



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:52 AM UTC

PDB ID : 9NVR / pdb_00009nvr
EMDB ID : EMD-49848
Title : Structure of Nanchung-Inactive-Calmodulin in complex with Afidopyropen, EDTA
Authors : Fedor, J.G.; Lee, S.-Y.
Deposited on : 2025-03-21
Resolution : 3.13 Å(reported)
Based on initial model : 5wo7

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:

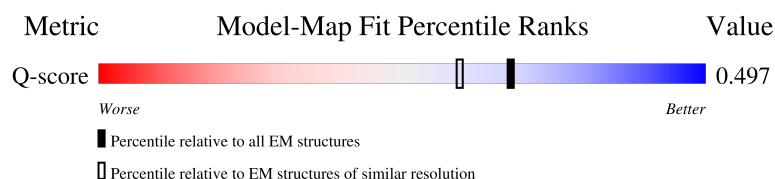
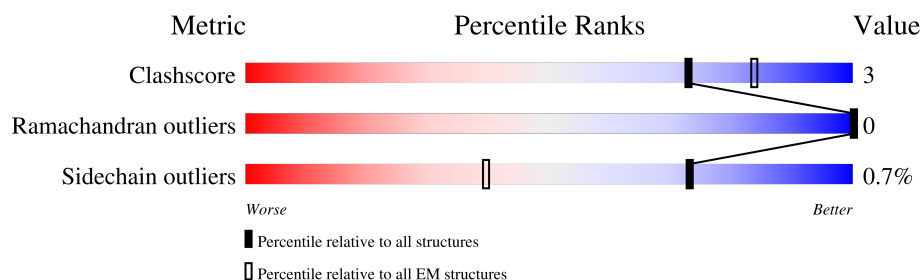
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.13 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	14478 (2.63 - 3.63)

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	
1	D	984	
2	E	149	
2	F	149	

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Mol	Chain	Length	Quality of chain
3	A	882	 74%7%19%
3	C	882	 74%7%19%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49206 atoms, of which 24512 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	679	Total	C	H	N	O	S	0	0
			10529	3428	5233	898	937	33		
1	D	679	Total	C	H	N	O	S	0	0
			10529	3428	5233	898	937	33		

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

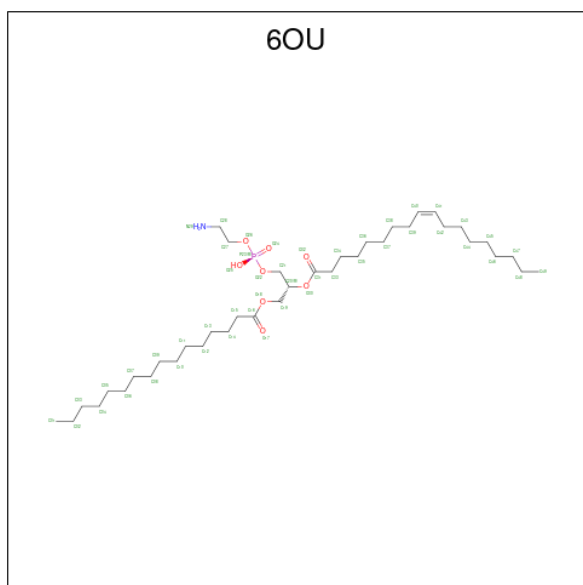
- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	131	Total	C	H	N	O	S	0	0
			1915	616	912	159	220	8		
2	F	131	Total	C	H	N	O	S	0	0
			1915	616	912	159	220	8		

- Molecule 3 is a protein called Nanchung.

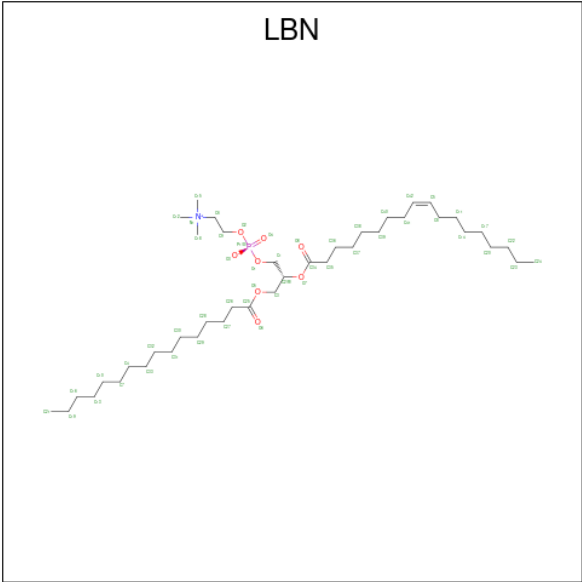
Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	717	Total	C	H	N	O	S	0	0
			11492	3737	5733	944	1022	56		
3	C	717	Total	C	H	N	O	S	0	0
			11492	3737	5733	944	1022	56		

- 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).



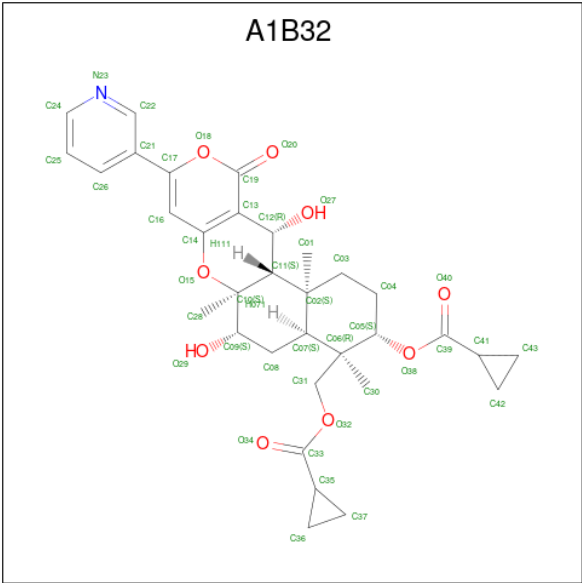
Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total 109	C 36	H 64	O 8	P 1	0	
4	B	1	Total 114	C 36	H 68	N 1	O 8	P 1	0
4	A	1	Total 102	C 32	H 60	N 1	O 8	P 1	0
4	A	1	Total 102	C 32	H 60	N 1	O 8	P 1	0
4	D	1	Total 109	C 36	H 64	O 8	P 1	0	
4	D	1	Total 114	C 36	H 68	N 1	O 8	P 1	0
4	C	1	Total 102	C 32	H 60	N 1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

