



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 AM UTC

PDB ID : 5JVD / pdb_00005jvd
Title : Tubulin-TUB092 complex
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Deposited on : 2016-05-11
Resolution : 2.39 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

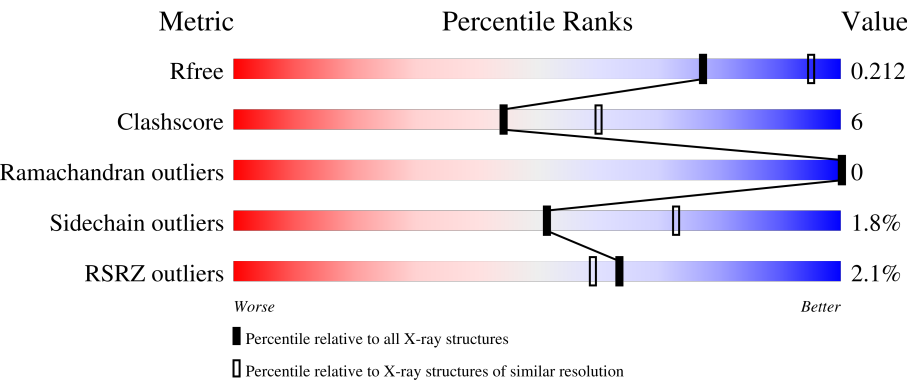
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	0% 83% 14% • •
1	C	451	0% 83% 14% •
2	B	445	0% 82% 14% •
2	D	445	2% 82% 12% • 5%

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Mol	Chain	Length	Quality of chain
3	E	143	3% 77% 8% 15%
4	F	384	4% 75% 14% 9%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17853 atoms, of which 36 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	0	0
			3422	2165	582	654	21			
1	C	439	Total	C	N	O	S	0	0	0
			3429	2170	583	655	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	1	0
			3346	2103	570	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3313	2082	563	642	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	0	0
			1008	622	182	199	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	348	Total	C	N	O	S	0	0	0
			2842	1821	487	520	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		
6	D	1	Total	Mg	0	0
			1	1		

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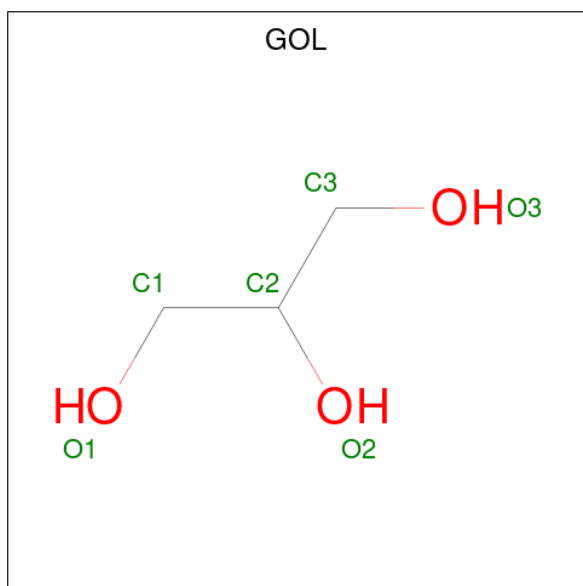
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

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

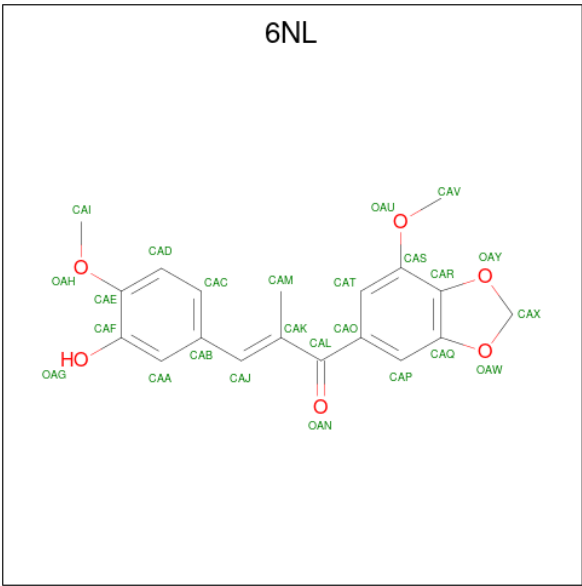
- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

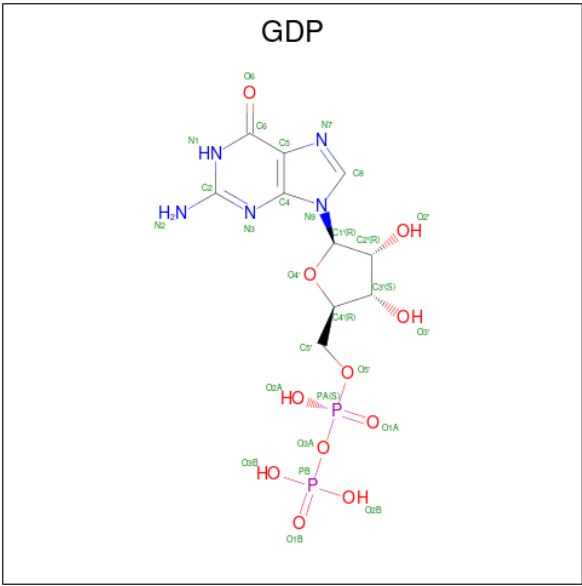
- Molecule 9 is (2E)-3-(3-hydroxy-4-methoxyphenyl)-1-(7-methoxy-2H-1,3-benzodioxol-5-yl)-

2-methylprop-2-en-1-one (CCD ID: 6NL) (formula: C₁₉H₁₈O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			43	19	18	6		
9	D	1	Total	C	H	O	0	0
			43	19	18	6		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



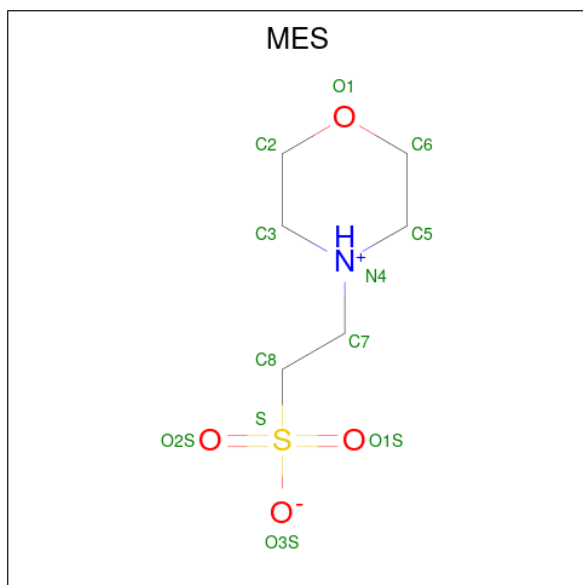
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			28	10	5	11		

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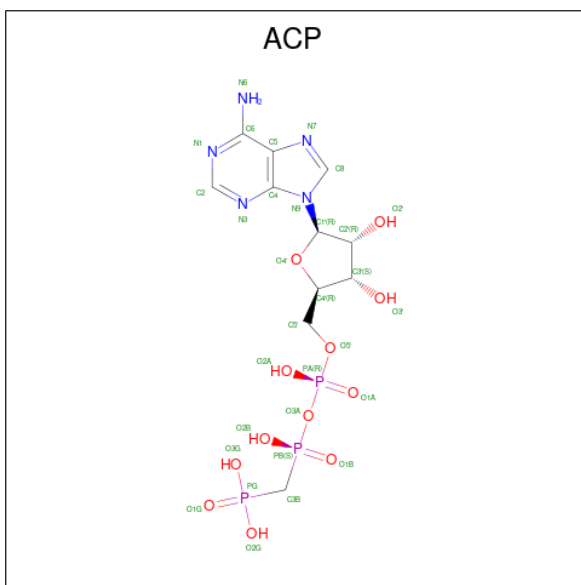
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

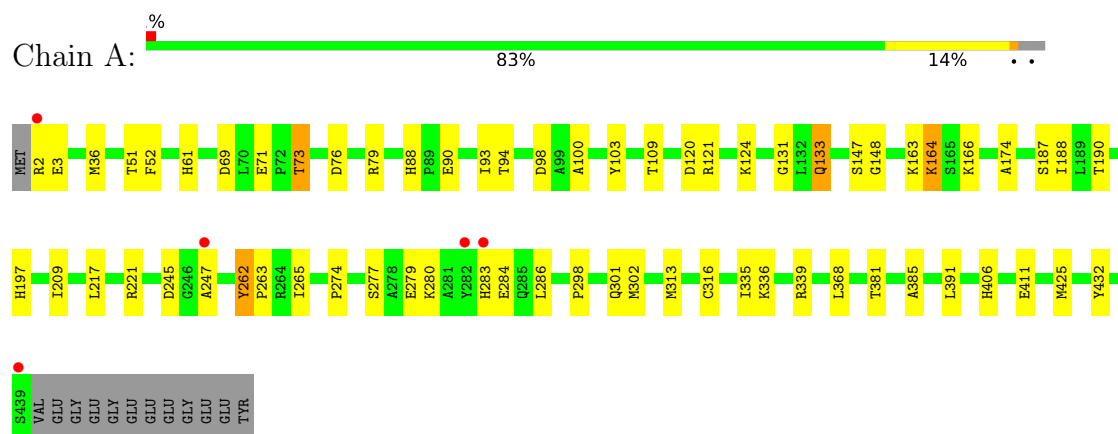
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	43	Total O 43 43	0	0
13	B	43	Total O 43 43	0	0
13	C	95	Total O 95 95	0	0
13	D	18	Total O 18 18	0	0
13	E	9	Total O 9 9	0	0
13	F	9	Total O 9 9	0	0

