



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:50 PM UTC

PDB ID : 9NVN / pdb_00009nvn
EMDB ID : EMD-49844
Title : Structure of Nanchung-Inactive-Calmodulin in apo state
Authors : Fedor, J.G.; Lee, S.-Y.
Deposited on : 2025-03-21
Resolution : 2.89 Å(reported)
Based on initial model : 8ET6

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:

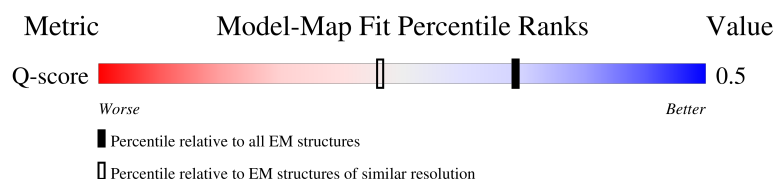
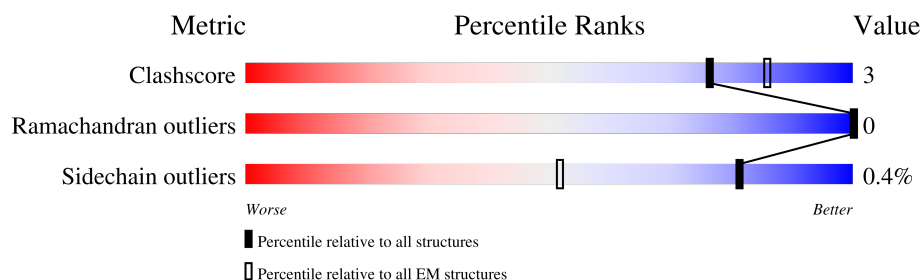
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.89 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	12148 (2.39 - 3.39)

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	B	984	 7% 63% 5% 32%
1	D	984	 6% 63% 5% 32%
2	E	74	 66% 62% 19% 19%
2	F	74	 65% 61% 20% 19%

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Mol	Chain	Length	Quality of chain
3	A	907	
3	C	907	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 46250 atoms, of which 22972 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 Inactive.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	668	Total	C	H	N	O	S	0	0
			9972	3294	4903	852	891	32		
1	D	668	Total	C	H	N	O	S	0	0
			9972	3294	4903	852	891	32		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	254	GLN	HIS	conflict	UNP A0A9P0HI19
B	401	ILE	LEU	conflict	UNP A0A9P0HI19
B	427	ILE	VAL	conflict	UNP A0A9P0HI19
B	445	LEU	ILE	conflict	UNP A0A9P0HI19
B	480	VAL	ILE	conflict	UNP A0A9P0HI19
B	487	ILE	MET	conflict	UNP A0A9P0HI19
B	607	VAL	ILE	conflict	UNP A0A9P0HI19
D	254	GLN	HIS	conflict	UNP A0A9P0HI19
D	401	ILE	LEU	conflict	UNP A0A9P0HI19
D	427	ILE	VAL	conflict	UNP A0A9P0HI19
D	445	LEU	ILE	conflict	UNP A0A9P0HI19
D	480	VAL	ILE	conflict	UNP A0A9P0HI19
D	487	ILE	MET	conflict	UNP A0A9P0HI19
D	607	VAL	ILE	conflict	UNP A0A9P0HI19

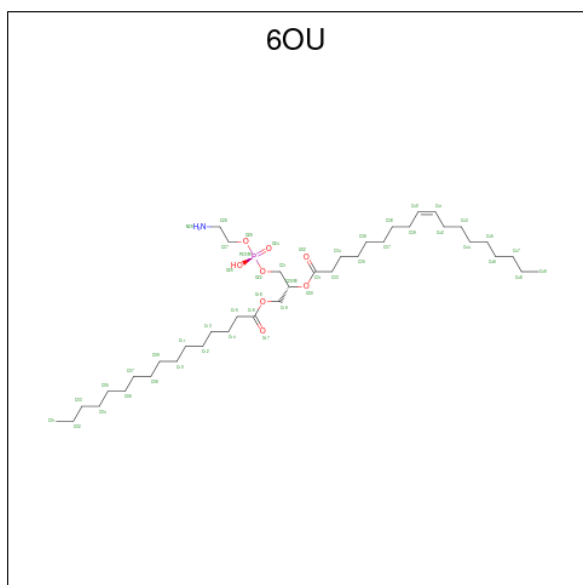
- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	60	Total	C	H	N	O	S	0	0
			739	254	334	63	85	3		
2	F	60	Total	C	H	N	O	S	0	0
			739	254	334	63	85	3		

- Molecule 3 is a protein called Nanchung.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	723	Total 11538	C 3757	H 5744	N 947	O 1034	S 56	0	0
3	C	723	Total 11538	C 3757	H 5744	N 947	O 1034	S 56	0	0

- Molecule 4 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



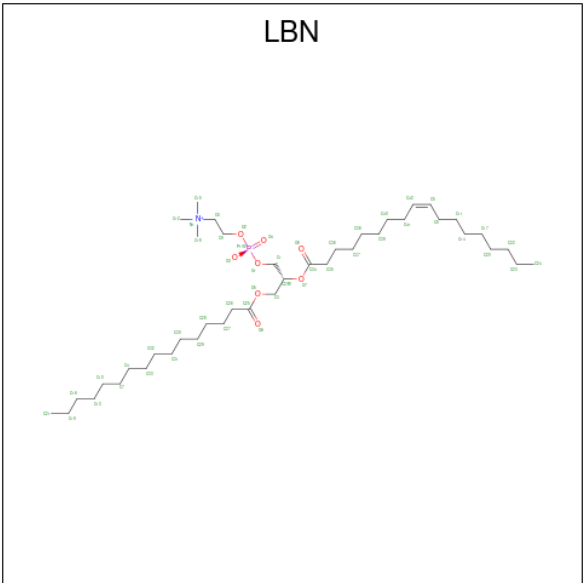
Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total 109	C 36	H 64	O 8	P 1	0	
4	B	1	Total 66	C 20	H 36	N 1	O 8	P 1	0
4	B	1	Total 83	C 27	H 47	O 8	P 1	0	
4	A	1	Total 114	C 36	H 68	N 1	O 8	P 1	0
4	A	1	Total 102	C 32	H 60	N 1	O 8	P 1	0
4	A	1	Total 102	C 32	H 60	N 1	O 8	P 1	0
4	D	1	Total 109	C 36	H 64	O 8	P 1	0	
4	D	1	Total 66	C 20	H 36	N 1	O 8	P 1	0
4	D	1	Total 83	C 27	H 47	O 8	P 1	0	

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Mol	Chain	Residues	Atoms						AltConf
4	C	1	Total	C	H	N	O	P	0
			114	36	68	1	8	1	
4	C	1	Total	C	H	N	O	P	0
			102	32	60	1	8	1	
4	C	1	Total	C	H	N	O	P	0
			102	32	60	1	8	1	

- Molecule 5 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P).

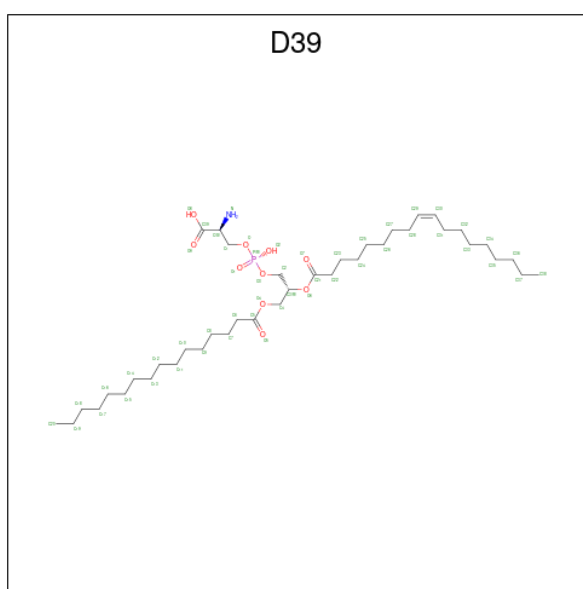


Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total 81	C 25	H 46	N 1	O 8	P 1	0
5	B	1	Total 41 C 15 H 26						0
5	B	1	Total 98	C 32	H 57	O 8	P 1	0	
5	D	1	Total 98	C 32	H 57	O 8	P 1	0	
5	D	1	Total 81	C 25	H 46	N 1	O 8	P 1	0
5	D	1	Total 41 C 15 H 26						0

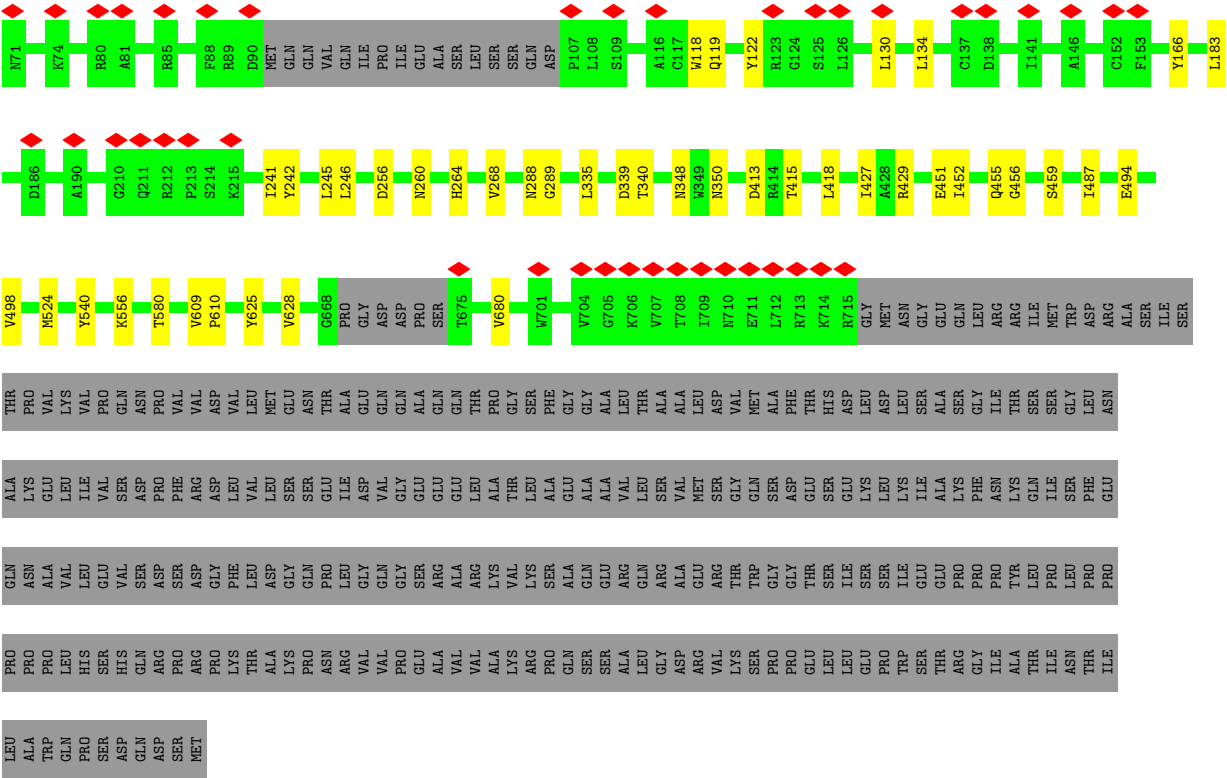
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	E	2	Total	Ca	0
			2	2	
6	A	1	Total	Ca	0
			1	1	
6	F	2	Total	Ca	0
			2	2	
6	C	1	Total	Ca	0
			1	1	

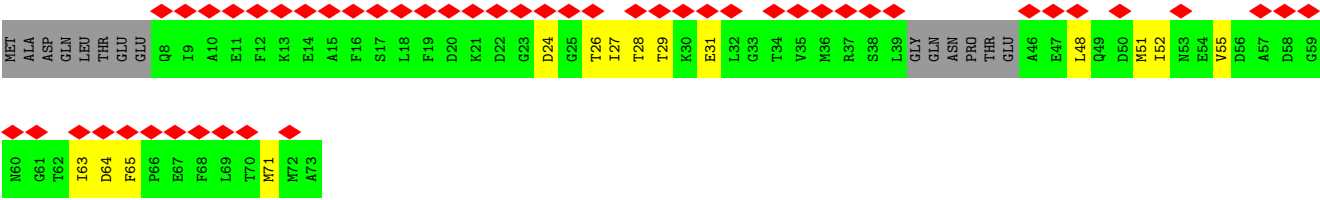
- Molecule 7 is (2 {S})-2-azanyl-3-[[[(2 {R})-3-hexadecanoyloxy-2-[({Z})-octadec-9-enoyl]oxypropoxy]-oxidanyl-phosphoryl]oxy-propanoic acid (CCD ID: D39) (formula: C₄₀H₇₆NO₁₀P).



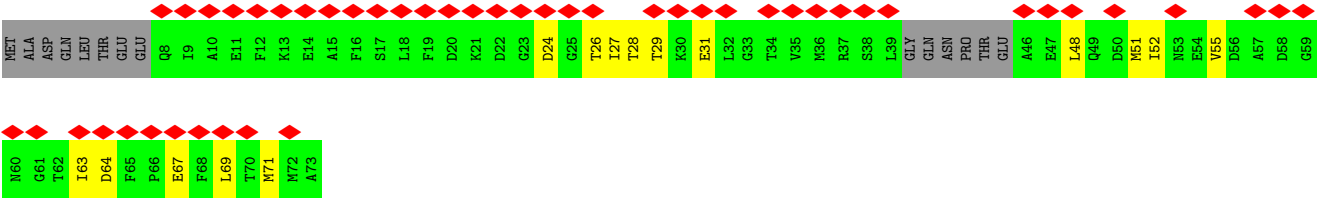
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			77	24	41	1	10	1	
7	C	1	Total	C	H	N	O	P	0
			77	24	41	1	10	1	



• Molecule 2: Calmodulin-1



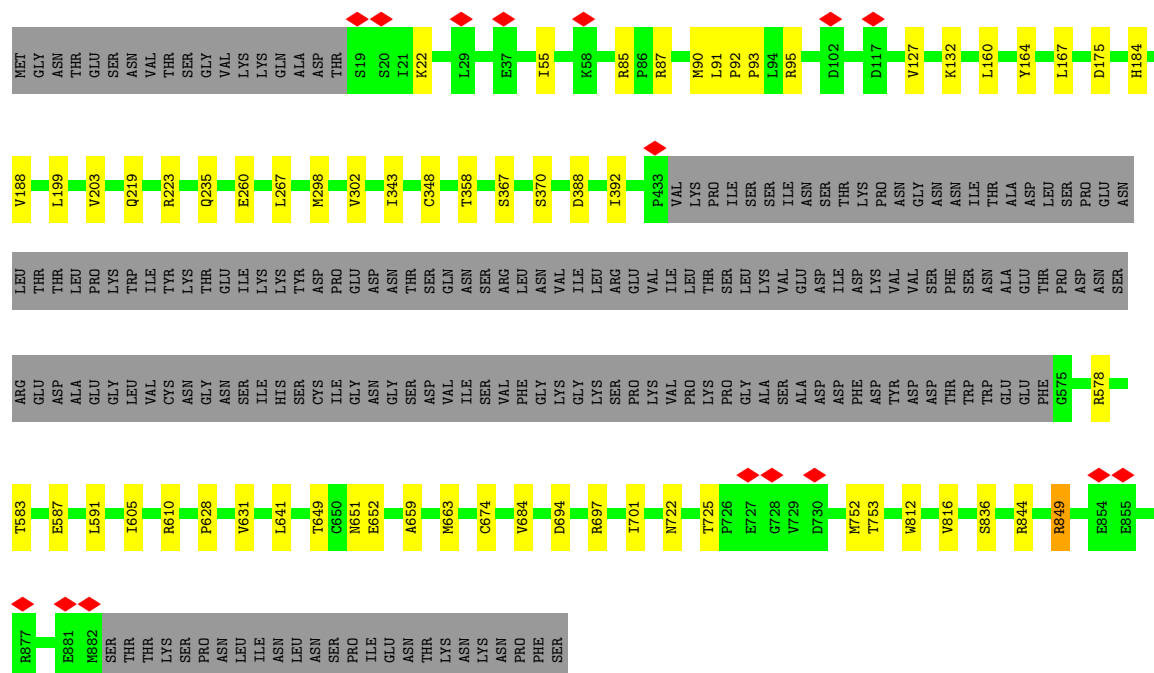
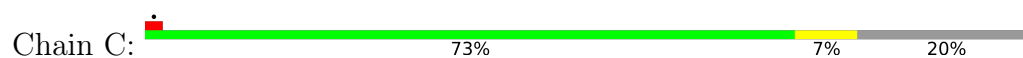
• Molecule 2: Calmodulin-1



• Molecule 3: Nanchung



- Molecule 3: Nanchung



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	328072	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)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.640	Depositor
Minimum map value	-1.699	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: D39, CA, LBN, 6OU

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	B	0.10	0/5159	0.22	0/7012
1	D	0.10	0/5159	0.22	0/7012
2	E	0.11	0/408	0.25	0/554
2	F	0.11	0/408	0.25	0/554
3	A	0.12	0/5929	0.26	1/8034 (0.0%)
3	C	0.11	0/5929	0.26	1/8034 (0.0%)
All	All	0.11	0/22992	0.24	2/31200 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	22	LYS	CD-CE-NZ	-6.55	90.95	111.90
3	A	22	LYS	CD-CE-NZ	-6.54	90.98	111.90

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	B	5069	4903	4915	27	0
1	D	5069	4903	4915	27	0
2	E	405	334	336	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	405	334	336	9	0
3	A	5794	5744	5749	33	0
3	C	5794	5744	5749	34	0
4	A	130	188	0	0	0
4	B	111	147	0	0	0
4	C	130	188	0	0	0
4	D	111	147	0	0	0
5	B	91	129	0	0	0
5	D	91	129	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	36	41	0	0	0
7	C	36	41	0	0	0
All	All	23278	22972	22000	135	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 3.