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



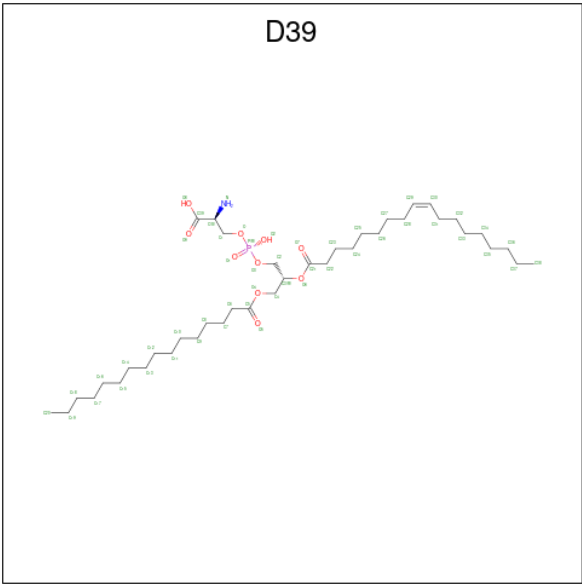
Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	H	N	O	P	0
			81	25	46	1	8	1	
5	D	1	Total	C	H	N	O	P	0
			81	25	46	1	8	1	

- Molecule 6 is Afidopyropen (CCD ID: A1B32) (formula: $C_{33}H_{39}NO_9$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			82	33	39	1	9	
6	C	1	Total	C	H	N	O	0
			82	33	39	1	9	

- 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).

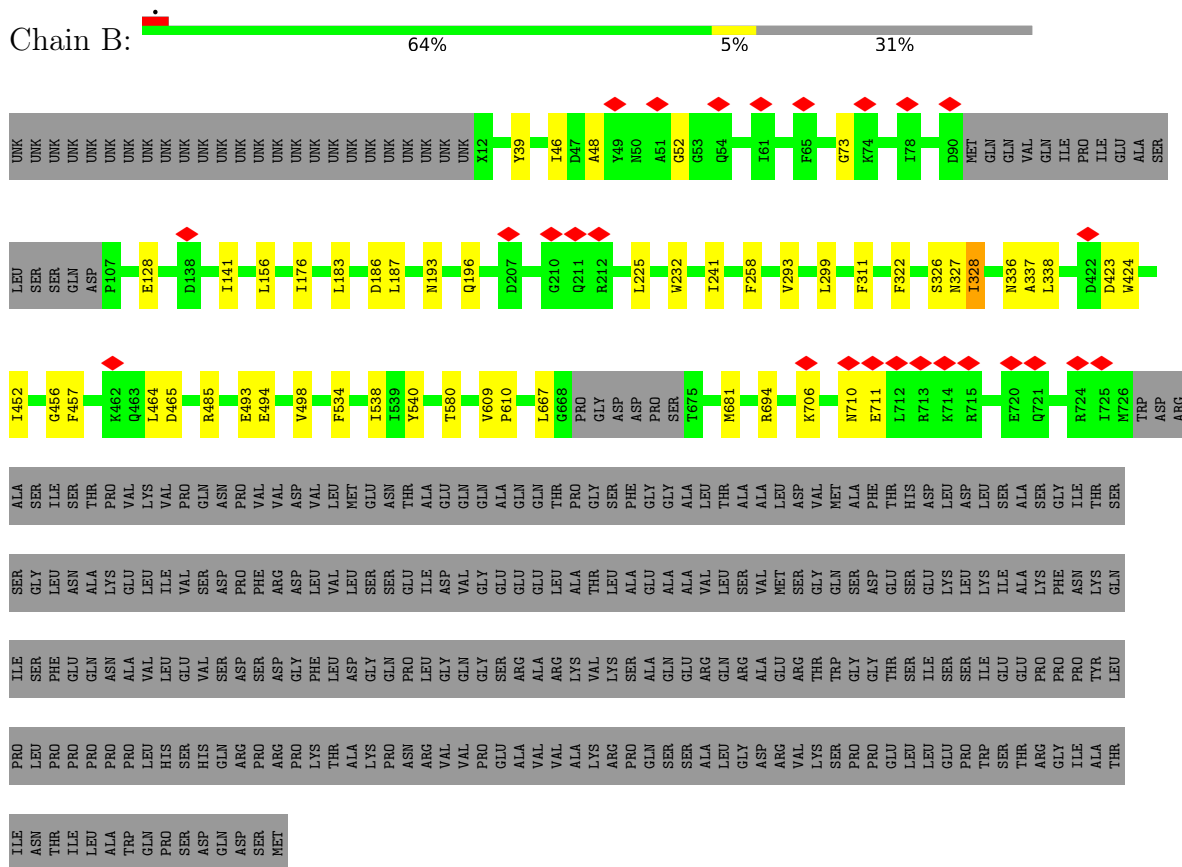


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
7	A	1	77	24	41	1	10	1	0
7	C	1	77	24	41	1	10	1	0