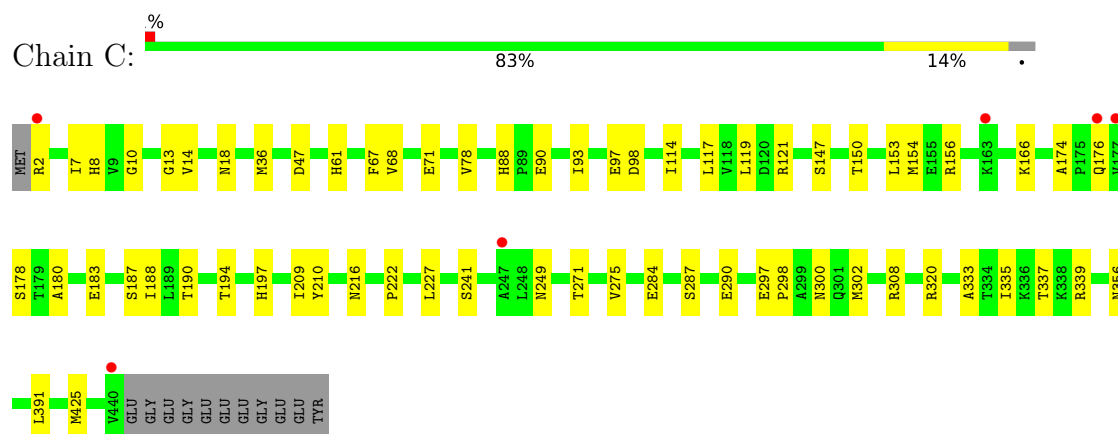
3 Residue-property plots [i](#)

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.

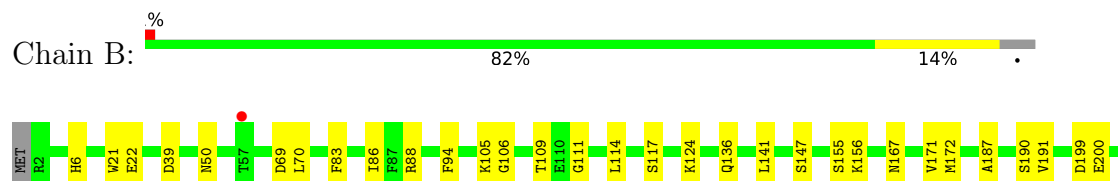
- Molecule 1: Tubulin alpha-1B chain

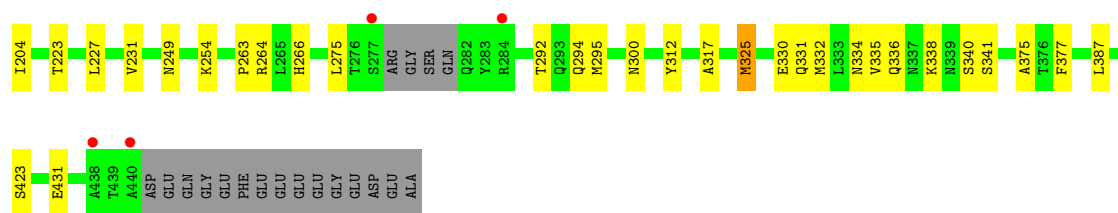


- Molecule 1: Tubulin alpha-1B chain

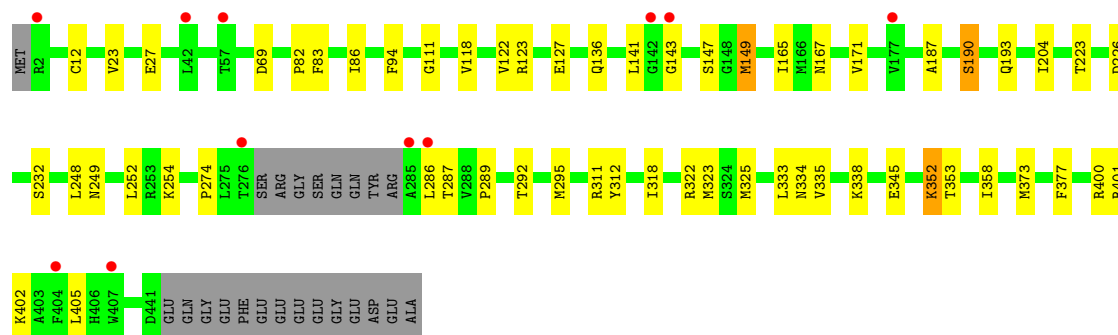
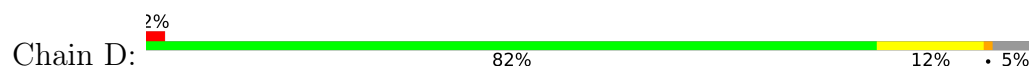


- Molecule 2: Tubulin beta-2B chain

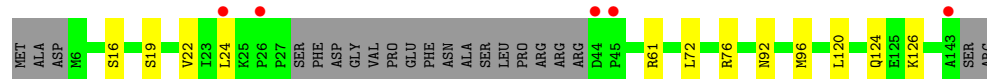




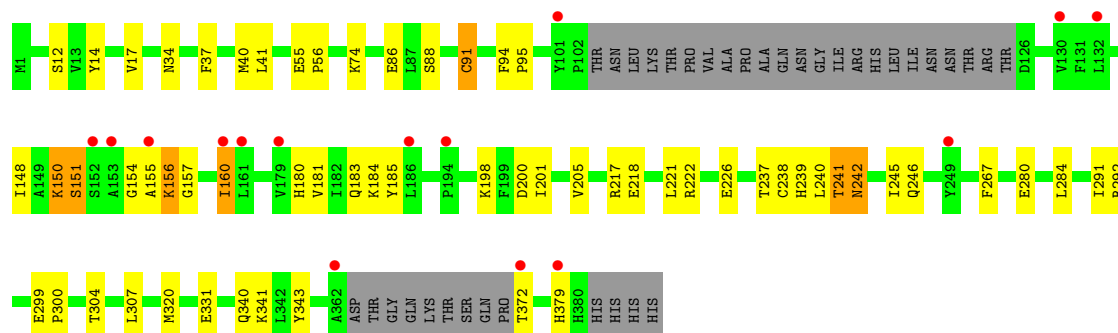
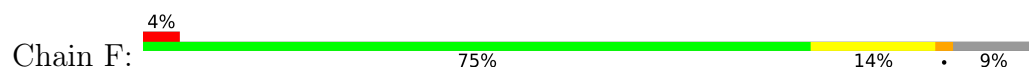
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.25Å 156.32Å 180.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 2.39 49.46 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.46-2.39) 99.6 (49.46-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.169 , 0.208 0.179 , 0.212	Depositor DCC
R_{free} test set	5816 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17853	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: GOL, MG, GTP, 6NL, CA, ACP, MES, GDP

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	0.37	0/3500	0.76	4/4752 (0.1%)
1	C	0.43	0/3507	0.75	0/4762
2	B	0.41	0/3423	0.73	0/4637
2	D	0.34	0/3386	0.72	1/4588 (0.0%)
3	E	0.36	0/1016	0.65	0/1348
4	F	0.28	0/2907	0.71	0/3926
All	All	0.37	0/17739	0.73	5/24013 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	TYR	CA-C-N	6.53	126.76	119.32
1	A	262	TYR	C-N-CA	6.53	126.76	119.32
1	A	174	ALA	CA-C-N	5.19	125.49	119.47
1	A	174	ALA	C-N-CA	5.19	125.49	119.47
2	D	358	ILE	N-CA-C	5.09	112.19	107.56

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	3422	0	3327	39	0
1	C	3429	0	3337	36	0
2	B	3346	0	3225	47	0
2	D	3313	0	3189	38	0
3	E	1008	0	1024	11	0
4	F	2842	0	2809	49	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	12	0	16	2	0
8	B	6	0	8	0	0
9	B	25	18	0	0	0
9	D	25	18	0	2	0
10	B	28	0	12	0	0
10	D	28	0	12	2	0
11	B	12	0	12	1	0
12	F	31	0	14	3	0
13	A	43	0	0	0	0
13	B	43	0	0	1	0
13	C	95	0	0	1	0
13	D	18	0	0	1	0
13	E	9	0	0	0	0
13	F	9	0	0	0	0
All	All	17817	36	17009	209	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 6.