All (135) 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:413:ASP:OD2	1:B:415:THR:OG1	2.15	0.64
1:D:413:ASP:OD2	1:D:415:THR:OG1	2.15	0.61
3:A:428:ARG:O	1:D:556:LYS:NZ	2.36	0.57
3:A:694:ASP:OD1	3:A:697:ARG:NH1	2.40	0.55
2:E:55:VAL:HG11	2:E:71:MET:HE2	1.88	0.54
1:D:339:ASP:OD1	1:D:340:THR:N	2.40	0.54
2:F:55:VAL:HG11	2:F:71:MET:HE2	1.88	0.54
3:C:694:ASP:OD1	3:C:697:ARG:NH1	2.40	0.54
1:B:339:ASP:OD1	1:B:340:THR:N	2.40	0.54
3:A:343:ILE:HD12	1:D:12:UNK:HA	1.91	0.53
1:B:609:VAL:HB	1:B:610:PRO:HD3	1.91	0.52
3:C:752:MET:O	3:C:753:THR:OG1	2.22	0.52
1:D:609:VAL:HB	1:D:610:PRO:HD3	1.91	0.52
3:A:184:HIS:O	3:A:188:VAL:HG23	2.11	0.51
3:A:722:ASN:O	3:A:725:THR:OG1	2.29	0.51
1:D:628:VAL:HG12	1:D:628:VAL:O	2.10	0.51
3:C:184:HIS:O	3:C:188:VAL:HG23	2.11	0.51
3:C:722:ASN:O	3:C:725:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:LEU:HA	2:E:51:MET:HE2	1.94	0.50
1:B:628:VAL:HG12	1:B:628:VAL:O	2.11	0.50
3:C:164:TYR:CB	3:C:167:LEU:HD23	2.42	0.50
3:A:164:TYR:CB	3:A:167:LEU:HD23	2.41	0.50
3:A:752:MET:O	3:A:753:THR:OG1	2.22	0.49
1:B:12:UNK:HA	3:C:343:ILE:HD12	1.94	0.49
3:A:348:CYS:SG	3:A:849:ARG:NH1	2.86	0.49
3:C:358:THR:HG22	3:C:358:THR:O	2.12	0.49
3:A:358:THR:O	3:A:358:THR:HG22	2.12	0.49
3:C:348:CYS:SG	3:C:849:ARG:NH1	2.86	0.49
1:B:348:ASN:ND2	1:B:350:ASN:OD1	2.45	0.49
3:C:587:GLU:O	3:C:591:LEU:HD23	2.12	0.49
1:D:118:TRP:NE1	1:D:122:TYR:O	2.42	0.49
3:C:199:LEU:HA	3:C:203:VAL:HG12	1.95	0.49
1:B:118:TRP:NE1	1:B:122:TYR:O	2.42	0.48
2:F:48:LEU:HA	2:F:51:MET:HE2	1.94	0.48
1:D:348:ASN:ND2	1:D:350:ASN:OD1	2.45	0.48
3:A:587:GLU:O	3:A:591:LEU:HD23	2.12	0.48
3:C:164:TYR:HB3	3:C:167:LEU:HD23	1.95	0.48
3:A:674:CYS:SG	3:A:684:VAL:HG21	2.54	0.48
3:A:836:SER:O	3:A:844:ARG:NH2	2.46	0.48
3:C:836:SER:O	3:C:844:ARG:NH2	2.46	0.48
1:B:288:ASN:OD1	1:B:289:GLY:N	2.47	0.48
1:D:242:TYR:CE2	1:D:246:LEU:HD11	2.49	0.48
1:B:242:TYR:CE2	1:B:246:LEU:HD11	2.49	0.48
3:C:674:CYS:SG	3:C:684:VAL:HG21	2.54	0.48
1:D:288:ASN:OD1	1:D:289:GLY:N	2.47	0.48
1:B:487:ILE:O	1:B:487:ILE:HG22	2.14	0.48
1:B:335:LEU:CD2	1:B:680:VAL:HG13	2.45	0.47
3:A:164:TYR:HB3	3:A:167:LEU:HD23	1.95	0.47
3:A:199:LEU:HA	3:A:203:VAL:HG12	1.95	0.47
1:B:540:TYR:OH	1:B:580:THR:HG21	2.15	0.47
3:A:388:ASP:HA	3:A:392:ILE:HD12	1.97	0.47
1:D:540:TYR:OH	1:D:580:THR:HG21	2.15	0.47
2:F:24:ASP:OD1	2:F:26:THR:N	2.47	0.47
1:D:335:LEU:CD2	1:D:680:VAL:HG13	2.45	0.47
1:B:451:GLU:O	1:B:455:GLN:NE2	2.49	0.46
3:C:388:ASP:HA	3:C:392:ILE:HD12	1.97	0.45
1:D:487:ILE:HG22	1:D:487:ILE:O	2.14	0.45
3:A:85:ARG:O	3:A:90:MET:HE2	2.17	0.45
1:D:451:GLU:O	1:D:455:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:ILE:O	1:D:456:GLY:N	2.42	0.45
3:C:85:ARG:O	3:C:90:MET:HE2	2.17	0.45
1:B:118:TRP:O	1:B:119:GLN:CB	2.65	0.45
2:E:29:THR:HG22	2:E:52:ILE:CD1	2.47	0.45
1:D:241:ILE:O	1:D:245:LEU:HD23	2.17	0.45
1:D:256:ASP:OD1	1:D:260:ASN:N	2.49	0.44
2:F:27:ILE:HG22	2:F:63:ILE:HG22	1.99	0.44
1:D:118:TRP:O	1:D:119:GLN:CB	2.65	0.44
1:B:241:ILE:O	1:B:245:LEU:HD23	2.17	0.44
1:B:256:ASP:OD1	1:B:260:ASN:N	2.49	0.44
2:E:24:ASP:OD1	2:E:26:THR:N	2.46	0.44
2:E:27:ILE:HG22	2:E:63:ILE:HG22	1.99	0.44
2:F:29:THR:HG22	2:F:52:ILE:CD1	2.47	0.44
2:F:64:ASP:N	2:F:67:GLU:OE1	2.47	0.44
1:D:13:UNK:HA	1:D:166:TYR:CE2	2.53	0.44
1:B:13:UNK:HA	1:B:166:TYR:CE2	2.53	0.43
3:A:92:PRO:N	3:A:93:PRO:CD	2.82	0.43
1:D:264:HIS:O	1:D:268:VAL:HG23	2.18	0.43
3:C:92:PRO:N	3:C:93:PRO:CD	2.82	0.43
3:A:649:THR:O	3:A:651:ASN:ND2	2.45	0.43
3:C:132:LYS:HA	3:C:132:LYS:HE2	2.01	0.43
3:A:367:SER:OG	3:A:370:SER:OG	2.33	0.43
1:D:335:LEU:HD23	1:D:680:VAL:HG13	2.01	0.43
1:B:418:LEU:O	1:B:429:ARG:NH2	2.52	0.43
1:B:494:GLU:O	1:B:498:VAL:HG23	2.19	0.43
3:A:132:LYS:HA	3:A:132:LYS:HE2	2.01	0.43
2:F:29:THR:HG22	2:F:52:ILE:HD13	2.01	0.43
3:A:583:THR:N	3:A:587:GLU:OE1	2.50	0.43
1:B:264:HIS:O	1:B:268:VAL:HG23	2.18	0.43
3:A:628:PRO:O	3:A:631:VAL:HG12	2.19	0.43
1:D:130:LEU:O	1:D:134:LEU:HD13	2.19	0.43
3:C:267:LEU:CD1	3:C:302:VAL:HG11	2.49	0.42
3:A:659:ALA:O	3:A:663:MET:HG3	2.19	0.42
3:C:605:ILE:HG13	3:C:641:LEU:HD11	2.01	0.42
3:A:267:LEU:CD1	3:A:302:VAL:HG11	2.49	0.42
1:D:418:LEU:O	1:D:429:ARG:NH2	2.52	0.42
3:C:659:ALA:O	3:C:663:MET:HG3	2.19	0.42
1:B:130:LEU:O	1:B:134:LEU:HD13	2.19	0.42
1:D:36:LEU:HD22	1:D:45:LEU:HD11	2.01	0.42
1:B:335:LEU:HD23	1:B:680:VAL:HG13	2.01	0.42
1:D:183:LEU:HD23	1:D:183:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ASP:OD1	3:C:223:ARG:NH1	2.53	0.42
3:C:628:PRO:O	3:C:631:VAL:HG12	2.19	0.42
1:B:183:LEU:HD23	1:B:183:LEU:O	2.20	0.42
3:A:578:ARG:NE	3:A:652:GLU:OE1	2.52	0.42
3:A:605:ILE:HG13	3:A:641:LEU:HD11	2.01	0.42
2:F:28:THR:H	2:F:31:GLU:HB2	1.85	0.42
1:D:494:GLU:O	1:D:498:VAL:HG23	2.19	0.42
3:C:649:THR:O	3:C:651:ASN:ND2	2.45	0.42
1:B:36:LEU:HD22	1:B:45:LEU:HD11	2.01	0.41
2:E:29:THR:HG22	2:E:52:ILE:HD13	2.01	0.41
3:C:127:VAL:O	3:C:127:VAL:HG13	2.20	0.41
1:B:524:MET:SD	1:B:625:TYR:CD2	3.13	0.41
1:D:524:MET:SD	1:D:625:TYR:CD2	3.13	0.41
3:C:219:GLN:NE2	3:C:235:GLN:O	2.53	0.41
3:C:260:GLU:OE1	3:C:298:MET:HE2	2.20	0.41
3:C:578:ARG:NE	3:C:652:GLU:OE1	2.52	0.41
2:E:28:THR:H	2:E:31:GLU:HB2	1.85	0.41
3:C:583:THR:N	3:C:587:GLU:OE1	2.50	0.41
3:A:55:ILE:HD12	3:A:160:LEU:HD11	2.01	0.41
3:C:55:ILE:HD12	3:C:160:LEU:HD11	2.01	0.41
1:B:701:TRP:HB3	2:E:71:MET:HE1	2.03	0.41
3:A:267:LEU:HD13	3:A:302:VAL:HG11	2.03	0.41
3:A:175:ASP:OD1	3:A:223:ARG:NH1	2.53	0.41
3:A:260:GLU:OE1	3:A:298:MET:HE2	2.20	0.41
3:C:87:ARG:NH2	3:C:95:ARG:O	2.54	0.41
2:F:69:LEU:C	2:F:69:LEU:HD23	2.46	0.40
3:C:367:SER:OG	3:C:370:SER:OG	2.33	0.40
2:E:64:ASP:OD1	2:E:65:PHE:N	2.51	0.40
3:C:267:LEU:HD13	3:C:302:VAL:HG11	2.03	0.40
1:B:108:LEU:HD13	1:B:167:LEU:HD22	2.03	0.40
3:A:127:VAL:O	3:A:127:VAL:HG13	2.21	0.40
3:A:87:ARG:NH2	3:A:95:ARG:O	2.54	0.40
3:C:91:LEU:HB3	3:C:93:PRO:HD2	2.04	0.40
3:A:812:TRP:O	3:A:816:VAL:HG23	2.22	0.40
3:C:812:TRP:O	3:C:816:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	B	657/984 (67%)	642 (98%)	15 (2%)	0	100	100
1	D	657/984 (67%)	642 (98%)	15 (2%)	0	100	100
2	E	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
2	F	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
3	A	719/907 (79%)	701 (98%)	18 (2%)	0	100	100
3	C	719/907 (79%)	700 (97%)	19 (3%)	0	100	100
All	All	2864/3930 (73%)	2795 (98%)	69 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	B	499/812 (62%)	497 (100%)	2 (0%)	84	94
1	D	499/812 (62%)	497 (100%)	2 (0%)	84	94
2	E	34/62 (55%)	34 (100%)	0	100	100
2	F	34/62 (55%)	34 (100%)	0	100	100
3	A	624/812 (77%)	621 (100%)	3 (0%)	81	93
3	C	624/812 (77%)	621 (100%)	3 (0%)	81	93
All	All	2314/3372 (69%)	2304 (100%)	10 (0%)	81	94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	427	ILE
1	B	459	SER
3	A	610	ARG
3	A	701	ILE
3	A	849	ARG
1	D	427	ILE
1	D	459	SER
3	C	610	ARG
3	C	701	ILE
3	C	849	ARG

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

Mol	Chain	Res	Type
1	B	193	ASN
1	B	430	GLN
3	A	53	HIS
3	A	76	GLN
3	A	88	HIS
3	A	796	ASN
1	D	430	GLN
3	C	53	HIS
3	C	76	GLN
3	C	88	HIS
3	C	796	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 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	LBN	D	1305	-	34,34,51	1.41	3 (8%)	40,42,59	0.97	2 (5%)
4	6OU	D	1304	-	35,35,48	1.10	5 (14%)	38,40,53	1.02	2 (5%)
4	6OU	A	1004	-	41,41,48	0.98	4 (9%)	44,46,53	1.18	3 (6%)
4	6OU	B	1003	-	35,35,48	1.11	5 (14%)	38,40,53	1.02	2 (5%)
7	D39	C	1002	-	34,35,51	1.41	5 (14%)	36,42,58	1.02	2 (5%)
4	6OU	B	1002	-	29,29,48	1.14	4 (13%)	32,34,53	1.10	2 (6%)
4	6OU	C	1004	-	41,41,48	0.98	4 (9%)	44,46,53	1.18	3 (6%)
4	6OU	C	1001	-	45,45,48	0.94	4 (8%)	48,50,53	0.86	2 (4%)
5	LBN	B	1005	-	14,14,51	0.64	0	13,13,59	1.19	1 (7%)
5	LBN	D	1306	-	14,14,51	0.64	0	13,13,59	1.19	1 (7%)
7	D39	A	1002	-	34,35,51	1.40	5 (14%)	36,42,58	1.03	2 (5%)
4	6OU	A	1001	-	45,45,48	0.94	4 (8%)	48,50,53	0.86	2 (4%)
4	6OU	D	1302	-	44,44,48	0.94	4 (9%)	47,49,53	0.89	2 (4%)
5	LBN	D	1301	-	40,40,51	1.28	3 (7%)	43,45,59	1.14	2 (4%)
4	6OU	C	1003	-	41,41,48	0.97	4 (9%)	44,46,53	1.16	4 (9%)
5	LBN	B	1006	-	40,40,51	1.27	3 (7%)	43,45,59	1.14	2 (4%)
4	6OU	D	1303	-	29,29,48	1.14	4 (13%)	32,34,53	1.10	2 (6%)
4	6OU	B	1001	-	44,44,48	0.94	4 (9%)	47,49,53	0.89	2 (4%)
5	LBN	B	1004	-	34,34,51	1.42	3 (8%)	40,42,59	0.97	2 (5%)
4	6OU	A	1003	-	41,41,48	0.98	4 (9%)	44,46,53	1.16	4 (9%)

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	LBN	D	1305	-	-	19/38/38/55	-
4	6OU	D	1304	-	-	16/37/37/52	-
4	6OU	A	1004	-	-	25/45/45/52	-
4	6OU	B	1003	-	-	16/37/37/52	-
7	D39	C	1002	-	-	23/41/41/57	-
4	6OU	B	1002	-	-	12/33/33/52	-
4	6OU	C	1004	-	-	25/45/45/52	-
4	6OU	C	1001	-	-	22/49/49/52	-
5	LBN	B	1005	-	-	8/12/12/55	-
5	LBN	D	1306	-	-	8/12/12/55	-
7	D39	A	1002	-	-	23/41/41/57	-
4	6OU	A	1001	-	-	22/49/49/52	-
4	6OU	D	1302	-	-	17/48/48/52	-
5	LBN	D	1301	-	-	27/44/44/55	-
4	6OU	C	1003	-	-	23/45/45/52	-
5	LBN	B	1006	-	-	27/44/44/55	-
4	6OU	D	1303	-	-	12/33/33/52	-
4	6OU	B	1001	-	-	17/48/48/52	-
5	LBN	B	1004	-	-	19/38/38/55	-
4	6OU	A	1003	-	-	23/45/45/52	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	LBN	P1-O2	5.13	1.79	1.59
5	D	1305	LBN	P1-O2	5.12	1.79	1.59
5	D	1301	LBN	P1-O2	5.11	1.79	1.59
5	B	1006	LBN	P1-O2	5.10	1.79	1.59
7	C	1002	D39	O6-C21	3.95	1.45	1.34
7	A	1002	D39	O6-C21	3.93	1.45	1.34
7	C	1002	D39	O4-C5	3.33	1.43	1.33
7	A	1002	D39	O4-C5	3.31	1.43	1.33
4	D	1304	6OU	P23-O26	2.81	1.65	1.54
4	B	1003	6OU	P23-O26	2.80	1.65	1.54
4	A	1001	6OU	O30-C20	-2.70	1.40	1.46
4	C	1001	6OU	O30-C20	-2.69	1.40	1.46
4	B	1002	6OU	O30-C20	-2.67	1.40	1.46
4	D	1303	6OU	O30-C20	-2.66	1.40	1.46
4	B	1003	6OU	O30-C20	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1004	6OU	O30-C20	-2.65	1.40	1.46
4	D	1304	6OU	O30-C20	-2.64	1.40	1.46
4	A	1003	6OU	O30-C20	-2.64	1.40	1.46
4	C	1003	6OU	O30-C20	-2.63	1.40	1.46
4	A	1004	6OU	O30-C20	-2.62	1.40	1.46
4	D	1302	6OU	O30-C20	-2.58	1.40	1.46
4	B	1001	6OU	O30-C20	-2.55	1.40	1.46
7	C	1002	D39	C6-C5	2.47	1.57	1.50
4	D	1303	6OU	O18-C16	2.46	1.40	1.33
7	A	1002	D39	C6-C5	2.46	1.57	1.50
4	C	1001	6OU	O18-C16	2.46	1.40	1.33
4	B	1003	6OU	O18-C16	2.46	1.40	1.33
4	B	1002	6OU	O18-C16	2.46	1.40	1.33
4	D	1302	6OU	O18-C16	2.45	1.40	1.33
4	A	1004	6OU	O18-C16	2.44	1.40	1.33
4	D	1304	6OU	O18-C16	2.44	1.40	1.33
4	C	1004	6OU	O18-C16	2.44	1.40	1.33
4	C	1003	6OU	O18-C16	2.42	1.40	1.33
4	A	1003	6OU	O18-C16	2.42	1.40	1.33
4	A	1001	6OU	O18-C16	2.42	1.40	1.33
4	B	1001	6OU	O18-C16	2.41	1.40	1.33
7	C	1002	D39	C22-C21	2.31	1.57	1.50
7	A	1002	D39	C22-C21	2.26	1.57	1.50
5	D	1301	LBN	P1-O1	2.21	1.68	1.59
5	B	1004	LBN	O2-C9	-2.20	1.36	1.44
5	D	1301	LBN	C1-C2	2.20	1.57	1.50
5	D	1305	LBN	O2-C9	-2.19	1.36	1.44
5	B	1006	LBN	P1-O1	2.18	1.67	1.59
5	B	1006	LBN	C1-C2	2.18	1.57	1.50
4	A	1003	6OU	O18-C19	-2.18	1.40	1.45
4	C	1001	6OU	O18-C19	-2.17	1.40	1.45
4	A	1001	6OU	O18-C19	-2.16	1.40	1.45
5	B	1004	LBN	P1-O1	2.16	1.67	1.59
4	B	1002	6OU	O30-C31	2.15	1.40	1.34
4	D	1304	6OU	O18-C19	-2.15	1.40	1.45
4	C	1003	6OU	O18-C19	-2.15	1.40	1.45
4	A	1001	6OU	O30-C31	2.15	1.40	1.34
4	D	1303	6OU	O18-C19	-2.15	1.40	1.45
4	B	1001	6OU	O18-C19	-2.15	1.40	1.45
4	B	1003	6OU	O18-C19	-2.15	1.40	1.45
4	D	1302	6OU	O30-C31	2.14	1.40	1.34
5	D	1305	LBN	P1-O1	2.14	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	6OU	O18-C19	-2.14	1.40	1.45
4	B	1001	6OU	O30-C31	2.14	1.40	1.34
4	D	1302	6OU	O18-C19	-2.14	1.40	1.45
4	C	1001	6OU	O30-C31	2.13	1.40	1.34
4	B	1003	6OU	O30-C31	2.13	1.40	1.34
4	D	1303	6OU	O30-C31	2.13	1.40	1.34
4	C	1003	6OU	O30-C31	2.12	1.40	1.34
4	C	1004	6OU	O18-C19	-2.12	1.40	1.45
4	A	1004	6OU	O30-C31	2.11	1.40	1.34
4	D	1304	6OU	O30-C31	2.11	1.40	1.34
4	A	1004	6OU	O18-C19	-2.10	1.40	1.45
4	A	1003	6OU	O30-C31	2.10	1.40	1.34
4	C	1004	6OU	O30-C31	2.09	1.40	1.34
7	C	1002	D39	P-O3	2.05	1.67	1.59
7	A	1002	D39	P-O3	2.02	1.67	1.59