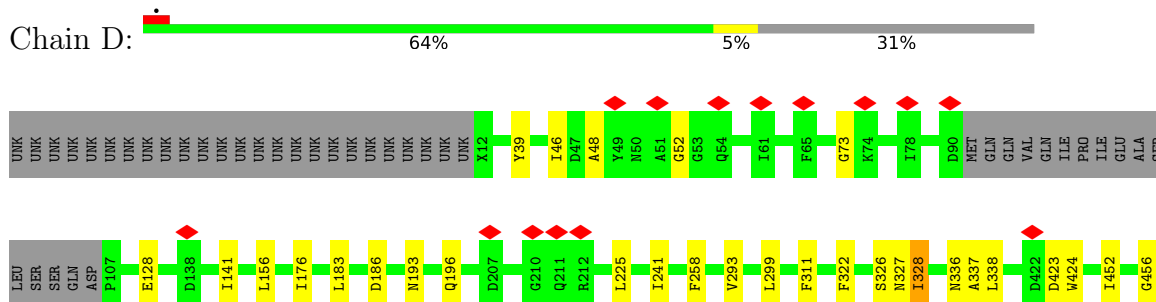
3 Residue-property plots

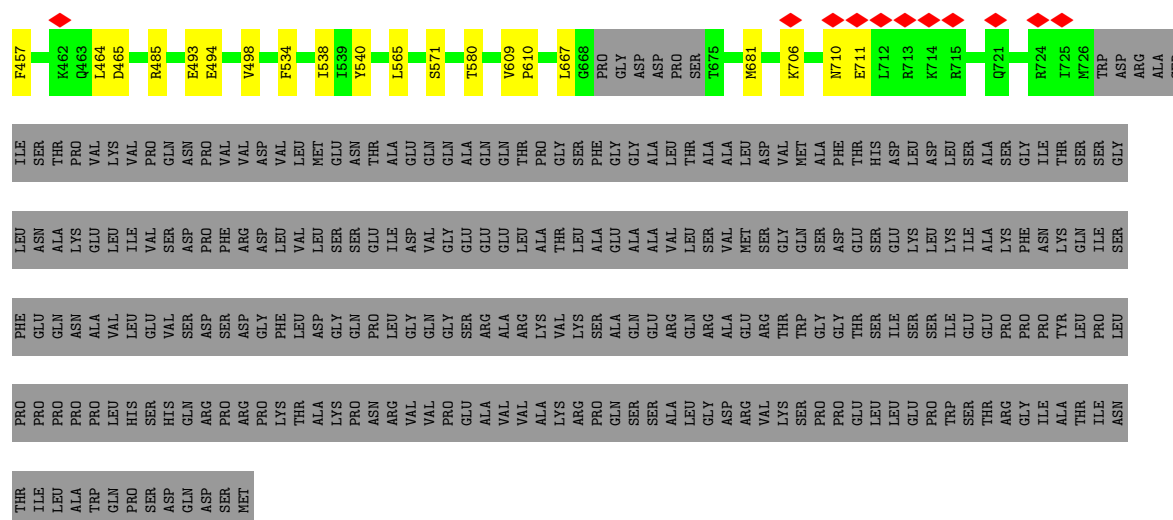
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Inactive

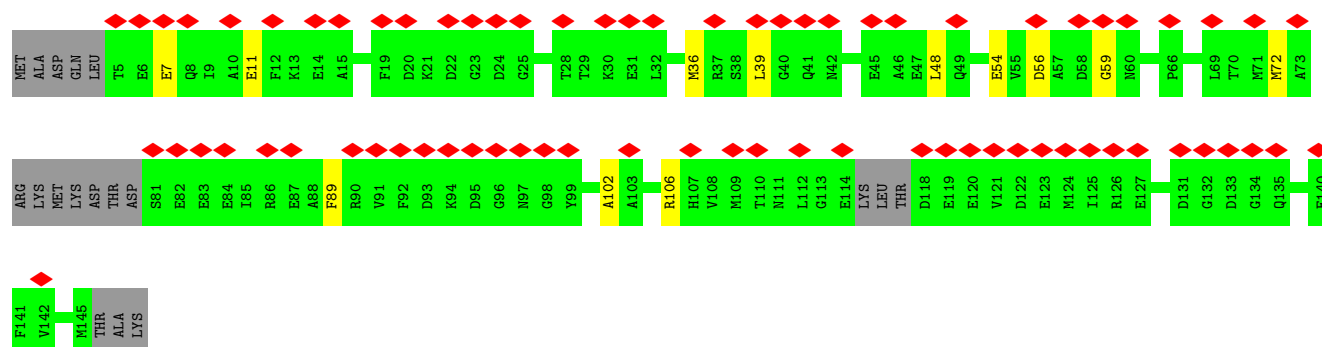


• Molecule 1: Inactive

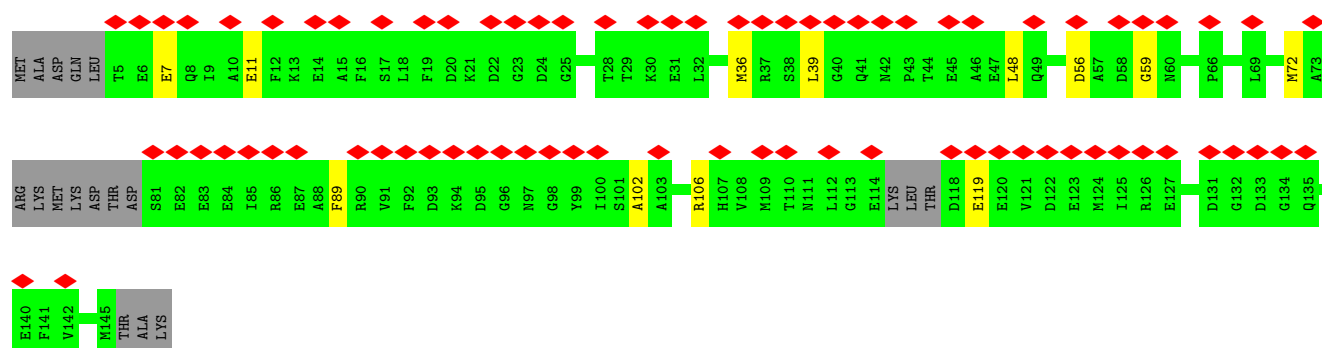
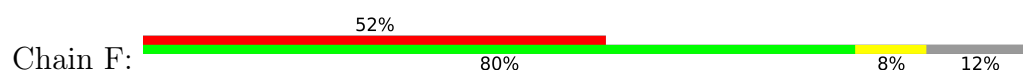




• Molecule 2: Calmodulin-1



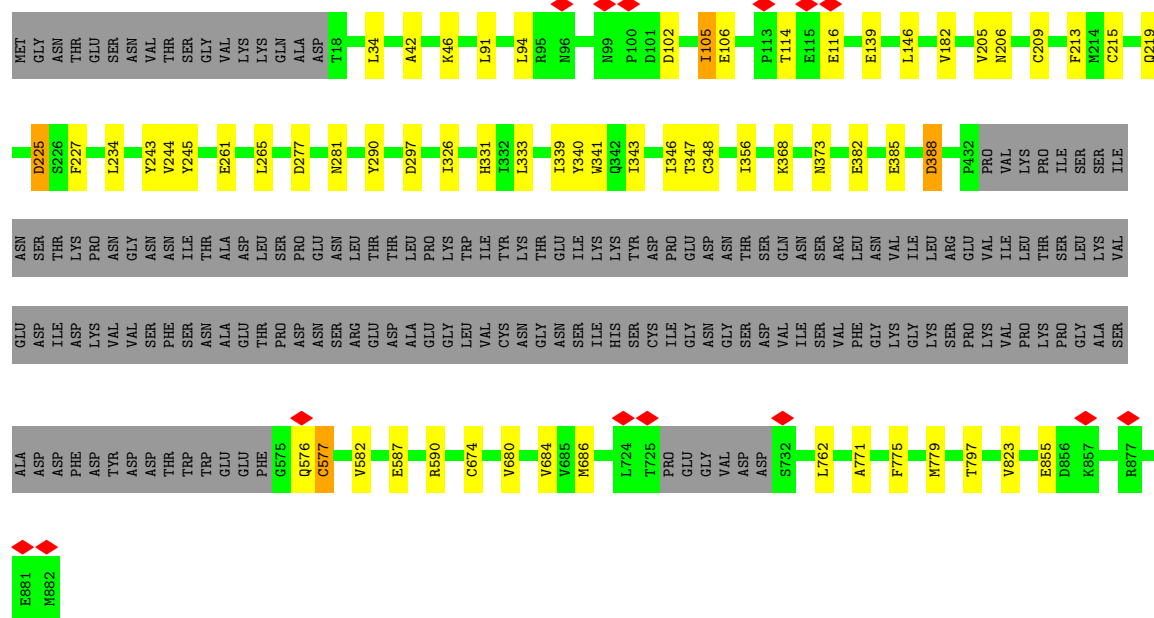
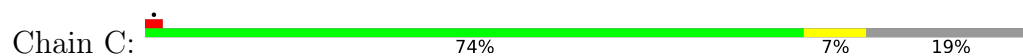
• Molecule 2: Calmodulin-1