All (209) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:ASN:ND2	2:B:338:LYS:HE3	1.73	1.02
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.03	0.91
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:151:SER:HB2	4:F:154:GLY:H	1.39	0.86
2:B:334:ASN:HD21	2:B:338:LYS:HE3	1.38	0.83
4:F:150:LYS:NZ	12:F:402:ACP:O2A	2.11	0.83
2:B:295:MET:HE3	2:B:375:ALA:HB1	1.58	0.83
4:F:155:ALA:HB1	4:F:156:LYS:HD3	1.64	0.80
4:F:320:MET:HE2	12:F:402:ACP:C2	2.13	0.78
2:B:334:ASN:CG	2:B:338:LYS:HE3	2.09	0.78
2:D:223:THR:N	2:D:226:ASP:OD2	2.15	0.77
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.18	0.76
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.32	0.74
1:A:164:LYS:HD2	1:A:164:LYS:N	2.04	0.72
1:A:221:ARG:HD3	2:B:325:MET:HB3	1.71	0.72
4:F:155:ALA:C	4:F:156:LYS:HE3	2.18	0.69
4:F:241:THR:OG1	12:F:402:ACP:O3'	2.00	0.69
4:F:156:LYS:HB2	4:F:156:LYS:HZ2	1.60	0.67
1:A:280:LYS:O	1:A:283:HIS:NE2	2.29	0.66
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.12	0.65
1:A:280:LYS:HB2	1:A:283:HIS:HE2	1.62	0.64
2:B:334:ASN:O	2:B:338:LYS:HD2	1.97	0.64
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.81	0.63
4:F:157:GLY:HA2	4:F:160:ILE:HD11	1.81	0.63
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.34	0.63
4:F:156:LYS:HB2	4:F:156:LYS:NZ	2.14	0.62
4:F:151:SER:HG	4:F:180:HIS:CE1	2.17	0.62
2:B:249:ASN:O	2:B:254:LYS:NZ	2.33	0.62
2:D:352:LYS:HG3	9:D:500:6NL:CAF	2.32	0.60
4:F:292:ARG:NH1	4:F:379:HIS:O	2.34	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.84	0.59
3:E:92:ASN:O	3:E:96:MET:HG2	2.02	0.59
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.67	0.59
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.85	0.58
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.84	0.58
2:B:294:GLN:OE1	13:B:601:HOH:O	2.17	0.58
1:C:190:THR:O	1:C:194:THR:HG23	2.04	0.58
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.86	0.58
1:C:241:SER:HA	1:C:249:ASN:HD21	1.69	0.57
4:F:148:ILE:HG22	4:F:183:GLN:O	2.04	0.57
2:B:332:MET:O	2:B:336:GLN:HG3	2.04	0.57
4:F:201:ILE:HG12	4:F:221:LEU:CD2	2.34	0.57
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.87	0.57
1:C:176:GLN:NE2	2:D:333:LEU:HD21	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HB2	1:A:283:HIS:NE2	2.20	0.56
8:A:504:GOL:O3	8:A:504:GOL:O1	2.19	0.56
1:A:166:LYS:HE2	1:A:197:HIS:O	2.06	0.55
2:B:50:ASN:H	2:B:50:ASN:ND2	2.04	0.55
2:B:88:ARG:HH22	2:B:124:LYS:HZ1	1.52	0.55
1:A:109:THR:OG1	1:A:411:GLU:OE2	2.19	0.55
4:F:200:ASP:N	4:F:241:THR:HG21	2.21	0.55
1:A:3:GLU:O	1:A:133:GLN:HG3	2.07	0.55
2:B:136:GLN:HA	2:B:167:ASN:O	2.06	0.54
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.89	0.54
1:C:98:ASP:OD2	2:D:254:LYS:NZ	2.41	0.54
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.89	0.54
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.89	0.54
3:E:72:LEU:O	3:E:76:ARG:HG2	2.07	0.54
1:C:47:ASP:OD2	13:C:601:HOH:O	2.18	0.54
1:C:320:ARG:HA	1:C:356:ASN:O	2.07	0.54
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.88	0.54
2:B:83:PHE:O	2:B:86:ILE:HG22	2.07	0.54
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	0.54
4:F:157:GLY:HA3	4:F:245:ILE:HD11	1.90	0.54
4:F:160:ILE:HD12	4:F:240:LEU:CD1	2.38	0.54
1:A:298:PRO:HA	1:A:301:GLN:CD	2.33	0.53
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.91	0.53
4:F:237:THR:O	4:F:246:GLN:NE2	2.35	0.53
4:F:239:HIS:C	4:F:240:LEU:HD23	2.34	0.53
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.91	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.52
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.44	0.52
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.74	0.52
4:F:155:ALA:O	4:F:156:LYS:HE3	2.09	0.52
2:D:83:PHE:O	2:D:86:ILE:HG22	2.09	0.52
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.45	0.52
1:A:2:ARG:HA	1:A:131:GLY:O	2.10	0.51
4:F:150:LYS:HG3	4:F:181:VAL:HG23	1.93	0.51
2:D:223:THR:OG1	2:D:226:ASP:OD2	2.27	0.51
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.93	0.51
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.76	0.51
2:B:264:ARG:HE	2:B:431:GLU:CD	2.18	0.51
1:A:221:ARG:NH1	2:B:325:MET:SD	2.84	0.50
1:C:209:ILE:HD11	1:C:302:MET:SD	2.51	0.50
2:D:143:GLY:HA3	10:D:501:GDP:O5'	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.92	0.50
4:F:88:SER:O	4:F:91:CYS:HB3	2.11	0.50
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.94	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.52	0.49
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.49
4:F:160:ILE:HD12	4:F:240:LEU:HD11	1.94	0.49
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.94	0.49
2:D:147:SER:HB2	2:D:190:SER:OG	2.13	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.49
4:F:222:ARG:O	4:F:241:THR:HG22	2.13	0.49
2:D:311:ARG:NH2	2:D:345:GLU:OE2	2.45	0.48
4:F:14:TYR:HA	4:F:17:VAL:HB	1.95	0.48
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.95	0.48
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.46	0.48
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.96	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.31	0.48
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.46	0.47
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.48	0.47
1:C:333:ALA:O	1:C:337:THR:HG23	2.15	0.47
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.96	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.15	0.47
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.96	0.47
2:B:156:LYS:HZ3	3:E:76:ARG:NE	2.12	0.47
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.96	0.47
2:D:141:LEU:HB3	2:D:187:ALA:HA	1.96	0.47
2:D:323:MET:HE2	2:D:373:MET:HG3	1.98	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.46
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.30	0.46
2:D:111:GLY:HA3	2:D:149:MET:HG3	1.97	0.46
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.97	0.46
1:C:10:GLY:O	1:C:14:VAL:HG23	2.16	0.46
4:F:155:ALA:HB1	4:F:156:LYS:CD	2.38	0.46
2:D:400:ARG:HG3	2:D:401:ARG:HG2	1.98	0.46
4:F:242:ASN:OD1	4:F:242:ASN:N	2.37	0.45
2:B:114:LEU:O	2:B:114:LEU:HG	2.16	0.45
2:B:105:LYS:HA	2:B:109:THR:OG1	2.17	0.45
4:F:201:ILE:HG12	4:F:221:LEU:HD23	1.98	0.45
2:B:50:ASN:H	2:B:50:ASN:HD22	1.64	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.17	0.45
1:C:147:SER:HB2	1:C:190:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:GLN:O	2:B:335:VAL:HG23	2.16	0.45
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.98	0.45
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.52	0.45
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.81	0.45
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.81	0.45
1:C:150:THR:O	1:C:154:MET:HG2	2.17	0.45
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.45
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.34	0.44
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.47	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.44
1:A:98:ASP:OD1	1:A:100:ALA:N	2.40	0.44
2:B:334:ASN:OD1	2:B:338:LYS:HE3	2.17	0.44
4:F:155:ALA:CB	4:F:156:LYS:HD3	2.43	0.44
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.52	0.44
2:D:69:ASP:O	2:D:94:PHE:HA	2.18	0.44
1:C:216:ASN:HB3	1:C:275:VAL:O	2.17	0.43
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.53	0.43
1:C:297:GLU:OE2	1:C:339:ARG:NH2	2.51	0.43
2:D:141:LEU:HA	2:D:147:SER:HB3	1.98	0.43
1:C:287:SER:OG	1:C:290:GLU:HG3	2.19	0.43
2:D:325:MET:HE3	2:D:325:MET:HB3	1.95	0.43
2:B:227:LEU:O	2:B:231:VAL:HG23	2.19	0.43
1:C:298:PRO:HG2	1:C:308:ARG:CZ	2.49	0.43
2:D:118:VAL:O	2:D:122:VAL:HG23	2.19	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.42
8:A:504:GOL:H31	3:E:61:ARG:HD2	2.00	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.42
2:B:199:ASP:O	2:B:266:HIS:HB2	2.19	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.42
2:D:352:LYS:HG3	9:D:500:6NL:CAA	2.49	0.42
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.54	0.42
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.01	0.42
2:B:223:THR:O	2:B:227:LEU:HD13	2.20	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.42
2:D:167:ASN:ND2	13:D:603:HOH:O	2.52	0.42
2:D:287:THR:HB	2:D:289:PRO:HD2	2.00	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.42
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.81	0.42
2:B:295:MET:HE1	2:B:317:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:SER:OG	4:F:34:ASN:ND2	2.48	0.42
2:D:123:ARG:O	2:D:127:GLU:HG2	2.19	0.42
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.53	0.42
3:E:120:LEU:O	3:E:124:GLN:HG3	2.20	0.42
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.55	0.42
2:D:23:VAL:O	2:D:27:GLU:HG3	2.19	0.42
2:B:39:ASP:OD1	2:B:39:ASP:N	2.53	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.41
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.02	0.41
1:A:209:ILE:HD11	1:A:302:MET:SD	2.61	0.41
4:F:55:GLU:HA	4:F:56:PRO:HD2	1.82	0.41
1:A:187:SER:CB	1:A:391:LEU:HD21	2.50	0.41
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.38	0.41
2:B:330:GLU:O	2:B:334:ASN:HB2	2.21	0.41
1:C:271:THR:HG23	1:C:300:ASN:O	2.19	0.41
2:D:295:MET:CG	2:D:377:PHE:HB2	2.50	0.41
2:B:275:LEU:HG	2:B:300:ASN:ND2	2.36	0.41
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.51	0.41
1:C:8:HIS:HB3	1:C:13:GLY:O	2.20	0.41
4:F:184:LYS:HE2	4:F:185:TYR:O	2.20	0.41
1:A:51:THR:HG22	1:A:52:PHE:CD1	2.54	0.41
2:B:156:LYS:NZ	3:E:76:ARG:NE	2.68	0.41
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.02	0.41
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.02	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.02	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.80	0.41
11:B:505:MES:H51	11:B:505:MES:H81	1.81	0.41
4:F:239:HIS:O	4:F:240:LEU:HD23	2.20	0.41
1:A:247:ALA:HB3	3:E:19:SER:OG	2.21	0.41
1:A:336:LYS:HG3	3:E:24:LEU:HD13	2.03	0.41
1:C:174:ALA:O	1:C:178:SER:HB3	2.21	0.41
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.84	0.41
4:F:240:LEU:HD12	4:F:245:ILE:HD13	2.03	0.41
1:A:245:ASP:HB3	3:E:16:SER:OG	2.22	0.40
1:A:265:ILE:HG21	1:A:313:MET:HE1	2.03	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.03	0.40
1:A:277:SER:OG	1:A:279:GLU:OE1	2.39	0.40
2:B:70:LEU:HA	2:B:70:LEU:HD23	1.86	0.40
2:B:187:ALA:O	2:B:191:VAL:HG23	2.22	0.40
2:B:199:ASP:C	2:B:200:GLU:HG3	2.46	0.40
4:F:155:ALA:CB	4:F:156:LYS:CE	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:352:LYS:HD3	2:D:353:THR:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	428 (98%)	8 (2%)	0	100	100
1	C	437/451 (97%)	429 (98%)	8 (2%)	0	100	100
2	B	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
2	D	418/445 (94%)	414 (99%)	4 (1%)	0	100	100
3	E	118/143 (82%)	116 (98%)	2 (2%)	0	100	100
4	F	342/384 (89%)	335 (98%)	7 (2%)	0	100	100
All	All	2173/2319 (94%)	2136 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	369/379 (97%)	362 (98%)	7 (2%)	50	71
1	C	370/379 (98%)	366 (99%)	4 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	368/383 (96%)	364 (99%)	4 (1%)	65	82
2	D	364/383 (95%)	357 (98%)	7 (2%)	50	71
3	E	109/127 (86%)	108 (99%)	1 (1%)	70	85
4	F	310/342 (91%)	299 (96%)	11 (4%)	32	53
All	All	1890/1993 (95%)	1856 (98%)	34 (2%)	51	73