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1003	6OU	C12-C11-C10	4.45	136.85	114.37
4	A	1003	6OU	C12-C11-C10	4.45	136.84	114.37
5	D	1301	LBN	C8-C5-C42	4.38	157.64	124.83
5	B	1006	LBN	C8-C5-C42	4.37	157.60	124.83
4	A	1004	6OU	C12-C11-C10	4.30	136.09	114.37
4	C	1004	6OU	C12-C11-C10	4.29	136.08	114.37
4	D	1303	6OU	O30-C31-C33	4.08	120.30	111.48
4	B	1002	6OU	O30-C31-C33	4.07	120.28	111.48
4	C	1004	6OU	O30-C31-C33	4.03	120.20	111.48
4	A	1004	6OU	O30-C31-C33	4.02	120.17	111.48
5	B	1005	LBN	C11-C8-C5	4.01	135.08	112.60
5	D	1306	LBN	C11-C8-C5	4.01	135.04	112.60
4	D	1304	6OU	O30-C31-C33	3.93	119.99	111.48
4	B	1003	6OU	O30-C31-C33	3.93	119.98	111.48
7	A	1002	D39	O6-C21-C22	3.75	119.59	111.48
7	C	1002	D39	O6-C21-C22	3.73	119.55	111.48
4	A	1001	6OU	O30-C31-C33	3.73	119.54	111.48
4	C	1001	6OU	O30-C31-C33	3.71	119.50	111.48
4	A	1003	6OU	O30-C31-C33	3.68	119.44	111.48
4	C	1003	6OU	O30-C31-C33	3.67	119.43	111.48
4	B	1001	6OU	O30-C31-C33	3.58	119.23	111.48
4	D	1302	6OU	O30-C31-C33	3.58	119.22	111.48
5	D	1301	LBN	O3-P1-O4	3.46	128.55	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	LBN	O3-P1-O4	3.46	128.53	112.44
5	B	1006	LBN	O3-P1-O4	3.46	128.52	112.44
5	D	1305	LBN	O3-P1-O4	3.45	128.48	112.44
4	C	1004	6OU	O18-C16-C15	2.83	120.47	111.83
4	A	1004	6OU	O18-C16-C15	2.83	120.45	111.83
4	D	1303	6OU	O18-C16-C15	2.73	120.17	111.83
4	B	1002	6OU	O18-C16-C15	2.73	120.17	111.83
4	D	1302	6OU	O18-C16-C15	2.72	120.11	111.83
4	B	1001	6OU	O18-C16-C15	2.71	120.10	111.83
4	C	1003	6OU	O18-C16-C15	2.70	120.08	111.83
4	A	1003	6OU	O18-C16-C15	2.70	120.06	111.83
7	A	1002	D39	O4-C5-C6	2.65	119.92	111.83
7	C	1002	D39	O4-C5-C6	2.64	119.90	111.83
4	C	1001	6OU	O18-C16-C15	2.59	119.72	111.83
4	A	1001	6OU	O18-C16-C15	2.59	119.72	111.83
4	D	1304	6OU	O18-C16-C15	2.55	119.61	111.83
4	B	1003	6OU	O18-C16-C15	2.52	119.53	111.83
5	D	1305	LBN	O2-P1-O4	-2.49	99.07	108.94
5	B	1004	LBN	O2-P1-O4	-2.49	99.08	108.94
4	C	1003	6OU	C20-O30-C31	-2.05	112.90	117.80
4	A	1003	6OU	C20-O30-C31	-2.03	112.94	117.80

There are no chirality outliers.

All (384) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1002	6OU	O26-C27-C28-N29
4	B	1002	6OU	O32-C31-O30-C20
4	B	1002	6OU	C33-C31-O30-C20
4	B	1003	6OU	C21-O22-P23-O24
4	B	1003	6OU	C33-C31-O30-C20
4	A	1001	6OU	O30-C20-C21-O22
4	A	1001	6OU	C21-O22-P23-O24
4	A	1001	6OU	C21-O22-P23-O25
4	A	1001	6OU	C21-O22-P23-O26
4	A	1001	6OU	O26-C27-C28-N29
4	A	1001	6OU	C33-C31-O30-C20
4	A	1003	6OU	C21-O22-P23-O24
4	A	1003	6OU	C21-O22-P23-O26
4	A	1003	6OU	C27-O26-P23-O22
4	A	1003	6OU	O32-C31-O30-C20
4	A	1003	6OU	C33-C31-O30-C20

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Mol	Chain	Res	Type	Atoms
4	A	1004	6OU	O30-C20-C21-O22
4	A	1004	6OU	C27-O26-P23-O22
4	A	1004	6OU	C27-O26-P23-O24
4	A	1004	6OU	C27-O26-P23-O25
4	A	1004	6OU	O26-C27-C28-N29
4	D	1303	6OU	O26-C27-C28-N29
4	D	1303	6OU	O32-C31-O30-C20
4	D	1303	6OU	C33-C31-O30-C20
4	D	1304	6OU	C21-O22-P23-O24
4	D	1304	6OU	C33-C31-O30-C20
4	C	1001	6OU	O30-C20-C21-O22
4	C	1001	6OU	C21-O22-P23-O24
4	C	1001	6OU	C21-O22-P23-O25
4	C	1001	6OU	C21-O22-P23-O26
4	C	1001	6OU	O26-C27-C28-N29
4	C	1001	6OU	C33-C31-O30-C20
4	C	1003	6OU	C21-O22-P23-O24
4	C	1003	6OU	C21-O22-P23-O26
4	C	1003	6OU	C27-O26-P23-O22
4	C	1003	6OU	O32-C31-O30-C20
4	C	1003	6OU	C33-C31-O30-C20
4	C	1004	6OU	O30-C20-C21-O22
4	C	1004	6OU	C27-O26-P23-O22
4	C	1004	6OU	C27-O26-P23-O24
4	C	1004	6OU	C27-O26-P23-O25
4	C	1004	6OU	O26-C27-C28-N29
5	B	1004	LBN	C9-O2-P1-O1
5	B	1004	LBN	C9-O2-P1-O3
5	B	1004	LBN	C9-O2-P1-O4
5	B	1004	LBN	N1-C6-C9-O2
5	B	1006	LBN	C1-O1-P1-O2
5	B	1006	LBN	C1-O1-P1-O3
5	B	1006	LBN	O7-C2-C3-O5
5	D	1301	LBN	C1-O1-P1-O2
5	D	1301	LBN	C1-O1-P1-O3
5	D	1301	LBN	O7-C2-C3-O5
5	D	1305	LBN	C9-O2-P1-O1
5	D	1305	LBN	C9-O2-P1-O3
5	D	1305	LBN	C9-O2-P1-O4
5	D	1305	LBN	N1-C6-C9-O2
7	A	1002	D39	O6-C3-C4-O4
7	A	1002	D39	N-C-C1-O

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Mol	Chain	Res	Type	Atoms
7	A	1002	D39	C39-C-C1-O
7	A	1002	D39	C-C1-O-P
7	A	1002	D39	C1-O-P-O3
7	C	1002	D39	O6-C3-C4-O4
7	C	1002	D39	N-C-C1-O
7	C	1002	D39	C39-C-C1-O
7	C	1002	D39	C-C1-O-P
7	C	1002	D39	C1-O-P-O3
4	B	1003	6OU	O17-C16-O18-C19
4	D	1304	6OU	O17-C16-O18-C19
5	B	1004	LBN	O6-C25-O5-C3
5	D	1305	LBN	O6-C25-O5-C3
4	A	1001	6OU	O32-C31-O30-C20
4	C	1001	6OU	O32-C31-O30-C20
4	B	1003	6OU	C15-C16-O18-C19
4	D	1304	6OU	C15-C16-O18-C19
4	A	1003	6OU	C15-C16-O18-C19
4	C	1003	6OU	C15-C16-O18-C19
5	B	1004	LBN	C26-C25-O5-C3
4	A	1003	6OU	O17-C16-O18-C19
4	C	1003	6OU	O17-C16-O18-C19
4	B	1003	6OU	O32-C31-O30-C20
4	D	1304	6OU	O32-C31-O30-C20
5	D	1305	LBN	C26-C25-O5-C3
4	A	1004	6OU	C33-C31-O30-C20
4	C	1004	6OU	C33-C31-O30-C20
4	A	1004	6OU	O32-C31-O30-C20
4	C	1004	6OU	O32-C31-O30-C20
4	A	1001	6OU	C20-C21-O22-P23
4	C	1001	6OU	C20-C21-O22-P23
7	A	1002	D39	N-C-C39-O8
7	C	1002	D39	N-C-C39-O8
7	A	1002	D39	C5-C6-C7-C8
7	C	1002	D39	C5-C6-C7-C8
5	B	1006	LBN	C35-C34-O7-C2
5	D	1301	LBN	C35-C34-O7-C2
4	B	1001	6OU	C15-C16-O18-C19
4	D	1302	6OU	C15-C16-O18-C19
5	B	1006	LBN	O8-C34-O7-C2
5	D	1301	LBN	O8-C34-O7-C2
5	D	1301	LBN	C34-C35-C36-C37
4	B	1001	6OU	O17-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
4	D	1302	6OU	O17-C16-O18-C19
5	B	1006	LBN	C34-C35-C36-C37
4	B	1001	6OU	C31-C33-C34-C35
4	D	1302	6OU	C31-C33-C34-C35
4	B	1001	6OU	C45-C46-C47-C48
4	D	1302	6OU	C45-C46-C47-C48
7	A	1002	D39	C23-C24-C25-C26
7	C	1002	D39	C23-C24-C25-C26
4	A	1003	6OU	C06-C07-C08-C09
4	C	1003	6OU	C06-C07-C08-C09
4	A	1001	6OU	C42-C43-C44-C45
4	C	1001	6OU	C42-C43-C44-C45
4	A	1003	6OU	C03-C04-C05-C06
4	C	1003	6OU	C03-C04-C05-C06
4	B	1003	6OU	C13-C14-C15-C16
4	B	1003	6OU	C31-C33-C34-C35
4	D	1304	6OU	C13-C14-C15-C16
4	D	1304	6OU	C31-C33-C34-C35
4	C	1003	6OU	C12-C13-C14-C15
4	A	1003	6OU	C12-C13-C14-C15
4	B	1001	6OU	C36-C37-C38-C39
4	D	1302	6OU	C36-C37-C38-C39
7	A	1002	D39	C25-C26-C27-C28
7	A	1002	D39	C22-C21-O6-C3
7	C	1002	D39	C22-C21-O6-C3
7	C	1002	D39	C25-C26-C27-C28
4	A	1003	6OU	C35-C36-C37-C38
4	C	1003	6OU	C35-C36-C37-C38
5	D	1301	LBN	C38-C39-C40-C41
4	A	1001	6OU	C12-C13-C14-C15
4	A	1001	6OU	C33-C34-C35-C36
4	C	1001	6OU	C12-C13-C14-C15
4	C	1001	6OU	C33-C34-C35-C36
5	B	1006	LBN	C38-C39-C40-C41
4	B	1001	6OU	C33-C31-O30-C20
4	D	1302	6OU	C33-C31-O30-C20
4	B	1001	6OU	C37-C38-C39-C40
4	D	1302	6OU	C37-C38-C39-C40
5	B	1005	LBN	C39-C40-C41-C42
5	D	1306	LBN	C39-C40-C41-C42
5	B	1006	LBN	C29-C30-C31-C32
5	D	1301	LBN	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
5	B	1004	LBN	C38-C39-C40-C41
5	D	1305	LBN	C38-C39-C40-C41
4	A	1001	6OU	C37-C38-C39-C40
4	C	1001	6OU	C37-C38-C39-C40
5	B	1006	LBN	C39-C40-C41-C42
5	D	1301	LBN	C39-C40-C41-C42
4	B	1002	6OU	C35-C36-C37-C38
4	D	1303	6OU	C35-C36-C37-C38
5	B	1004	LBN	C35-C34-O7-C2
5	D	1305	LBN	C35-C34-O7-C2
4	A	1004	6OU	C05-C06-C07-C08
4	C	1004	6OU	C05-C06-C07-C08
5	D	1301	LBN	C26-C27-C28-C29
5	B	1006	LBN	C26-C27-C28-C29
4	A	1001	6OU	C41-C42-C43-C44
4	C	1001	6OU	C41-C42-C43-C44
5	B	1004	LBN	C39-C40-C41-C42
5	B	1006	LBN	C14-C11-C8-C5
5	D	1301	LBN	C14-C11-C8-C5
5	D	1305	LBN	C39-C40-C41-C42
4	A	1004	6OU	C19-C20-C21-O22
4	C	1004	6OU	C19-C20-C21-O22
5	B	1006	LBN	O1-C1-C2-C3
5	D	1301	LBN	O1-C1-C2-C3
4	D	1302	6OU	O32-C31-O30-C20
4	C	1004	6OU	C04-C05-C06-C07
4	A	1004	6OU	C31-C33-C34-C35
4	C	1004	6OU	C31-C33-C34-C35
4	A	1004	6OU	C04-C05-C06-C07
4	B	1001	6OU	O32-C31-O30-C20
7	A	1002	D39	O7-C21-O6-C3
7	C	1002	D39	O7-C21-O6-C3
5	B	1004	LBN	C34-C35-C36-C37
5	D	1305	LBN	C34-C35-C36-C37
4	B	1002	6OU	O18-C19-C20-C21
4	D	1303	6OU	O18-C19-C20-C21
5	B	1006	LBN	C1-C2-C3-O5
5	D	1301	LBN	C1-C2-C3-O5
4	B	1001	6OU	C07-C08-C09-C10
4	D	1302	6OU	C07-C08-C09-C10
5	B	1005	LBN	C14-C11-C8-C5
5	D	1306	LBN	C14-C11-C8-C5

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Mol	Chain	Res	Type	Atoms
4	A	1003	6OU	C08-C09-C10-C11
4	C	1003	6OU	C08-C09-C10-C11
4	A	1001	6OU	C02-C03-C04-C05
4	C	1001	6OU	C02-C03-C04-C05
4	C	1004	6OU	C13-C14-C15-C16
4	A	1003	6OU	C04-C05-C06-C07
4	A	1004	6OU	C09-C10-C11-C12
4	C	1003	6OU	C04-C05-C06-C07
4	C	1004	6OU	C09-C10-C11-C12
4	A	1004	6OU	C36-C37-C38-C39
4	C	1004	6OU	C36-C37-C38-C39
4	A	1004	6OU	C13-C14-C15-C16
5	B	1006	LBN	C27-C28-C29-C30
5	D	1301	LBN	C27-C28-C29-C30
4	A	1004	6OU	C06-C07-C08-C09
4	A	1004	6OU	C35-C36-C37-C38
4	C	1004	6OU	C35-C36-C37-C38
4	C	1004	6OU	C06-C07-C08-C09
5	D	1301	LBN	C35-C36-C37-C38
5	B	1006	LBN	C35-C36-C37-C38
4	B	1003	6OU	C35-C36-C37-C38
4	D	1304	6OU	C35-C36-C37-C38
4	B	1001	6OU	C41-C42-C43-C44
4	D	1302	6OU	C41-C42-C43-C44
4	B	1002	6OU	C15-C16-O18-C19
4	D	1303	6OU	C15-C16-O18-C19
5	B	1005	LBN	C34-C35-C36-C37
5	D	1306	LBN	C34-C35-C36-C37
4	B	1003	6OU	C19-C20-C21-O22
4	A	1001	6OU	C19-C20-C21-O22
4	D	1304	6OU	C19-C20-C21-O22
4	C	1001	6OU	C19-C20-C21-O22
4	A	1001	6OU	C35-C36-C37-C38
4	C	1001	6OU	C35-C36-C37-C38
4	A	1004	6OU	C12-C13-C14-C15
4	C	1004	6OU	C12-C13-C14-C15
4	B	1001	6OU	O18-C19-C20-C21
4	D	1302	6OU	O18-C19-C20-C21
7	A	1002	D39	N-C-C39-O9
7	C	1002	D39	N-C-C39-O9
5	B	1006	LBN	O1-C1-C2-O7
5	D	1301	LBN	O1-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
4	C	1003	6OU	C05-C06-C07-C08
4	A	1003	6OU	C05-C06-C07-C08
5	D	1301	LBN	C31-C32-C33-C4
5	B	1006	LBN	C31-C32-C33-C4
5	B	1006	LBN	C37-C38-C39-C40
5	D	1301	LBN	C37-C38-C39-C40
4	B	1002	6OU	C37-C38-C39-C40
4	B	1001	6OU	C09-C10-C11-C12
4	D	1302	6OU	C09-C10-C11-C12
4	D	1303	6OU	C37-C38-C39-C40
5	B	1004	LBN	O1-C1-C2-C3
5	D	1305	LBN	O1-C1-C2-C3
4	A	1004	6OU	C34-C35-C36-C37
4	C	1004	6OU	C34-C35-C36-C37
4	B	1003	6OU	C21-O22-P23-O25
4	D	1304	6OU	C21-O22-P23-O25
4	B	1002	6OU	O17-C16-O18-C19
4	D	1303	6OU	O17-C16-O18-C19
7	A	1002	D39	C6-C5-O4-C4
7	C	1002	D39	C6-C5-O4-C4
5	B	1004	LBN	O8-C34-O7-C2
5	D	1305	LBN	O8-C34-O7-C2
5	B	1004	LBN	O1-C1-C2-O7
5	D	1305	LBN	O1-C1-C2-O7
7	A	1002	D39	C2-C3-C4-O4
7	C	1002	D39	C2-C3-C4-O4
5	B	1006	LBN	C28-C29-C30-C31
5	D	1301	LBN	C28-C29-C30-C31
4	D	1304	6OU	C42-C43-C44-C45
4	B	1003	6OU	C42-C43-C44-C45
4	B	1001	6OU	O18-C19-C20-O30
4	B	1002	6OU	O18-C19-C20-O30
4	A	1003	6OU	O18-C19-C20-O30
4	D	1302	6OU	O18-C19-C20-O30
4	D	1303	6OU	O18-C19-C20-O30
4	C	1003	6OU	O18-C19-C20-O30
5	D	1301	LBN	C33-C4-C7-C10
5	B	1006	LBN	C33-C4-C7-C10
5	B	1004	LBN	C37-C38-C39-C40
4	D	1303	6OU	C33-C34-C35-C36
5	D	1305	LBN	C37-C38-C39-C40
4	B	1002	6OU	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	D	1302	6OU	C43-C44-C45-C46
4	B	1002	6OU	C12-C13-C14-C15
5	B	1006	LBN	C32-C33-C4-C7
4	B	1001	6OU	C43-C44-C45-C46
4	D	1303	6OU	C12-C13-C14-C15
5	D	1301	LBN	C32-C33-C4-C7
4	A	1004	6OU	C07-C08-C09-C10
4	C	1004	6OU	C07-C08-C09-C10
5	B	1006	LBN	C30-C31-C32-C33
5	D	1301	LBN	C30-C31-C32-C33
4	B	1003	6OU	O30-C20-C21-O22
4	D	1304	6OU	O30-C20-C21-O22
4	A	1004	6OU	C01-C02-C03-C04
4	C	1004	6OU	C01-C02-C03-C04
4	A	1003	6OU	C09-C10-C11-C12
4	C	1003	6OU	C09-C10-C11-C12
5	D	1305	LBN	C25-C26-C27-C28
7	A	1002	D39	O5-C5-O4-C4
7	C	1002	D39	O5-C5-O4-C4
5	B	1004	LBN	C25-C26-C27-C28
4	A	1001	6OU	C40-C41-C42-C43
4	C	1001	6OU	C40-C41-C42-C43
4	A	1001	6OU	C27-O26-P23-O25
4	A	1003	6OU	C27-O26-P23-O24
4	C	1001	6OU	C27-O26-P23-O25
4	C	1003	6OU	C27-O26-P23-O24
5	B	1004	LBN	C1-O1-P1-O4
5	B	1006	LBN	C9-O2-P1-O4
5	D	1301	LBN	C9-O2-P1-O4
5	D	1305	LBN	C1-O1-P1-O4
7	A	1002	D39	C1-O-P-O1
7	A	1002	D39	C1-O-P-O2
7	C	1002	D39	C1-O-P-O1
7	C	1002	D39	C1-O-P-O2
4	A	1003	6OU	C34-C35-C36-C37
4	B	1001	6OU	C19-C20-O30-C31
4	D	1302	6OU	C19-C20-O30-C31
4	C	1003	6OU	C34-C35-C36-C37
4	C	1004	6OU	C08-C09-C10-C11
7	A	1002	D39	C27-C28-C29-C30
7	C	1002	D39	C27-C28-C29-C30
4	A	1004	6OU	C08-C09-C10-C11