• Molecule 3: Nanchung



- Molecule 3: Nanchung



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	58231	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	2.198	Depositor
Minimum map value	-1.363	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	302.40002, 302.40002, 302.40002	wwPDB
Map dimensions	280, 280, 280	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, 6OU, LBN, A1B32

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	0.12	0/5388	0.28	2/7299 (0.0%)
1	D	0.12	0/5388	0.28	2/7299 (0.0%)
2	E	0.09	0/1012	0.23	0/1360
2	F	0.09	0/1012	0.23	0/1360
3	A	0.14	0/5891	0.30	0/7975
3	C	0.14	0/5891	0.30	0/7975
All	All	0.13	0/24582	0.28	4/33268 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	GLY	CA-C-N	7.73	130.64	120.28
1	D	73	GLY	C-N-CA	7.73	130.64	120.28
1	B	73	GLY	CA-C-N	7.71	130.60	120.28
1	B	73	GLY	C-N-CA	7.71	130.60	120.28

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	5296	5233	5246	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5296	5233	5246	33	0
2	E	1003	912	910	9	0
2	F	1003	912	910	9	0
3	A	5759	5733	5736	42	0
3	C	5759	5733	5736	41	0
4	A	84	120	0	0	0
4	B	91	132	0	0	0
4	C	84	120	0	0	0
4	D	91	132	0	0	0
5	B	35	46	0	0	0
5	D	35	46	0	0	0
6	A	43	39	0	0	0
6	C	43	39	0	0	0
7	A	36	41	0	0	0
7	C	36	41	0	0	0
All	All	24694	24512	23784	162	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 (162) 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:156:LEU:O	1:B:156:LEU:HD23	1.98	0.64
1:B:328:ILE:HD11	3:C:213:PHE:CZ	2.34	0.63
1:D:156:LEU:HD23	1:D:156:LEU:O	1.98	0.63
3:A:213:PHE:CZ	1:D:328:ILE:HD11	2.34	0.62
3:A:213:PHE:HZ	1:D:328:ILE:HD11	1.66	0.60
3:C:385:GLU:OE1	3:C:385:GLU:N	2.36	0.59
3:A:385:GLU:N	3:A:385:GLU:OE1	2.36	0.59
1:D:39:TYR:OH	1:D:128:GLU:OE2	2.16	0.58
1:B:328:ILE:HD11	3:C:213:PHE:HZ	1.66	0.58
1:B:39:TYR:OH	1:B:128:GLU:OE2	2.16	0.57
3:A:333:LEU:HD21	3:A:356:ILE:HD11	1.88	0.55
1:B:580:THR:HG22	1:B:609:VAL:HG11	1.89	0.55
1:D:580:THR:HG22	1:D:609:VAL:HG11	1.89	0.55
3:A:368:LYS:O	3:A:373:ASN:ND2	2.40	0.54
3:A:225:ASP:N	3:A:225:ASP:OD1	2.40	0.54
3:C:225:ASP:OD1	3:C:225:ASP:N	2.40	0.54
1:D:48:ALA:O	1:D:52:GLY:N	2.38	0.54
3:C:368:LYS:O	3:C:373:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:333:LEU:HD21	3:C:356:ILE:HD11	1.88	0.54
1:B:423:ASP:OD1	1:B:424:TRP:N	2.42	0.53
1:B:494:GLU:O	1:B:498:VAL:HG23	2.09	0.53
3:A:587:GLU:OE1	3:A:590:ARG:NH1	2.38	0.53
3:A:341:TRP:CD1	3:A:348:CYS:HG	2.27	0.53
3:C:587:GLU:OE1	3:C:590:ARG:NH1	2.38	0.52
1:B:48:ALA:O	1:B:52:GLY:N	2.38	0.52
3:A:114:THR:HG22	3:A:116:GLU:H	1.74	0.52
1:D:423:ASP:OD1	1:D:424:TRP:N	2.42	0.52
1:D:326:SER:O	1:D:327:ASN:HB2	2.10	0.51
3:C:114:THR:HG22	3:C:116:GLU:H	1.74	0.51
1:D:494:GLU:O	1:D:498:VAL:HG23	2.09	0.51
1:B:485:ARG:NH2	1:B:493:GLU:OE2	2.42	0.51
2:E:102:ALA:O	2:E:106:ARG:NH1	2.44	0.51
3:C:674:CYS:SG	3:C:684:VAL:HG21	2.51	0.51
3:A:762:LEU:HD22	3:A:771:ALA:HB1	1.93	0.51
1:D:225:LEU:HD12	1:D:225:LEU:N	2.26	0.51
2:F:39:LEU:HD22	1:D:711:GLU:HG2	1.93	0.50
3:C:762:LEU:HD22	3:C:771:ALA:HB1	1.93	0.50
1:B:225:LEU:HD12	1:B:225:LEU:N	2.26	0.50
1:B:326:SER:O	1:B:327:ASN:HB2	2.10	0.50
2:F:102:ALA:O	2:F:106:ARG:NH1	2.44	0.50
3:C:823:VAL:HG12	3:C:823:VAL:O	2.12	0.50
3:A:245:TYR:O	3:A:290:TYR:OH	2.20	0.49
3:A:674:CYS:SG	3:A:684:VAL:HG21	2.51	0.49
3:A:823:VAL:HG12	3:A:823:VAL:O	2.12	0.49
3:A:855:GLU:OE1	3:A:855:GLU:N	2.43	0.49
3:C:91:LEU:HD13	3:C:227:PHE:CE1	2.48	0.49
3:C:206:ASN:O	3:C:206:ASN:ND2	2.47	0.48
1:D:485:ARG:NH2	1:D:493:GLU:OE2	2.42	0.48
1:D:706:LYS:O	1:D:710:ASN:ND2	2.42	0.48
3:A:91:LEU:HD13	3:A:227:PHE:CE1	2.48	0.48
3:A:206:ASN:O	3:A:206:ASN:ND2	2.47	0.47
3:A:388:ASP:N	3:A:388:ASP:OD1	2.46	0.47
3:A:105:ILE:O	3:A:106:GLU:HB2	2.15	0.47
1:D:540:TYR:OH	1:D:580:THR:HG21	2.14	0.47
1:D:452:ILE:HD11	1:D:457:PHE:CD2	2.50	0.47
1:B:540:TYR:OH	1:B:580:THR:HG21	2.14	0.47
3:C:146:LEU:HD22	3:C:182:VAL:HB	1.96	0.47
3:C:855:GLU:OE1	3:C:855:GLU:N	2.43	0.47
3:A:146:LEU:HD22	3:A:182:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:MET:N	2:F:72:MET:HE2	2.30	0.47
1:B:706:LYS:O	1:B:710:ASN:ND2	2.42	0.47
3:A:244:VAL:HG23	3:A:244:VAL:O	2.16	0.46
1:D:464:LEU:O	1:D:465:ASP:HB2	2.15	0.46
3:C:105:ILE:O	3:C:106:GLU:HB2	2.15	0.46
3:C:245:TYR:O	3:C:290:TYR:OH	2.20	0.46
3:A:341:TRP:NE1	3:A:348:CYS:HG	2.13	0.46
1:B:183:LEU:HD23	1:B:183:LEU:O	2.15	0.46
3:C:34:LEU:C	3:C:34:LEU:HD23	2.41	0.46
2:E:72:MET:N	2:E:72:MET:HE2	2.30	0.46
1:D:338:LEU:HD12	1:D:338:LEU:O	2.16	0.46
1:B:452:ILE:HD11	1:B:457:PHE:CD2	2.50	0.46
3:C:244:VAL:O	3:C:244:VAL:HG23	2.16	0.46
1:B:338:LEU:HD12	1:B:338:LEU:O	2.16	0.46
2:F:89:PHE:C	2:F:89:PHE:CD1	2.94	0.46
1:D:183:LEU:HD23	1:D:183:LEU:O	2.15	0.46
