



Full wwPDB EM Validation Report ⓘ

Apr 8, 2026 – 10:32 PM UTC

PDB ID : 9UAR / pdb_00009uar
EMDB ID : EMD-63990
Title : CTP synthase DON-state
Authors : Guo, C.J.
Deposited on : 2025-04-01
Resolution : 1.99 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

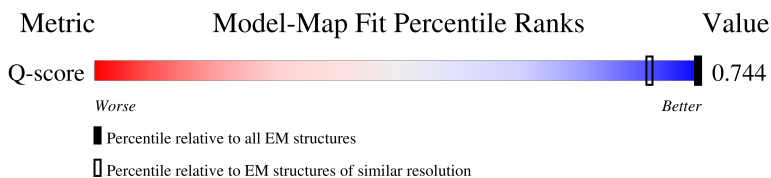
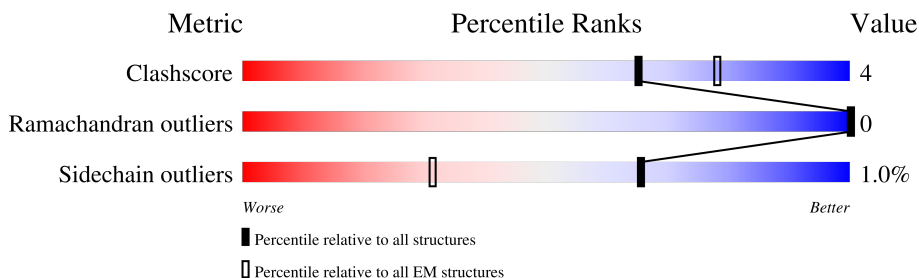
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 1.99 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1416 (1.50 - 2.49)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	<div> <div>10%</div> <div>90%</div> <div>9%</div> </div>
1	B	556	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
1	C	556	<div> <div>10%</div> <div>89%</div> <div>10%</div> </div>
1	D	556	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>

2 Entry composition [i](#)

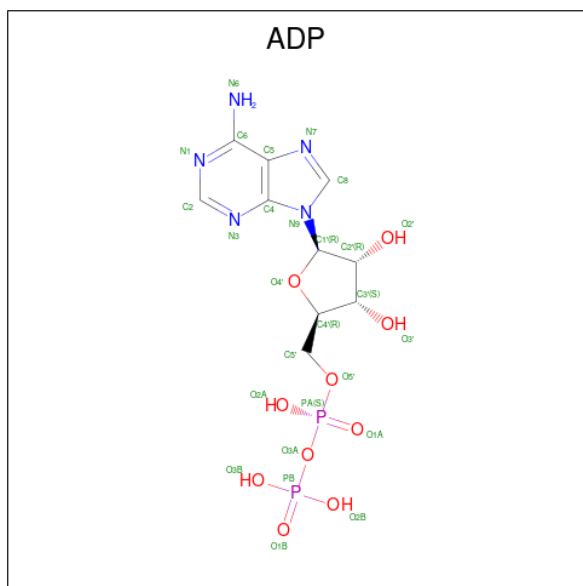
There are 7 unique types of molecules in this entry. The entry contains 18848 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CTP synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	556	Total	C	N	O	S	0	0
			4384	2779	770	813	22		
1	B	556	Total	C	N	O	S	0	0
			4384	2779	770	813	22		
1	C	556	Total	C	N	O	S	0	0
			4384	2779	770	813	22		
1	D	556	Total	C	N	O	S	0	0
			4384	2779	770	813	22		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



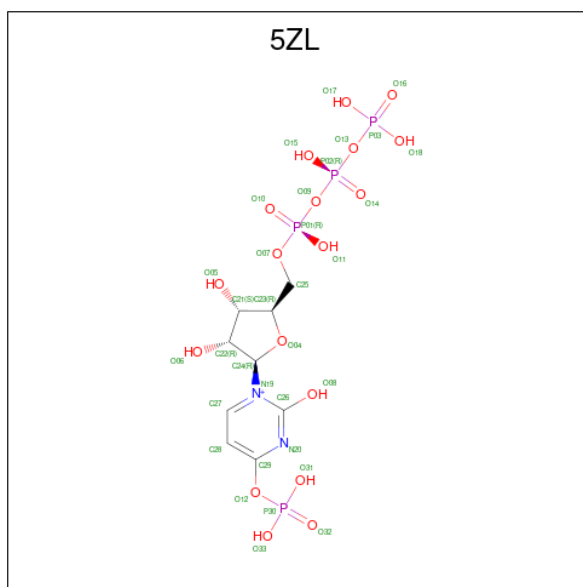
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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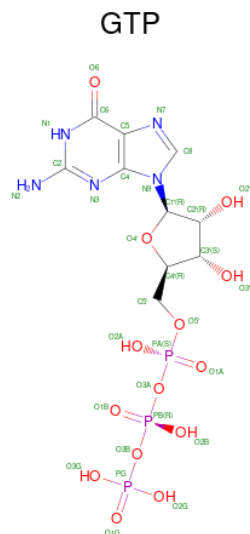
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-3,4-bis(oxidanyl)-5-(2-oxidanyl-4-phosphonooxy-pyrimidin-1-yl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: 5ZL) (formula: C₉H₁₇N₂O₁₈P₄) (labeled as "Ligand of Interest" by depositor).



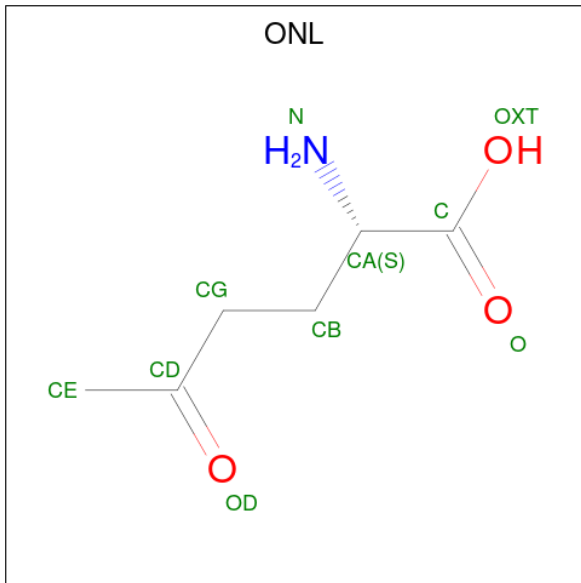
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			33	9	2	18	4	
3	B	1	Total	C	N	O	P	0
			33	9	2	18	4	
3	C	1	Total	C	N	O	P	0
			33	9	2	18	4	
3	D	1	Total	C	N	O	P	0
			33	9	2	18	4	

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 5-OXO-L-NORLEUCINE (CCD ID: ONL) (formula: $\text{C}_6\text{H}_{11}\text{NO}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			10	6	1	3	
5	B	1	Total	C	N	O	0
			10	6	1	3	
5	C	1	Total	C	N	O	0
			10	6	1	3	
5	D	1	Total	C	N	O	0
			10	6	1	3	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	4	Total	Mg	0
			4	4	
6	B	4	Total	Mg	0
			4	4	
6	C	4	Total	Mg	0
			4	4	
6	D	4	Total	Mg	0
			4	4	

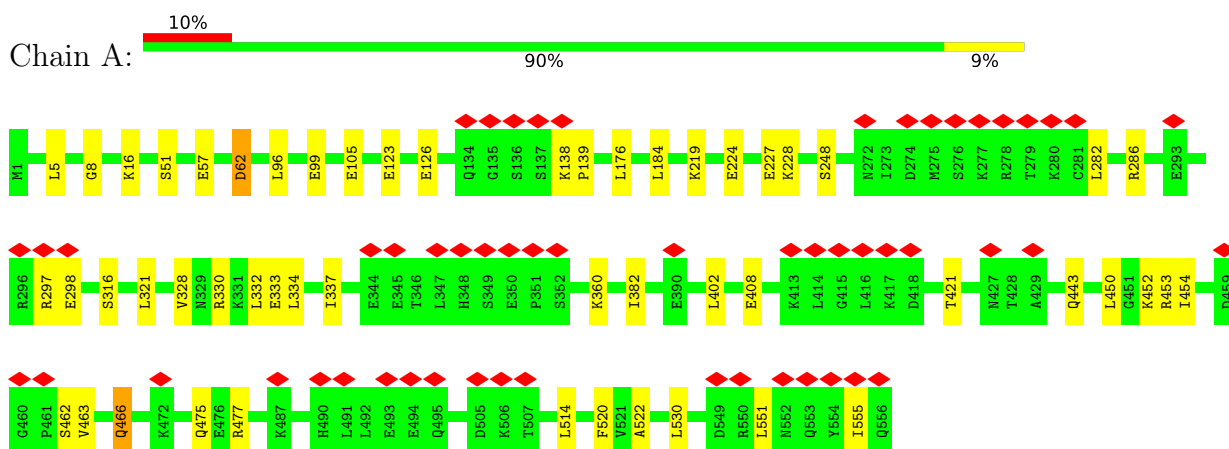
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	225	Total	O	0
			225	225	
7	B	220	Total	O	0
			220	220	
7	C	222	Total	O	0
			222	222	
7	D	221	Total	O	0
			221	221	

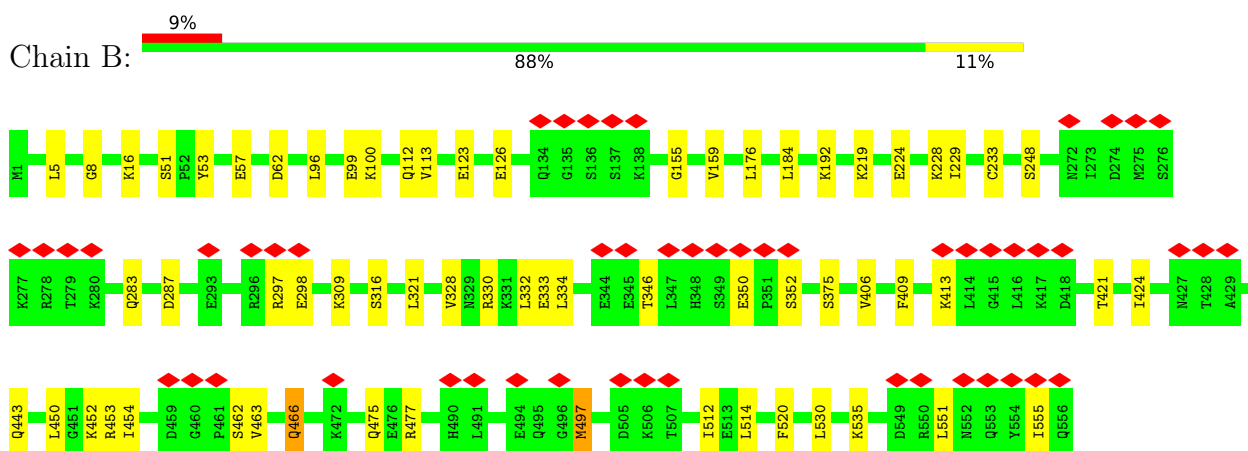
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

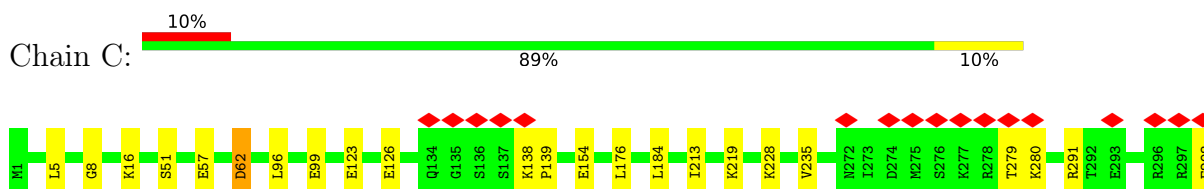
- Molecule 1: CTP synthase

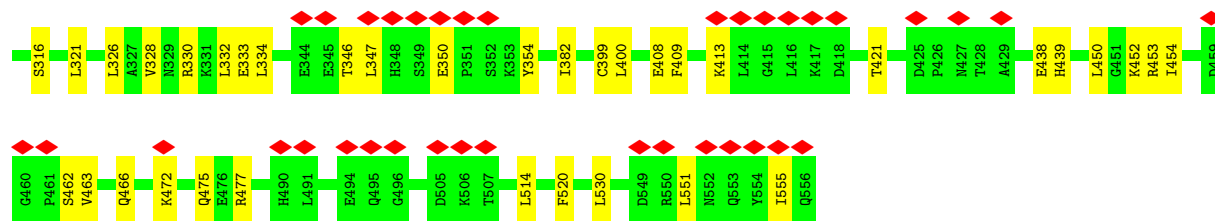


- Molecule 1: CTP synthase

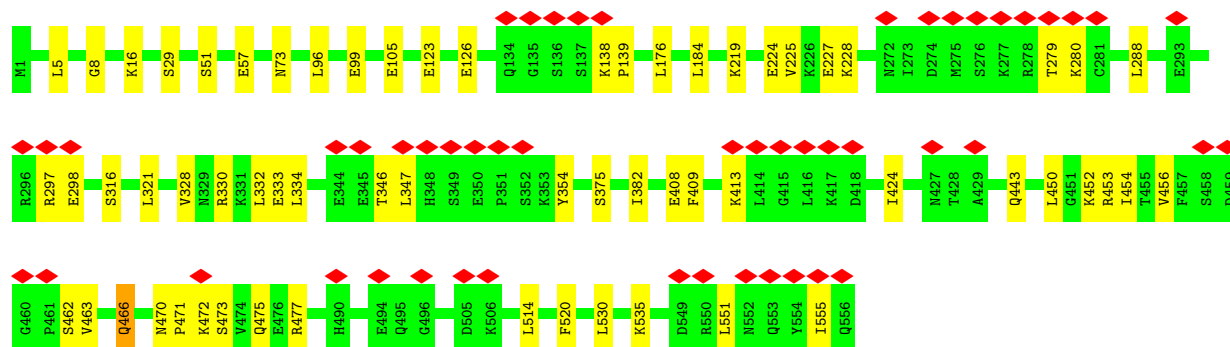
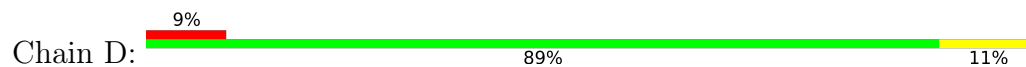


- Molecule 1: CTP synthase





• Molecule 1: CTP synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	894213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.841	Depositor
Minimum map value	-1.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	271.488, 271.488, 271.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.707, 0.707, 0.707	Depositor

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: ONL, GTP, MG, ADP, 5ZL

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	0.13	0/4473	0.29	0/6055
1	B	0.13	0/4473	0.31	0/6055
1	C	0.13	0/4473	0.31	0/6055
1	D	0.13	0/4473	0.30	0/6055
All	All	0.13	0/17892	0.30	0/24220

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	4384	0	4431	31	0
1	B	4384	0	4431	40	0
1	C	4384	0	4431	36	0
1	D	4384	0	4431	38	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	0	0
3	C	33	0	0	0	0
3	D	33	0	0	1	0
4	A	32	0	12	0	0
4	B	32	0	12	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0
5	A	10	0	10	0	0
5	B	10	0	10	0	0
5	C	10	0	10	0	0
5	D	10	0	10	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
7	A	225	0	0	4	0
7	B	220	0	0	3	0
7	C	222	0	0	2	0
7	D	221	0	0	4	0
All	All	18848	0	17860	143	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 4.