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Mol	Chain	Res	Type	Atoms
5	D	1306	LBN	C8-C11-C14-C17
5	B	1005	LBN	C8-C11-C14-C17
4	B	1001	6OU	C34-C35-C36-C37
4	D	1302	6OU	C34-C35-C36-C37
4	C	1001	6OU	C07-C08-C09-C10
4	A	1001	6OU	C07-C08-C09-C10
4	A	1001	6OU	O18-C19-C20-O30
4	C	1001	6OU	O18-C19-C20-O30
4	B	1001	6OU	C42-C43-C44-C45
4	D	1302	6OU	C42-C43-C44-C45
4	A	1001	6OU	C11-C12-C13-C14
4	C	1001	6OU	C11-C12-C13-C14
4	C	1003	6OU	C31-C33-C34-C35
4	A	1003	6OU	C31-C33-C34-C35
5	B	1006	LBN	C13-C10-C7-C4
5	D	1301	LBN	C13-C10-C7-C4
7	A	1002	D39	C21-C22-C23-C24
7	C	1002	D39	C21-C22-C23-C24
4	A	1003	6OU	O30-C20-C21-O22
4	C	1003	6OU	O30-C20-C21-O22
5	B	1004	LBN	C35-C36-C37-C38
5	D	1305	LBN	C35-C36-C37-C38
4	B	1003	6OU	C40-C41-C42-C43
4	D	1304	6OU	C40-C41-C42-C43
4	A	1001	6OU	C04-C05-C06-C07
7	A	1002	D39	O3-C2-C3-C4
7	C	1002	D39	O3-C2-C3-C4
4	C	1001	6OU	C04-C05-C06-C07
5	B	1006	LBN	C40-C41-C42-C5
5	D	1301	LBN	C40-C41-C42-C5
4	C	1004	6OU	C10-C11-C12-C13
4	A	1004	6OU	C10-C11-C12-C13
4	C	1004	6OU	C33-C34-C35-C36
4	A	1004	6OU	C33-C34-C35-C36
5	D	1306	LBN	C35-C36-C37-C38
4	A	1003	6OU	C38-C39-C40-C41
4	C	1003	6OU	C38-C39-C40-C41
5	B	1006	LBN	C42-C5-C8-C11
5	D	1301	LBN	C42-C5-C8-C11
5	B	1005	LBN	C35-C36-C37-C38
5	B	1005	LBN	C42-C5-C8-C11
5	B	1005	LBN	C40-C41-C42-C5

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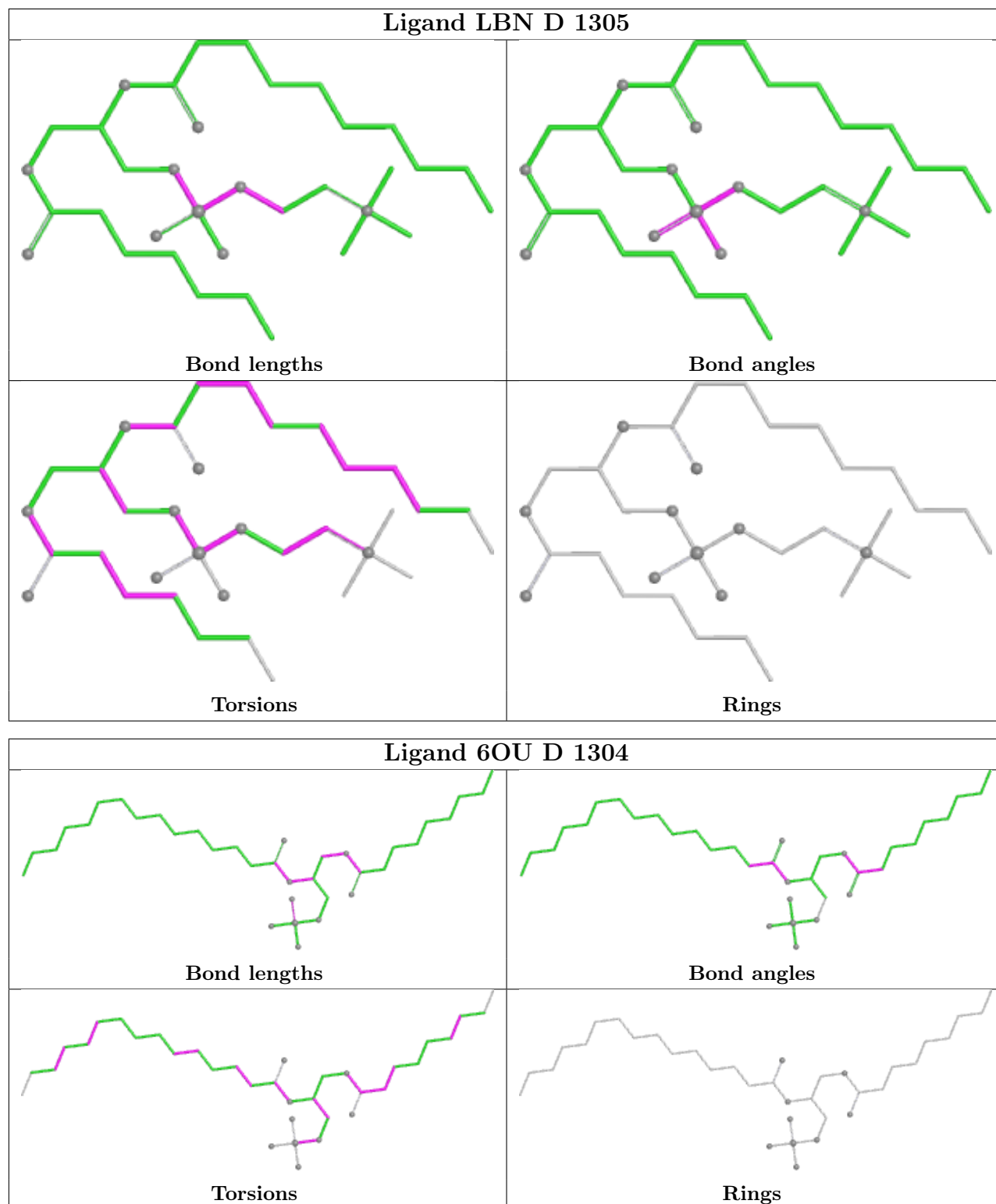
Mol	Chain	Res	Type	Atoms
5	D	1306	LBN	C40-C41-C42-C5
5	B	1004	LBN	C9-C6-N1-C12
5	D	1305	LBN	C9-C6-N1-C12
4	A	1004	6OU	C14-C15-C16-O18
4	C	1004	6OU	C14-C15-C16-O18
5	D	1306	LBN	C42-C5-C8-C11
7	A	1002	D39	O6-C21-C22-C23
7	A	1002	D39	C7-C8-C9-C10
7	C	1002	D39	C7-C8-C9-C10
7	C	1002	D39	O6-C21-C22-C23
4	B	1003	6OU	C09-C10-C11-C12
4	D	1304	6OU	C09-C10-C11-C12
5	B	1005	LBN	C36-C37-C38-C39
5	D	1306	LBN	C36-C37-C38-C39
4	A	1003	6OU	O18-C19-C20-C21
4	C	1003	6OU	O18-C19-C20-C21
4	B	1003	6OU	C14-C15-C16-O18
4	D	1304	6OU	C14-C15-C16-O18
7	A	1002	D39	O7-C21-C22-C23
7	C	1002	D39	O7-C21-C22-C23
4	B	1002	6OU	C14-C15-C16-O18
4	D	1303	6OU	C14-C15-C16-O18
4	C	1004	6OU	C14-C15-C16-O17
4	A	1004	6OU	C14-C15-C16-O17
4	B	1003	6OU	C14-C15-C16-O17
4	D	1304	6OU	C14-C15-C16-O17
4	A	1003	6OU	C19-C20-C21-O22
4	C	1003	6OU	C19-C20-C21-O22
5	B	1004	LBN	C26-C27-C28-C29
5	D	1305	LBN	C26-C27-C28-C29
5	B	1006	LBN	O5-C25-C26-C27
5	D	1301	LBN	O5-C25-C26-C27

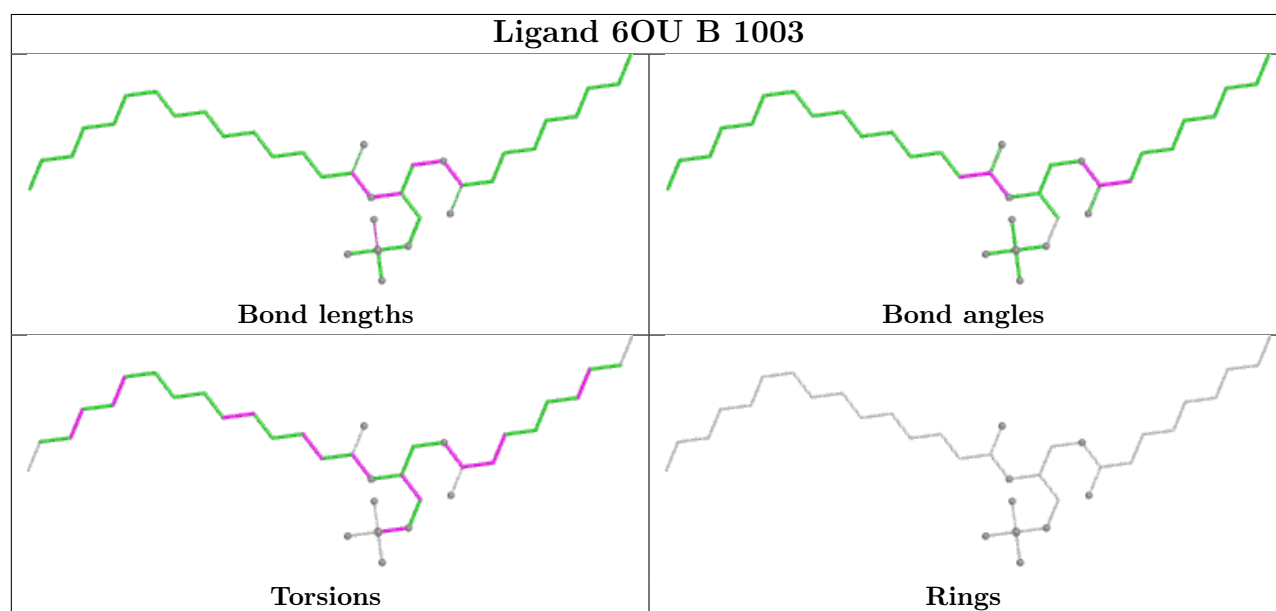
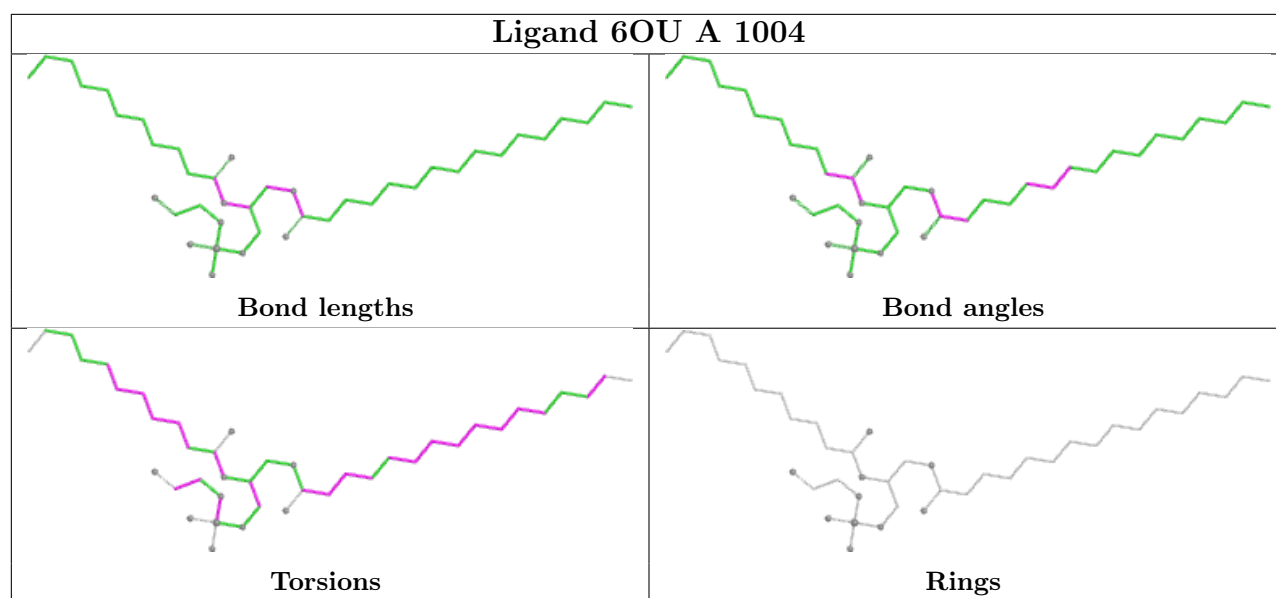
There are no ring outliers.

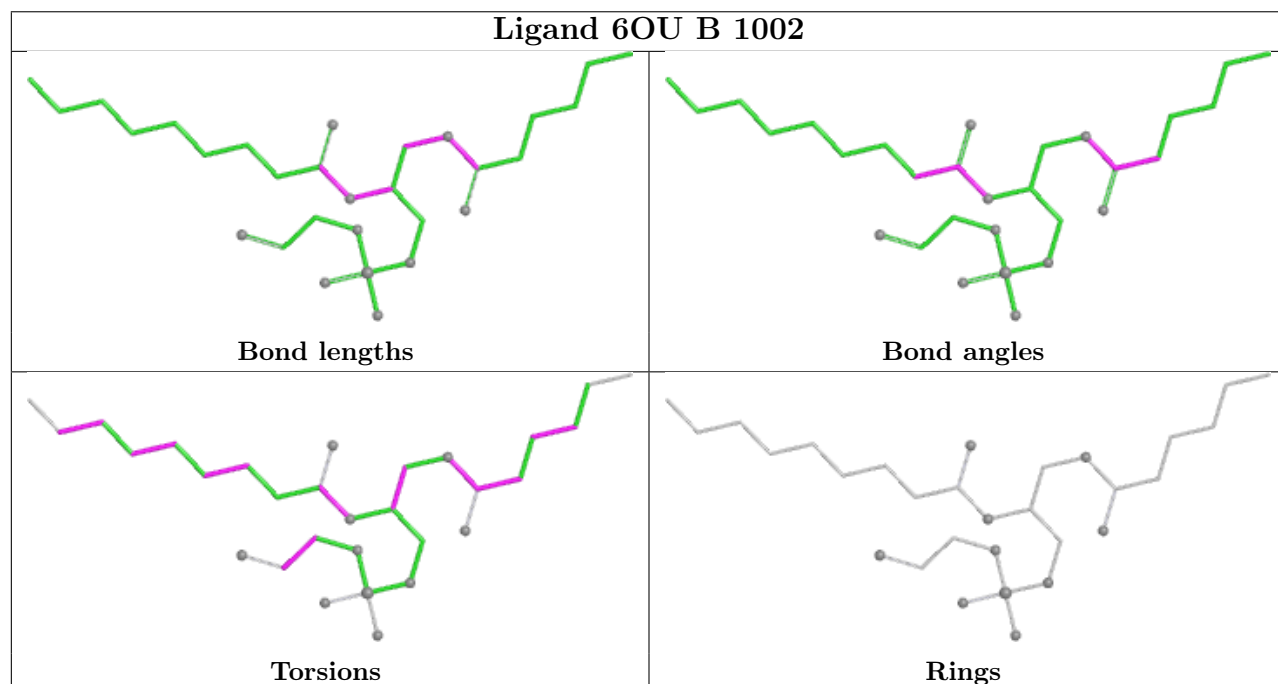
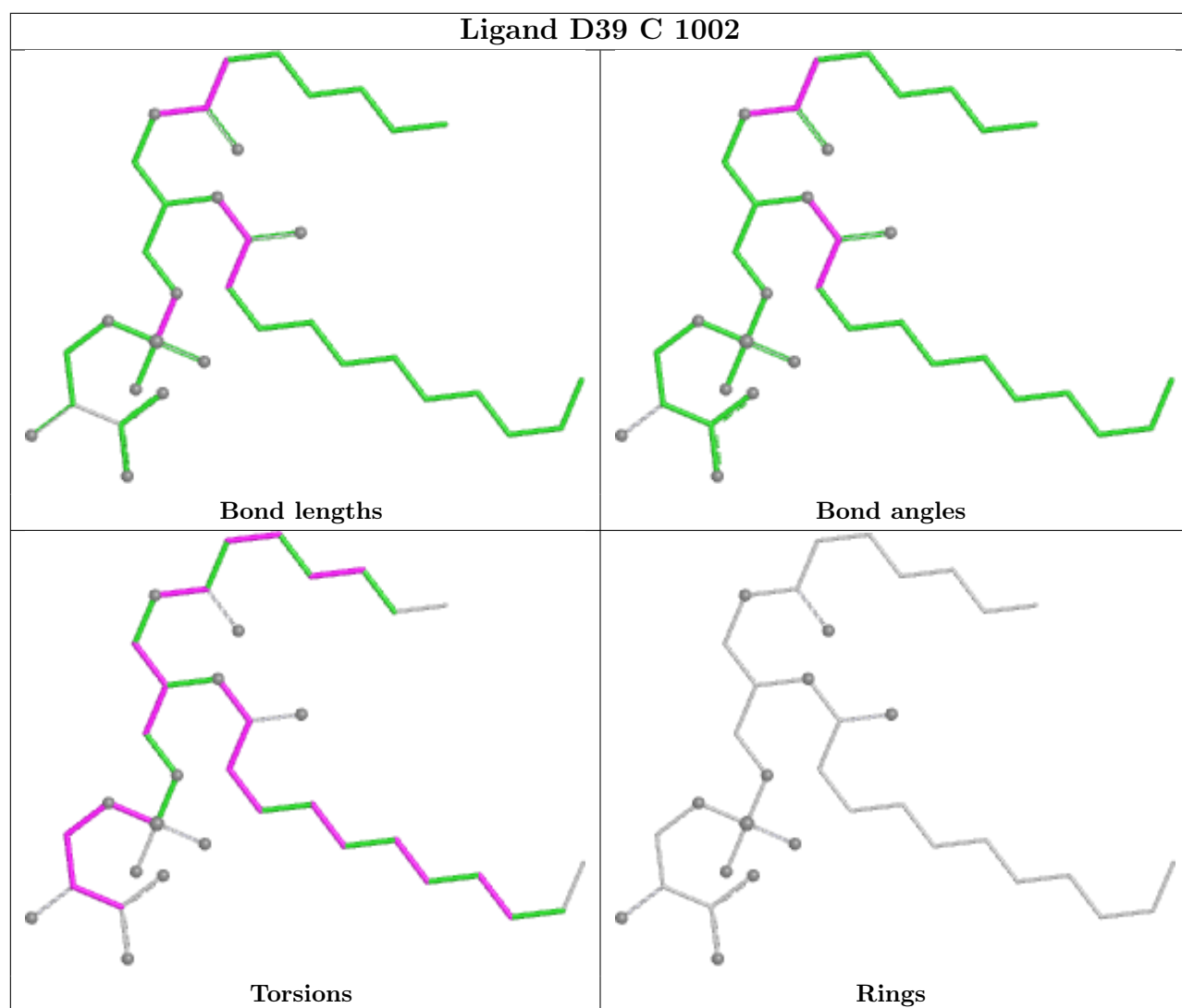
No monomer is involved in short contacts.