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

Mol	Chain	Res	Type
1	A	73	THR
1	A	133	GLN
1	A	163	LYS
1	A	164	LYS
1	A	284	GLU
1	A	316	CYS
1	A	381	THR
2	B	117	SER
2	B	325	MET
2	B	341	SER
2	B	423	SER
1	C	2	ARG
1	C	68	VAL
1	C	97	GLU
1	C	284	GLU
2	D	149	MET
2	D	190	SER
2	D	232	SER
2	D	248	LEU
2	D	249	ASN
2	D	322	ARG
2	D	352	LYS
3	E	22	VAL
4	F	12	SER
4	F	86	GLU
4	F	91	CYS
4	F	150	LYS
4	F	151	SER
4	F	156	LYS
4	F	160	ILE
4	F	241	THR
4	F	242	ASN

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Mol	Chain	Res	Type
4	F	341	LYS
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
1	A	393	HIS
2	B	11	GLN
2	B	15	GLN
2	B	50	ASN
2	B	167	ASN
2	B	300	ASN
2	B	331	GLN
2	B	436	GLN
1	C	249	ASN
1	C	283	HIS
1	C	393	HIS
2	D	11	GLN
2	D	15	GLN
2	D	50	ASN
2	D	249	ASN
2	D	406	HIS
3	E	84	GLN
3	E	103	GLN
4	F	269	GLN
4	F	348	GLN

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 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	501	6	33,34,34	1.03	1 (3%)	50,54,54	1.59	11 (22%)
8	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.38	0
8	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.47	0
10	GDP	B	502	6	29,30,30	1.18	3 (10%)	45,47,47	1.77	8 (17%)
8	GOL	B	504	-	5,5,5	0.37	0	5,5,5	0.39	0
11	MES	B	505	-	12,12,12	2.32	1 (8%)	15,16,16	1.76	3 (20%)
10	GDP	D	501	6	29,30,30	1.14	2 (6%)	45,47,47	1.80	6 (13%)
5	GTP	A	501	6	33,34,34	1.06	2 (6%)	50,54,54	1.57	10 (20%)
9	6NL	B	501	-	27,27,27	1.04	1 (3%)	36,38,38	1.51	6 (16%)
12	ACP	F	402	6	31,33,33	1.78	3 (9%)	47,52,52	1.18	6 (12%)
9	6NL	D	500	-	27,27,27	0.98	1 (3%)	36,38,38	1.65	7 (19%)

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	C	501	6	-	8/22/38/38	0/3/3/3
8	GOL	A	504	-	-	0/4/4/4	-
8	GOL	A	505	-	-	2/4/4/4	-
10	GDP	B	502	6	-	4/16/32/32	0/3/3/3
8	GOL	B	504	-	-	2/4/4/4	-
11	MES	B	505	-	-	0/6/14/14	0/1/1/1
10	GDP	D	501	6	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
9	6NL	B	501	-	-	0/16/22/22	0/3/3/3
12	ACP	F	402	6	-	4/19/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	6NL	D	500	-	-	0/16/22/22	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	MES	C8-S	-7.77	1.66	1.77
12	F	402	ACP	PB-O3A	5.97	1.65	1.58
12	F	402	ACP	PA-O3A	5.92	1.65	1.59
9	B	501	6NL	CAJ-CAK	3.73	1.38	1.34
5	C	501	GTP	PB-O3B	3.63	1.63	1.59
9	D	500	6NL	CAJ-CAK	3.31	1.37	1.34
10	D	501	GDP	C5-C4	3.08	1.47	1.38
10	B	502	GDP	C5-C4	2.97	1.46	1.38
5	A	501	GTP	PB-O3B	2.95	1.62	1.59
5	A	501	GTP	PA-O3A	2.59	1.62	1.59
10	D	501	GDP	C6-N1	-2.52	1.34	1.38
12	F	402	ACP	C8-N9	2.41	1.41	1.37
10	B	502	GDP	C6-N1	-2.40	1.34	1.38
10	B	502	GDP	PA-O3A	2.25	1.61	1.59

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	501	GDP	C5-C4-N3	-6.16	118.59	128.39
10	B	502	GDP	C5-C4-N3	-5.50	119.64	128.39
10	D	501	GDP	C2-N3-C4	5.12	121.12	112.30
10	B	502	GDP	C2-N3-C4	4.97	120.86	112.30
9	D	500	6NL	CAX-OAY-CAR	-4.86	99.27	105.05
5	C	501	GTP	C2-N3-C4	4.71	120.41	112.30
5	A	501	GTP	C5-C4-N3	-4.67	120.96	128.39
5	C	501	GTP	C5-C4-N3	-4.65	120.98	128.39
11	B	505	MES	C5-N4-C3	4.63	118.81	108.84
5	A	501	GTP	C2-N3-C4	4.53	120.09	112.30
10	D	501	GDP	N9-C4-N3	4.50	134.95	125.95
9	D	500	6NL	CAX-OAW-CAQ	-4.43	99.38	105.32
10	B	502	GDP	N9-C4-N3	3.99	133.92	125.95
10	B	502	GDP	C6-C5-N7	3.90	137.38	130.29
9	D	500	6NL	OAH-CAE-CAF	3.66	120.03	114.55
9	B	501	6NL	CAX-OAY-CAR	-3.62	100.73	105.05
9	B	501	6NL	OAH-CAE-CAF	3.52	119.83	114.55
12	F	402	ACP	O1G-PG-C3B	-3.51	103.72	111.37
10	D	501	GDP	C6-C5-N7	3.43	136.54	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	6NL	CAX-OAW-CAQ	-2.99	101.31	105.32
5	C	501	GTP	O2A-PA-O3A	2.95	115.24	107.27
5	A	501	GTP	N9-C4-N3	2.91	131.78	125.95
5	C	501	GTP	N9-C4-N3	2.91	131.78	125.95
5	C	501	GTP	N9-C8-N7	-2.90	108.03	113.40
5	A	501	GTP	N9-C8-N7	-2.83	108.16	113.40
10	D	501	GDP	C4-C5-N7	-2.78	106.26	110.67
5	A	501	GTP	O2A-PA-O3A	2.69	114.54	107.27
5	A	501	GTP	C2-N1-C6	-2.65	120.31	125.11
5	C	501	GTP	C8-N7-C5	2.63	108.94	104.26
10	B	502	GDP	C4-C5-N7	-2.62	106.53	110.67
9	B	501	6NL	OAH-CAE-CAD	-2.60	119.92	124.30
5	A	501	GTP	C8-N7-C5	2.57	108.83	104.26
9	D	500	6NL	OAH-CAE-CAD	-2.55	120.00	124.30
5	C	501	GTP	C2-N1-C6	-2.54	120.50	125.11
9	D	500	6NL	CAT-CAS-CAR	-2.54	117.40	120.22
9	B	501	6NL	CAT-CAS-CAR	-2.49	117.45	120.22
9	B	501	6NL	CAB-CAA-CAF	-2.46	119.06	120.79
12	F	402	ACP	PB-O3A-PA	-2.43	124.43	132.37
5	A	501	GTP	O6-C6-C5	-2.41	120.16	126.53
5	C	501	GTP	C5-C6-N1	2.41	119.38	113.25
5	A	501	GTP	C5-C6-N1	2.39	119.34	113.25
11	B	505	MES	O1S-S-C8	2.39	110.34	106.73
5	C	501	GTP	O2B-PB-O3A	2.36	113.65	107.27
10	B	502	GDP	O6-C6-C5	-2.35	120.32	126.53
12	F	402	ACP	O2B-PB-O1B	2.33	117.54	109.95
12	F	402	ACP	N3-C2-N1	-2.25	125.17	128.58
5	C	501	GTP	O6-C6-C5	-2.25	120.59	126.53
10	B	502	GDP	C5-C6-N1	2.11	118.63	113.25
12	F	402	ACP	C4-C5-N7	2.11	113.00	110.58
11	B	505	MES	C6-C5-N4	-2.11	106.92	110.12
5	A	501	GTP	O2G-PG-O3B	2.10	111.69	104.64
9	D	500	6NL	CAB-CAA-CAF	-2.09	119.32	120.79
10	B	502	GDP	O2A-PA-O3A	2.06	112.85	107.27
12	F	402	ACP	O2G-PG-C3B	-2.06	101.41	106.40
10	D	501	GDP	C8-N7-C5	2.02	107.87	104.26
9	D	500	6NL	OAU-CAS-CAR	2.02	118.60	115.14
5	C	501	GTP	N1-C2-N3	-2.02	119.63	123.32

There are no chirality outliers.