All (143) 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:B:497:MET:HE2	1:B:512:ILE:HD12	1.77	0.66
1:B:452:LYS:HD3	1:B:477:ARG:HG2	1.81	0.62
1:A:328:VAL:HG23	1:A:330:ARG:HG2	1.81	0.61
1:A:184:LEU:HD13	1:A:219:LYS:HE2	1.83	0.60
1:A:452:LYS:HD3	1:A:477:ARG:HG2	1.84	0.60
1:B:328:VAL:HG23	1:B:330:ARG:HG2	1.82	0.60
1:C:452:LYS:HD3	1:C:477:ARG:HG2	1.84	0.60
1:D:328:VAL:HG23	1:D:330:ARG:HG2	1.82	0.60
1:D:452:LYS:HD3	1:D:477:ARG:HG2	1.85	0.59
1:D:184:LEU:HD13	1:D:219:LYS:HE2	1.85	0.59
1:C:328:VAL:HG23	1:C:330:ARG:HG2	1.86	0.58
1:A:443:GLN:NE2	7:A:704:HOH:O	2.29	0.58
1:B:283:GLN:NE2	1:B:287:ASP:OD1	2.36	0.57
1:C:184:LEU:HD13	1:C:219:LYS:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LEU:HD13	1:C:334:LEU:HD11	1.86	0.57
1:D:454:ILE:HD13	1:D:475:GLN:OE1	2.05	0.57
1:D:321:LEU:HD13	1:D:334:LEU:HD11	1.88	0.56
1:B:321:LEU:HD13	1:B:334:LEU:HD11	1.88	0.56
1:C:123:GLU:HA	1:C:126:GLU:HG3	1.88	0.56
1:B:184:LEU:HD13	1:B:219:LYS:HE2	1.88	0.55
1:B:450:LEU:O	1:B:453:ARG:NH1	2.41	0.54
1:A:321:LEU:HD13	1:A:334:LEU:HD11	1.88	0.54
1:D:279:THR:HG22	1:D:280:LYS:HG2	1.89	0.54
1:D:443:GLN:NE2	7:D:704:HOH:O	2.29	0.54
1:A:454:ILE:HD13	1:A:475:GLN:OE1	2.07	0.54
1:C:96:LEU:O	1:C:99:GLU:HG3	2.07	0.54
1:B:406:VAL:HA	1:B:497:MET:HE1	1.88	0.53
1:B:454:ILE:HD13	1:B:475:GLN:OE1	2.09	0.53
1:A:96:LEU:O	1:A:99:GLU:HG3	2.09	0.53
1:D:450:LEU:O	1:D:453:ARG:NH1	2.42	0.53
1:B:8:GLY:HA3	1:B:16:LYS:HD3	1.91	0.53
1:A:450:LEU:O	1:A:453:ARG:NH1	2.41	0.52
1:B:229:ILE:O	1:B:233:CYS:HB2	2.09	0.52
1:C:450:LEU:O	1:C:453:ARG:NH1	2.41	0.52
1:C:454:ILE:HD13	1:C:475:GLN:OE1	2.09	0.52
1:B:375:SER:HB3	1:B:424:ILE:HG12	1.91	0.52
1:D:96:LEU:O	1:D:99:GLU:HG3	2.10	0.51
1:B:99:GLU:OE2	1:B:100:LYS:HG3	2.10	0.51
1:A:8:GLY:HA3	1:A:16:LYS:HD3	1.93	0.51
1:B:462:SER:O	1:B:466:GLN:HG2	2.11	0.51
1:B:463:VAL:HG13	1:B:555:ILE:HD11	1.93	0.51
1:C:5:LEU:HD23	1:C:176:LEU:HD13	1.92	0.51
1:B:443:GLN:NE2	7:B:704:HOH:O	2.28	0.50
1:C:8:GLY:HA3	1:C:16:LYS:HD3	1.94	0.50
1:A:5:LEU:HD23	1:A:176:LEU:HD13	1.92	0.50
1:B:123:GLU:HA	1:B:126:GLU:HG3	1.94	0.50
1:A:297:ARG:HB2	1:A:330:ARG:HA	1.94	0.49
1:C:462:SER:O	1:C:466:GLN:HG2	2.12	0.49
1:C:463:VAL:HG13	1:C:555:ILE:HD11	1.93	0.49
1:D:5:LEU:HD23	1:D:176:LEU:HD13	1.93	0.49
1:D:8:GLY:HA3	1:D:16:LYS:HD3	1.93	0.49
1:B:5:LEU:HD23	1:B:176:LEU:HD13	1.94	0.49
1:C:463:VAL:HG11	1:C:551:LEU:HD21	1.95	0.48
1:D:463:VAL:HG13	1:D:555:ILE:HD11	1.95	0.48
1:B:57:GLU:CD	1:B:316:SER:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:SER:O	1:A:466:GLN:HG2	2.14	0.47
1:A:332:LEU:HD21	1:A:334:LEU:HD13	1.96	0.47
1:A:463:VAL:HG13	1:A:555:ILE:HD11	1.95	0.47
1:B:332:LEU:HD21	1:B:334:LEU:HD13	1.95	0.47
1:C:332:LEU:HD21	1:C:334:LEU:HD13	1.94	0.47
1:A:463:VAL:HG11	1:A:551:LEU:HD21	1.96	0.47
1:D:57:GLU:CD	1:D:316:SER:H	2.20	0.47
1:D:228:LYS:NZ	7:D:716:HOH:O	2.48	0.47
1:D:462:SER:O	1:D:466:GLN:HG2	2.14	0.47
1:D:463:VAL:HG11	1:D:551:LEU:HD21	1.97	0.47
1:C:57:GLU:CD	1:C:316:SER:H	2.19	0.46
1:C:291:ARG:HB3	1:C:326:LEU:HD11	1.96	0.46
1:A:123:GLU:HA	1:A:126:GLU:HG3	1.97	0.46
1:B:298:GLU:HG2	1:B:333:GLU:HG3	1.98	0.46
1:C:228:LYS:NZ	7:C:716:HOH:O	2.47	0.46
1:A:452:LYS:HE2	1:A:530:LEU:HD21	1.98	0.46
1:A:282:LEU:O	1:A:286:ARG:HG3	2.16	0.45
1:D:298:GLU:HG2	1:D:333:GLU:HG3	1.98	0.45
1:D:123:GLU:HA	1:D:126:GLU:HG3	1.98	0.45
1:C:279:THR:O	1:C:280:LYS:HG3	2.16	0.45
1:C:438:GLU:HG2	1:C:439:HIS:CD2	2.52	0.45
1:A:57:GLU:CD	1:A:316:SER:H	2.21	0.45
1:D:138:LYS:HD2	1:D:139:PRO:HD2	1.98	0.45
1:B:452:LYS:HE2	1:B:530:LEU:HD21	1.98	0.44
1:C:399:CYS:HB3	1:C:400:LEU:H	1.69	0.44
1:C:514:LEU:HB3	1:C:520:PHE:HB3	2.00	0.44
1:A:228:LYS:NZ	7:A:718:HOH:O	2.49	0.44
1:B:192:LYS:HE3	3:D:603:5ZL:O17	2.18	0.44
1:B:463:VAL:HG11	1:B:551:LEU:HD21	1.99	0.44
1:C:452:LYS:HE2	1:C:530:LEU:HD21	2.00	0.44
1:A:514:LEU:HB3	1:A:520:PHE:HB3	2.00	0.44
1:D:347:LEU:HD13	1:D:354:TYR:CD1	2.52	0.44
1:B:228:LYS:NZ	7:B:720:HOH:O	2.51	0.44
1:B:297:ARG:HB2	1:B:330:ARG:HA	2.00	0.44
1:C:298:GLU:HG2	1:C:333:GLU:HG3	2.00	0.44
1:B:113:VAL:HG23	1:C:154:GLU:HG3	1.99	0.44
1:D:452:LYS:HE2	1:D:530:LEU:HD21	1.99	0.44
1:C:138:LYS:HD2	1:C:139:PRO:HD2	2.00	0.43
1:D:409:PHE:CE1	1:D:413:LYS:HG3	2.54	0.43
1:D:332:LEU:HD21	1:D:334:LEU:HD13	2.00	0.43
1:A:298:GLU:HG2	1:A:333:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LEU:HD12	1:D:334:LEU:HA	1.92	0.43
1:A:382:ILE:HG23	1:A:408:GLU:HB2	2.01	0.42
1:B:334:LEU:HD12	1:B:334:LEU:HA	1.93	0.42
1:D:514:LEU:HB3	1:D:520:PHE:HB3	2.00	0.42
1:C:219:LYS:HG2	7:C:775:HOH:O	2.19	0.42
1:A:337:ILE:HD13	1:A:360:LYS:HE2	2.01	0.42
1:B:53:TYR:CZ	1:B:309:LYS:HE3	2.54	0.42
1:A:219:LYS:HG2	7:A:781:HOH:O	2.19	0.42
1:D:224:GLU:OE1	1:D:225:VAL:HG23	2.20	0.42
1:B:452:LYS:CD	1:B:477:ARG:HG2	2.49	0.42
1:C:346:THR:O	1:C:350:GLU:N	2.48	0.42
1:D:382:ILE:HG23	1:D:408:GLU:HB2	2.02	0.42
1:D:346:THR:HG22	1:D:354:TYR:HB2	2.02	0.42
1:A:138:LYS:HD2	1:A:139:PRO:HD2	2.01	0.41
1:D:470:ASN:N	1:D:471:PRO:HD3	2.35	0.41
1:B:155:GLY:O	1:B:159:VAL:HG23	2.20	0.41
1:B:224:GLU:H	1:B:224:GLU:CD	2.27	0.41
1:C:347:LEU:HD13	1:C:354:TYR:CD1	2.55	0.41
1:D:297:ARG:HB2	1:D:330:ARG:HA	2.02	0.41
1:A:62:ASP:OD1	1:A:452:LYS:HE3	2.21	0.41
1:A:402:LEU:HB2	1:A:522:ALA:HB1	2.02	0.41
1:B:96:LEU:O	1:B:99:GLU:HG3	2.21	0.41
1:B:346:THR:O	1:B:350:GLU:N	2.46	0.41
1:D:73:ASN:ND2	7:D:712:HOH:O	2.41	0.41
1:D:472:LYS:HD2	1:D:472:LYS:HA	1.83	0.41
1:A:219:LYS:NZ	7:A:717:HOH:O	2.48	0.41
1:C:62:ASP:OD1	1:C:452:LYS:HE3	2.21	0.41
1:C:409:PHE:CE1	1:C:413:LYS:HG3	2.56	0.41
1:D:375:SER:HB3	1:D:424:ILE:HG12	2.01	0.41
1:A:224:GLU:HA	1:A:227:GLU:HG3	2.02	0.41
1:B:112:GLN:HB3	1:C:154:GLU:OE2	2.21	0.41
1:C:472:LYS:HA	1:C:472:LYS:HD2	1.63	0.41
1:D:288:LEU:HD23	1:D:288:LEU:HA	1.91	0.41
1:D:456:VAL:HG12	1:D:473:SER:HB3	2.02	0.41
1:B:62:ASP:OD1	1:B:452:LYS:HE3	2.21	0.41
1:B:514:LEU:HB3	1:B:520:PHE:HB3	2.02	0.41
1:B:535:LYS:HE3	1:B:535:LYS:HB3	1.88	0.41
1:C:279:THR:C	1:C:280:LYS:HG3	2.46	0.41
1:D:535:LYS:HE3	1:D:535:LYS:HB3	1.88	0.41
1:B:219:LYS:HG2	7:B:780:HOH:O	2.21	0.40
1:C:213:ILE:HD12	1:C:235:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:GLU:HA	1:D:227:GLU:HG3	2.01	0.40
1:D:219:LYS:HG2	7:D:787:HOH:O	2.19	0.40
1:C:382:ILE:HG23	1:C:408:GLU:HB2	2.03	0.40
1:C:452:LYS:CD	1:C:477:ARG:HG2	2.50	0.40
1:A:452:LYS:CD	1:A:477:ARG:HG2	2.50	0.40
1:B:409:PHE:CE1	1:B:413:LYS:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	554/556 (100%)	548 (99%)	6 (1%)	0	100	100
1	B	554/556 (100%)	546 (99%)	8 (1%)	0	100	100
1	C	554/556 (100%)	547 (99%)	7 (1%)	0	100	100
1	D	554/556 (100%)	544 (98%)	10 (2%)	0	100	100
All	All	2216/2224 (100%)	2185 (99%)	31 (1%)	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 PDB entries followed by that with respect to all EM entries.

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	486/486 (100%)	480 (99%)	6 (1%)	63	70
1	B	486/486 (100%)	480 (99%)	6 (1%)	63	70
1	C	486/486 (100%)	483 (99%)	3 (1%)	78	85
1	D	486/486 (100%)	482 (99%)	4 (1%)	73	80
All	All	1944/1944 (100%)	1925 (99%)	19 (1%)	65	75

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	62	ASP
1	A	105	GLU
1	A	248	SER
1	A	421	THR
1	A	466	GLN
1	B	51	SER
1	B	248	SER
1	B	352	SER
1	B	421	THR
1	B	466	GLN
1	B	497	MET
1	C	51	SER
1	C	62	ASP
1	C	421	THR
1	D	29	SER
1	D	51	SER
1	D	105	GLU
1	D	466	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	A	430	ASN
1	B	83	HIS
1	B	122	GLN
1	B	173	ASN
1	B	259	ASN
1	B	386	GLN
1	B	412	ASN

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Mol	Chain	Res	Type
1	B	430	ASN
1	C	83	HIS
1	C	495	GLN
1	D	122	GLN
1	D	412	ASN
1	D	430	ASN

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 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	ONL	B	604	-	8,9,9	0.77	0	8,11,11	1.50	2 (25%)
5	ONL	D	605	-	8,9,9	0.77	0	8,11,11	1.50	2 (25%)
2	ADP	C	602	6	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)
4	GTP	C	604	6	33,34,34	0.98	2 (6%)	50,54,54	1.68	10 (20%)
2	ADP	A	601	6	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)
5	ONL	A	604	-	8,9,9	0.77	0	8,11,11	1.50	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	D	602	6	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)
3	5ZL	B	602	6	29,34,34	3.64	17 (58%)	41,54,54	2.22	10 (24%)
3	5ZL	A	602	6	29,34,34	3.64	17 (58%)	41,54,54	2.22	10 (24%)
4	GTP	B	603	6	33,34,34	0.98	2 (6%)	50,54,54	1.68	10 (20%)
2	ADP	B	601	6	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)
4	GTP	A	603	6	33,34,34	0.98	2 (6%)	50,54,54	1.68	10 (20%)
3	5ZL	C	603	6	29,34,34	3.64	17 (58%)	41,54,54	2.22	10 (24%)
5	ONL	C	605	-	8,9,9	0.77	0	8,11,11	1.50	2 (25%)
4	GTP	D	604	6	33,34,34	0.98	2 (6%)	50,54,54	1.68	10 (20%)
3	5ZL	D	603	6	29,34,34	3.64	17 (58%)	41,54,54	2.22	10 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ONL	B	604	-	-	1/9/9/9	-
5	ONL	D	605	-	-	1/9/9/9	-
2	ADP	C	602	6	-	0/16/32/32	0/3/3/3
4	GTP	C	604	6	-	5/22/38/38	0/3/3/3
2	ADP	A	601	6	-	0/16/32/32	0/3/3/3
5	ONL	A	604	-	-	1/9/9/9	-
2	ADP	D	602	6	-	0/16/32/32	0/3/3/3
3	5ZL	B	602	6	-	9/25/43/43	0/2/2/2
3	5ZL	A	602	6	-	9/25/43/43	0/2/2/2
4	GTP	B	603	6	-	4/22/38/38	0/3/3/3
2	ADP	B	601	6	-	0/16/32/32	0/3/3/3
4	GTP	A	603	6	-	4/22/38/38	0/3/3/3
3	5ZL	C	603	6	-	9/25/43/43	0/2/2/2
5	ONL	C	605	-	-	1/9/9/9	-
4	GTP	D	604	6	-	4/22/38/38	0/3/3/3
3	5ZL	D	603	6	-	8/25/43/43	0/2/2/2