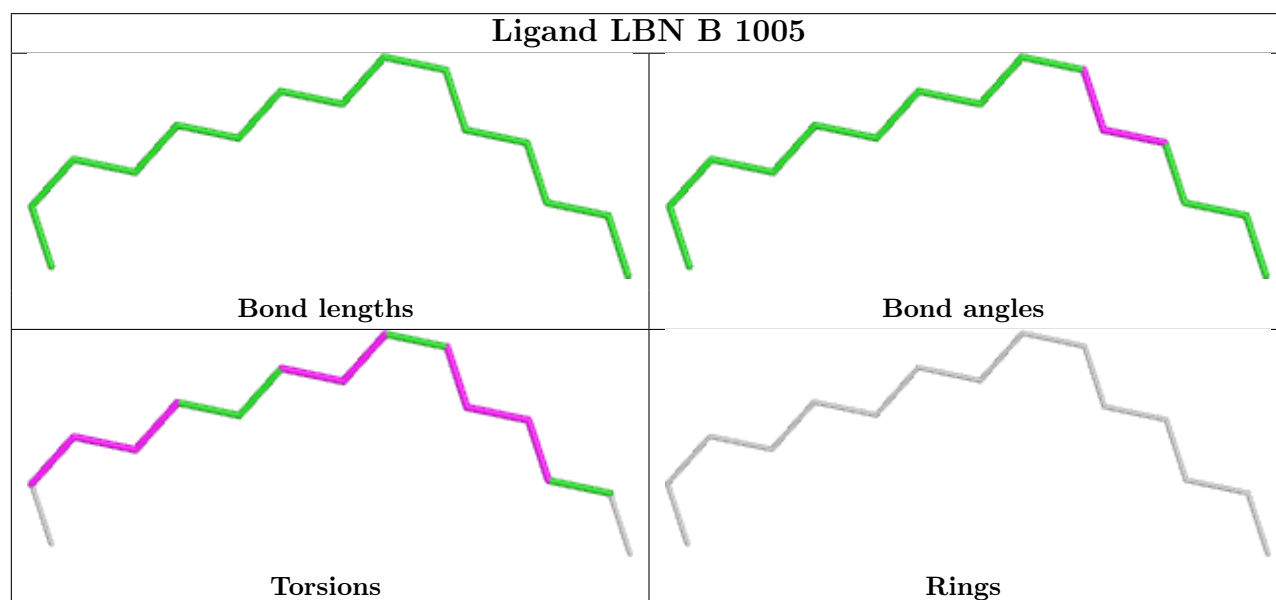
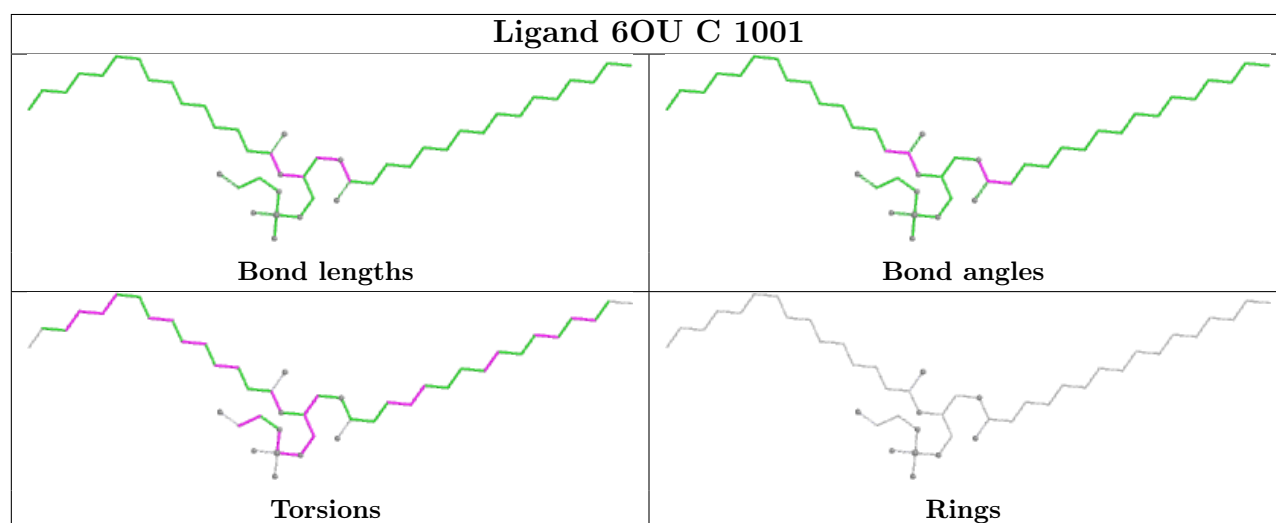
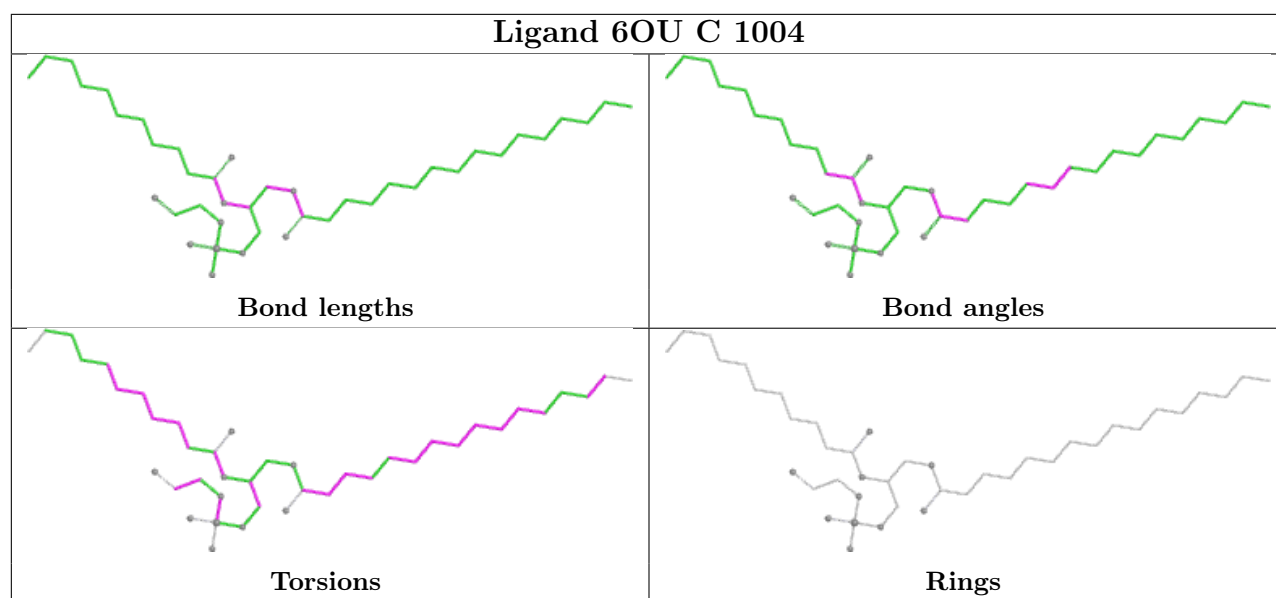
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

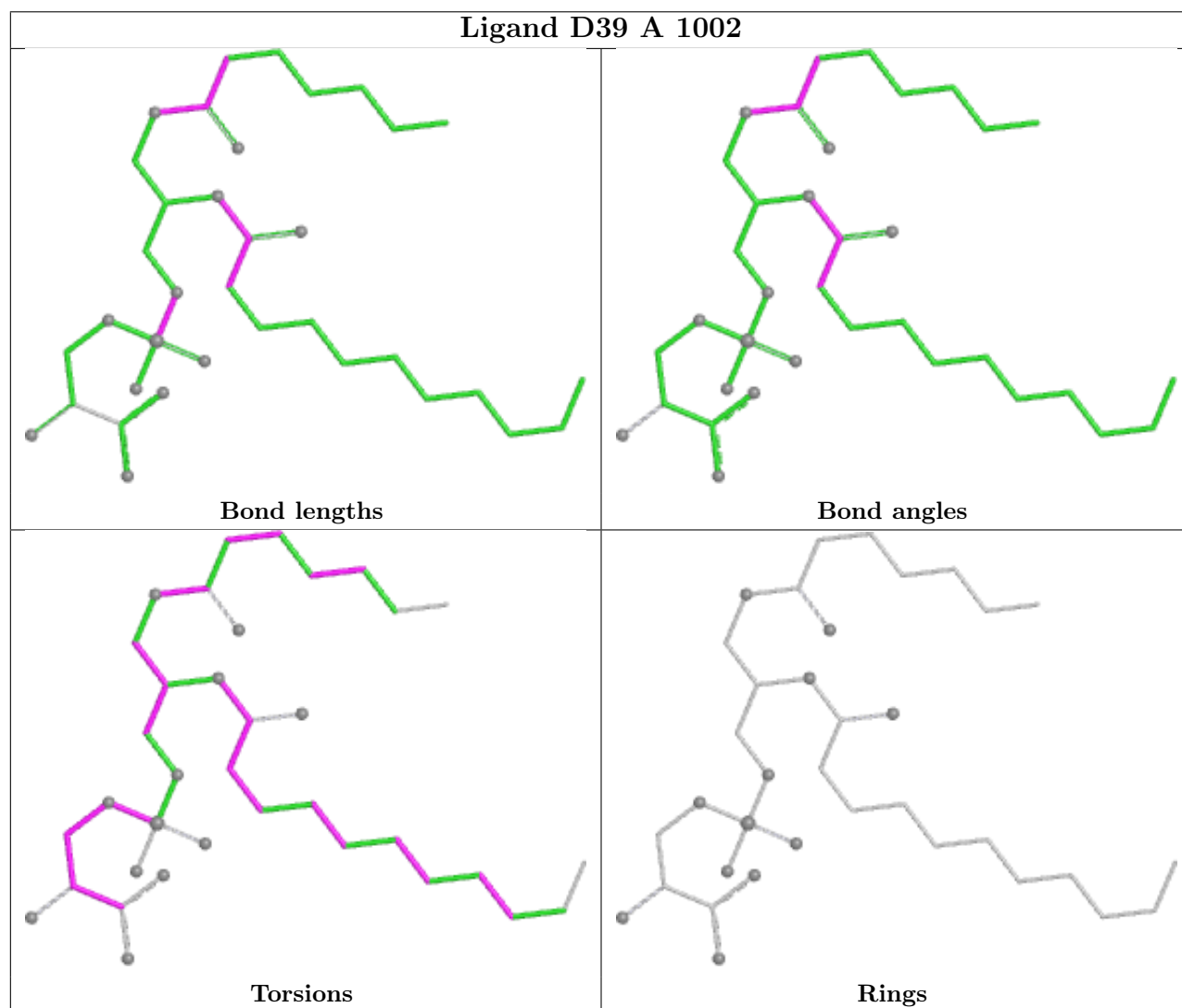
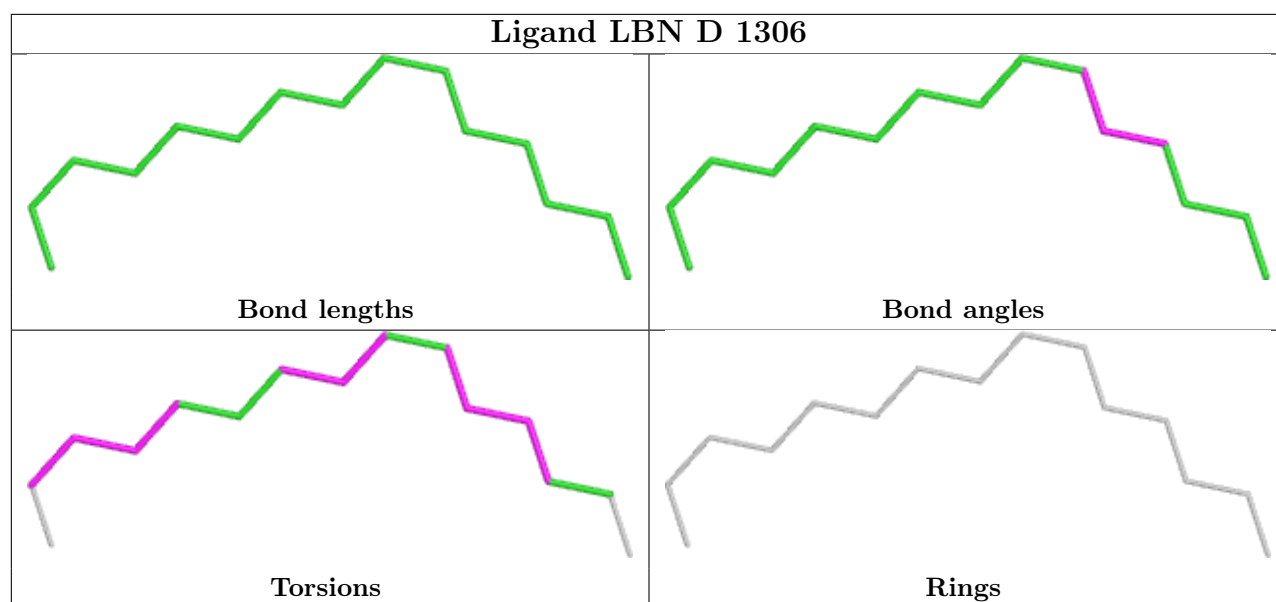
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