All (33) torsion outliers are listed below:

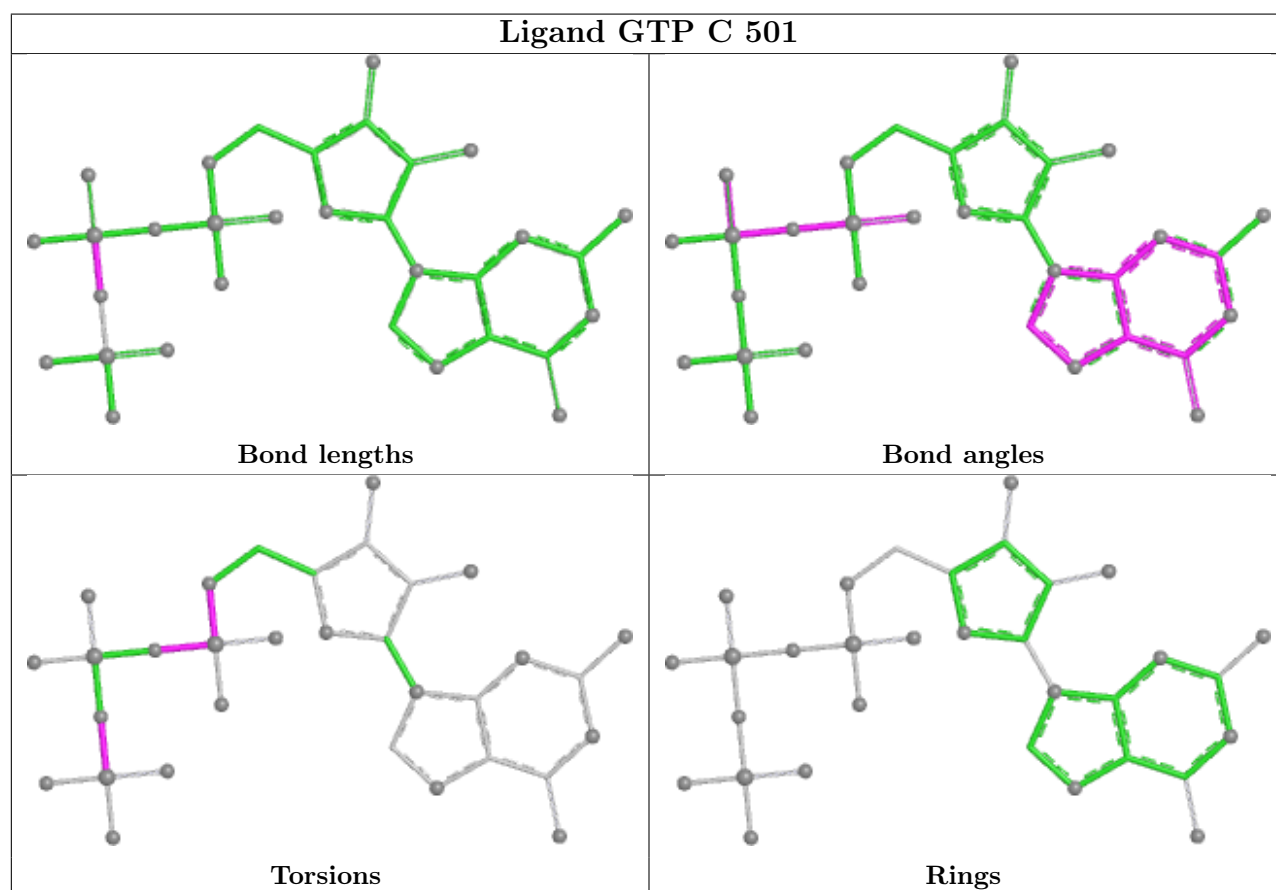
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	504	GOL	O1-C1-C2-C3
10	B	502	GDP	C5'-O5'-PA-O3A
10	B	502	GDP	C5'-O5'-PA-O1A
10	B	502	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O1A
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O2B
12	F	402	ACP	PG-C3B-PB-O3A
8	A	505	GOL	O1-C1-C2-C3
8	A	505	GOL	O1-C1-C2-O2
8	B	504	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O1G
10	B	502	GDP	PB-O3A-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
12	F	402	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O1A
10	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A

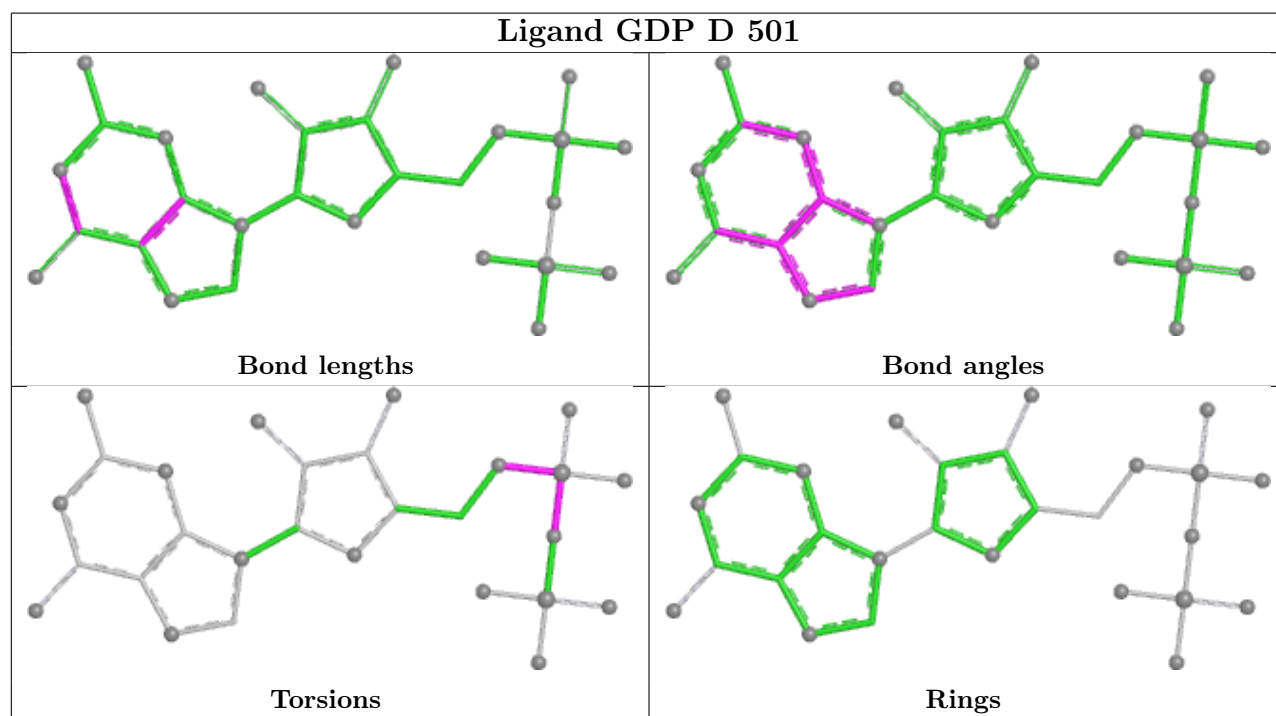
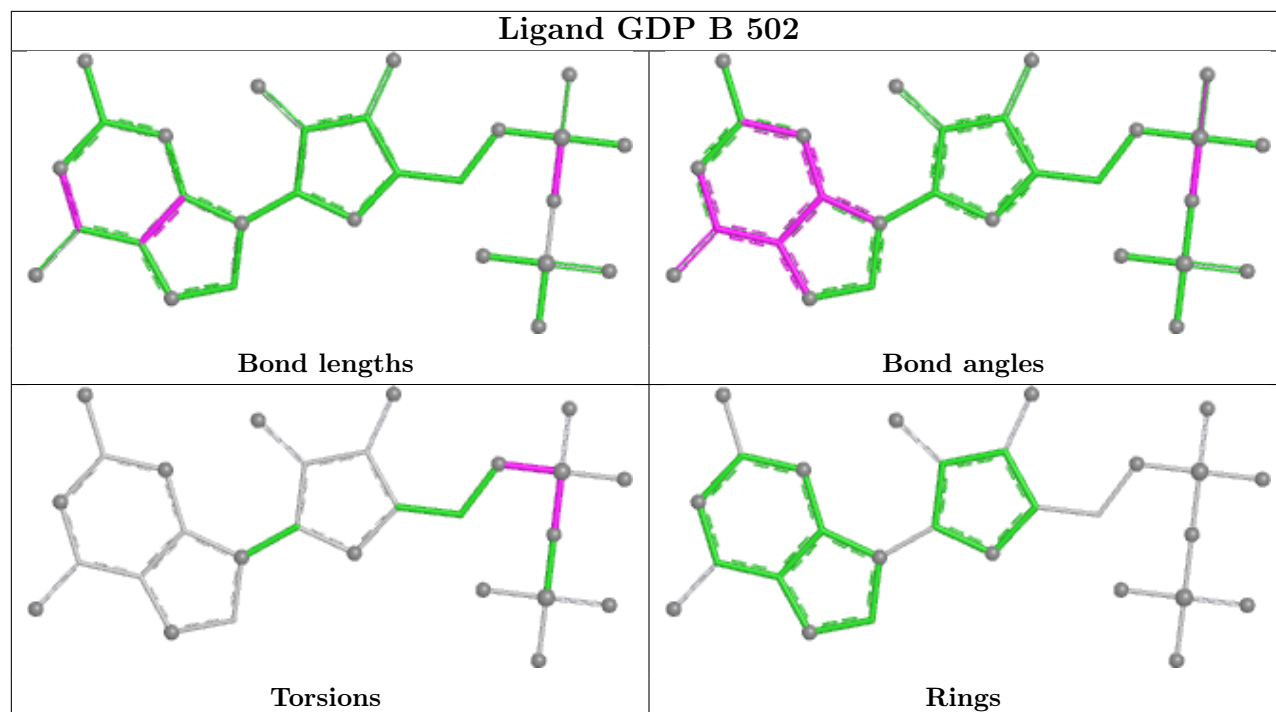
There are no ring outliers.