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	5ZL	O04-C24	8.72	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	5ZL	O04-C24	8.72	1.52	1.40
3	A	602	5ZL	O04-C24	8.72	1.52	1.40
3	D	603	5ZL	O04-C24	8.72	1.52	1.40
3	C	603	5ZL	C27-N19	7.82	1.46	1.36
3	A	602	5ZL	C27-N19	7.82	1.46	1.36
3	D	603	5ZL	C27-N19	7.81	1.46	1.36
3	B	602	5ZL	C27-N19	7.81	1.46	1.36
3	A	602	5ZL	P01-O09	7.10	1.67	1.59
3	C	603	5ZL	P01-O09	7.10	1.67	1.59
3	D	603	5ZL	P01-O09	7.08	1.67	1.59
3	B	602	5ZL	C29-N20	7.06	1.45	1.33
3	B	602	5ZL	P01-O09	7.05	1.67	1.59
3	C	603	5ZL	C29-N20	7.05	1.45	1.33
3	A	602	5ZL	C29-N20	7.05	1.45	1.33
3	D	603	5ZL	C29-N20	7.04	1.45	1.33
3	D	603	5ZL	P02-O09	6.90	1.67	1.59
3	A	602	5ZL	P02-O09	6.89	1.66	1.59
3	C	603	5ZL	P02-O09	6.88	1.66	1.59
3	B	602	5ZL	P02-O09	6.88	1.66	1.59
2	A	601	ADP	C5-C4	4.69	1.47	1.39
2	C	602	ADP	C5-C4	4.68	1.47	1.39
2	D	602	ADP	C5-C4	4.68	1.47	1.39
2	B	601	ADP	C5-C4	4.68	1.47	1.39
3	A	602	5ZL	C24-N19	-3.08	1.41	1.50
3	B	602	5ZL	C24-N19	-3.08	1.41	1.50
3	D	603	5ZL	C24-N19	-3.07	1.41	1.50
3	C	603	5ZL	C24-N19	-3.07	1.41	1.50
3	B	602	5ZL	P30-O12	3.00	1.65	1.59
3	A	602	5ZL	P30-O12	2.99	1.65	1.59
3	C	603	5ZL	P30-O12	2.99	1.65	1.59
3	D	603	5ZL	P30-O12	2.99	1.65	1.59
3	A	602	5ZL	P03-O18	-2.81	1.44	1.54
3	C	603	5ZL	P03-O18	-2.81	1.44	1.54
3	D	603	5ZL	P03-O18	-2.81	1.44	1.54
3	B	602	5ZL	P03-O18	-2.80	1.44	1.54
3	B	602	5ZL	C22-C21	-2.73	1.46	1.53
2	A	601	ADP	C5-C6	2.72	1.48	1.41
2	B	601	ADP	C5-C6	2.72	1.48	1.41
3	A	602	5ZL	C22-C21	-2.72	1.46	1.53
3	D	603	5ZL	C22-C21	-2.72	1.46	1.53
2	C	602	ADP	C5-C6	2.72	1.48	1.41
3	C	603	5ZL	C22-C21	-2.72	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	ADP	C5-C6	2.72	1.48	1.41
3	D	603	5ZL	P30-O31	-2.69	1.44	1.54
3	A	602	5ZL	P30-O31	-2.69	1.44	1.54
3	C	603	5ZL	P30-O31	-2.69	1.44	1.54
3	B	602	5ZL	P30-O31	-2.68	1.44	1.54
3	B	602	5ZL	P02-O13	2.55	1.62	1.59
3	A	602	5ZL	P02-O13	2.54	1.62	1.59
3	C	603	5ZL	P02-O13	2.53	1.62	1.59
3	B	602	5ZL	O04-C23	2.52	1.50	1.45
3	D	603	5ZL	O04-C23	2.52	1.50	1.45
3	A	602	5ZL	O04-C23	2.52	1.50	1.45
3	C	603	5ZL	O04-C23	2.52	1.50	1.45
3	D	603	5ZL	P02-O13	2.47	1.62	1.59
3	C	603	5ZL	C27-C28	2.39	1.43	1.38
3	D	603	5ZL	C27-C28	2.38	1.43	1.38
3	A	602	5ZL	C27-C28	2.38	1.43	1.38
3	B	602	5ZL	C27-C28	2.38	1.43	1.38
3	D	603	5ZL	P03-O17	-2.35	1.46	1.54
3	C	603	5ZL	P03-O17	-2.33	1.46	1.54
3	A	602	5ZL	P03-O17	-2.33	1.46	1.54
3	B	602	5ZL	P03-O17	-2.32	1.46	1.54
2	C	602	ADP	C5-N7	-2.30	1.34	1.39
2	D	602	ADP	C5-N7	-2.30	1.34	1.39
2	A	601	ADP	C5-N7	-2.30	1.34	1.39
2	B	601	ADP	C5-N7	-2.30	1.34	1.39
3	A	602	5ZL	P30-O33	-2.28	1.46	1.54
3	B	602	5ZL	P30-O33	-2.28	1.46	1.54
3	C	603	5ZL	P30-O33	-2.28	1.46	1.54
3	D	603	5ZL	P30-O33	-2.28	1.46	1.54
2	A	601	ADP	C8-N7	2.16	1.35	1.31
2	C	602	ADP	C8-N7	2.15	1.35	1.31
2	B	601	ADP	C8-N7	2.15	1.35	1.31
2	D	602	ADP	C8-N7	2.15	1.35	1.31
4	B	603	GTP	PA-O3A	2.13	1.61	1.59
4	C	604	GTP	PA-O3A	2.12	1.61	1.59
4	A	603	GTP	PA-O3A	2.12	1.61	1.59
4	D	604	GTP	PA-O3A	2.12	1.61	1.59
4	C	604	GTP	C2-N3	2.12	1.38	1.33
4	A	603	GTP	C2-N3	2.11	1.38	1.33
4	B	603	GTP	C2-N3	2.11	1.38	1.33
4	D	604	GTP	C2-N3	2.11	1.38	1.33
3	A	602	5ZL	P02-O15	-2.06	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	5ZL	P01-O11	-2.06	1.45	1.55
3	C	603	5ZL	P02-O15	-2.06	1.45	1.55
3	D	603	5ZL	P02-O15	-2.06	1.45	1.55
3	B	602	5ZL	P01-O11	-2.05	1.45	1.55
3	C	603	5ZL	P01-O11	-2.05	1.45	1.55
3	B	602	5ZL	P02-O15	-2.05	1.45	1.55
3	D	603	5ZL	P01-O11	-2.05	1.45	1.55

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	5ZL	C26-N20-C29	8.02	119.82	114.49
3	A	602	5ZL	C26-N20-C29	8.02	119.82	114.49
3	D	603	5ZL	C26-N20-C29	8.00	119.81	114.49
3	B	602	5ZL	C26-N20-C29	7.95	119.78	114.49
3	D	603	5ZL	C23-O04-C24	-7.29	103.25	109.92
3	B	602	5ZL	C23-O04-C24	-7.28	103.26	109.92
3	A	602	5ZL	C23-O04-C24	-7.28	103.26	109.92
3	C	603	5ZL	C23-O04-C24	-7.27	103.27	109.92
2	A	601	ADP	C5-C4-N3	-5.81	118.72	126.72
2	D	602	ADP	C5-C4-N3	-5.80	118.73	126.72
2	B	601	ADP	C5-C4-N3	-5.80	118.73	126.72
2	C	602	ADP	C5-C4-N3	-5.80	118.73	126.72
4	A	603	GTP	C5-C4-N3	-5.18	120.15	128.39
4	C	604	GTP	C5-C4-N3	-5.17	120.16	128.39
4	B	603	GTP	C5-C4-N3	-5.17	120.16	128.39
4	D	604	GTP	C5-C4-N3	-5.17	120.16	128.39
4	A	603	GTP	C2-N3-C4	5.09	121.07	112.30
4	B	603	GTP	C2-N3-C4	5.08	121.06	112.30
4	C	604	GTP	C2-N3-C4	5.08	121.05	112.30
4	D	604	GTP	C2-N3-C4	5.08	121.05	112.30
2	A	601	ADP	N3-C4-N9	4.73	135.21	127.17
2	D	602	ADP	N3-C4-N9	4.72	135.20	127.17
2	B	601	ADP	N3-C4-N9	4.72	135.20	127.17
2	C	602	ADP	N3-C4-N9	4.72	135.19	127.17
2	D	602	ADP	C2-N3-C4	3.75	120.99	111.83
2	A	601	ADP	C2-N3-C4	3.75	120.99	111.83
2	C	602	ADP	C2-N3-C4	3.75	120.99	111.83
2	B	601	ADP	C2-N3-C4	3.75	120.99	111.83
2	A	601	ADP	C4-C5-N7	-3.46	106.63	110.58
2	D	602	ADP	C4-C5-N7	-3.46	106.63	110.58
2	C	602	ADP	C4-C5-N7	-3.45	106.63	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C4-C5-N7	-3.45	106.64	110.58
2	C	602	ADP	N3-C2-N1	-3.43	123.39	128.58
2	A	601	ADP	N3-C2-N1	-3.42	123.40	128.58
2	D	602	ADP	N3-C2-N1	-3.42	123.40	128.58
2	B	601	ADP	N3-C2-N1	-3.42	123.40	128.58
4	C	604	GTP	N9-C4-N3	3.32	132.60	125.95
4	B	603	GTP	N9-C4-N3	3.32	132.59	125.95
4	A	603	GTP	N9-C4-N3	3.32	132.59	125.95
4	D	604	GTP	N9-C4-N3	3.31	132.58	125.95
5	D	605	ONL	OXT-C-O	-3.18	116.88	124.08
5	B	604	ONL	OXT-C-O	-3.17	116.88	124.08
5	C	605	ONL	OXT-C-O	-3.17	116.89	124.08
5	A	604	ONL	OXT-C-O	-3.17	116.90	124.08
4	C	604	GTP	C2-N1-C6	-2.89	119.87	125.11
4	D	604	GTP	C2-N1-C6	-2.89	119.88	125.11
4	B	603	GTP	C2-N1-C6	-2.89	119.88	125.11
4	A	603	GTP	C2-N1-C6	-2.88	119.88	125.11
3	B	602	5ZL	O31-P30-O12	2.86	113.77	105.32
3	C	603	5ZL	O31-P30-O12	2.85	113.75	105.32
3	A	602	5ZL	O31-P30-O12	2.85	113.74	105.32
3	D	603	5ZL	O31-P30-O12	2.85	113.74	105.32
2	A	601	ADP	C4-N9-C8	2.83	108.71	105.74
2	D	602	ADP	C4-N9-C8	2.83	108.71	105.74
2	B	601	ADP	C4-N9-C8	2.83	108.71	105.74
2	C	602	ADP	C4-N9-C8	2.83	108.71	105.74
4	D	604	GTP	N9-C8-N7	-2.79	108.23	113.40
4	C	604	GTP	N9-C8-N7	-2.78	108.24	113.40
4	A	603	GTP	N9-C8-N7	-2.78	108.25	113.40
4	B	603	GTP	N9-C8-N7	-2.78	108.25	113.40
4	D	604	GTP	C8-N7-C5	2.67	109.03	104.26
4	C	604	GTP	C8-N7-C5	2.67	109.01	104.26
4	A	603	GTP	C8-N7-C5	2.66	109.00	104.26
4	B	603	GTP	C8-N7-C5	2.66	109.00	104.26
4	B	603	GTP	C5-C6-N1	2.65	119.99	113.25
4	D	604	GTP	C5-C6-N1	2.65	119.99	113.25
4	C	604	GTP	C5-C6-N1	2.64	119.98	113.25
4	A	603	GTP	C5-C6-N1	2.64	119.98	113.25
3	A	602	5ZL	O33-P30-O12	2.61	113.03	105.32
3	D	603	5ZL	O33-P30-O12	2.60	113.02	105.32
3	B	602	5ZL	O33-P30-O12	2.60	113.02	105.32
3	C	603	5ZL	O33-P30-O12	2.60	113.01	105.32
2	D	602	ADP	C5-N7-C8	2.60	107.53	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	C5-N7-C8	2.60	107.53	103.45
2	C	602	ADP	C5-N7-C8	2.60	107.53	103.45
2	B	601	ADP	C5-N7-C8	2.59	107.52	103.45
3	D	603	5ZL	O18-P03-O13	2.56	113.22	104.64
3	A	602	5ZL	O18-P03-O13	2.54	113.14	104.64
3	B	602	5ZL	O18-P03-O13	2.53	113.11	104.64
3	C	603	5ZL	O18-P03-O13	2.53	113.11	104.64
5	A	604	ONL	CB-CG-CD	-2.43	110.97	114.77
5	B	604	ONL	CB-CG-CD	-2.42	110.99	114.77
4	A	603	GTP	O6-C6-C5	-2.42	120.14	126.53
4	D	604	GTP	O6-C6-C5	-2.42	120.15	126.53
4	B	603	GTP	O6-C6-C5	-2.42	120.15	126.53
4	C	604	GTP	O6-C6-C5	-2.42	120.15	126.53
5	D	605	ONL	CB-CG-CD	-2.41	111.01	114.77
3	C	603	5ZL	O17-P03-O13	2.41	112.71	104.64
3	B	602	5ZL	O17-P03-O13	2.40	112.70	104.64
3	A	602	5ZL	O17-P03-O13	2.40	112.69	104.64
5	C	605	ONL	CB-CG-CD	-2.40	111.02	114.77
3	A	602	5ZL	O11-P01-O09	2.33	113.58	107.27
3	D	603	5ZL	O11-P01-O09	2.33	113.58	107.27
3	B	602	5ZL	O11-P01-O09	2.32	113.55	107.27
3	C	603	5ZL	O11-P01-O09	2.32	113.53	107.27
3	D	603	5ZL	O17-P03-O13	2.31	112.38	104.64
3	C	603	5ZL	O11-P01-O10	-2.26	101.95	112.44
3	D	603	5ZL	O11-P01-O10	-2.25	101.96	112.44
3	A	602	5ZL	O11-P01-O10	-2.25	101.97	112.44
3	B	602	5ZL	O11-P01-O10	-2.25	101.97	112.44
3	B	602	5ZL	O12-C29-C28	2.14	121.41	116.98
3	D	603	5ZL	O12-C29-C28	2.13	121.38	116.98
3	C	603	5ZL	O12-C29-C28	2.13	121.38	116.98
4	C	604	GTP	O3G-PG-O3B	2.12	111.76	104.64
3	A	602	5ZL	O12-C29-C28	2.12	121.38	116.98
3	C	603	5ZL	O15-P02-O14	-2.11	102.63	112.44
3	A	602	5ZL	O15-P02-O14	-2.11	102.64	112.44
3	B	602	5ZL	O15-P02-O14	-2.11	102.65	112.44
4	A	603	GTP	O3G-PG-O3B	2.10	111.67	104.64
3	D	603	5ZL	O15-P02-O14	-2.10	102.69	112.44
4	B	603	GTP	O3G-PG-O3B	2.09	111.66	104.64
4	D	604	GTP	O3G-PG-O3B	2.09	111.66	104.64
4	A	603	GTP	N1-C2-N3	-2.05	119.57	123.32
2	C	602	ADP	C6-C5-N7	2.05	136.04	132.09
4	B	603	GTP	N1-C2-N3	-2.05	119.58	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	ADP	C6-C5-N7	2.05	136.03	132.09
2	A	601	ADP	C6-C5-N7	2.04	136.03	132.09
4	D	604	GTP	N1-C2-N3	-2.04	119.58	123.32
2	B	601	ADP	C6-C5-N7	2.04	136.03	132.09
4	C	604	GTP	N1-C2-N3	-2.04	119.58	123.32
2	C	602	ADP	N9-C8-N7	-2.03	111.06	113.94
2	D	602	ADP	N9-C8-N7	-2.03	111.06	113.94
2	A	601	ADP	N9-C8-N7	-2.03	111.06	113.94
2	B	601	ADP	N9-C8-N7	-2.03	111.06	113.94

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	5ZL	C22-C24-N19-C27
3	A	602	5ZL	O04-C24-N19-C27
3	B	602	5ZL	C22-C24-N19-C27
3	B	602	5ZL	O04-C24-N19-C27
3	C	603	5ZL	C22-C24-N19-C27
3	C	603	5ZL	O04-C24-N19-C27
3	D	603	5ZL	C22-C24-N19-C27
3	D	603	5ZL	O04-C24-N19-C27
5	A	604	ONL	CA-CB-CG-CD
5	B	604	ONL	CA-CB-CG-CD
5	C	605	ONL	CA-CB-CG-CD
5	D	605	ONL	CA-CB-CG-CD
4	A	603	GTP	C3'-C4'-C5'-O5'
4	B	603	GTP	C3'-C4'-C5'-O5'
4	C	604	GTP	C3'-C4'-C5'-O5'
4	D	604	GTP	C3'-C4'-C5'-O5'
4	A	603	GTP	O4'-C4'-C5'-O5'
4	B	603	GTP	O4'-C4'-C5'-O5'
4	C	604	GTP	O4'-C4'-C5'-O5'
4	D	604	GTP	O4'-C4'-C5'-O5'
3	D	603	5ZL	P01-O09-P02-O14
3	B	602	5ZL	N20-C29-O12-P30
3	A	602	5ZL	P01-O09-P02-O14
3	B	602	5ZL	P01-O09-P02-O14
3	C	603	5ZL	P01-O09-P02-O14
4	A	603	GTP	PA-O3A-PB-O1B
4	B	603	GTP	PA-O3A-PB-O1B
4	C	604	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	D	604	GTP	PA-O3A-PB-O1B
3	A	602	5ZL	N20-C29-O12-P30
3	C	603	5ZL	N20-C29-O12-P30
3	D	603	5ZL	N20-C29-O12-P30
3	A	602	5ZL	P02-O09-P01-O11
3	A	602	5ZL	P03-O13-P02-O14
3	B	602	5ZL	P02-O09-P01-O11
3	B	602	5ZL	P03-O13-P02-O14
3	C	603	5ZL	P02-O09-P01-O11
3	C	603	5ZL	P03-O13-P02-O14
3	D	603	5ZL	P02-O09-P01-O11
3	D	603	5ZL	P03-O13-P02-O14
3	A	602	5ZL	C28-C29-O12-P30
3	C	603	5ZL	C28-C29-O12-P30
3	D	603	5ZL	C28-C29-O12-P30
3	B	602	5ZL	C28-C29-O12-P30
3	A	602	5ZL	P02-O09-P01-O10
3	A	602	5ZL	P03-O13-P02-O15
3	B	602	5ZL	P02-O09-P01-O10
3	B	602	5ZL	P03-O13-P02-O15
3	C	603	5ZL	P02-O09-P01-O10
3	C	603	5ZL	P03-O13-P02-O15
3	D	603	5ZL	P02-O09-P01-O10
4	A	603	GTP	PA-O3A-PB-O2B
4	B	603	GTP	PA-O3A-PB-O2B
4	C	604	GTP	PG-O3B-PB-O2B
4	C	604	GTP	PA-O3A-PB-O2B
4	D	604	GTP	PA-O3A-PB-O2B