1:D:336:ASN:OD1	1:D:337:ALA:N	2.49	0.46
3:A:34:LEU:C	3:A:34:LEU:HD23	2.41	0.46
1:B:336:ASN:OD1	1:B:337:ALA:N	2.49	0.45
1:D:141:ILE:HD12	1:D:141:ILE:N	2.32	0.45
1:D:452:ILE:O	1:D:456:GLY:N	2.46	0.45
1:B:464:LEU:O	1:B:465:ASP:HB2	2.15	0.45
2:F:7:GLU:O	2:F:11:GLU:N	2.41	0.45
1:B:667:LEU:C	1:B:667:LEU:HD12	2.42	0.45
3:C:205:VAL:HG12	3:C:206:ASN:H	1.81	0.45
1:D:667:LEU:C	1:D:667:LEU:HD12	2.42	0.45
1:B:258:PHE:O	1:B:293:VAL:HG22	2.17	0.45
1:B:452:ILE:O	1:B:456:GLY:N	2.46	0.45
1:B:141:ILE:HD12	1:B:141:ILE:N	2.32	0.45
3:A:42:ALA:O	3:A:46:LYS:N	2.44	0.45
3:A:205:VAL:HG12	3:A:206:ASN:H	1.82	0.45
2:E:89:PHE:C	2:E:89:PHE:CD1	2.94	0.45
1:D:258:PHE:O	1:D:293:VAL:HG22	2.17	0.45
3:C:388:ASP:N	3:C:388:ASP:OD1	2.46	0.45
3:A:219:GLN:NE2	3:A:234:LEU:HD13	2.32	0.44
3:C:341:TRP:CD1	3:C:348:CYS:HG	2.35	0.44
2:F:119:GLU:OE1	2:F:119:GLU:N	2.46	0.44
3:C:326:ILE:HD11	3:C:382:GLU:HB3	2.00	0.44
3:C:219:GLN:NE2	3:C:234:LEU:HD13	2.32	0.44
3:A:582:VAL:HG13	3:A:582:VAL:O	2.18	0.44
2:F:36:MET:CE	2:F:48:LEU:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:582:VAL:HG13	3:C:582:VAL:O	2.18	0.44
2:E:36:MET:CE	2:E:48:LEU:HD11	2.48	0.43
1:D:193:ASN:ND2	1:D:196:GLN:OE1	2.51	0.43
3:A:326:ILE:HD11	3:A:382:GLU:HB3	2.00	0.43
3:C:243:TYR:O	3:C:244:VAL:HG22	2.19	0.43
1:B:193:ASN:ND2	1:B:196:GLN:OE1	2.51	0.43
3:A:674:CYS:HB2	3:A:680:VAL:HG21	2.00	0.43
3:C:775:PHE:CE2	3:C:779:MET:HE3	2.54	0.43
3:A:243:TYR:O	3:A:244:VAL:HG22	2.19	0.43
1:B:452:ILE:HD11	1:B:457:PHE:HD2	1.84	0.42
3:A:686:MET:HE1	3:A:797:THR:HG22	2.02	0.42
3:C:42:ALA:O	3:C:46:LYS:N	2.44	0.42
1:B:176:ILE:CD1	1:B:241:ILE:HG21	2.49	0.42
1:D:452:ILE:HD11	1:D:457:PHE:HD2	1.84	0.42
3:C:277:ASP:OD1	3:C:281:ASN:N	2.53	0.42
1:B:46:ILE:N	1:B:46:ILE:HD12	2.34	0.42
3:C:686:MET:HE1	3:C:797:THR:HG22	2.01	0.42
3:C:94:LEU:HD12	3:C:94:LEU:O	2.19	0.42
3:A:576:GLN:O	3:A:577:CYS:SG	2.78	0.42
1:B:183:LEU:HA	1:B:186:ASP:OD2	2.20	0.42
3:A:339:ILE:HG23	3:A:347:THR:OG1	2.20	0.42
1:D:46:ILE:HD12	1:D:46:ILE:N	2.34	0.42
1:D:176:ILE:CD1	1:D:241:ILE:HG21	2.49	0.42
3:C:576:GLN:O	3:C:577:CYS:SG	2.78	0.42
3:C:576:GLN:OE1	3:C:576:GLN:N	2.53	0.42
3:A:576:GLN:N	3:A:576:GLN:OE1	2.53	0.42
3:A:94:LEU:O	3:A:94:LEU:HD12	2.19	0.42
3:A:775:PHE:CE2	3:A:779:MET:HE3	2.54	0.42
1:D:183:LEU:HA	1:D:186:ASP:OD2	2.20	0.41
1:D:322:PHE:HD2	1:D:681:MET:HE3	1.85	0.41
3:A:139:GLU:OE1	3:A:139:GLU:N	2.39	0.41
3:C:343:ILE:O	3:C:346:ILE:HG22	2.20	0.41
2:E:36:MET:HE1	2:E:48:LEU:HD11	2.03	0.41
2:E:7:GLU:O	2:E:11:GLU:N	2.41	0.41
1:B:609:VAL:HB	1:B:610:PRO:HD3	2.03	0.41
3:A:343:ILE:O	3:A:346:ILE:HG22	2.20	0.41
3:C:674:CYS:HB2	3:C:680:VAL:HG21	2.00	0.41
1:B:299:LEU:HD11	1:B:311:PHE:CE1	2.56	0.41
3:A:297:ASP:OD1	3:A:331:HIS:NE2	2.54	0.41
1:D:609:VAL:HB	1:D:610:PRO:HD3	2.03	0.41
3:C:339:ILE:HG23	3:C:347:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:PHE:HD2	1:B:681:MET:HE3	1.85	0.41
3:A:38:LEU:HD23	3:A:38:LEU:O	2.21	0.41
3:C:340:TYR:HB2	3:C:348:CYS:SG	2.61	0.41
1:B:187:LEU:HD23	1:B:187:LEU:O	2.21	0.41
1:B:694:ARG:NH1	2:E:54:GLU:OE2	2.54	0.41
1:D:534:PHE:CZ	1:D:538:ILE:HD11	2.56	0.41
3:C:297:ASP:OD1	3:C:331:HIS:NE2	2.54	0.41
2:E:56:ASP:OD1	2:E:59:GLY:N	2.54	0.41
2:F:36:MET:HE1	2:F:48:LEU:HD11	2.03	0.41
2:F:56:ASP:OD1	2:F:59:GLY:N	2.54	0.41
1:B:534:PHE:CZ	1:B:538:ILE:HD11	2.56	0.40
1:B:711:GLU:HG2	2:E:39:LEU:HD22	2.02	0.40
3:A:277:ASP:OD1	3:A:281:ASN:N	2.53	0.40
1:D:299:LEU:HD11	1:D:311:PHE:CE1	2.56	0.40
3:C:762:LEU:HD22	3:C:771:ALA:CB	2.51	0.40
3:A:340:TYR:HB2	3:A:348:CYS:SG	2.61	0.40
3:C:139:GLU:OE1	3:C:139:GLU:N	2.39	0.40
3:C:265:LEU:HD23	3:C:265:LEU:O	2.21	0.40
3:A:265:LEU:O	3:A:265:LEU:HD23	2.21	0.40
1:D:565:LEU:O	1:D:571:SER:OG	2.31	0.40
1:B:225:LEU:HD22	1:B:232:TRP:CE3	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	B	668/984 (68%)	651 (98%)	17 (2%)	0	100	100
1	D	668/984 (68%)	651 (98%)	17 (2%)	0	100	100
2	E	125/149 (84%)	121 (97%)	4 (3%)	0	100	100
2	F	125/149 (84%)	121 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	711/882 (81%)	690 (97%)	21 (3%)	0	100	100
3	C	711/882 (81%)	690 (97%)	21 (3%)	0	100	100
All	All	3008/4030 (75%)	2924 (97%)	84 (3%)	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	543/812 (67%)	542 (100%)	1 (0%)	87	87
1	D	543/812 (67%)	542 (100%)	1 (0%)	87	87
2	E	105/127 (83%)	105 (100%)	0	100	100
2	F	105/127 (83%)	105 (100%)	0	100	100
3	A	620/787 (79%)	612 (99%)	8 (1%)	61	73
3	C	620/787 (79%)	612 (99%)	8 (1%)	61	73
All	All	2536/3452 (74%)	2518 (99%)	18 (1%)	73	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	328	ILE
3	A	102	ASP
3	A	105	ILE
3	A	209	CYS
3	A	215	CYS
3	A	225	ASP
3	A	261	GLU
3	A	388	ASP
3	A	577	CYS
1	D	328	ILE
3	C	102	ASP
3	C	105	ILE