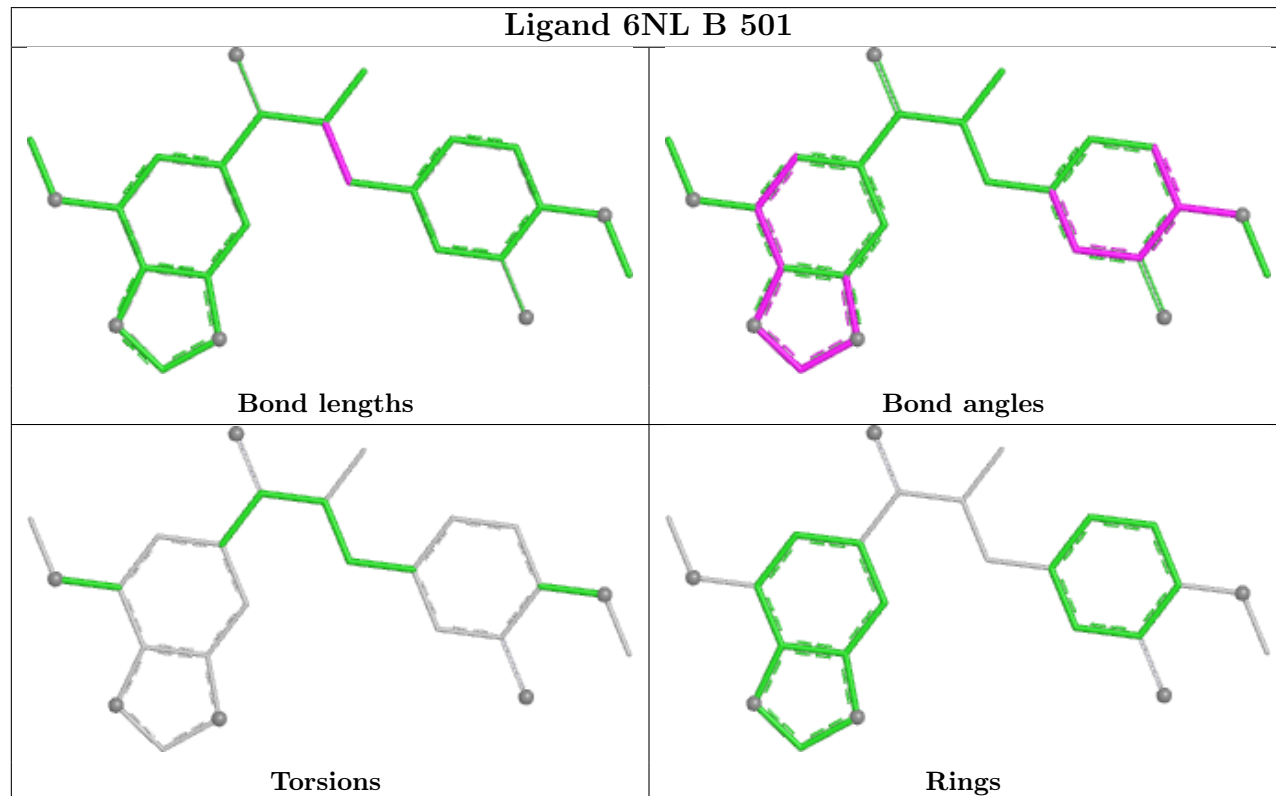
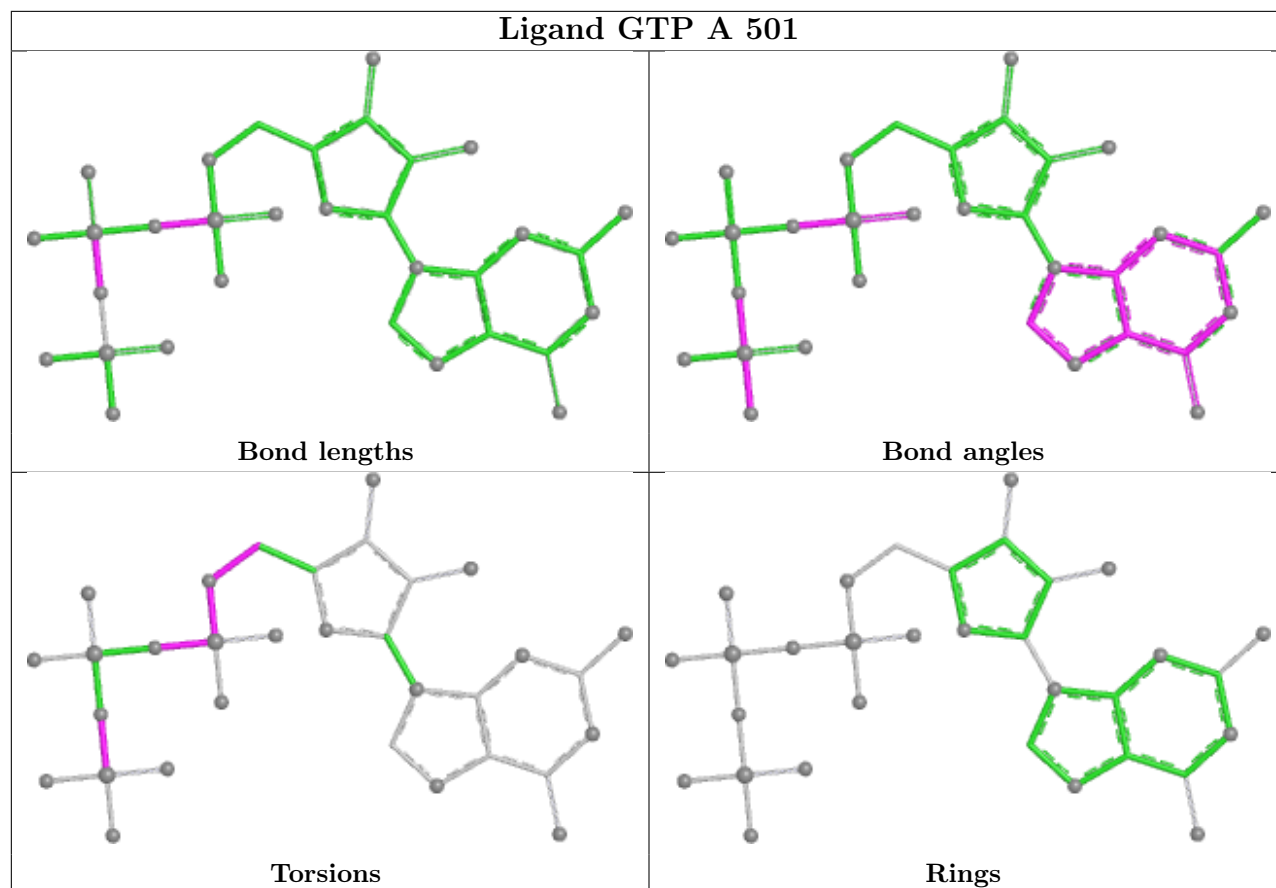
5 monomers are involved in 10 short contacts:

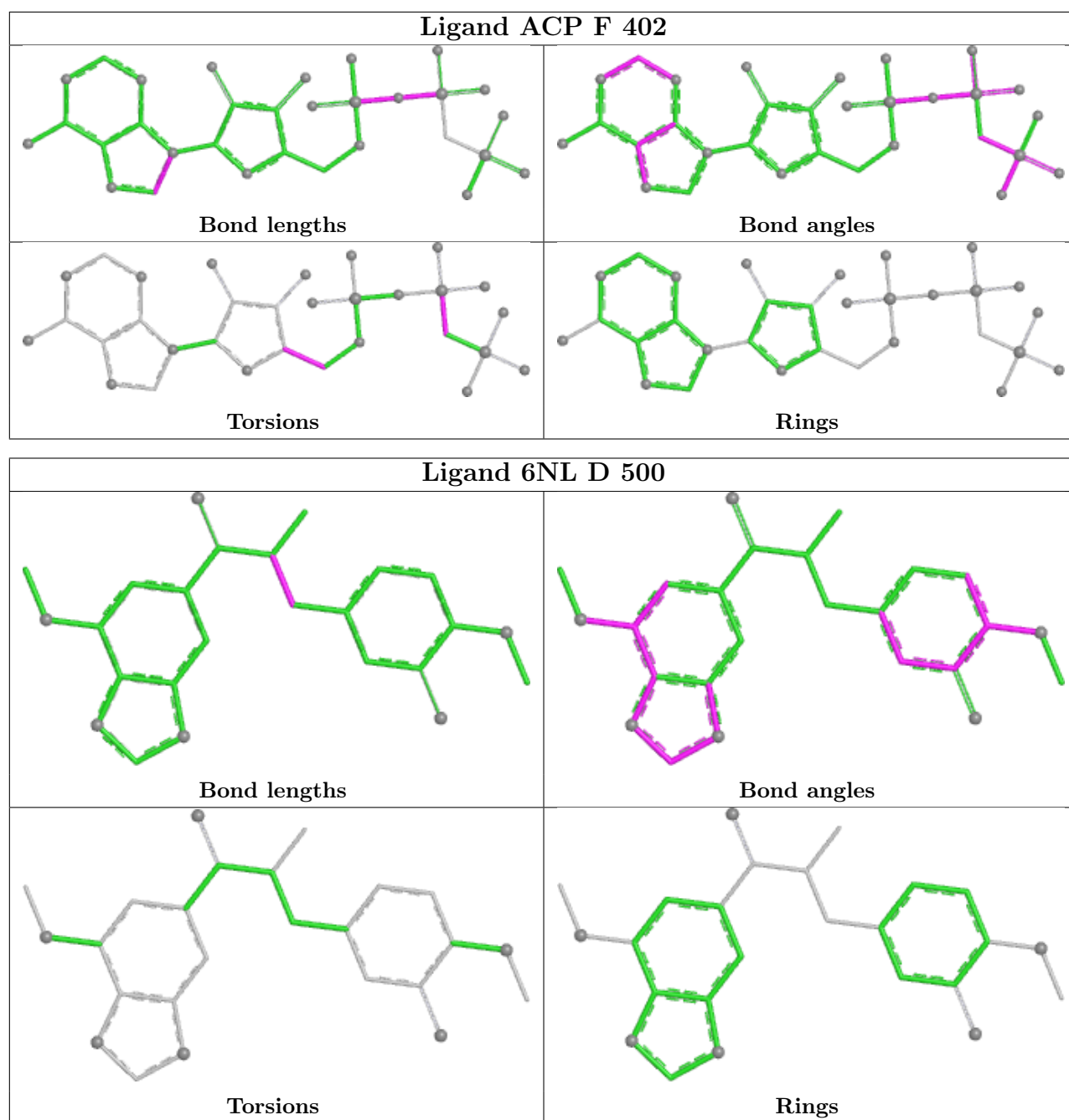
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	504	GOL	2	0
11	B	505	MES	1	0
10	D	501	GDP	2	0
12	F	402	ACP	3	0
9	D	500	6NL	2	0

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 [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%)	-0.03	5 (1%) 78 74	44, 66, 105, 177	0
1	C	439/451 (97%)	-0.22	6 (1%) 73 69	38, 53, 84, 110	0
2	B	425/445 (95%)	-0.12	5 (1%) 76 73	27, 58, 96, 134	2 (0%)
2	D	422/445 (94%)	0.20	11 (2%) 57 53	45, 76, 113, 144	3 (0%)
3	E	122/143 (85%)	0.30	5 (4%) 41 37	50, 80, 116, 130	0
4	F	348/384 (90%)	0.39	15 (4%) 40 36	56, 95, 164, 186	0
All	All	2194/2319 (94%)	0.04	47 (2%) 63 59	27, 69, 128, 186	5 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	440	ALA	6.1
2	D	285	ALA	4.7
1	C	440	VAL	4.0
2	D	276	THR	4.0
3	E	143	ALA	3.9
2	D	286	LEU	3.4
4	F	362	ALA	3.3
1	A	282	TYR	3.2
4	F	152	SER	3.2
4	F	155	ALA	3.2
1	A	283	HIS	3.1
2	B	277	SER	3.1
2	D	143	GLY	3.0
2	D	2	ARG	3.0
1	C	177	VAL	2.9
4	F	194	PRO	2.9
1	C	247	ALA	2.9
4	F	372	THR	2.9
2	B	57	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	407	TRP	2.7
3	E	26	PRO	2.7
2	D	57	THR	2.6
1	C	176	GLN	2.6
2	D	177	VAL	2.6
4	F	160	ILE	2.6
1	C	2	ARG	2.5
3	E	45	PRO	2.5
4	F	161	LEU	2.4
4	F	249	TYR	2.4
1	A	2	ARG	2.3
3	E	24	LEU	2.2
4	F	130	VAL	2.2
4	F	132	LEU	2.2
4	F	379	HIS	2.2
4	F	179	VAL	2.2
2	D	404	PHE	2.2
3	E	44	ASP	2.1
2	B	438	ALA	2.1
2	D	42	LEU	2.1
2	B	284	ARG	2.1
1	A	247	ALA	2.1
1	A	439	SER	2.1
4	F	186	LEU	2.1
2	D	142	GLY	2.1
1	C	163	LYS	2.0
4	F	153	ALA	2.0
4	F	101	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

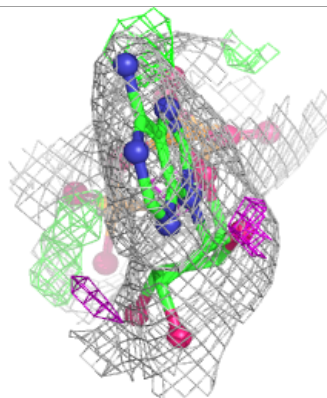
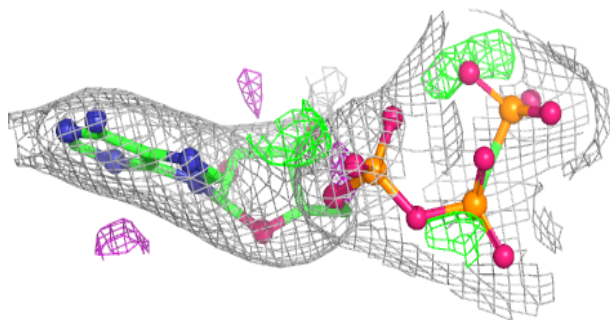
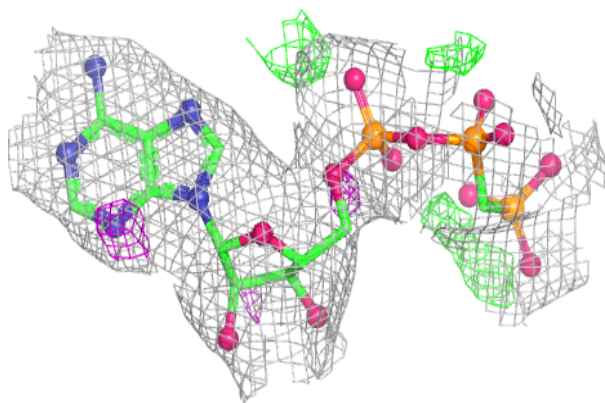
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	502	1/1	0.65	0.14	74,74,74,74	0
7	CA	B	506	1/1	0.65	0.29	163,163,163,163	0
8	GOL	A	505	6/6	0.87	0.17	83,85,91,94	0
8	GOL	A	504	6/6	0.88	0.15	87,89,94,97	0
6	MG	F	401	1/1	0.89	0.08	104,104,104,104	0
12	ACP	F	402	31/31	0.89	0.10	86,105,139,156	0
8	GOL	B	504	6/6	0.90	0.18	103,106,108,110	0
6	MG	D	502	1/1	0.92	0.12	75,75,75,75	0
7	CA	E	201	1/1	0.92	0.12	111,111,111,111	0
10	GDP	D	501	28/28	0.93	0.09	56,68,83,92	0
7	CA	A	503	1/1	0.93	0.06	89,89,89,89	0
11	MES	B	505	12/12	0.95	0.09	49,63,77,78	0
9	6NL	D	500	25/25	0.96	0.08	42,59,84,85	0
9	6NL	B	501	25/25	0.96	0.07	36,50,60,67	0
10	GDP	B	502	28/28	0.98	0.05	35,43,50,61	0
5	GTP	A	501	32/32	0.98	0.05	39,48,55,73	0
6	MG	B	503	1/1	0.99	0.06	45,45,45,45	0
7	CA	C	503	1/1	0.99	0.03	78,78,78,78	0
5	GTP	C	501	32/32	0.99	0.05	31,40,53,68	0
6	MG	C	502	1/1	1.00	0.03	39,39,39,39	0

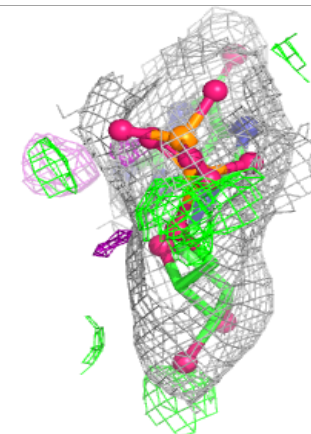
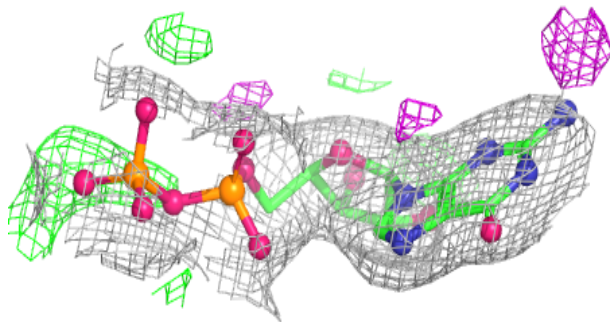
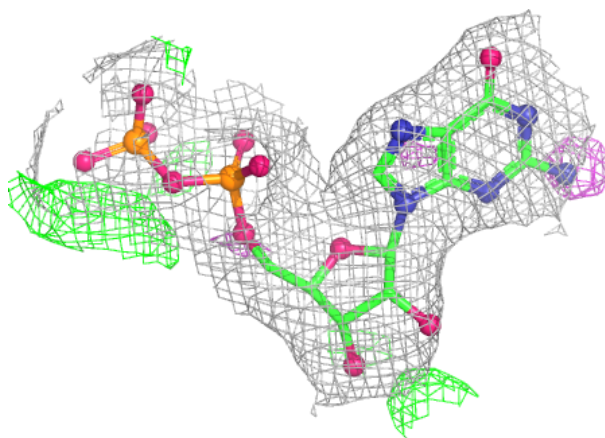
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