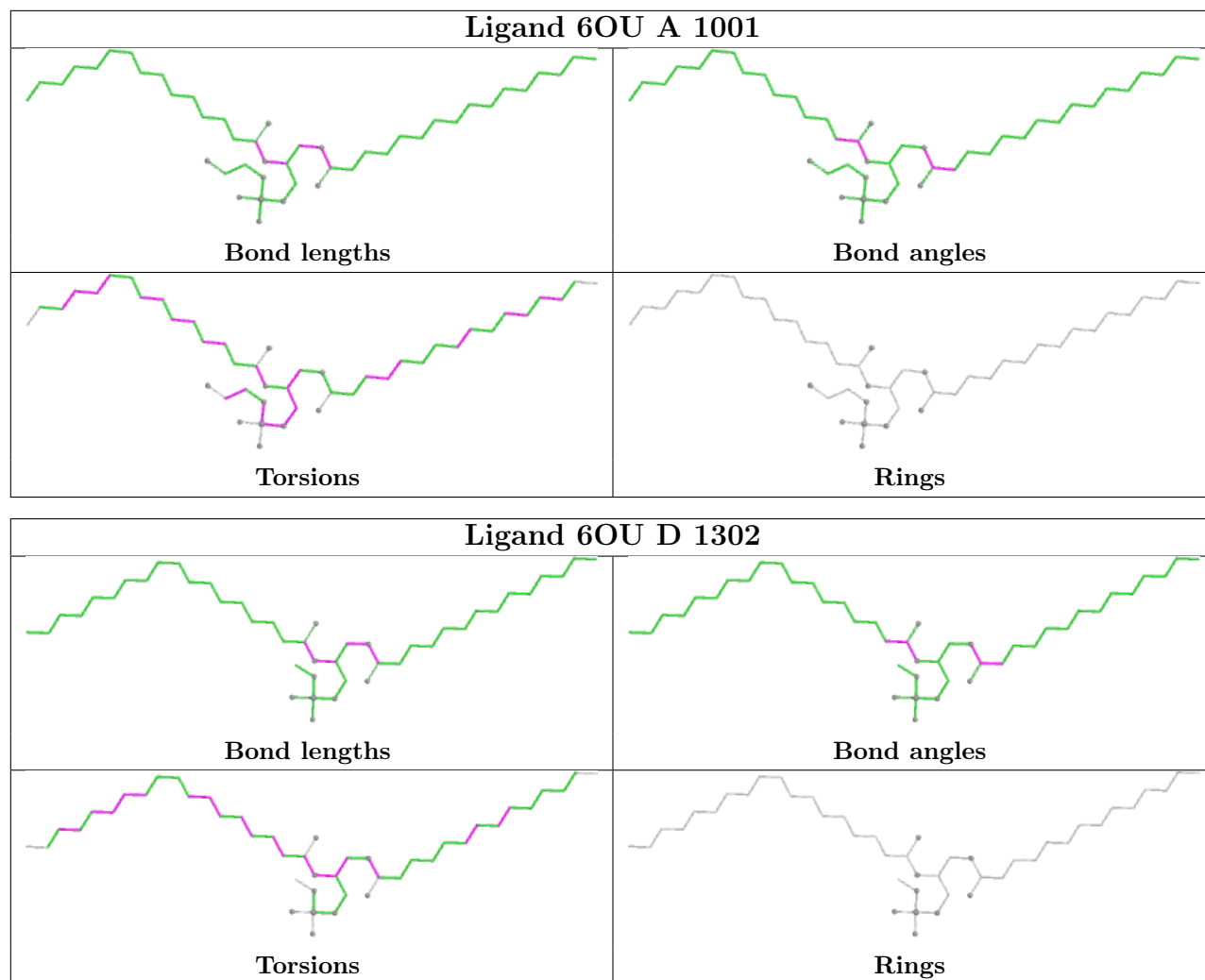


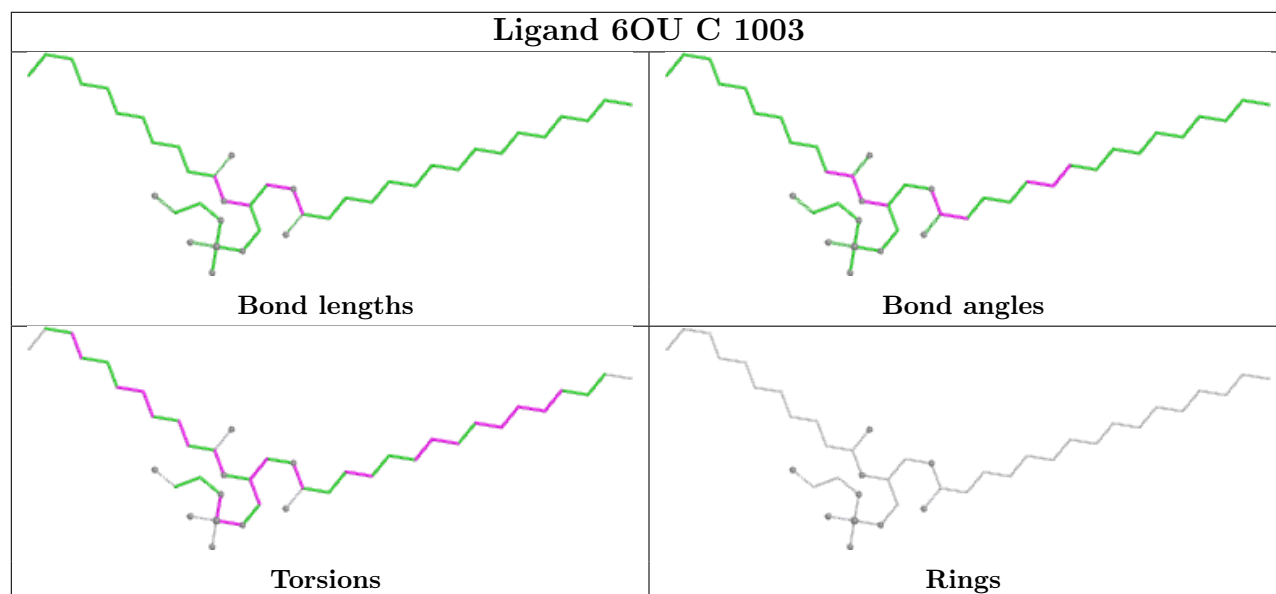
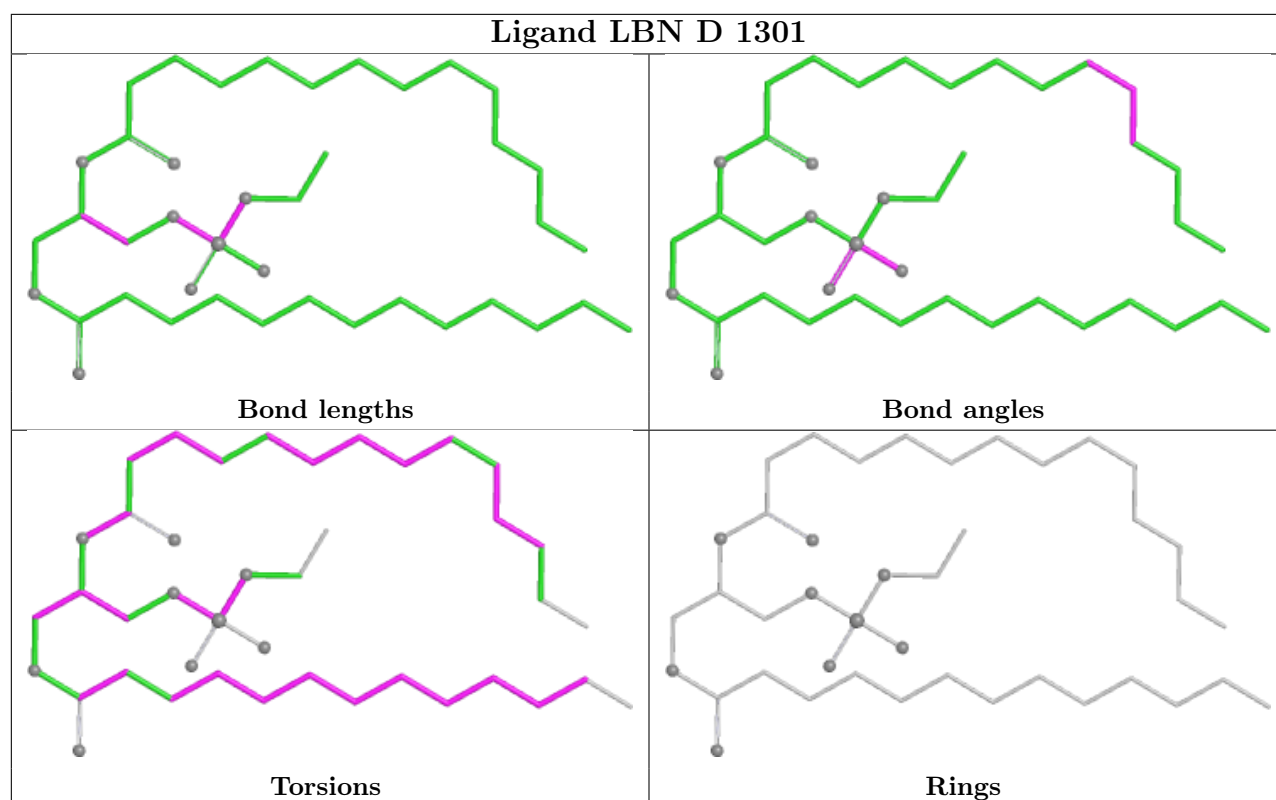


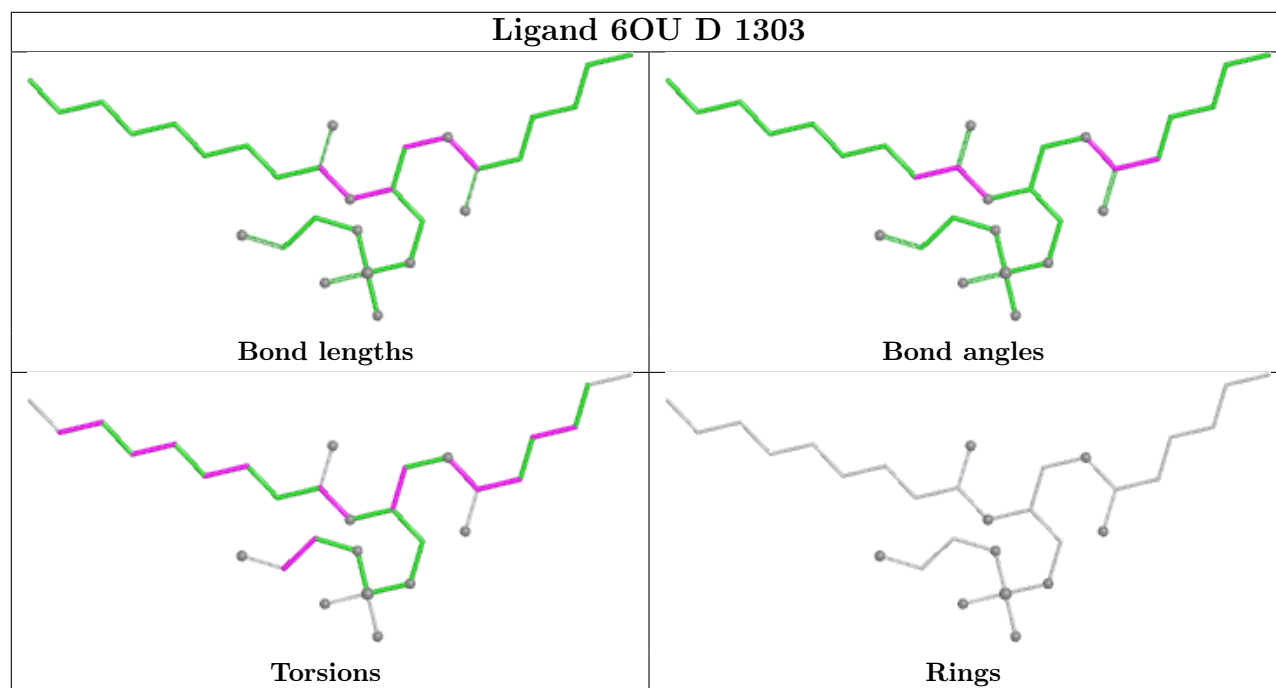
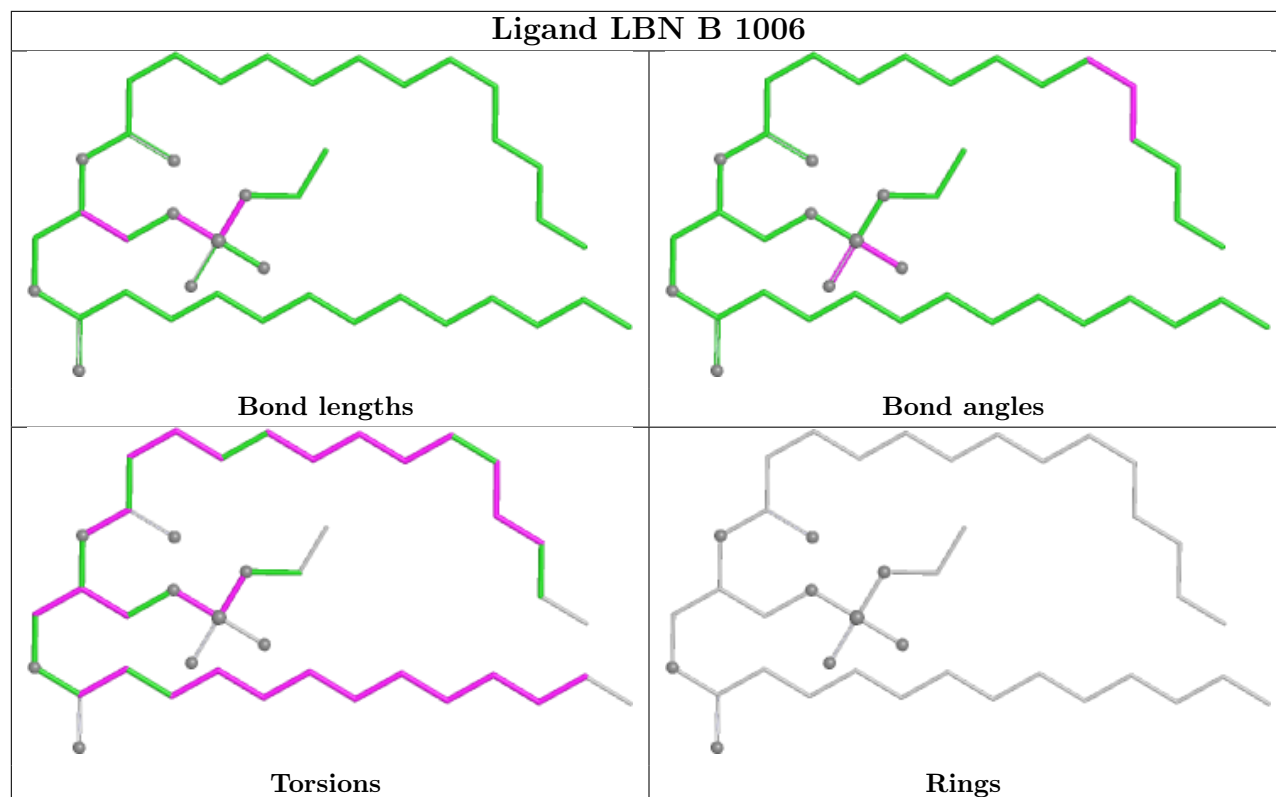


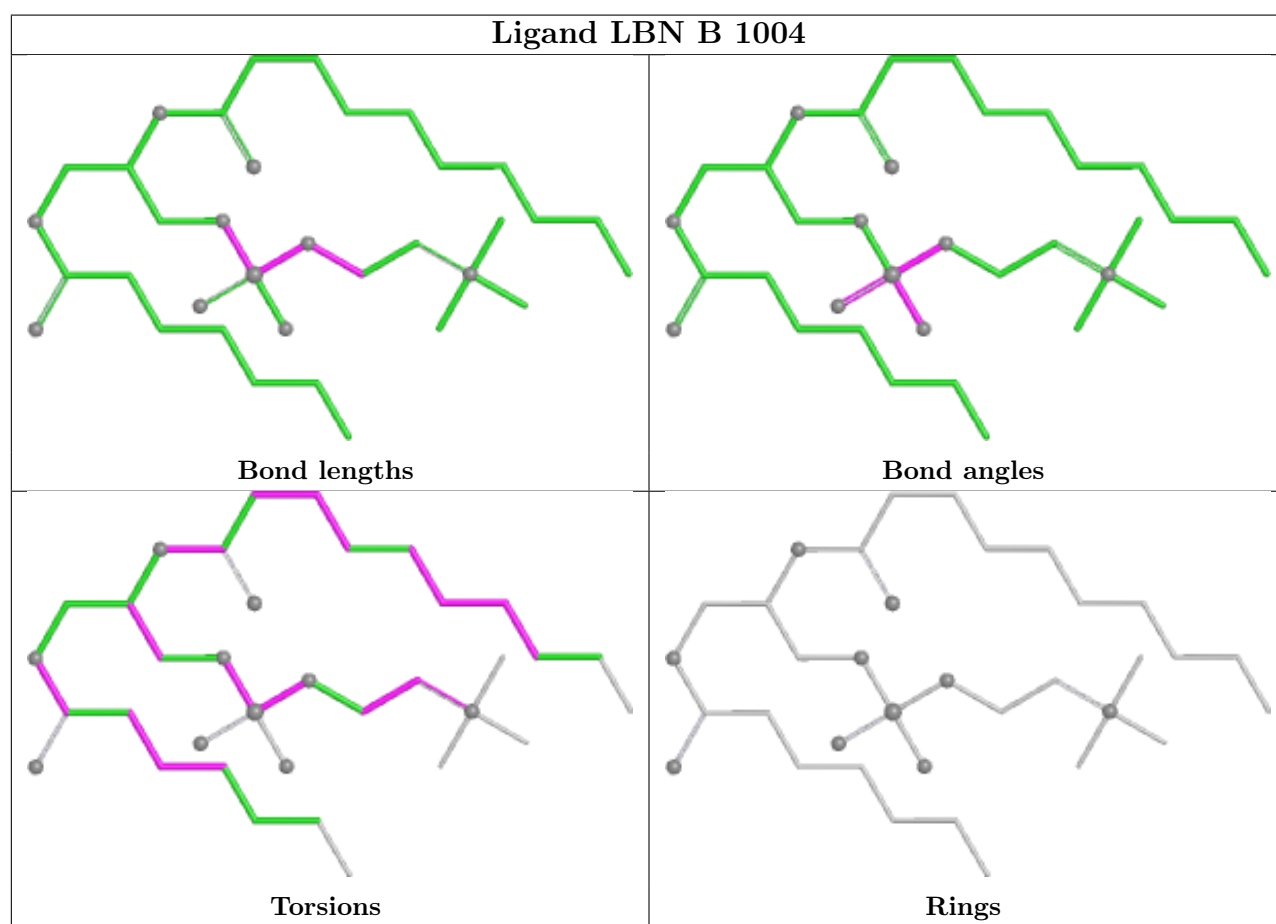
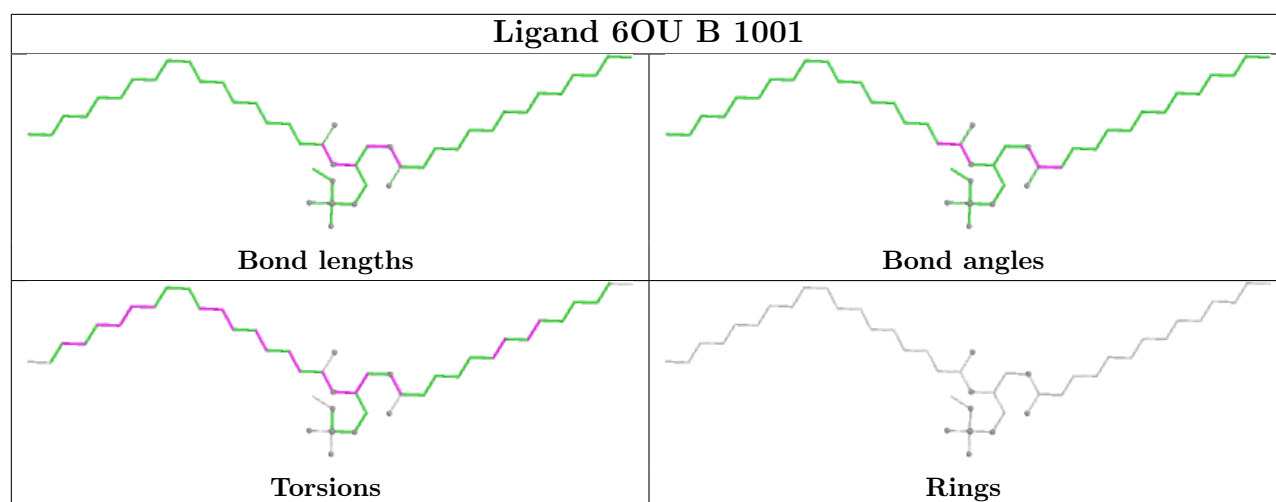


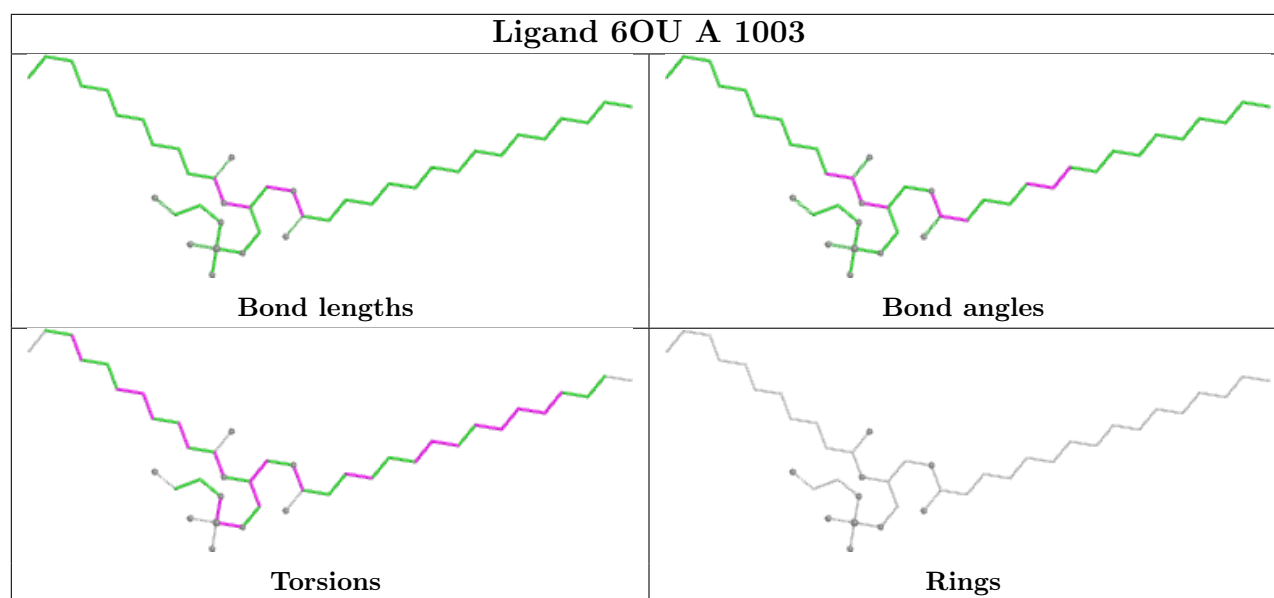












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	16:UNK	C	31:CYS	N	14.29
1	D	16:UNK	C	31:CYS	N	14.29

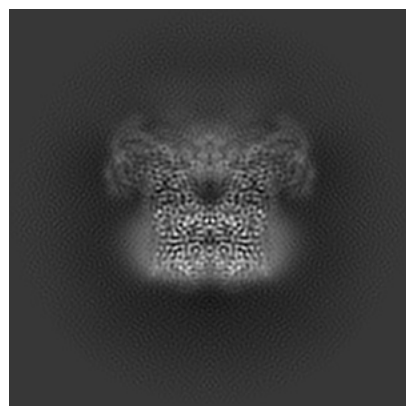
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49844. These allow visual inspection of the internal detail of the map and identification of artifacts.