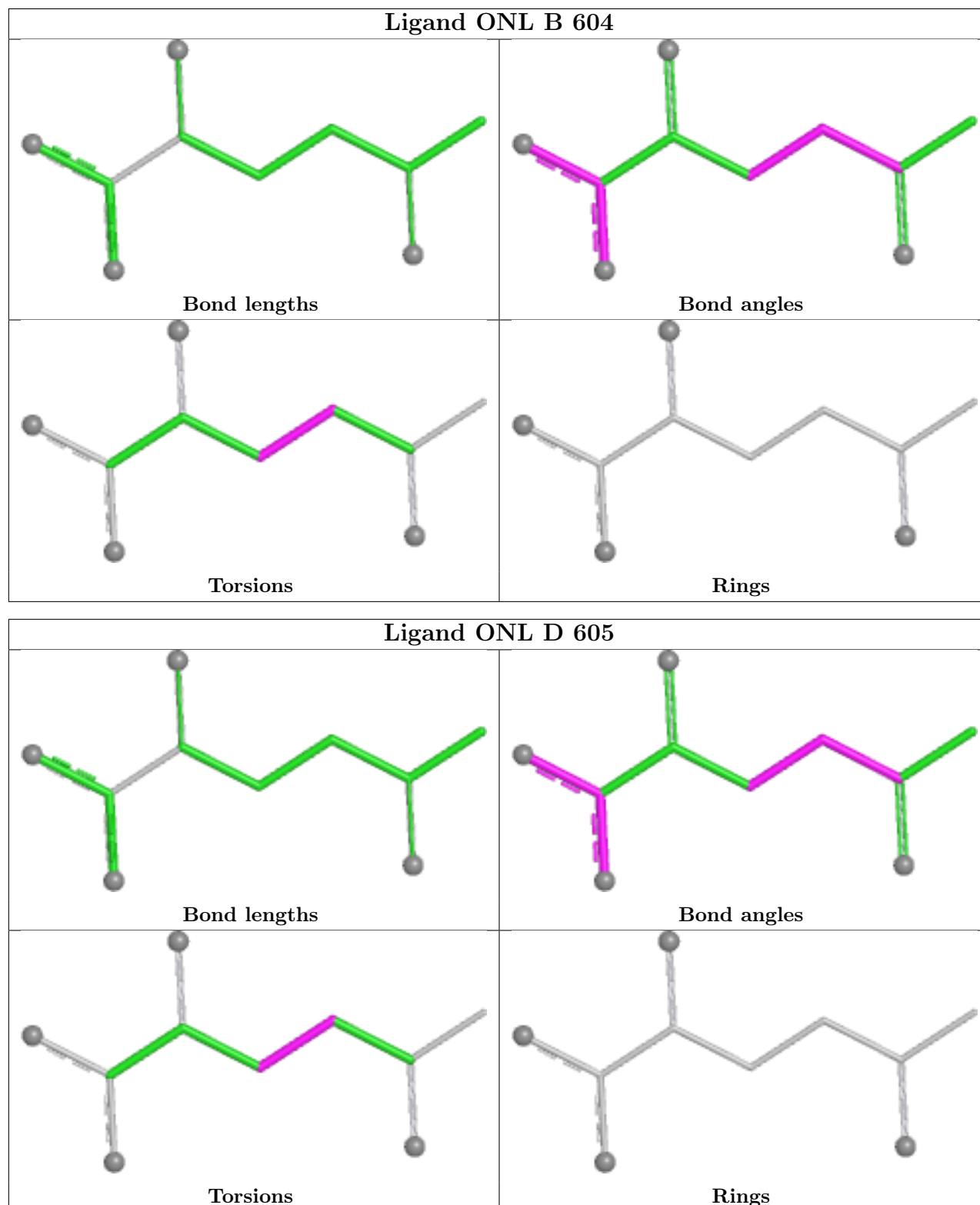
There are no ring outliers.

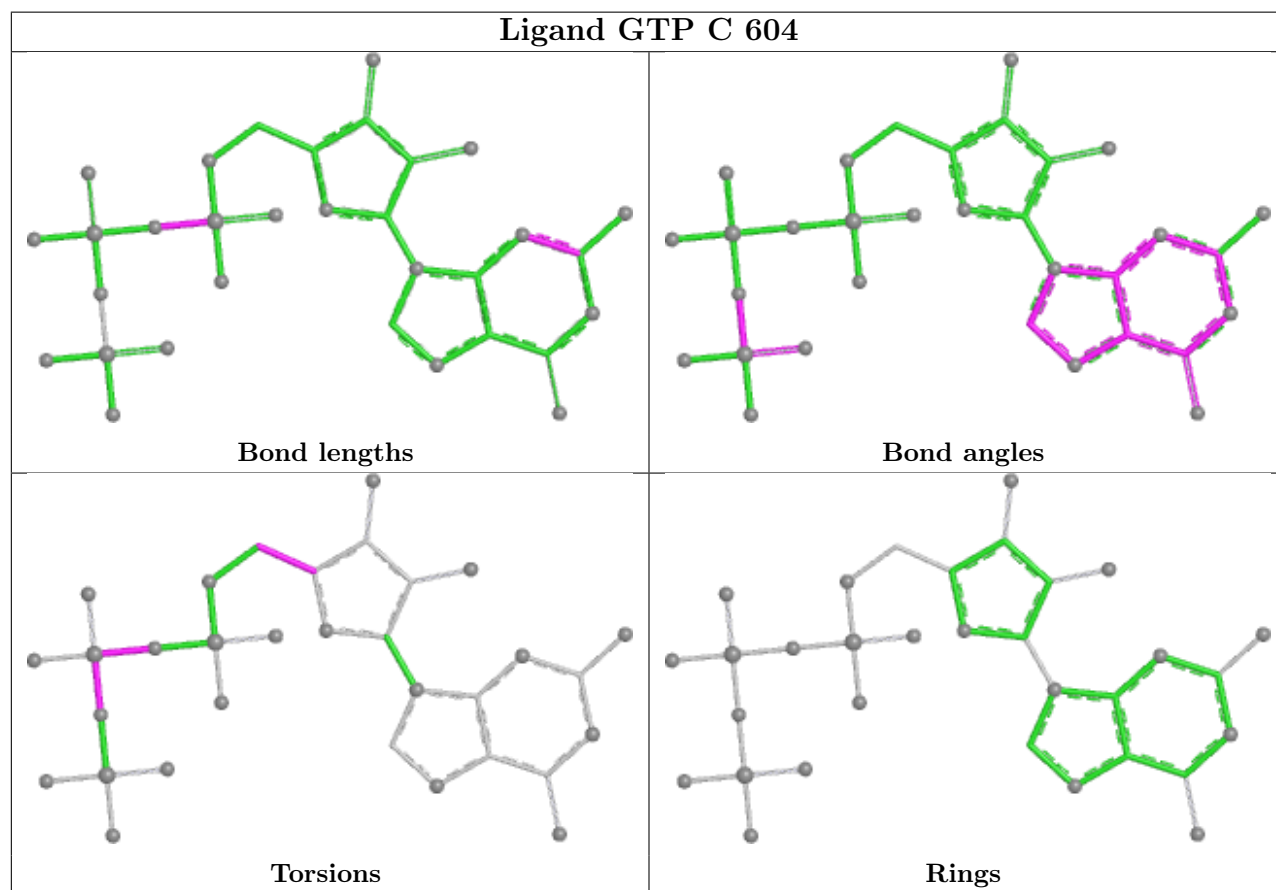
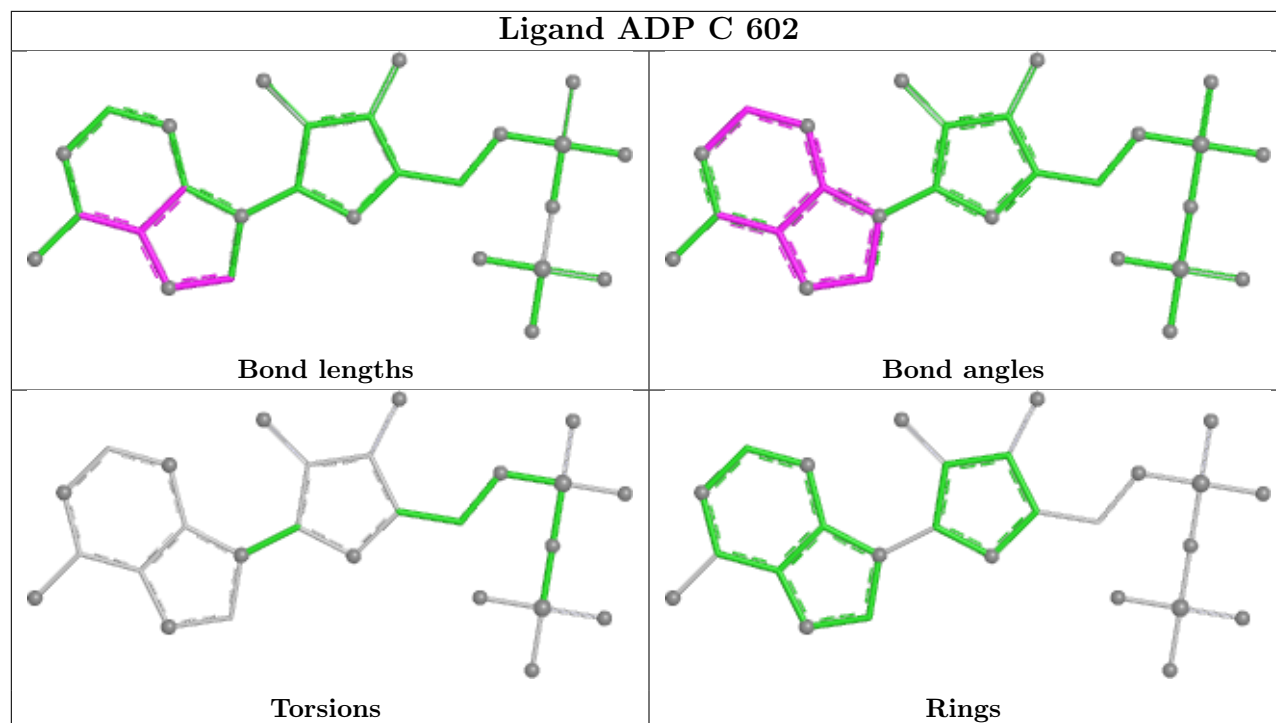
1 monomer is involved in 1 short contact:

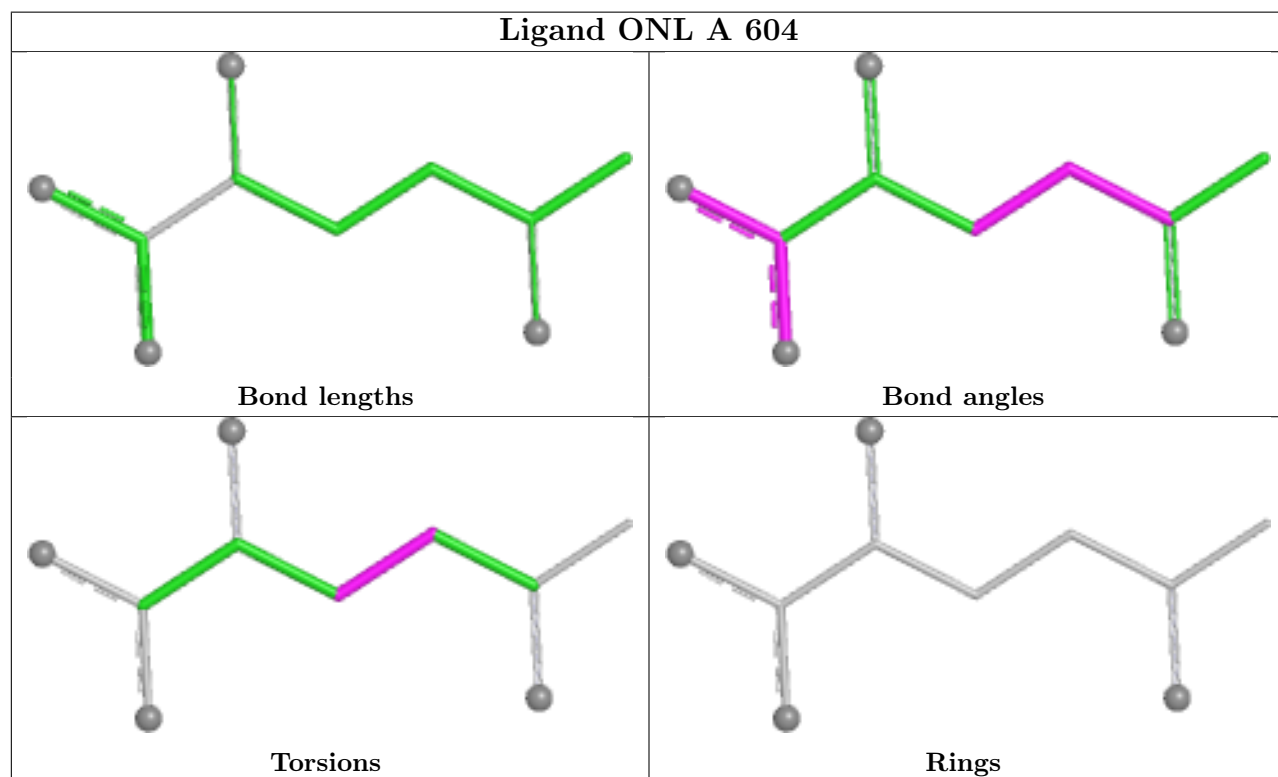
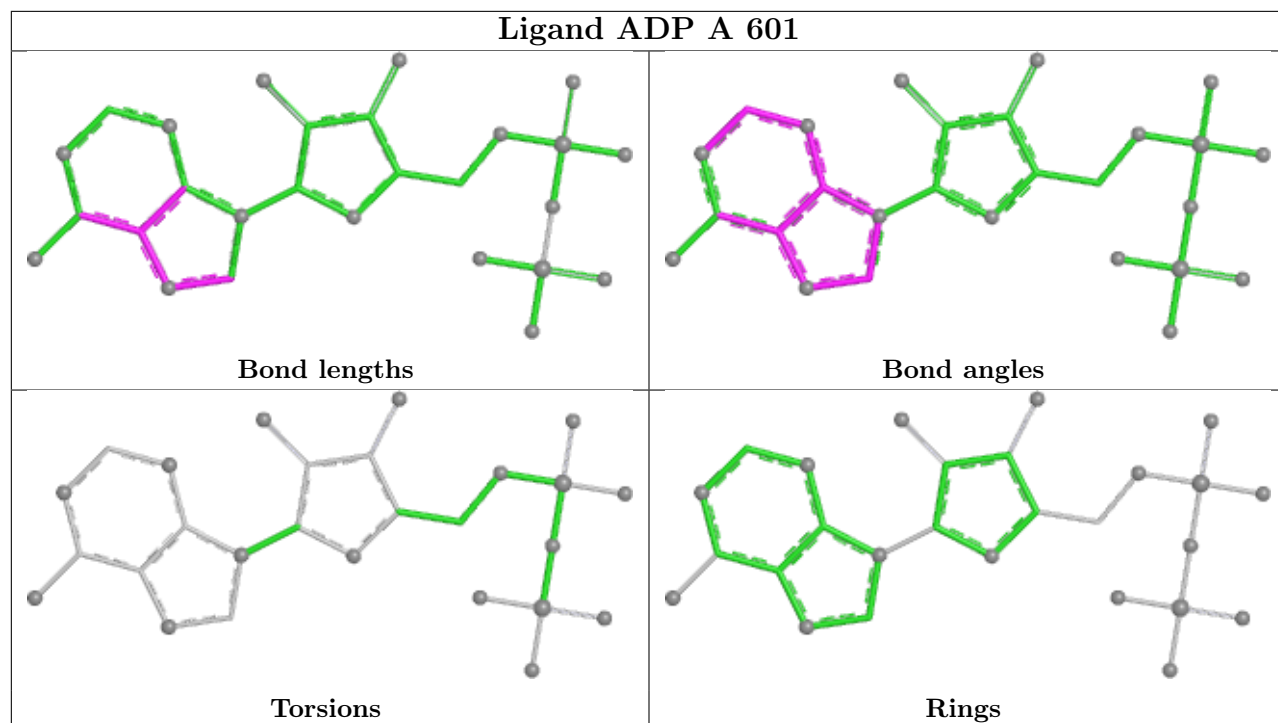
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	5ZL	1	0