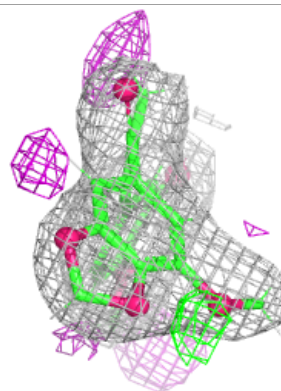
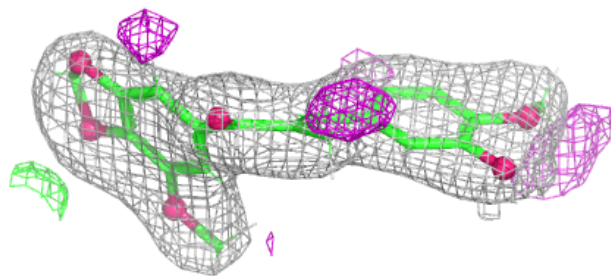
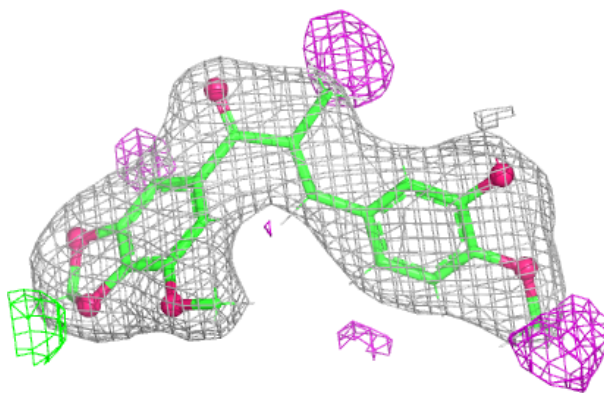
**Electron density around GDP D 501:**

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

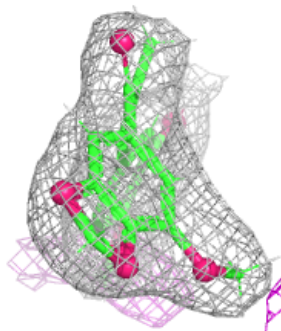
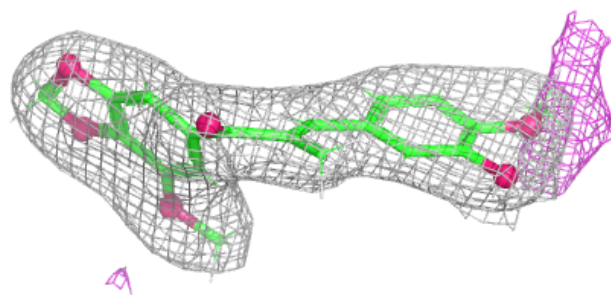
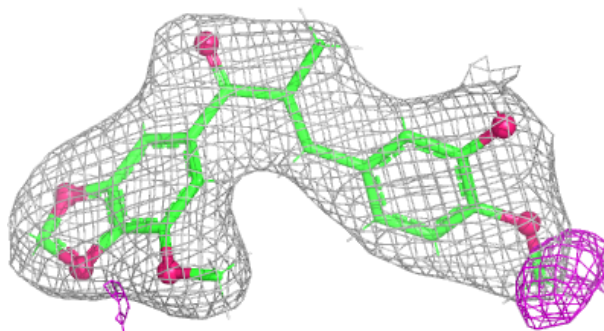


Electron density around 6NL D 500:

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

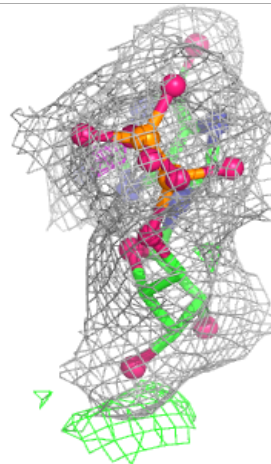
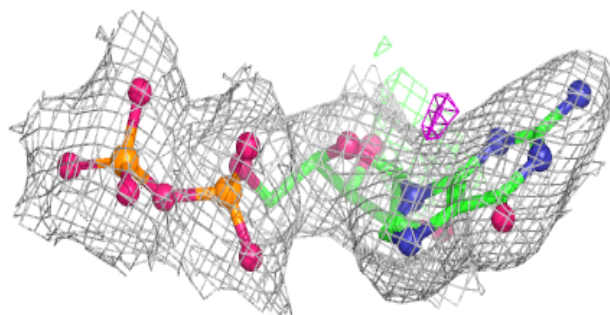
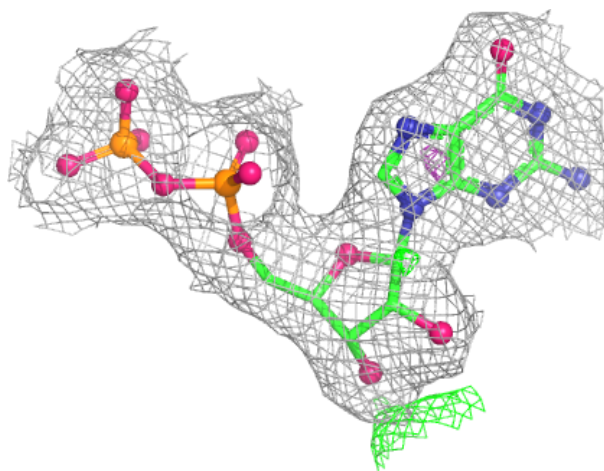
**Electron density around 6NL B 501:**

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



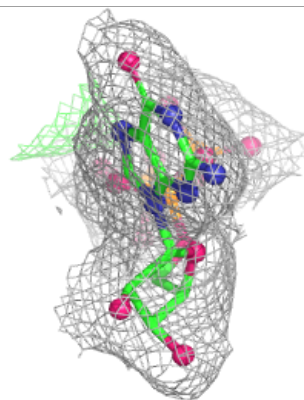
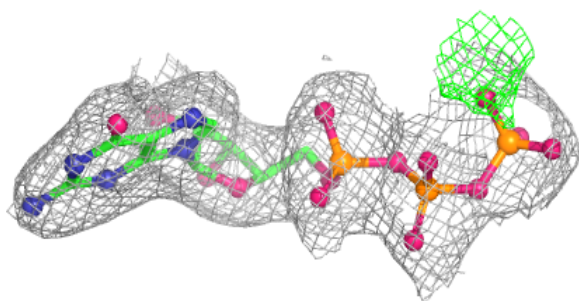
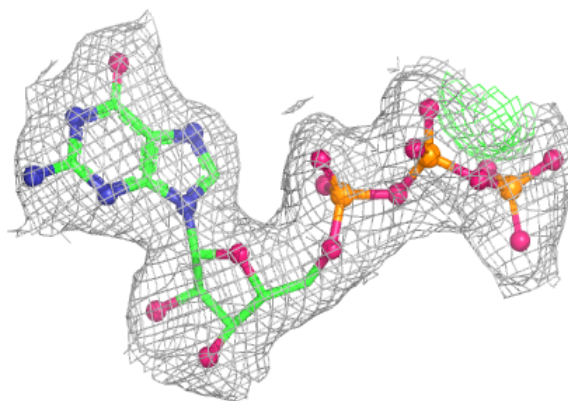
Electron density around GDP B 502:

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

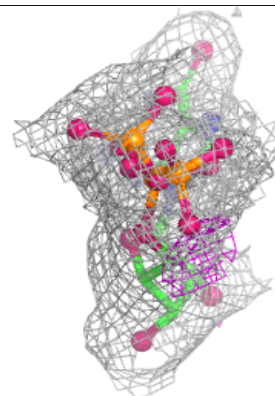
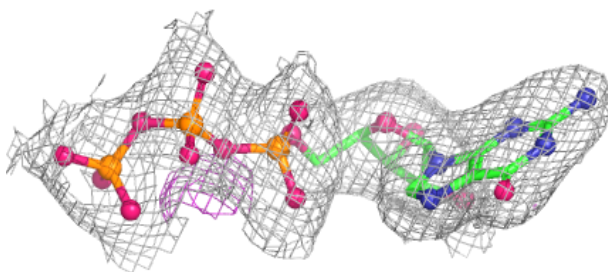
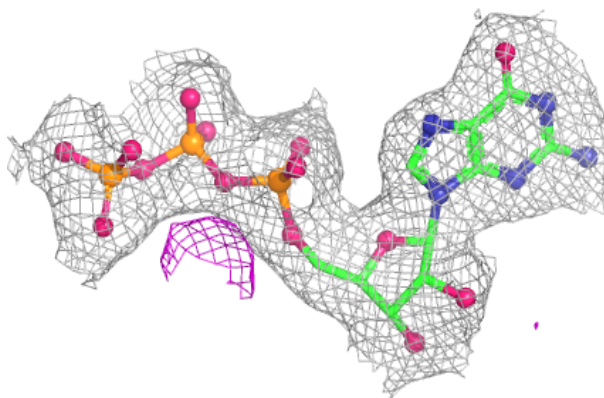


Electron density around GTP A 501:

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

**Electron density around 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.