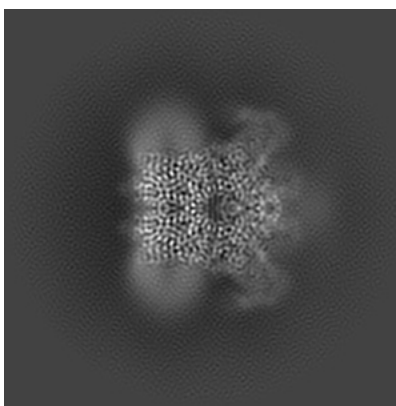
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

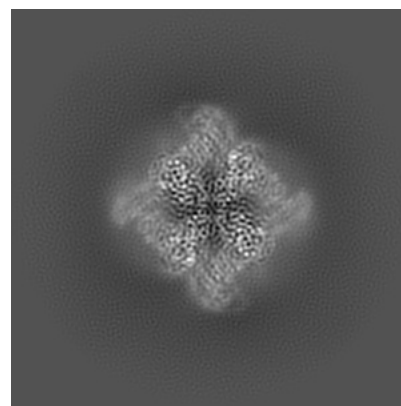
6.1.1 Primary map



X

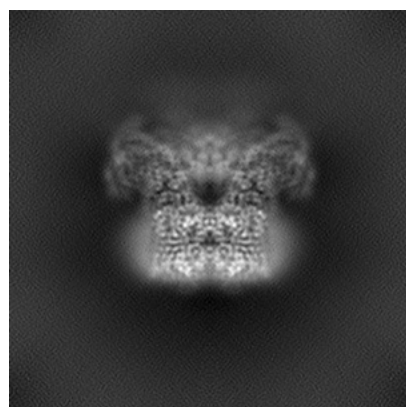


Y

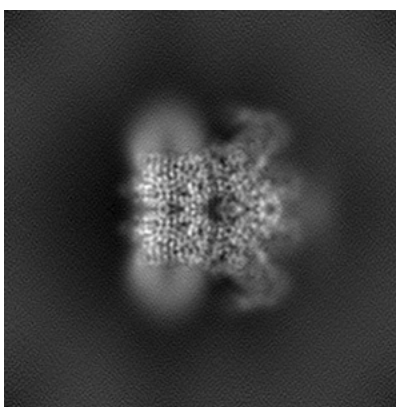


Z

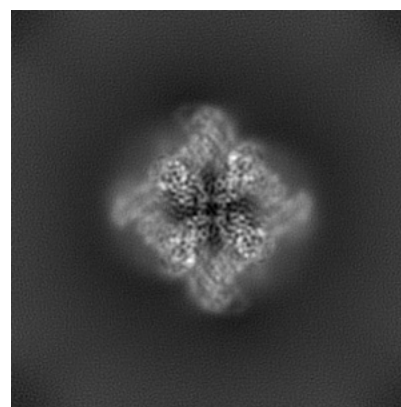
6.1.2 Raw map



X



Y

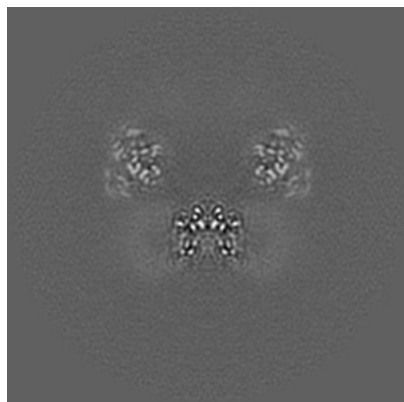


Z

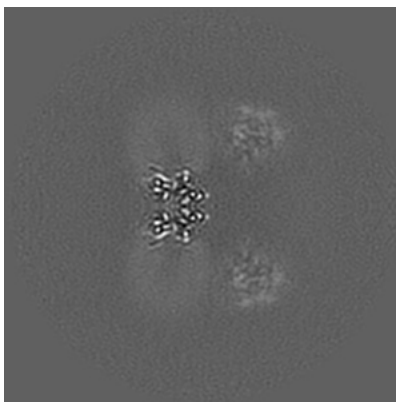
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

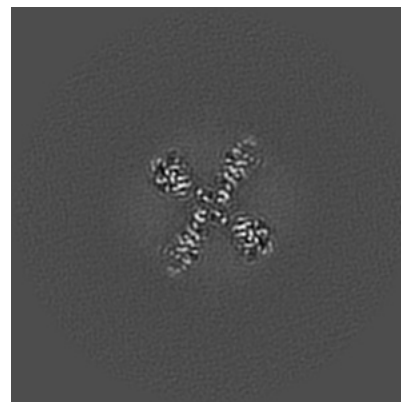
6.2.1 Primary map



X Index: 128

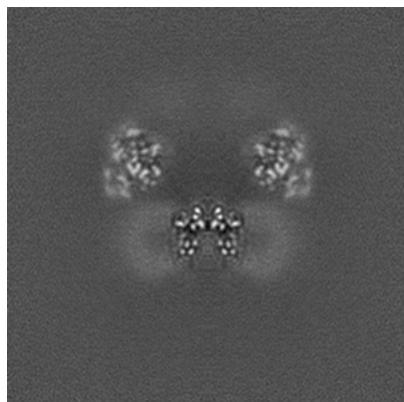


Y Index: 128

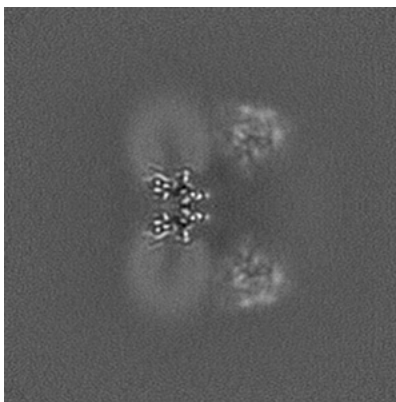


Z Index: 128

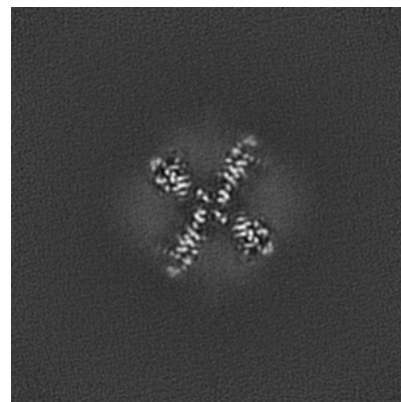
6.2.2 Raw map



X Index: 128



Y Index: 128

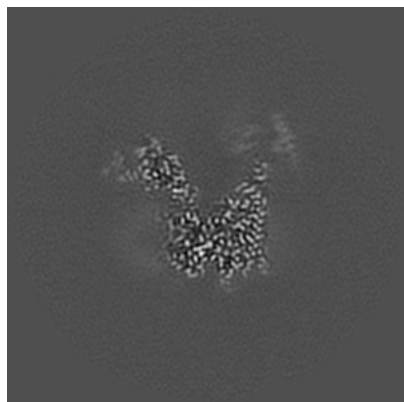


Z Index: 128

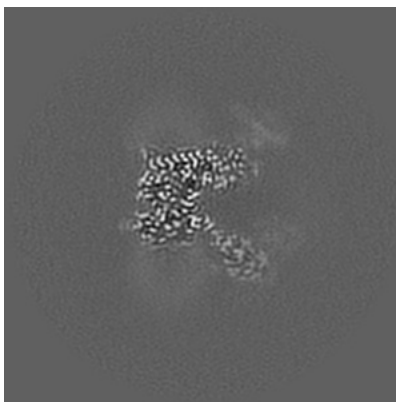
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

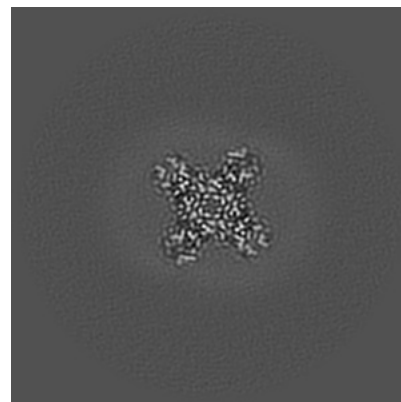
6.3.1 Primary map



X Index: 141

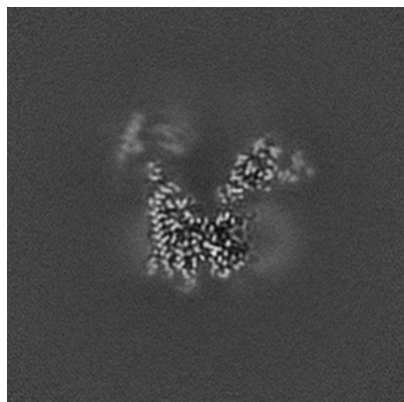


Y Index: 114

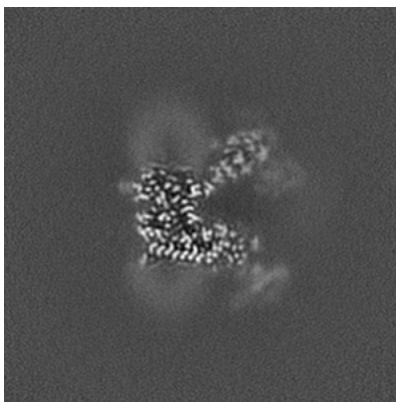


Z Index: 99

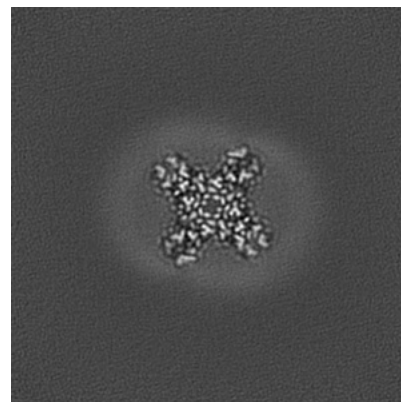
6.3.2 Raw map



X Index: 115



Y Index: 142

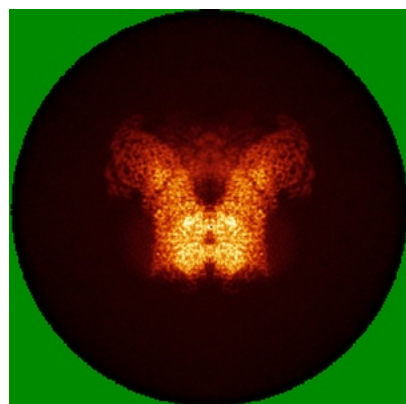


Z Index: 99

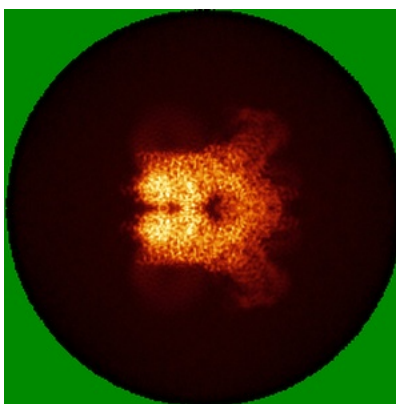
The images above show the largest variance slices of the map in three orthogonal directions.

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

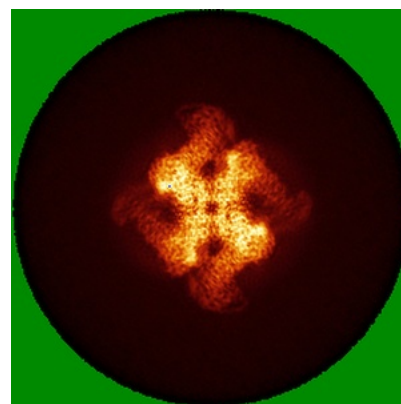
6.4.1 Primary map



X

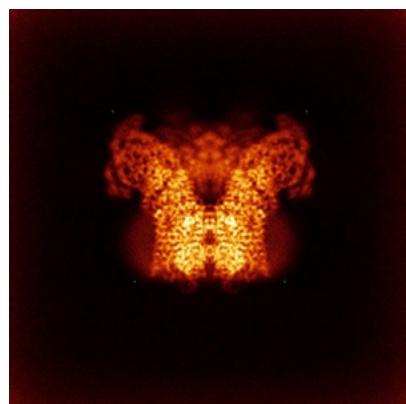


Y

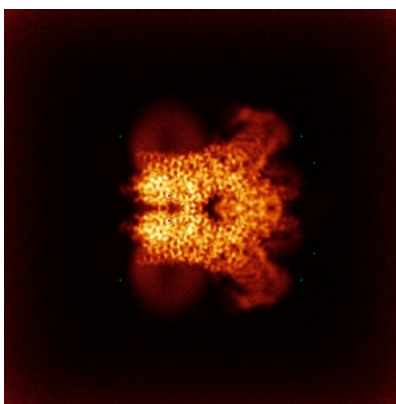


Z

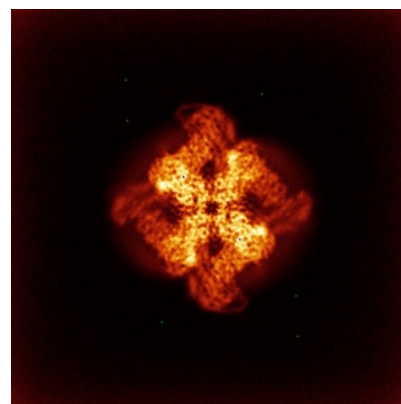
6.4.2 Raw map



X



Y

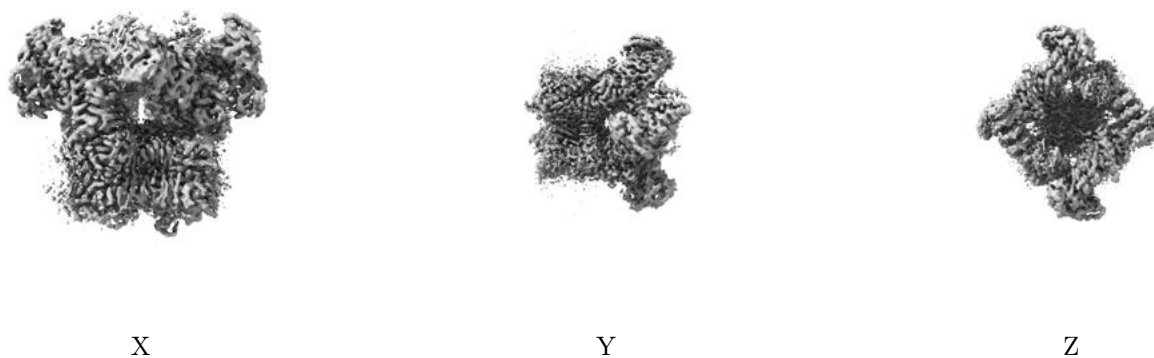


Z

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.

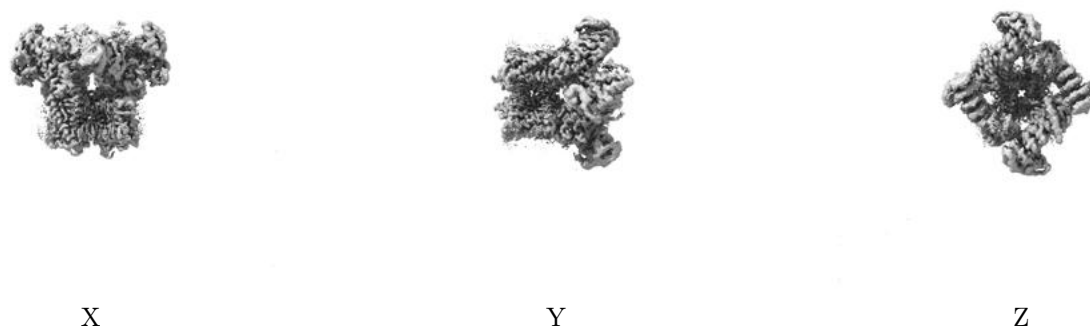
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

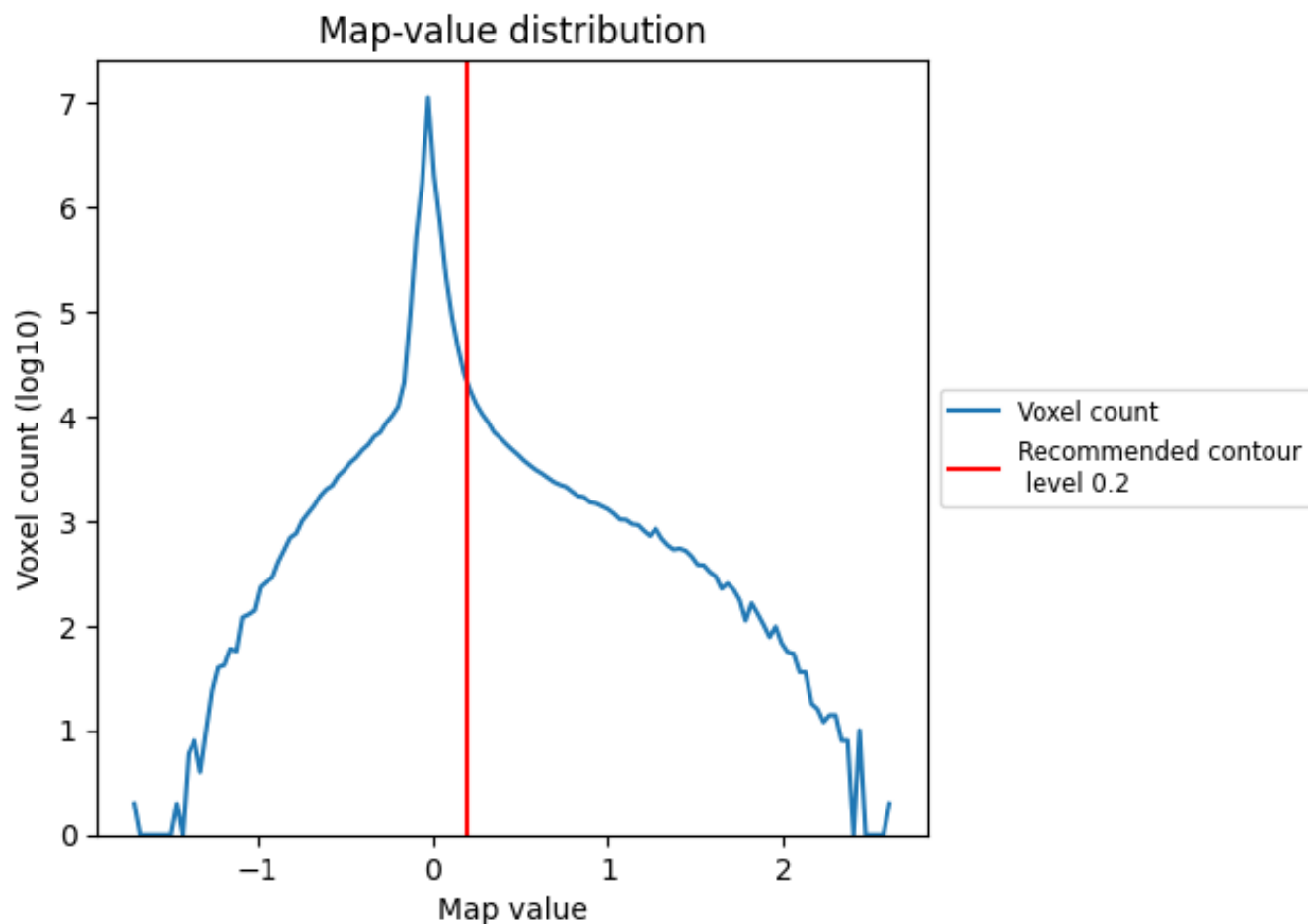
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