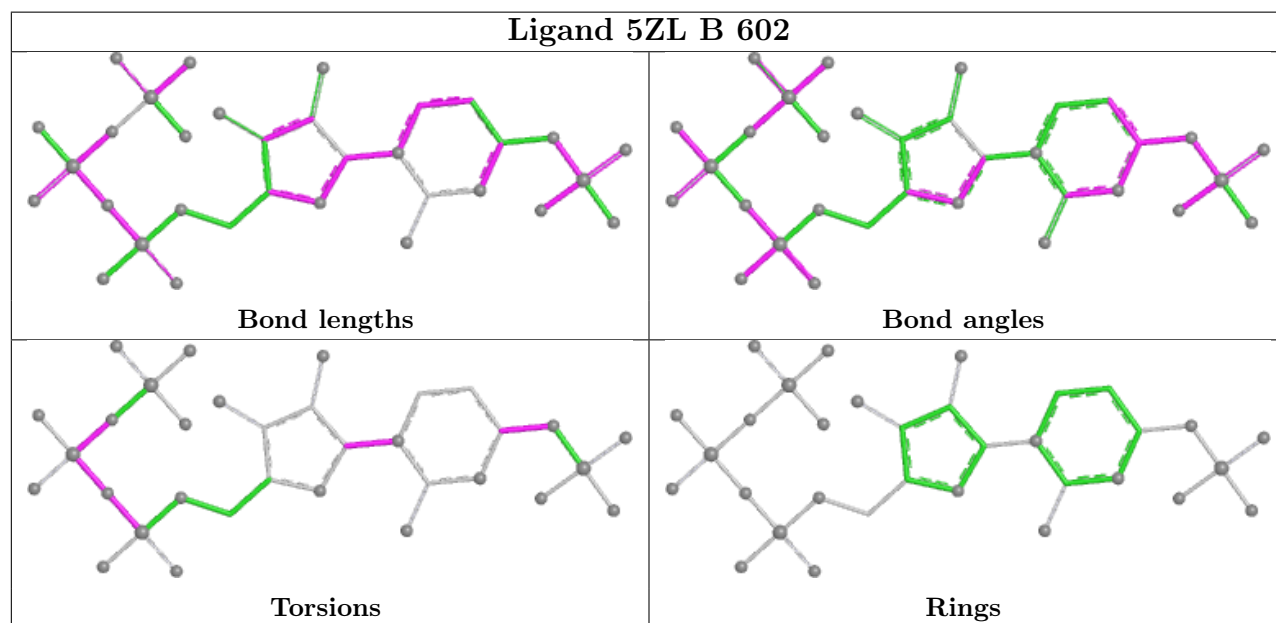
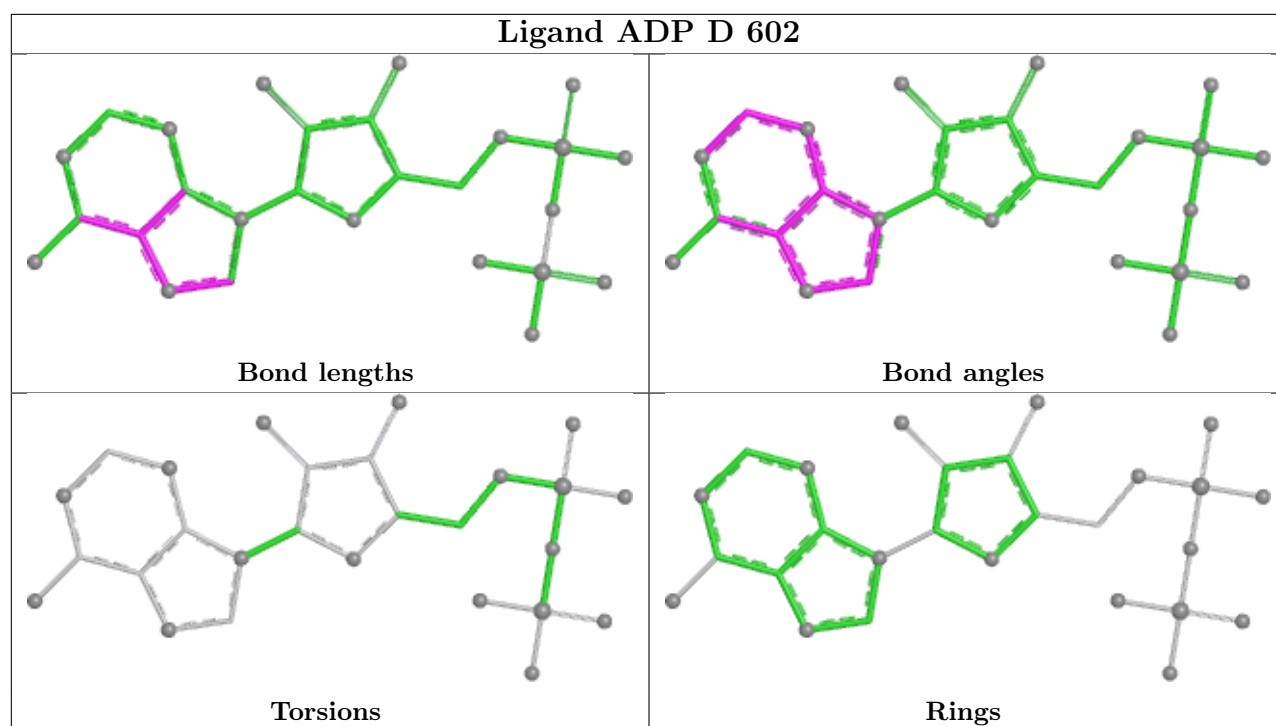
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

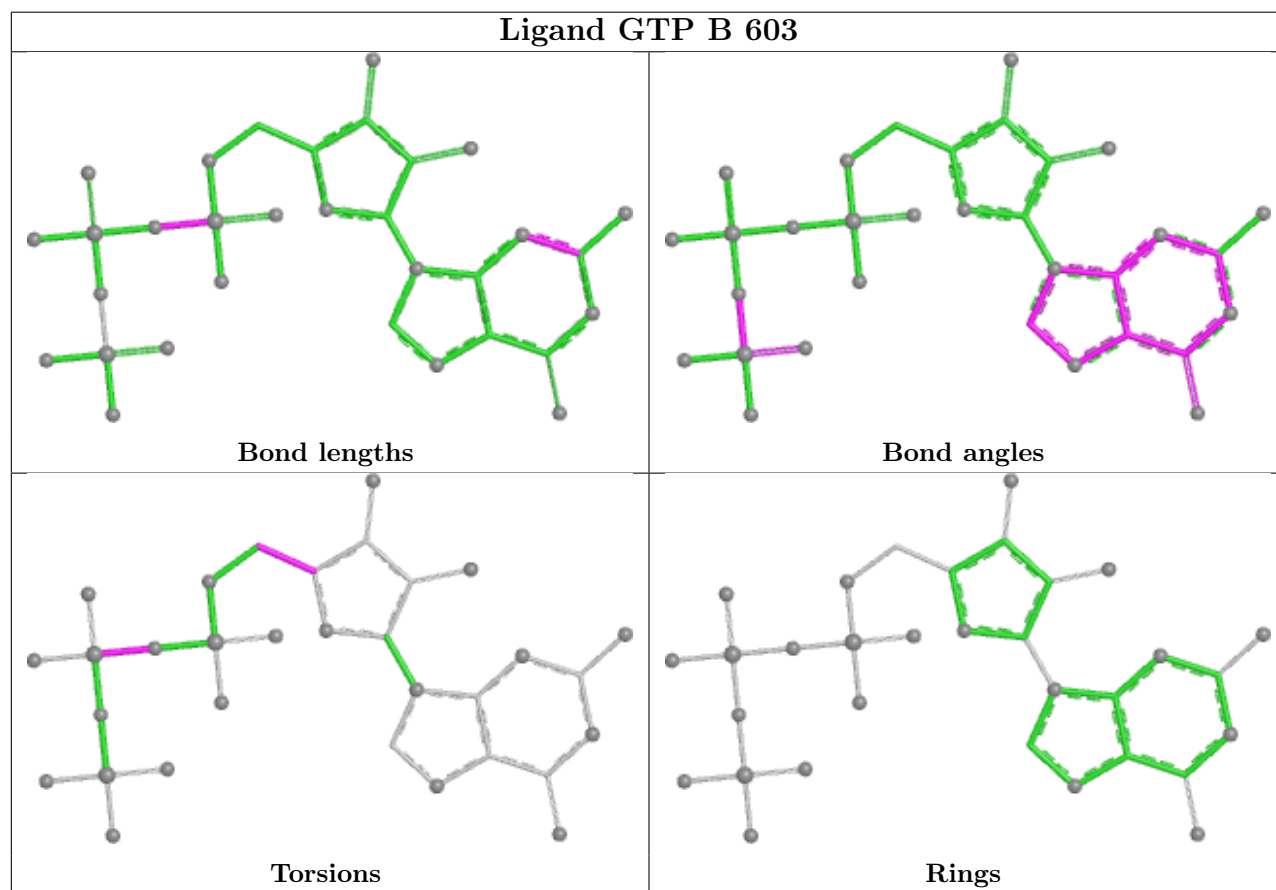
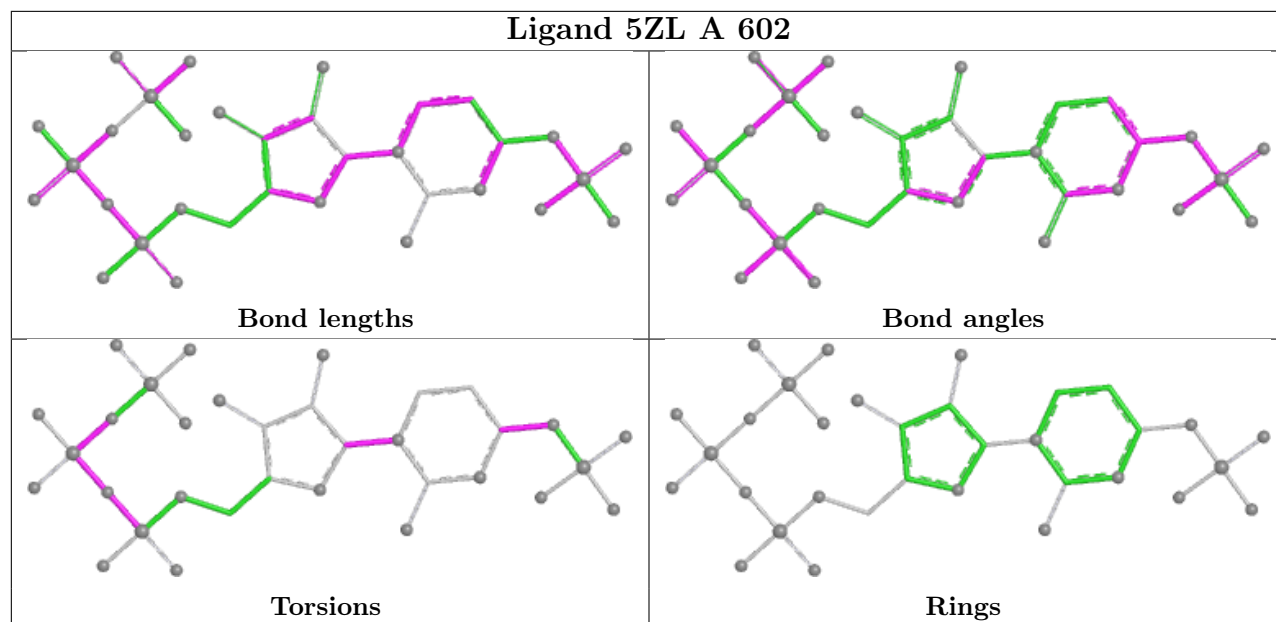
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

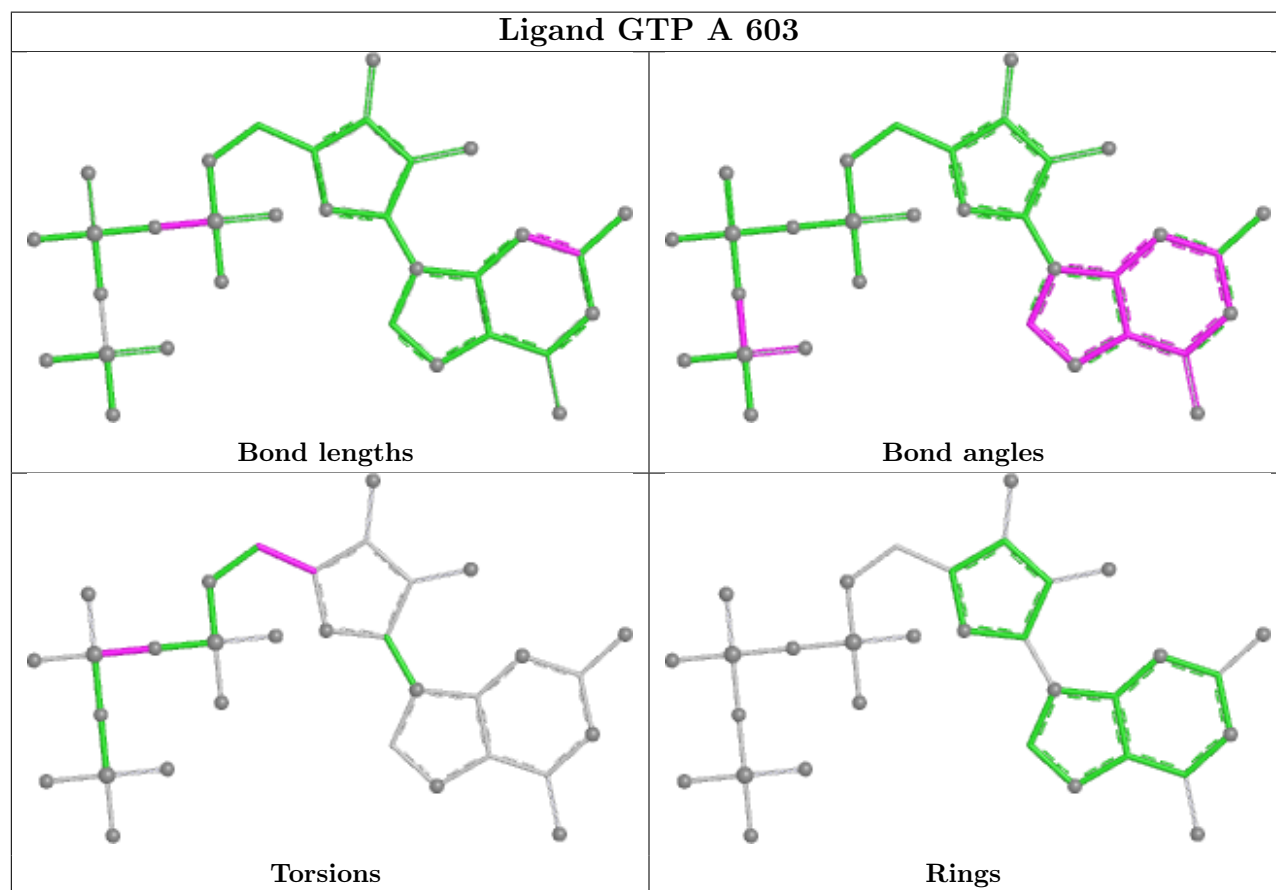
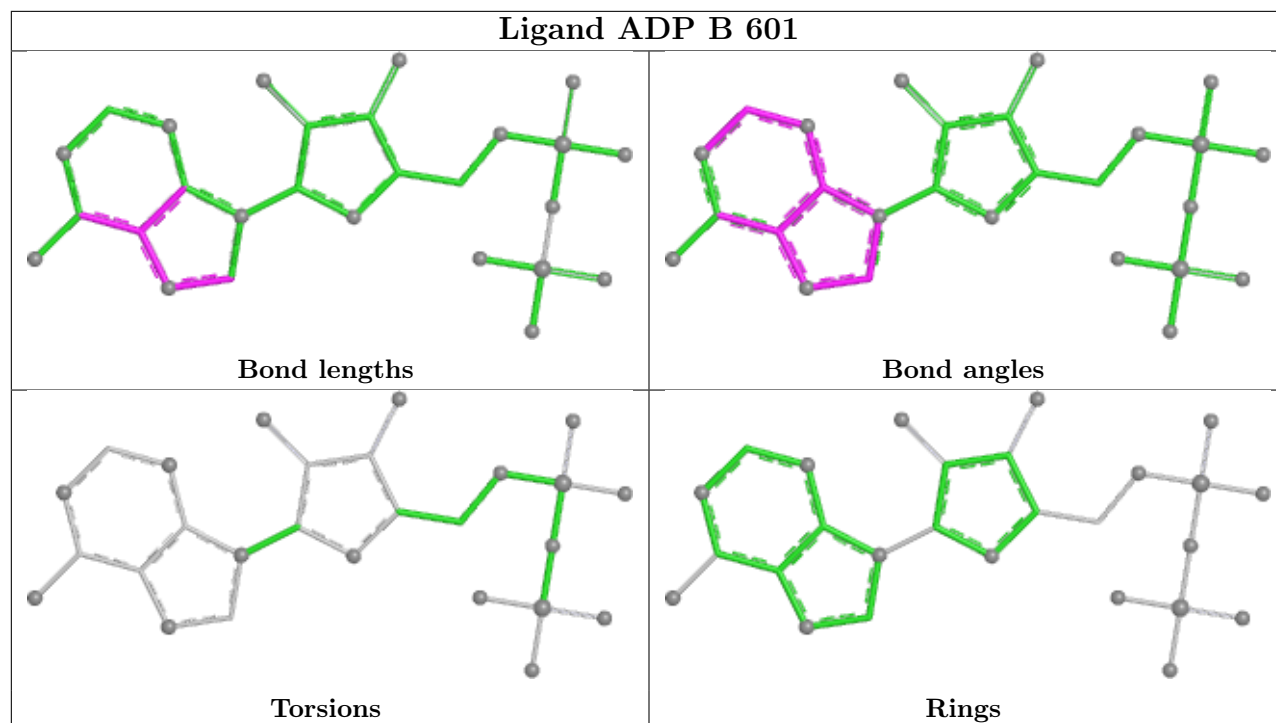