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Mol	Chain	Res	Type
3	C	209	CYS
3	C	215	CYS
3	C	225	ASP
3	C	261	GLU
3	C	388	ASP
3	C	577	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	155	ASN
1	B	185	GLN
1	B	208	GLN
2	E	107	HIS
3	A	88	HIS
3	A	169	ASN
3	A	806	ASN
2	F	107	HIS
1	D	155	ASN
1	D	185	GLN
1	D	208	GLN
1	D	693	GLN
3	C	88	HIS
3	C	169	ASN
3	C	806	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

14 ligands are modelled in this entry.

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	1003	-	34,34,51	1.38	3 (8%)	40,42,59	1.03	4 (10%)
4	6OU	B	1001	-	44,44,48	0.94	4 (9%)	47,49,53	0.89	2 (4%)
4	6OU	D	1002	-	45,45,48	0.94	4 (8%)	48,50,53	0.86	2 (4%)
6	A1B32	A	901	-	48,49,49	1.81	8 (16%)	69,78,78	3.27	34 (49%)
4	6OU	C	902	-	41,41,48	0.98	4 (9%)	44,46,53	1.14	3 (6%)
4	6OU	A	904	-	41,41,48	0.98	4 (9%)	44,46,53	1.19	4 (9%)
4	6OU	C	904	-	41,41,48	0.99	4 (9%)	44,46,53	1.19	4 (9%)
4	6OU	A	902	-	41,41,48	0.98	4 (9%)	44,46,53	1.14	3 (6%)
4	6OU	B	1002	-	45,45,48	0.94	4 (8%)	48,50,53	0.86	2 (4%)
6	A1B32	C	901	-	48,49,49	1.81	8 (16%)	69,78,78	3.27	34 (49%)
7	D39	A	903	-	34,35,51	1.41	5 (14%)	36,42,58	1.06	2 (5%)
7	D39	C	903	-	34,35,51	1.40	5 (14%)	36,42,58	1.06	2 (5%)
5	LBN	B	1003	-	34,34,51	1.38	3 (8%)	40,42,59	1.03	4 (10%)
4	6OU	D	1001	-	44,44,48	0.93	4 (9%)	47,49,53	0.89	2 (4%)