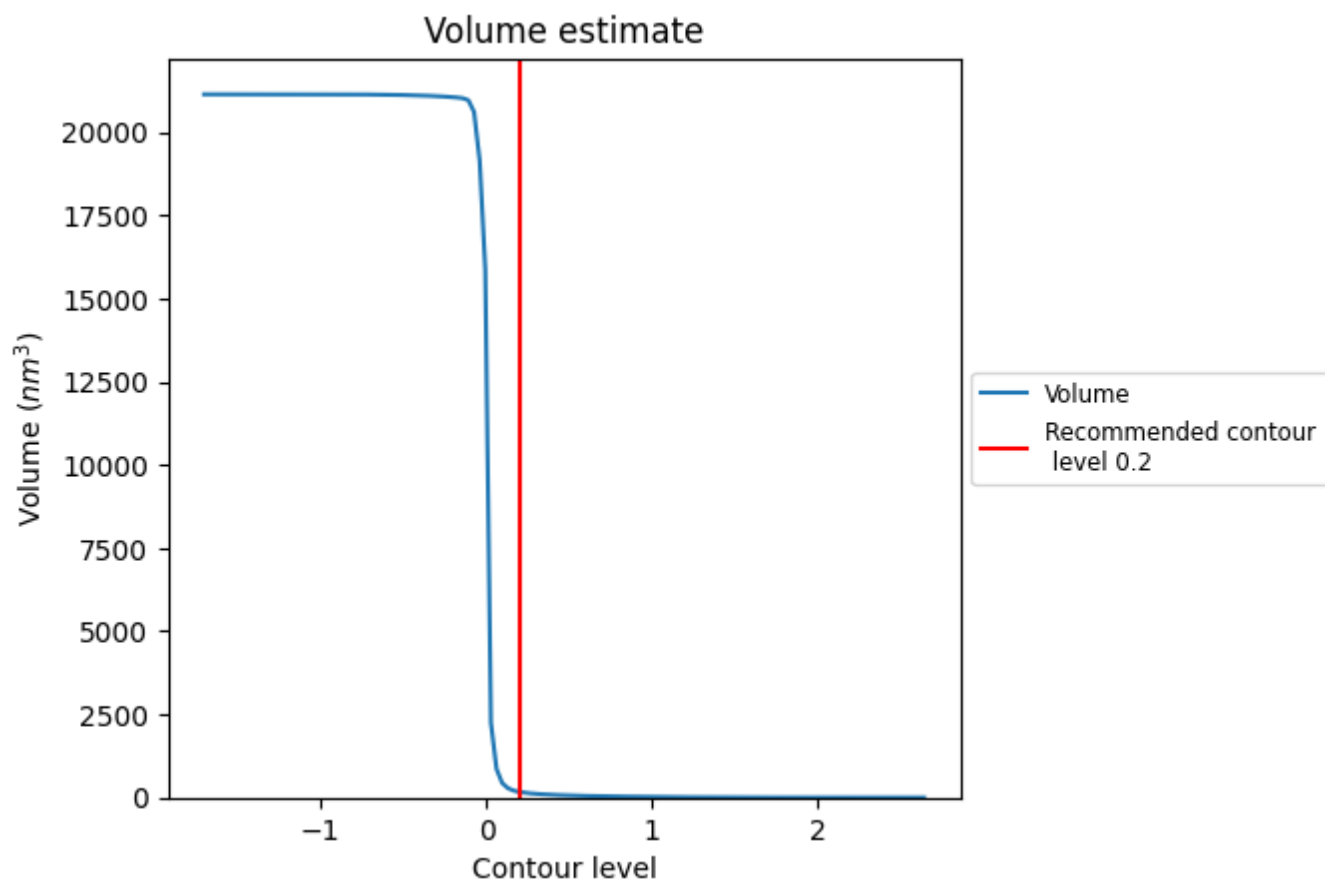
This section contains the results of statistical analysis of the map.

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.

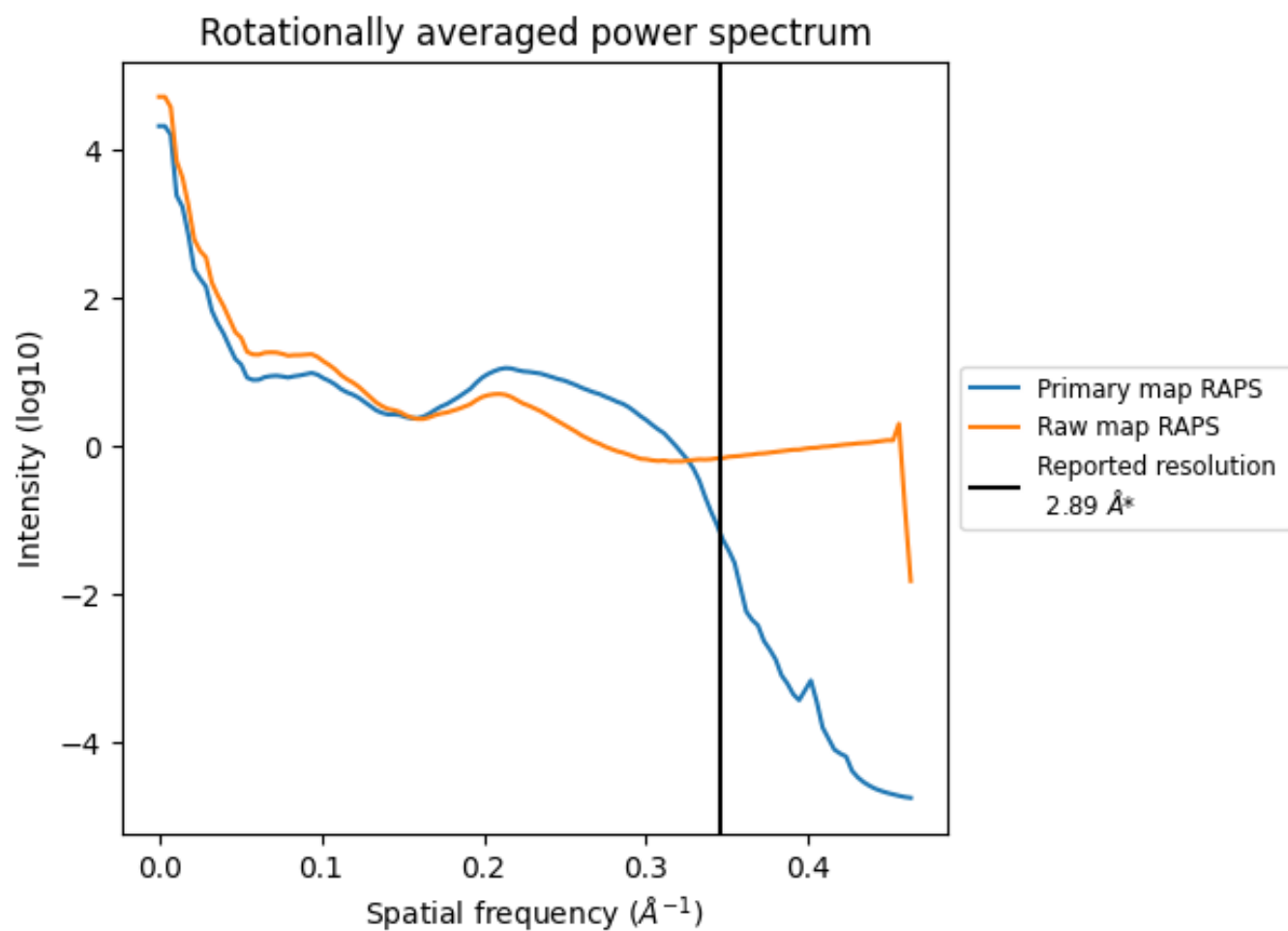
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 153 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 ⓘ

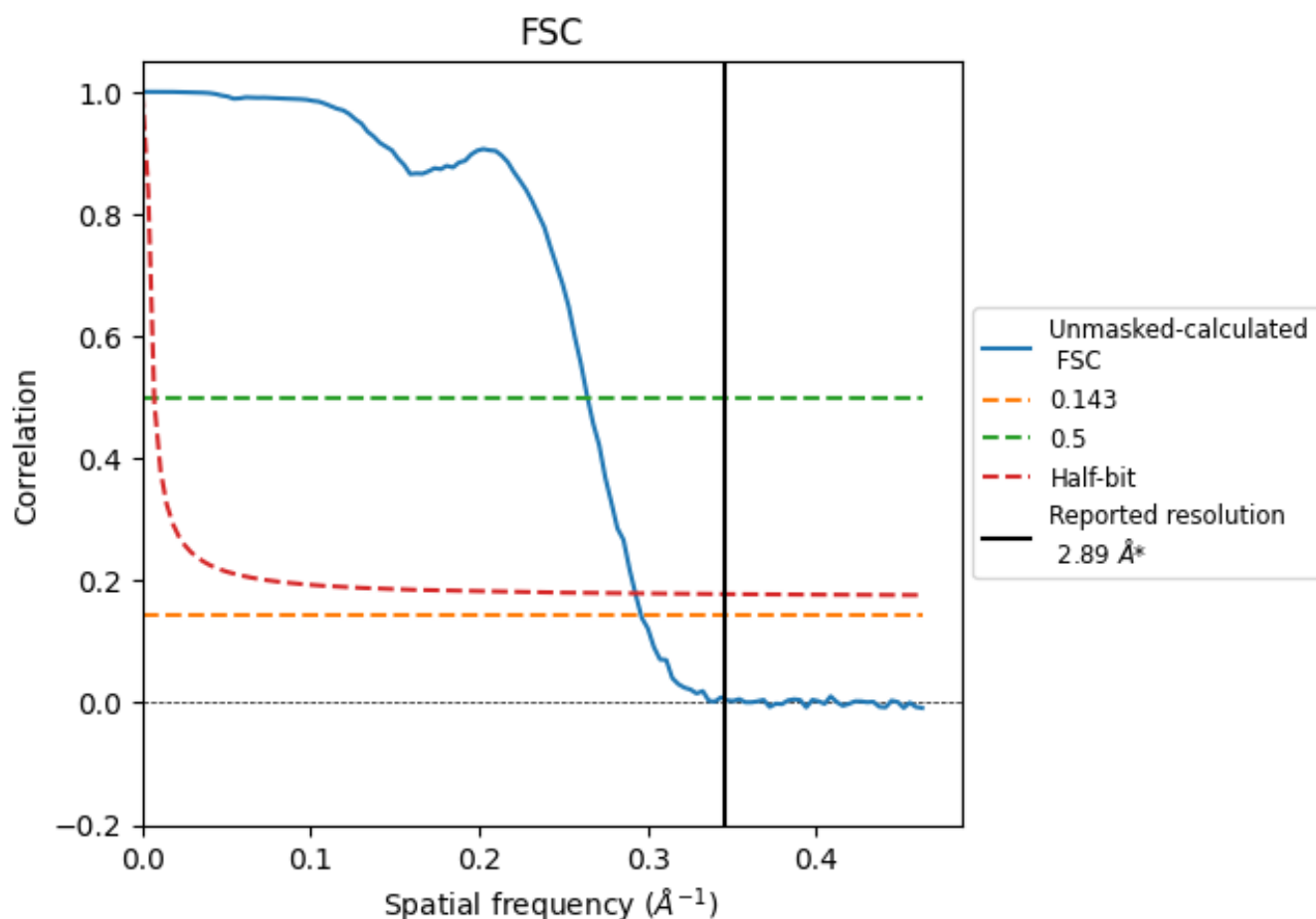


*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

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 0.346 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

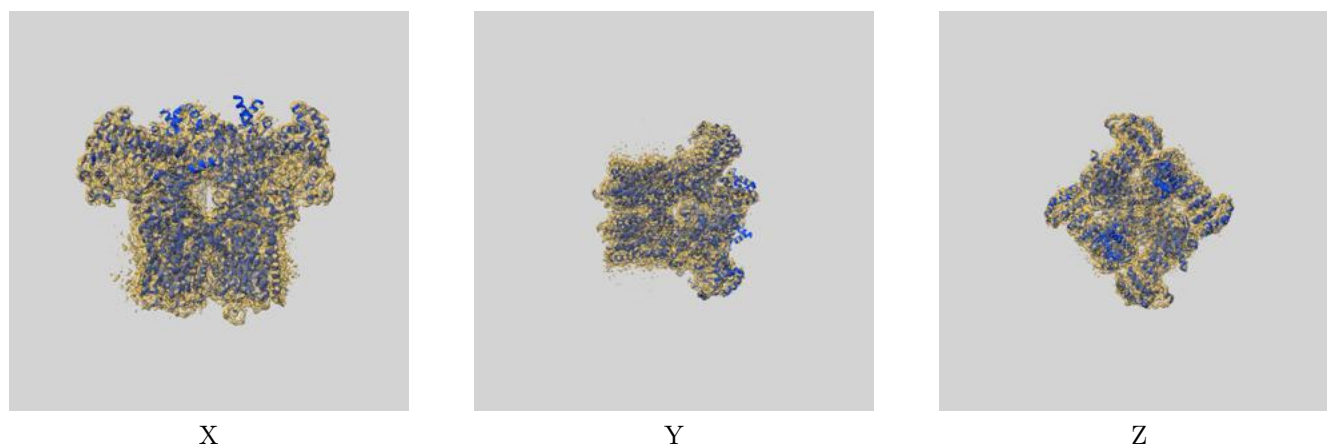
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.78	3.42

*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 3.38 differs from the reported value 2.89 by more than 10 %

9 Map-model fit [i](#)

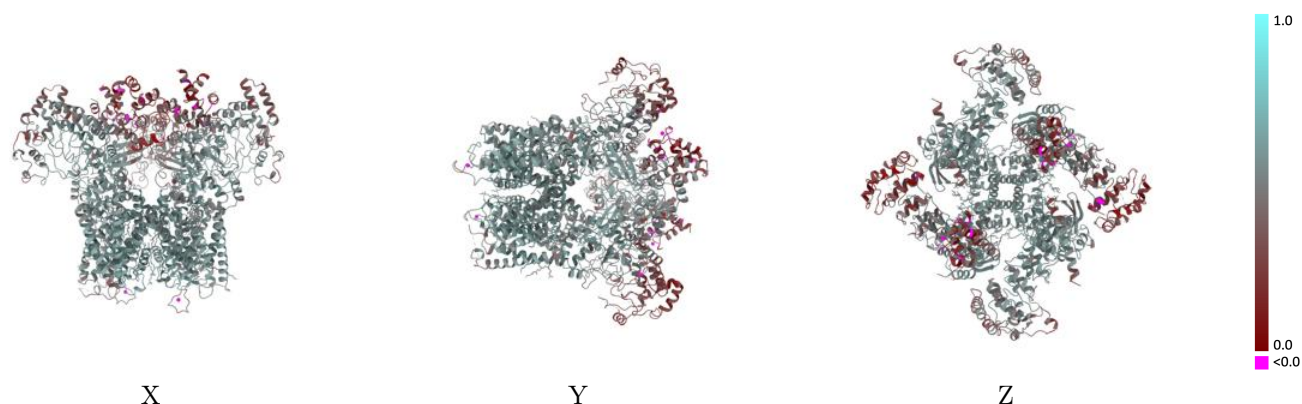
This section contains information regarding the fit between EMDB map EMD-49844 and PDB model 9NVN. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 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](#)

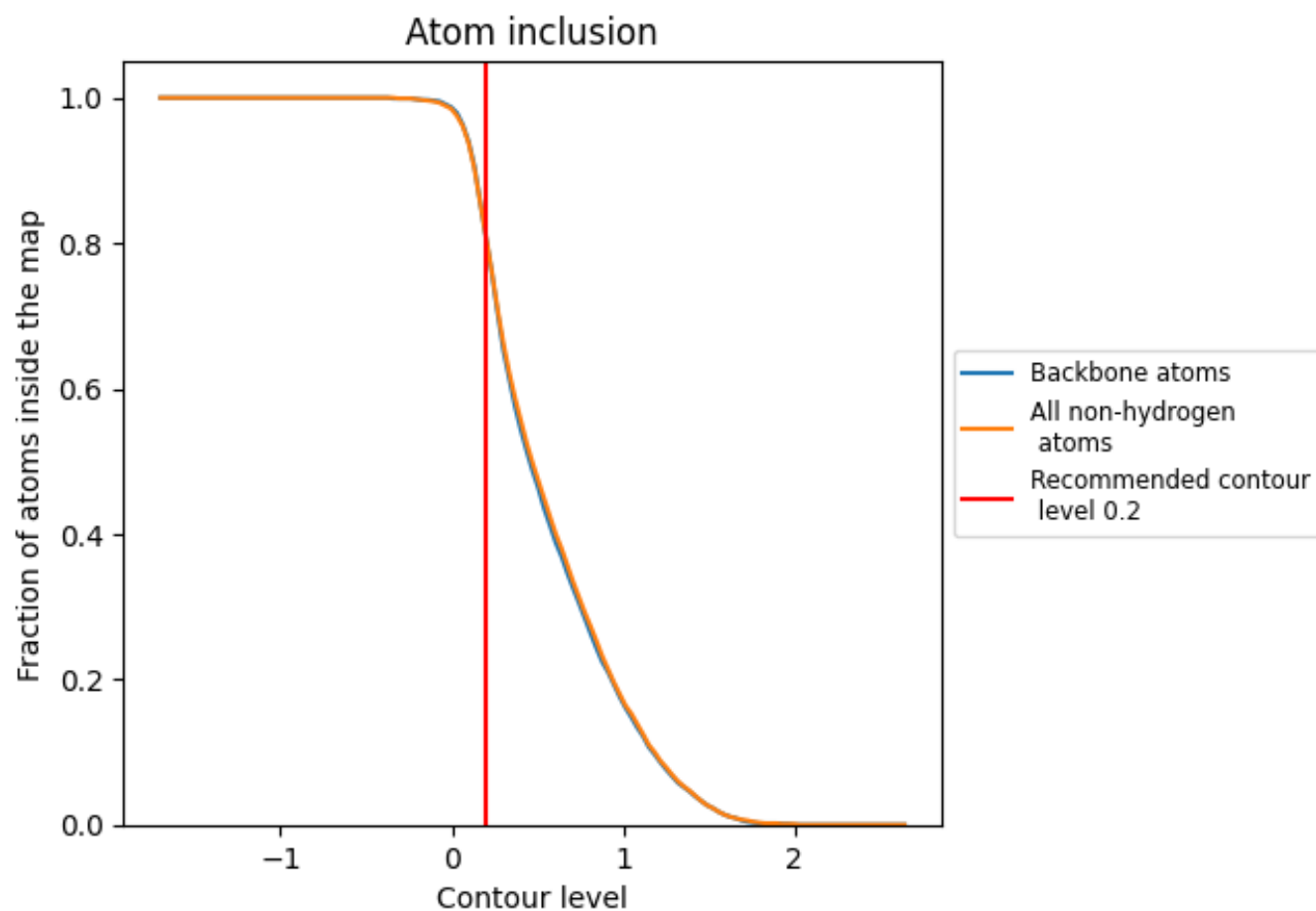


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.5000
A	0.8650	0.5340
B	0.7980	0.4870
C	0.8620	0.5320
D	0.8000	0.4860
E	0.2020	0.2020
F	0.2060	0.2090

1.0

0.0

<0.0