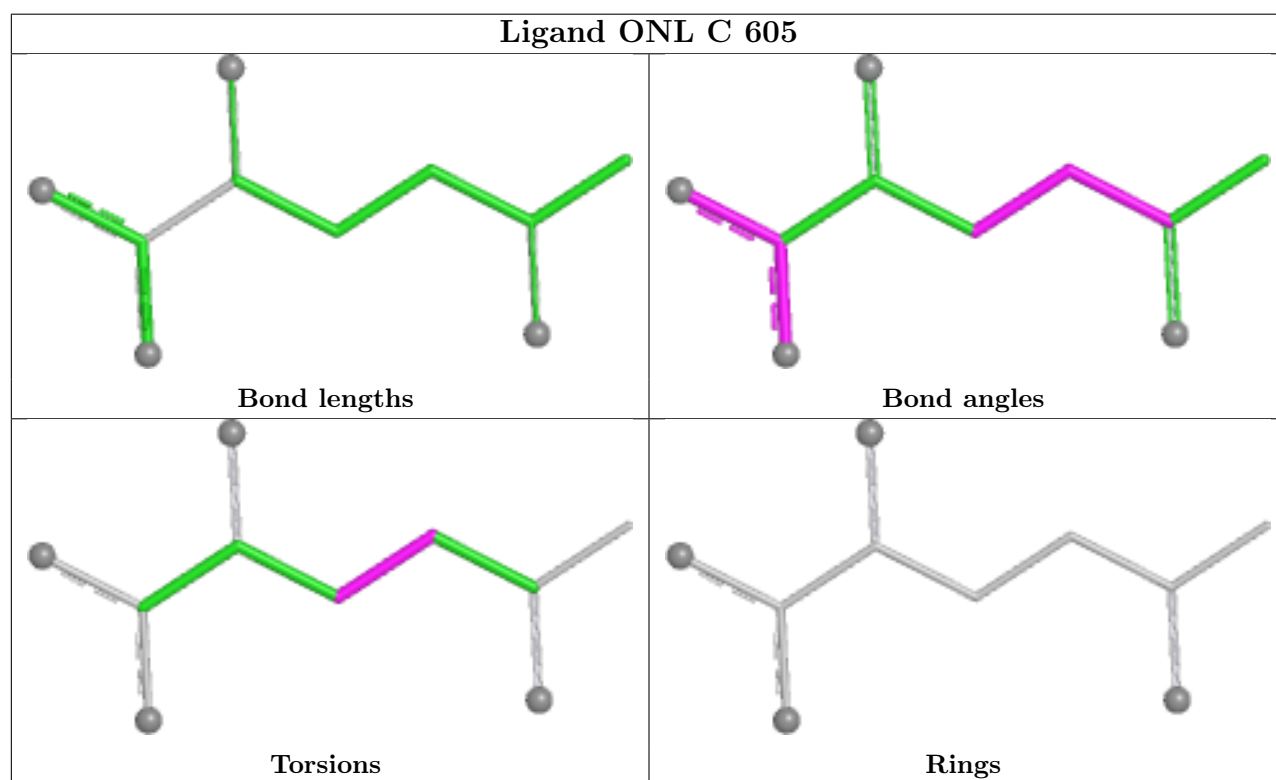
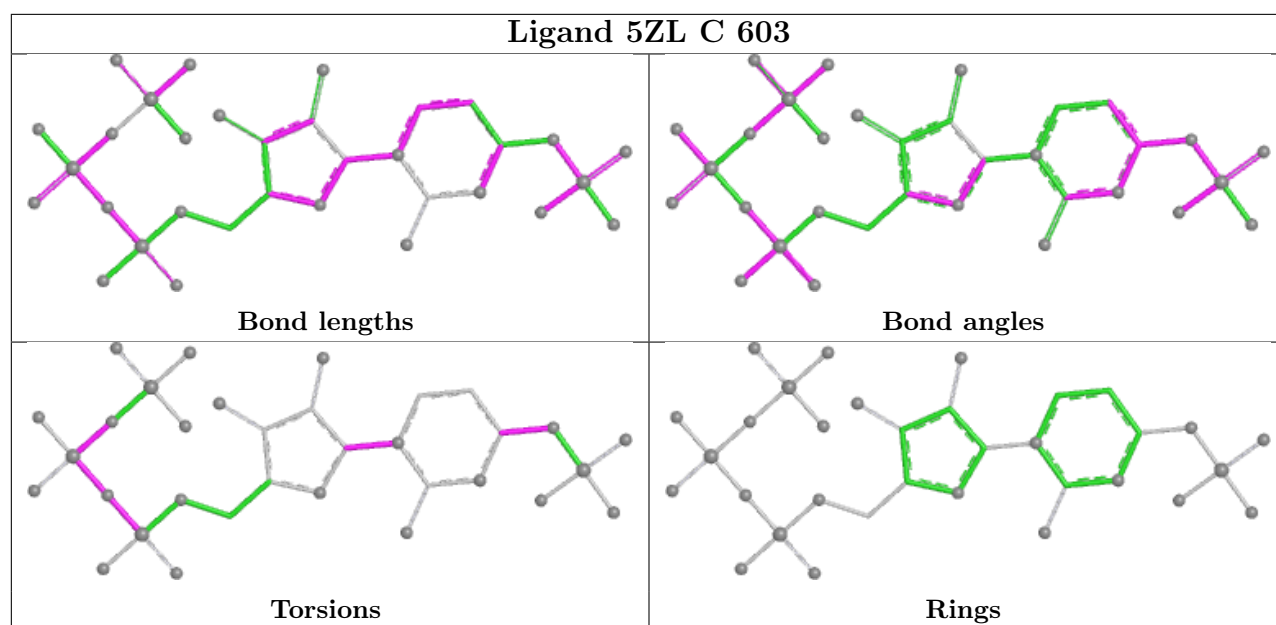


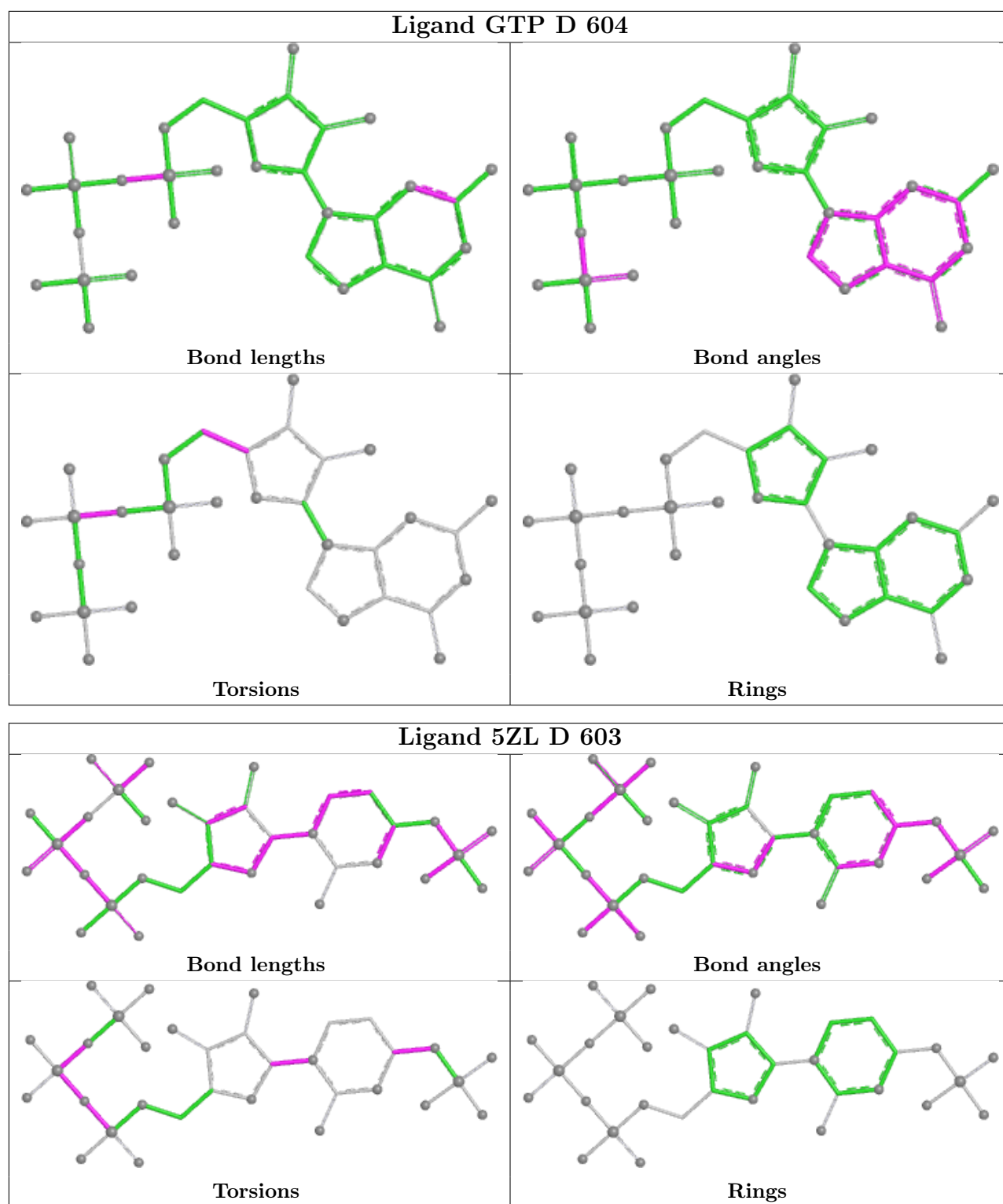












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

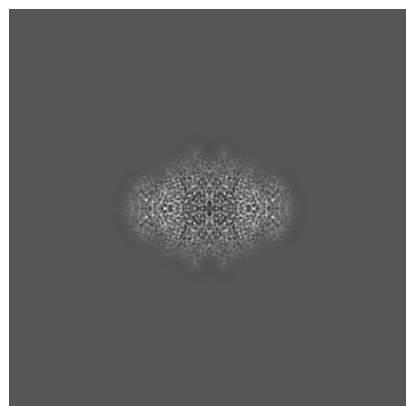
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63990. These allow visual inspection of the internal detail of the map and identification of artifacts.

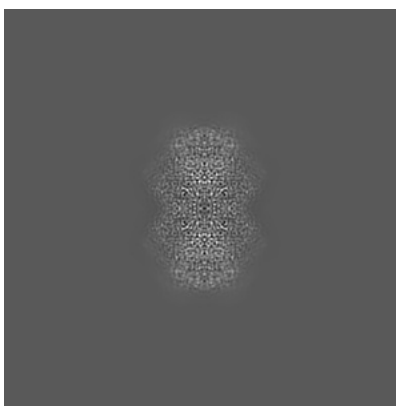
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

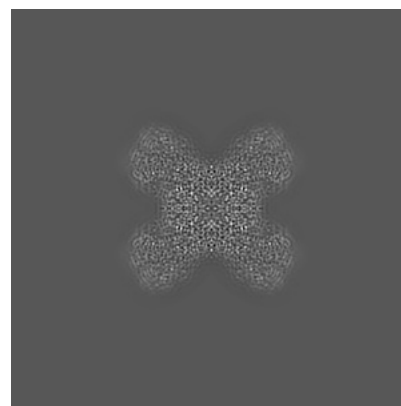
6.1.1 Primary map



X

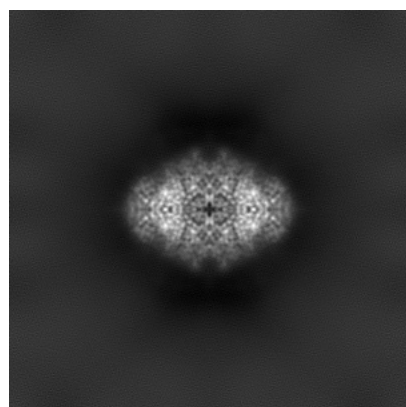


Y

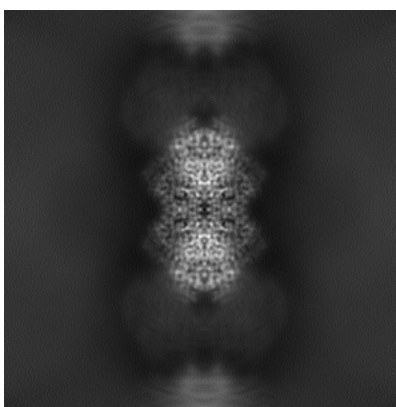


Z

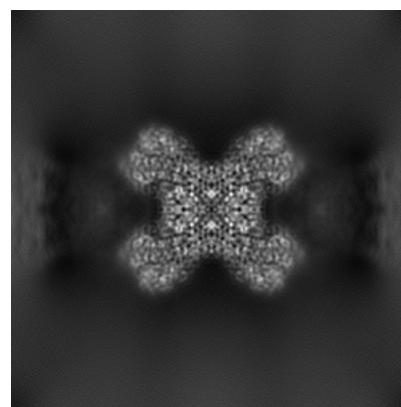
6.1.2 Raw map



X



Y

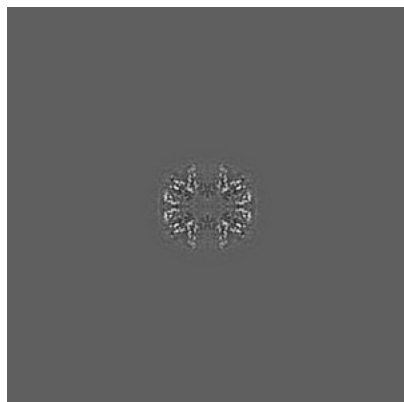


Z

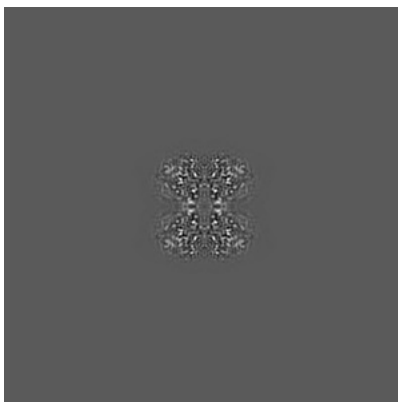
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

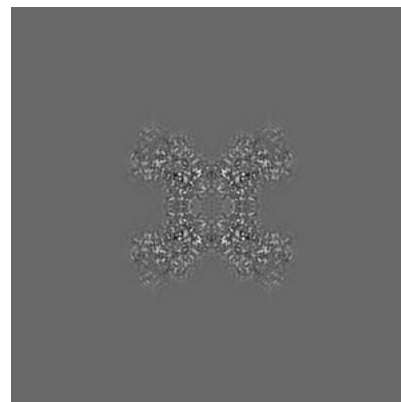
6.2.1 Primary map



X Index: 192

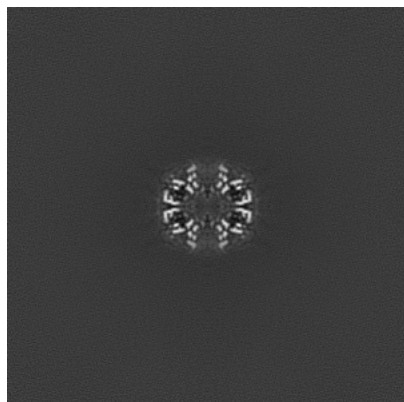


Y Index: 192

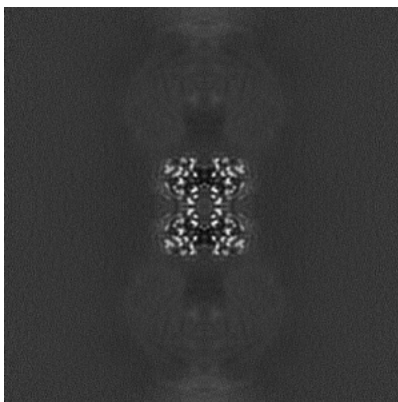


Z Index: 192

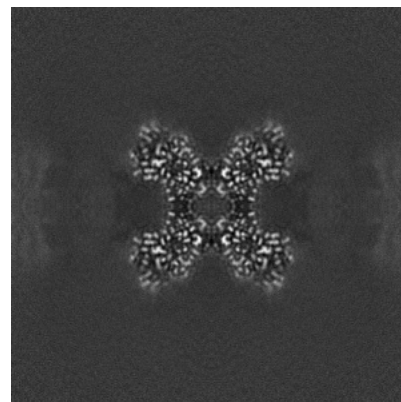
6.2.2 Raw map



X Index: 192



Y Index: 192

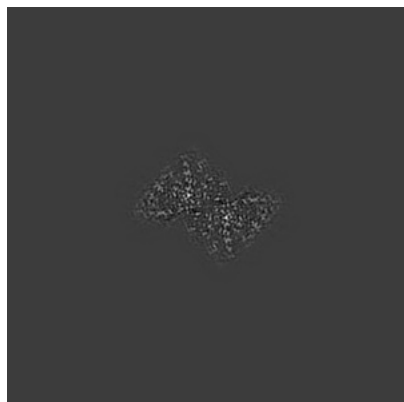


Z Index: 192

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 221

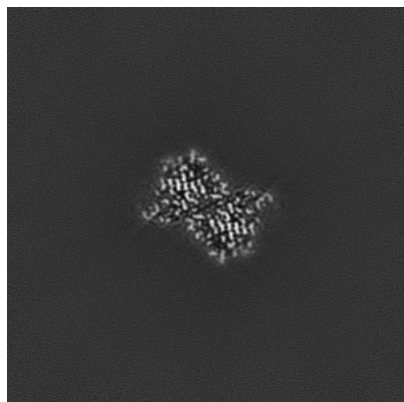


Y Index: 160

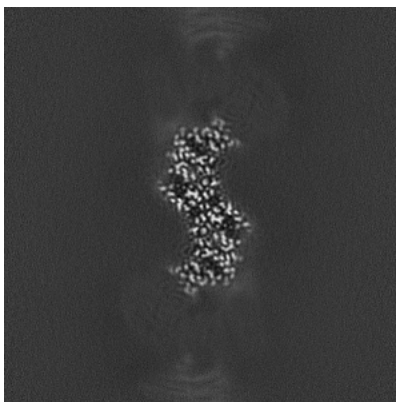


Z Index: 198

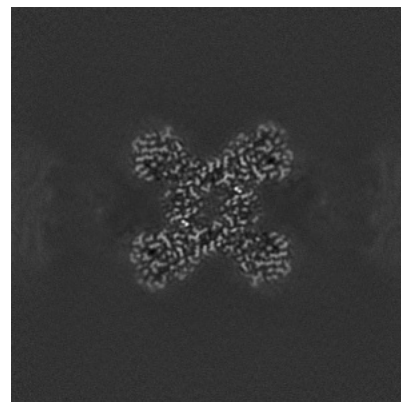
6.3.2 Raw map



X Index: 211



Y Index: 224

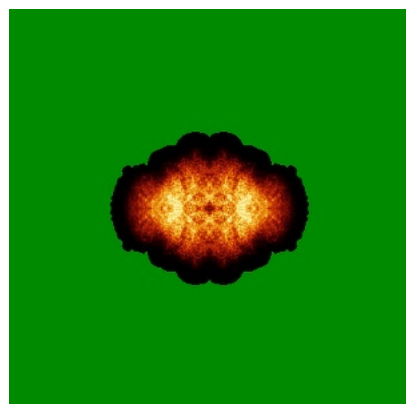


Z Index: 198

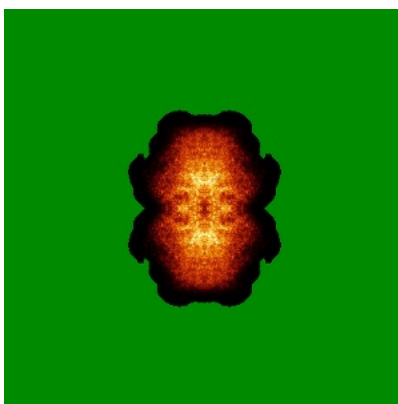
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