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	1003	-	-	14/38/38/55	-
4	6OU	B	1001	-	-	16/48/48/52	-
4	6OU	D	1002	-	-	24/49/49/52	-
6	A1B32	A	901	-	-	9/22/85/85	0/7/7/7
4	6OU	C	902	-	-	19/45/45/52	-
4	6OU	A	904	-	-	26/45/45/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6OU	C	904	-	-	26/45/45/52	-
4	6OU	A	902	-	-	19/45/45/52	-
4	6OU	B	1002	-	-	24/49/49/52	-
6	A1B32	C	901	-	-	9/22/85/85	0/7/7/7
7	D39	A	903	-	-	18/41/41/57	-
7	D39	C	903	-	-	18/41/41/57	-
5	LBN	B	1003	-	-	15/38/38/55	-
4	6OU	D	1001	-	-	16/48/48/52	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	901	A1B32	C02-C11	6.27	1.66	1.57
6	C	901	A1B32	C02-C11	6.27	1.66	1.57
6	C	901	A1B32	C08-C09	5.09	1.61	1.53
6	A	901	A1B32	C08-C09	5.09	1.61	1.53
5	B	1003	LBN	P1-O2	4.95	1.78	1.59
5	D	1003	LBN	P1-O2	4.94	1.78	1.59
7	A	903	D39	O6-C21	3.92	1.45	1.34
7	C	903	D39	O6-C21	3.89	1.45	1.34
6	A	901	A1B32	C11-C12	3.45	1.60	1.54
6	C	901	A1B32	C11-C12	3.43	1.60	1.54
7	A	903	D39	O4-C5	3.36	1.43	1.33
7	C	903	D39	O4-C5	3.35	1.43	1.33
6	A	901	A1B32	C21-C17	3.23	1.55	1.48
6	C	901	A1B32	C21-C17	3.20	1.55	1.48
6	A	901	A1B32	C22-C21	2.71	1.43	1.39
6	C	901	A1B32	C22-C21	2.71	1.43	1.39
4	C	904	6OU	O30-C20	-2.67	1.40	1.46
4	B	1002	6OU	O30-C20	-2.66	1.40	1.46
4	D	1002	6OU	O30-C20	-2.66	1.40	1.46
4	C	902	6OU	O30-C20	-2.66	1.40	1.46
4	A	904	6OU	O30-C20	-2.64	1.40	1.46
4	A	902	6OU	O30-C20	-2.63	1.40	1.46
4	B	1001	6OU	O30-C20	-2.62	1.40	1.46
4	D	1001	6OU	O30-C20	-2.62	1.40	1.46
6	A	901	A1B32	C16-C14	2.59	1.49	1.41
6	C	901	A1B32	C30-C06	2.59	1.58	1.54
6	C	901	A1B32	C16-C14	2.55	1.49	1.41
6	A	901	A1B32	C30-C06	2.53	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	6OU	O18-C16	2.46	1.40	1.33
4	D	1001	6OU	O18-C16	2.45	1.40	1.33
4	C	902	6OU	O18-C16	2.45	1.40	1.33
4	B	1002	6OU	O18-C16	2.45	1.40	1.33
4	C	904	6OU	O18-C16	2.45	1.40	1.33
4	A	902	6OU	O18-C16	2.44	1.40	1.33
7	C	903	D39	C6-C5	2.44	1.57	1.50
7	A	903	D39	C6-C5	2.43	1.57	1.50
4	D	1002	6OU	O18-C16	2.42	1.40	1.33
4	A	904	6OU	O18-C16	2.42	1.40	1.33
7	C	903	D39	C22-C21	2.31	1.57	1.50
7	A	903	D39	C22-C21	2.29	1.57	1.50
5	B	1003	LBN	O2-C9	-2.25	1.35	1.44
5	D	1003	LBN	O2-C9	-2.24	1.35	1.44
6	C	901	A1B32	C31-C06	2.22	1.57	1.53
6	A	901	A1B32	C31-C06	2.22	1.57	1.53
4	B	1002	6OU	O18-C19	-2.19	1.40	1.45
4	A	904	6OU	O18-C19	-2.18	1.40	1.45
4	D	1002	6OU	O18-C19	-2.16	1.40	1.45
4	C	904	6OU	O30-C31	2.15	1.40	1.34
4	A	902	6OU	O18-C19	-2.15	1.40	1.45
4	B	1002	6OU	O30-C31	2.15	1.40	1.34
4	D	1002	6OU	O30-C31	2.14	1.40	1.34
4	C	904	6OU	O18-C19	-2.13	1.40	1.45
4	C	902	6OU	O18-C19	-2.13	1.40	1.45
4	B	1001	6OU	O18-C19	-2.12	1.40	1.45
4	D	1001	6OU	O18-C19	-2.12	1.40	1.45
4	A	902	6OU	O30-C31	2.11	1.40	1.34
4	A	904	6OU	O30-C31	2.10	1.40	1.34
4	B	1001	6OU	O30-C31	2.10	1.40	1.34
4	C	902	6OU	O30-C31	2.09	1.40	1.34
5	B	1003	LBN	P1-O1	2.09	1.67	1.59
4	D	1001	6OU	O30-C31	2.09	1.40	1.34
5	D	1003	LBN	P1-O1	2.07	1.67	1.59
7	A	903	D39	P-O3	2.04	1.67	1.59
7	C	903	D39	P-O3	2.04	1.67	1.59

