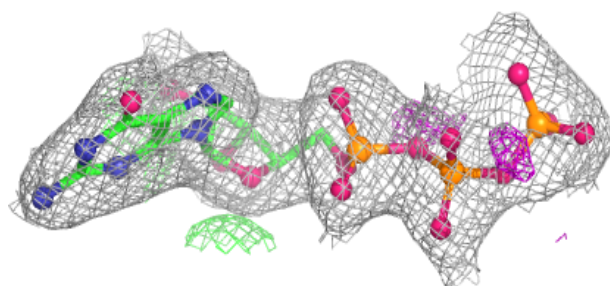
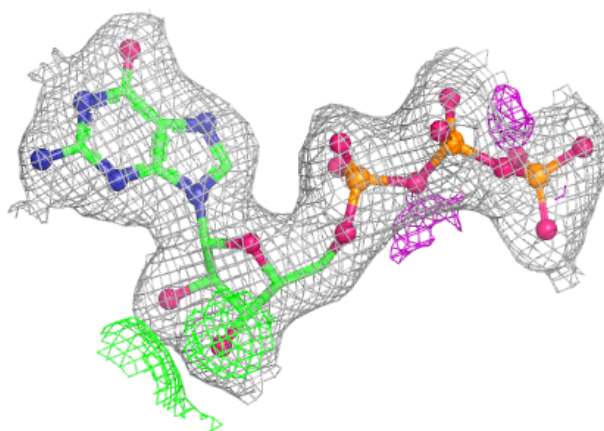
Electron density around GDP B 501:

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and green (positive)

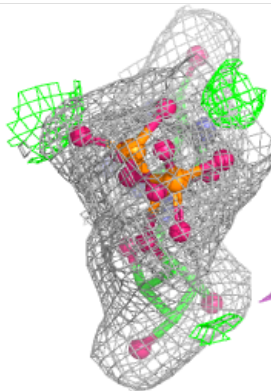
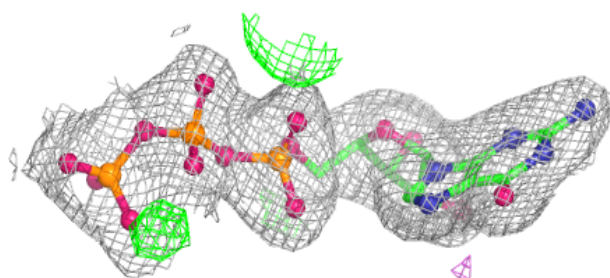
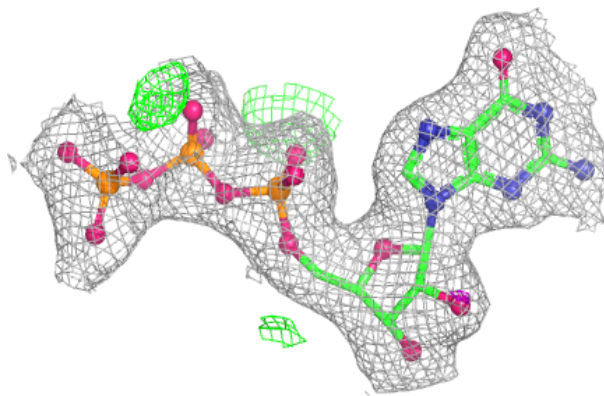


Electron density around GTP A 501:

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

**Electron density around 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.