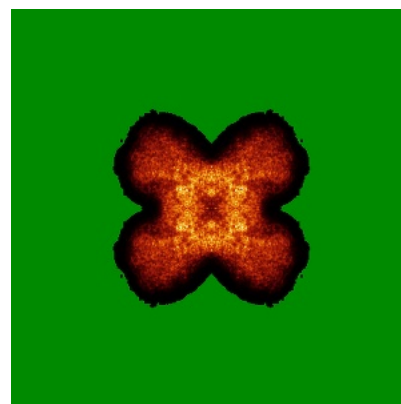
6.4.1 Primary map



X

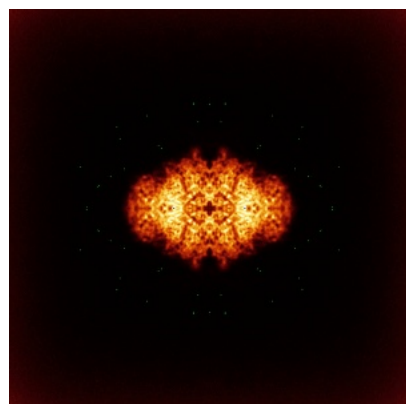


Y

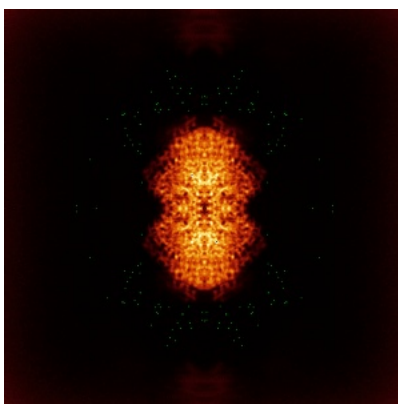


Z

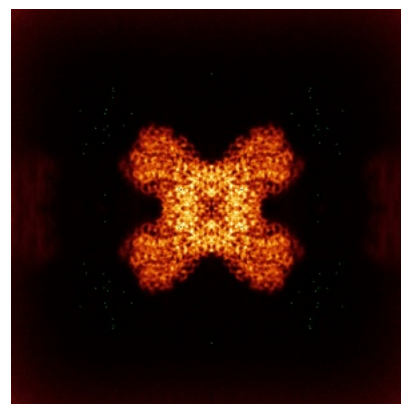
6.4.2 Raw map



X



Y

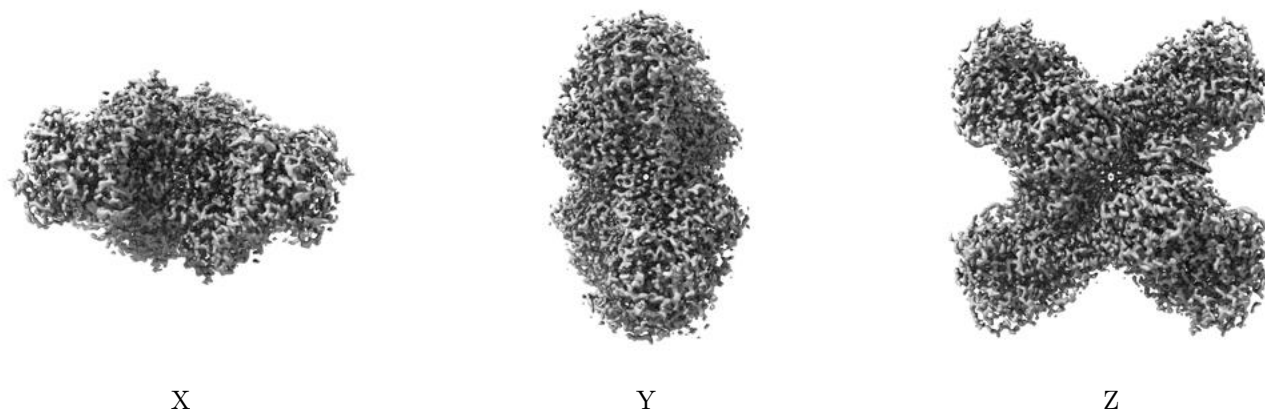


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

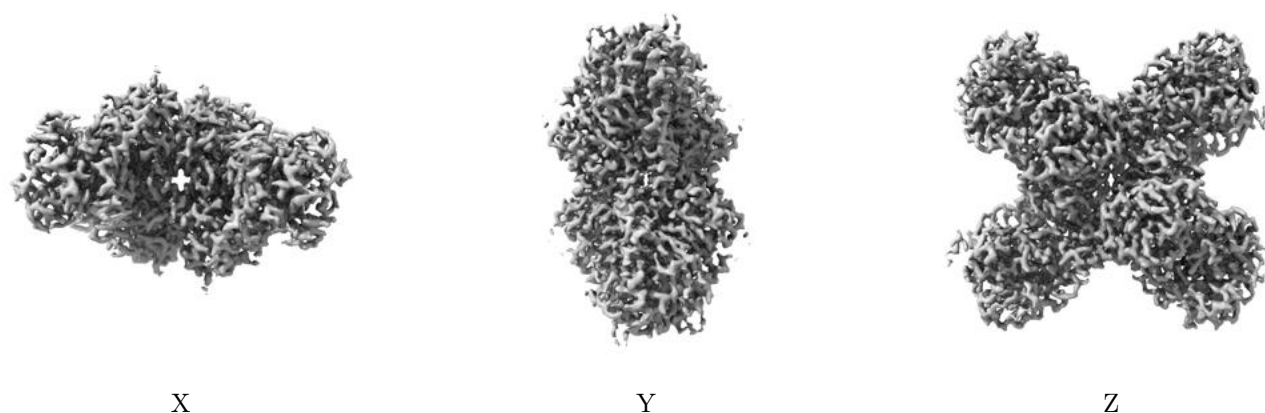
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

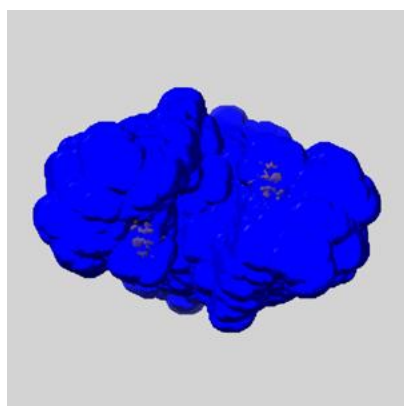
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

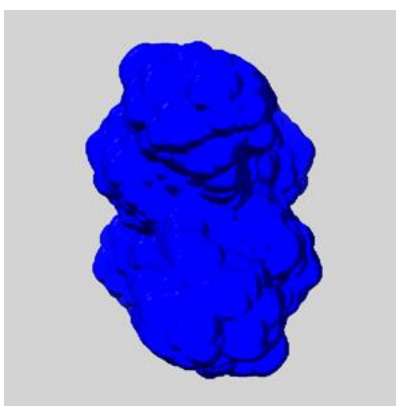
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

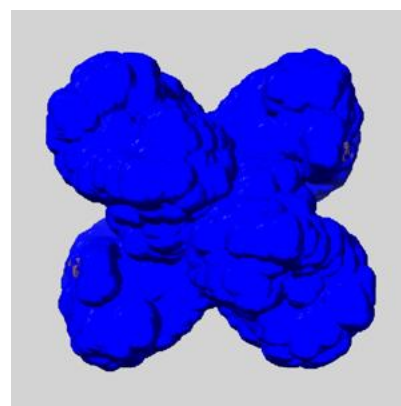
6.6.1 emd_63990_msk_1.map [i](#)



X



Y

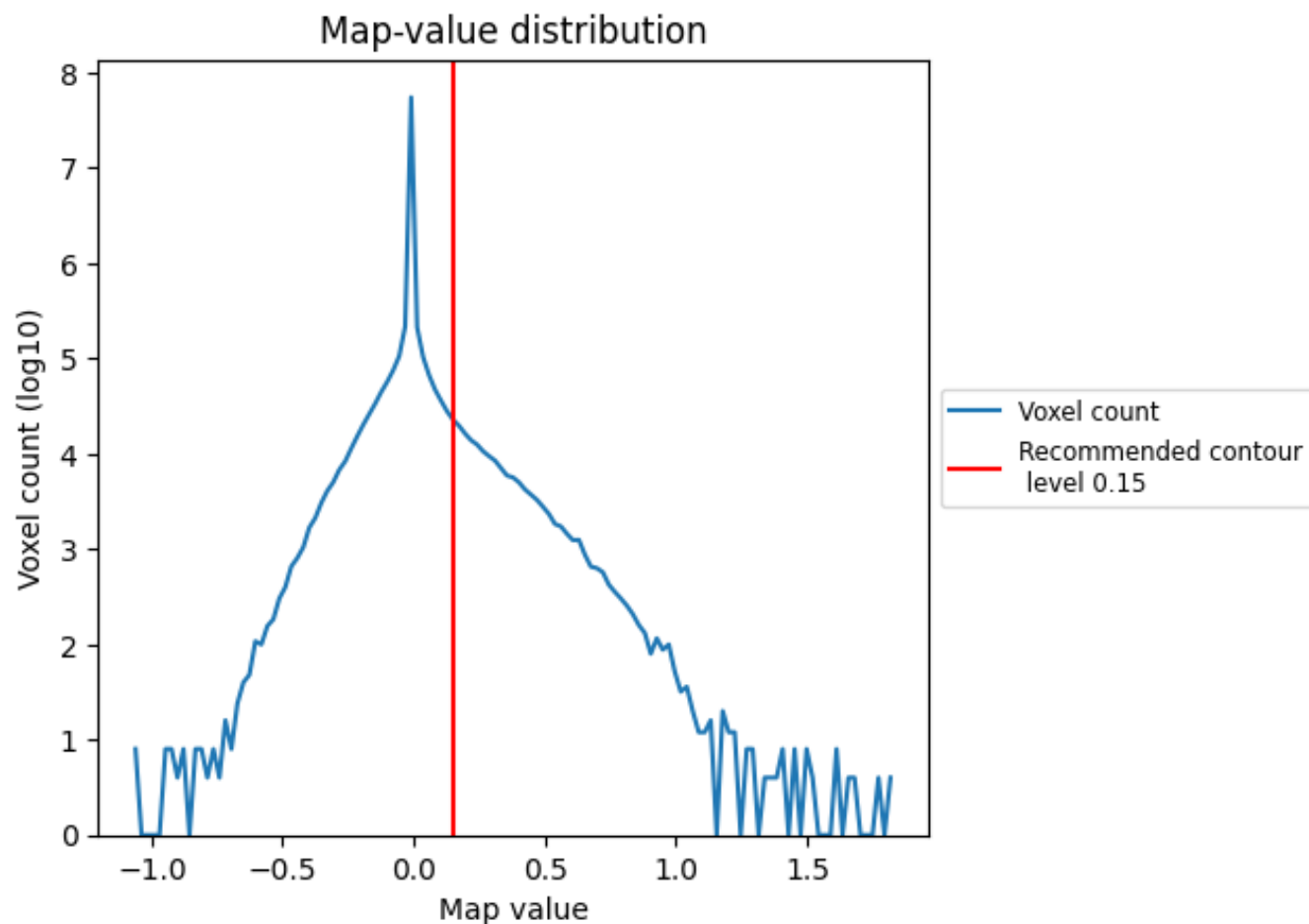


Z

7 Map analysis [i](#)

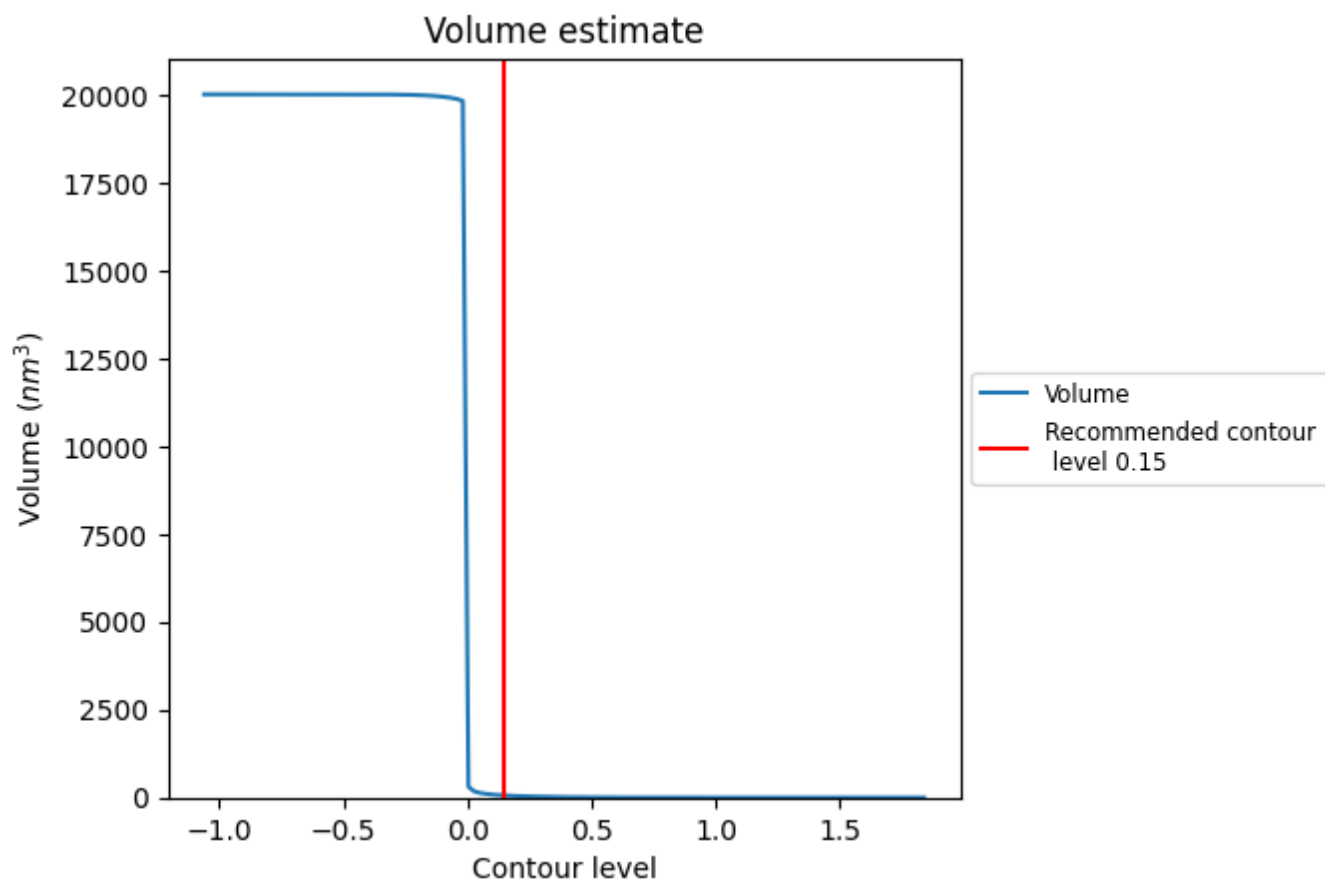
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

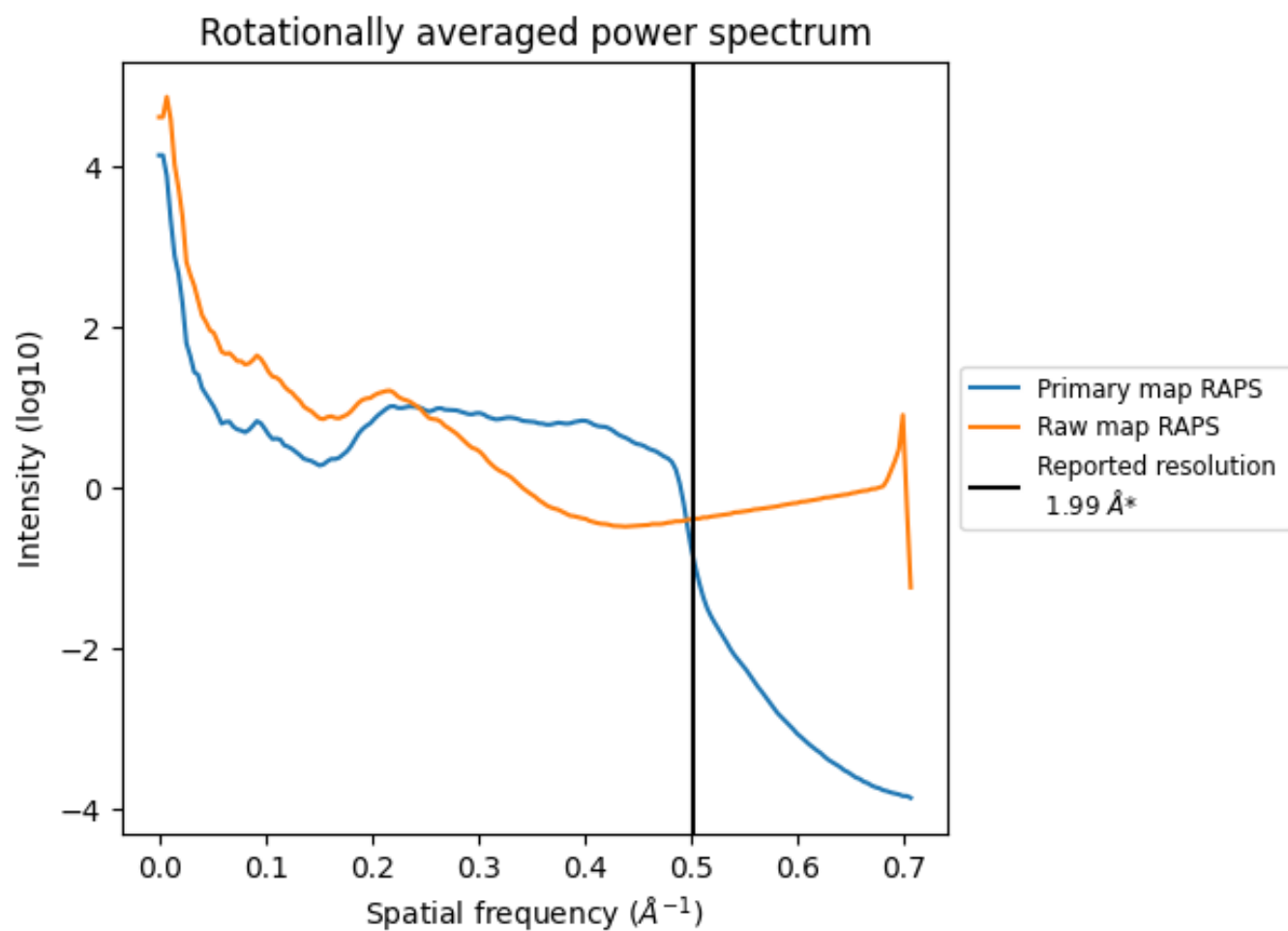
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 53 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

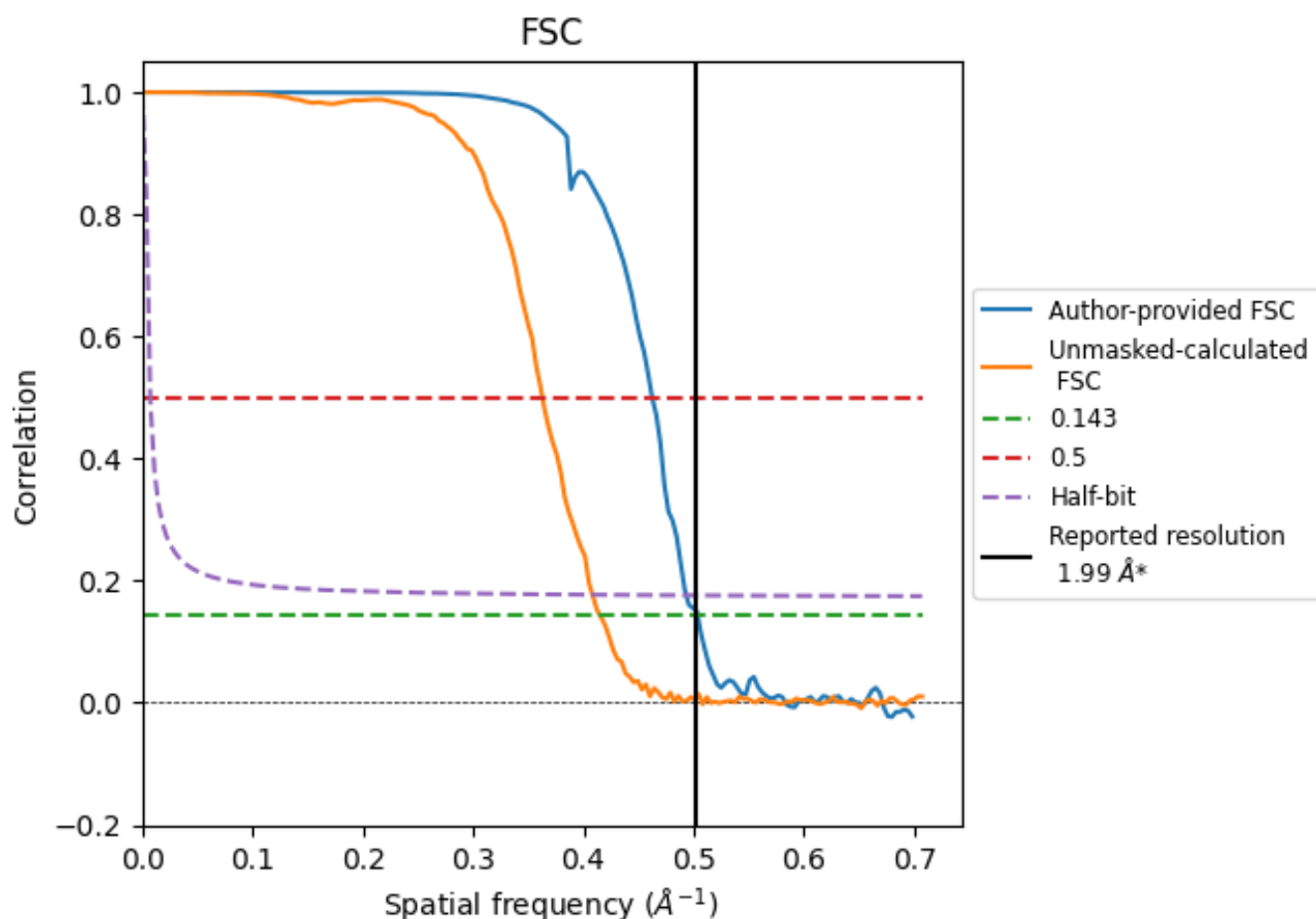


*Reported resolution corresponds to spatial frequency of 0.503 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.503 \AA^{-1}

8.2 Resolution estimates [i](#)

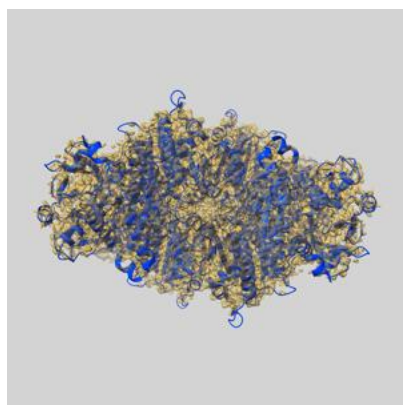
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.99	-	-
Author-provided FSC curve	1.99	2.16	2.03
Unmasked-calculated*	2.41	2.76	2.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.41 differs from the reported value 1.99 by more than 10 %

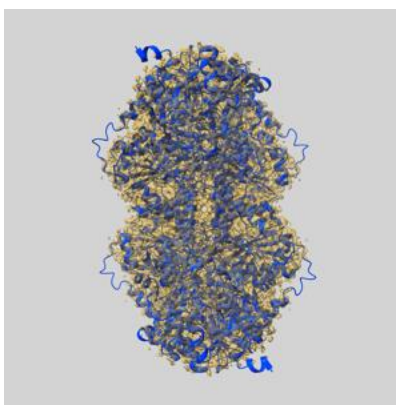
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63990 and PDB model 9UAR. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

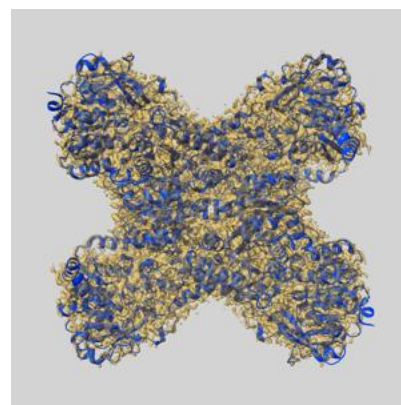
9.1 Map-model overlay [i](#)



X



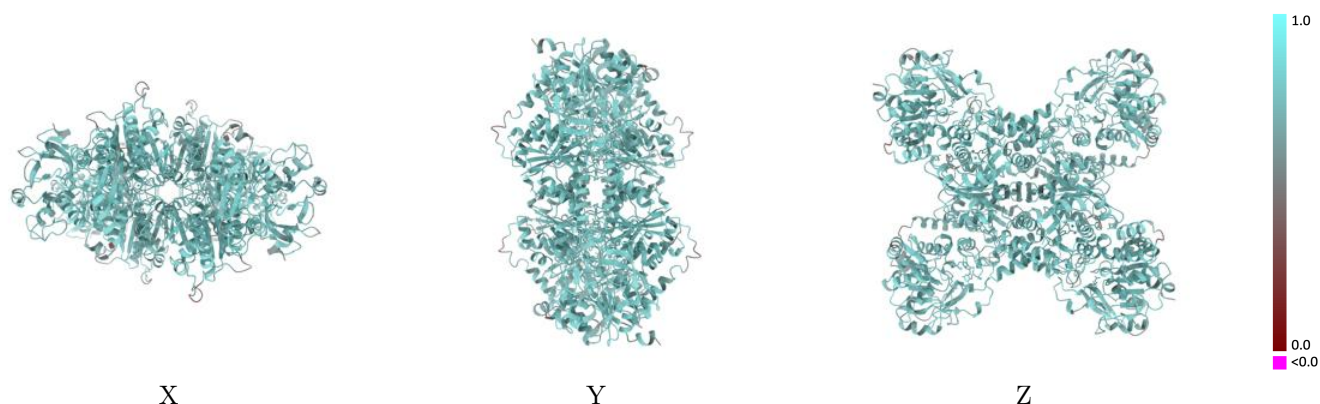
Y



Z

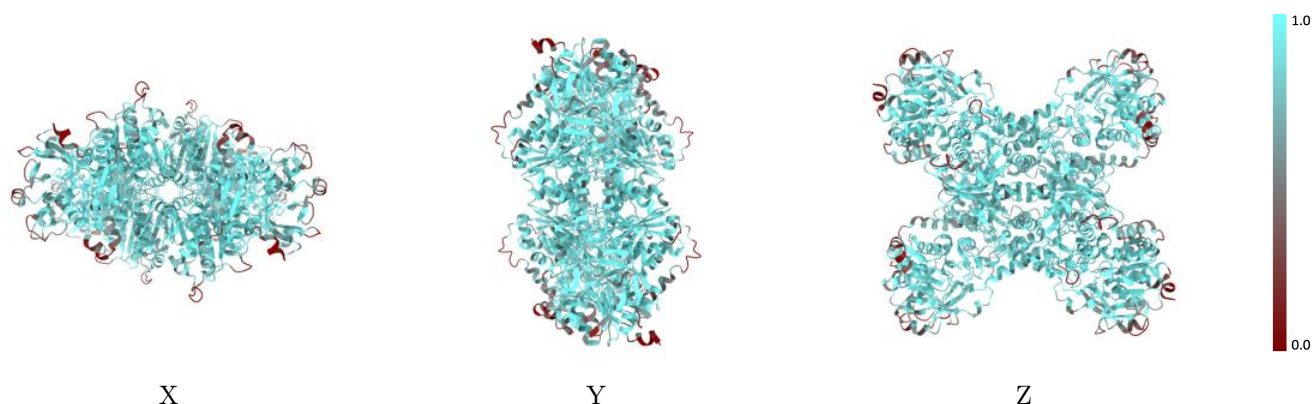
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



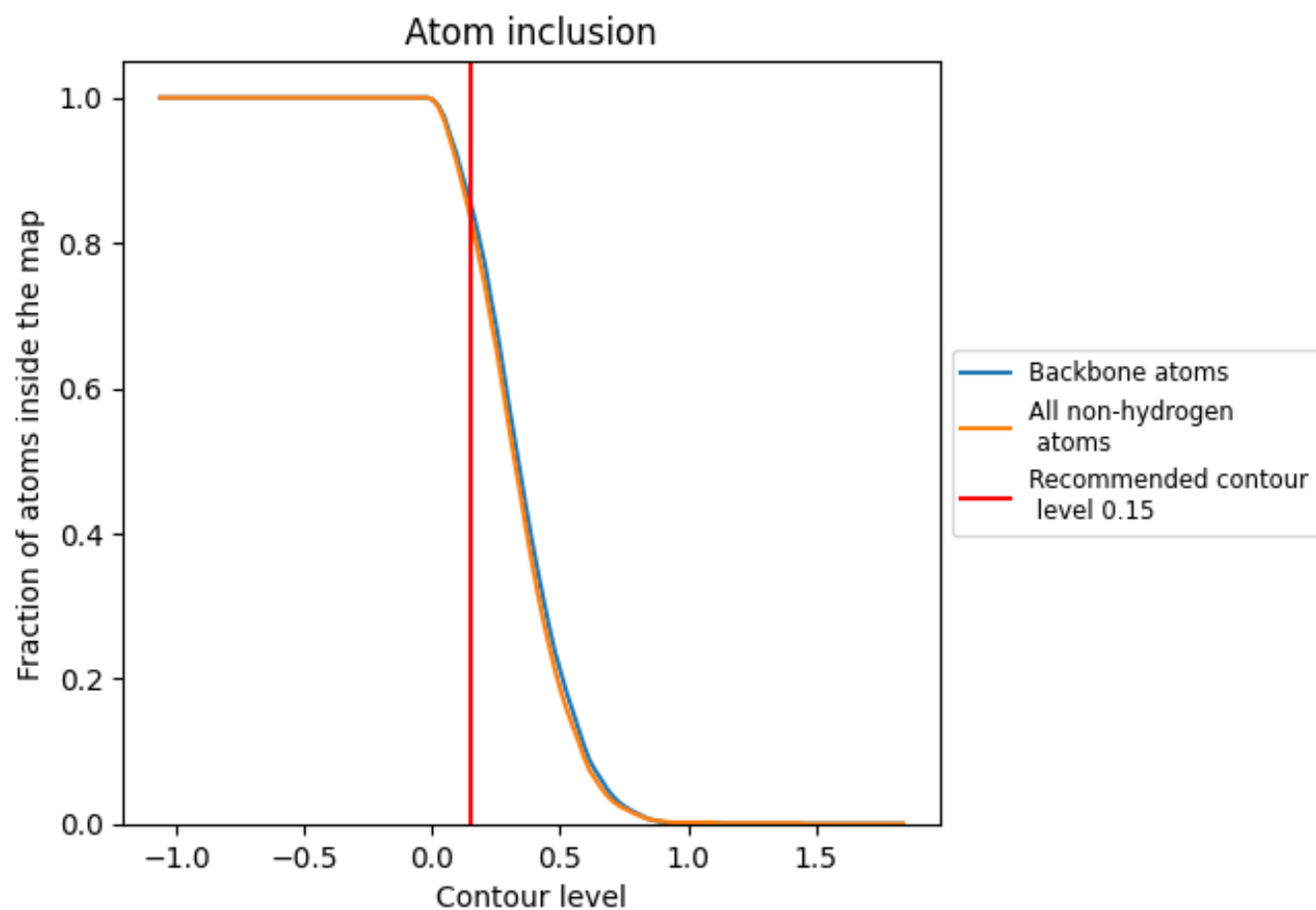
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8360	<div></div> 0.7440
A	<div></div> 0.8350	<div></div> 0.7440
B	<div></div> 0.8380	<div></div> 0.7440
C	<div></div> 0.8370	<div></div> 0.7420
D	<div></div> 0.8420	<div></div> 0.7450