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	901	A1B32	C28-C10-C09	-7.70	100.43	111.61
6	A	901	A1B32	C28-C10-C09	-7.68	100.45	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	901	A1B32	C16-C14-C13	-7.60	115.53	122.34
6	C	901	A1B32	C16-C14-C13	-7.57	115.55	122.34
6	C	901	A1B32	O38-C39-C41	7.12	125.01	111.79
6	A	901	A1B32	O38-C39-C41	7.12	125.01	111.79
6	C	901	A1B32	C01-C02-C07	-6.98	100.06	112.94
6	A	901	A1B32	C01-C02-C07	-6.96	100.08	112.94
6	A	901	A1B32	C26-C21-C22	-6.87	109.96	117.61
6	C	901	A1B32	C26-C21-C22	-6.87	109.96	117.61
6	C	901	A1B32	O15-C14-C16	6.44	122.94	115.08
6	A	901	A1B32	O15-C14-C16	6.40	122.89	115.08
6	A	901	A1B32	C06-C07-C02	6.17	124.97	117.01
6	C	901	A1B32	C06-C07-C02	6.16	124.96	117.01
6	C	901	A1B32	O27-C12-C13	-5.90	99.79	110.13
6	A	901	A1B32	O27-C12-C13	-5.89	99.80	110.13
6	C	901	A1B32	C08-C07-C06	-5.88	107.47	114.36
6	A	901	A1B32	C08-C07-C06	-5.87	107.48	114.36
6	A	901	A1B32	C07-C02-C11	4.83	114.86	106.83
6	C	901	A1B32	C07-C02-C11	4.82	114.85	106.83
6	C	901	A1B32	O18-C17-C16	-4.79	116.07	121.02
6	A	901	A1B32	O18-C17-C16	-4.73	116.13	121.02
6	A	901	A1B32	O38-C39-O40	-4.58	115.67	123.95
6	C	901	A1B32	O38-C39-O40	-4.58	115.68	123.95
6	A	901	A1B32	C30-C06-C07	-4.47	104.69	112.94
6	C	901	A1B32	C30-C06-C07	-4.46	104.70	112.94
4	A	902	6OU	C12-C11-C10	4.38	136.51	114.37
4	C	904	6OU	C12-C11-C10	4.38	136.50	114.37
4	C	902	6OU	C12-C11-C10	4.38	136.49	114.37
4	A	904	6OU	C12-C11-C10	4.37	136.48	114.37
6	A	901	A1B32	C25-C26-C21	4.31	124.60	120.36
6	C	901	A1B32	C25-C26-C21	4.29	124.58	120.36
7	C	903	D39	O6-C21-C22	3.94	120.00	111.48
7	A	903	D39	O6-C21-C22	3.93	119.99	111.48
4	D	1002	6OU	O30-C31-C33	3.88	119.87	111.48
4	B	1002	6OU	O30-C31-C33	3.87	119.86	111.48
6	C	901	A1B32	C17-C16-C14	3.80	123.69	119.00
4	A	904	6OU	O30-C31-C33	3.79	119.68	111.48
6	A	901	A1B32	C17-C16-C14	3.77	123.66	119.00
4	C	904	6OU	O30-C31-C33	3.77	119.63	111.48
6	C	901	A1B32	C01-C02-C11	3.67	122.28	113.19
6	A	901	A1B32	C01-C02-C11	3.66	122.25	113.19
4	D	1001	6OU	O30-C31-C33	3.61	119.30	111.48
4	A	902	6OU	O30-C31-C33	3.61	119.28	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	902	6OU	O30-C31-C33	3.61	119.28	111.48
4	B	1001	6OU	O30-C31-C33	3.61	119.28	111.48
6	A	901	A1B32	C30-C06-C05	3.49	116.41	109.75
6	C	901	A1B32	C30-C06-C05	3.47	116.39	109.75
5	D	1003	LBN	O3-P1-O4	3.44	128.47	112.44
5	B	1003	LBN	O3-P1-O4	3.44	128.45	112.44
6	A	901	A1B32	C01-C02-C03	-3.39	102.92	108.31
6	C	901	A1B32	C01-C02-C03	-3.38	102.92	108.31
6	A	901	A1B32	O29-C09-C10	-3.35	107.58	111.89
6	C	901	A1B32	O29-C09-C10	-3.33	107.60	111.89
6	C	901	A1B32	O32-C31-C06	3.33	116.25	109.28
6	A	901	A1B32	O32-C31-C06	3.30	116.20	109.28
6	A	901	A1B32	C05-O38-C39	-3.17	112.67	118.20
6	C	901	A1B32	C05-O38-C39	-3.16	112.67	118.20
6	C	901	A1B32	C07-C08-C09	3.14	117.97	111.38
6	A	901	A1B32	C07-C08-C09	3.12	117.94	111.38
6	A	901	A1B32	O15-C10-C28	3.05	112.28	105.93
6	C	901	A1B32	O15-C10-C28	3.04	112.25	105.93
6	C	901	A1B32	O18-C19-C13	2.90	121.33	117.51
6	A	901	A1B32	O18-C19-C13	2.85	121.26	117.51
6	C	901	A1B32	O18-C17-C21	2.83	115.32	111.68
6	A	901	A1B32	O18-C17-C21	2.81	115.29	111.68
4	A	904	6OU	O18-C16-C15	2.79	120.35	111.83
4	C	904	6OU	O18-C16-C15	2.78	120.31	111.83
4	A	902	6OU	O18-C16-C15	2.76	120.27	111.83
4	C	902	6OU	O18-C16-C15	2.76	120.26	111.83
4	B	1001	6OU	O18-C16-C15	2.75	120.22	111.83
5	D	1003	LBN	C2-O7-C34	2.75	124.38	117.80
4	D	1001	6OU	O18-C16-C15	2.74	120.20	111.83
5	B	1003	LBN	C2-O7-C34	2.74	124.35	117.80
6	C	901	A1B32	O29-C09-C08	-2.70	103.63	109.12
6	A	901	A1B32	O29-C09-C08	-2.69	103.64	109.12
6	C	901	A1B32	C03-C04-C05	2.67	115.71	110.66
6	A	901	A1B32	C03-C04-C05	2.65	115.67	110.66
6	C	901	A1B32	O32-C33-C35	-2.65	107.56	112.00
6	A	901	A1B32	C08-C09-C10	2.64	117.95	111.31
6	C	901	A1B32	C04-C03-C02	-2.64	108.29	112.74
6	C	901	A1B32	C08-C09-C10	2.63	117.92	111.31
6	A	901	A1B32	C04-C03-C02	-2.63	108.31	112.74
6	A	901	A1B32	O32-C33-C35	-2.62	107.61	112.00
7	A	903	D39	O4-C5-C6	2.62	119.82	111.83
7	C	903	D39	O4-C5-C6	2.62	119.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	901	A1B32	C08-C07-C02	-2.55	107.78	111.01
6	C	901	A1B32	C08-C07-C02	-2.55	107.79	111.01
5	D	1003	LBN	O2-P1-O4	-2.52	98.94	108.94
5	B	1003	LBN	O2-P1-O4	-2.52	98.96	108.94
4	D	1002	6OU	O18-C16-C15	2.40	119.15	111.83
4	B	1002	6OU	O18-C16-C15	2.38	119.11	111.83
6	C	901	A1B32	C21-C22-N23	2.37	127.03	123.50
4	C	904	6OU	C20-O30-C31	-2.35	112.17	117.80
4	A	904	6OU	C20-O30-C31	-2.35	112.17	117.80
6	A	901	A1B32	C21-C22-N23	2.35	126.99	123.50
6	C	901	A1B32	C17-O18-C19	-2.33	120.22	122.82
6	A	901	A1B32	C17-O18-C19	-2.32	120.24	122.82
6	C	901	A1B32	C26-C21-C17	2.32	124.45	120.77
6	A	901	A1B32	C26-C21-C17	2.31	124.44	120.77
5	D	1003	LBN	C3-C2-C1	-2.06	106.99	111.78
5	B	1003	LBN	C3-C2-C1	-2.04	107.02	111.78

There are no chirality outliers.

All (253) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	6OU	C27-O26-P23-O25
4	B	1002	6OU	C21-O22-P23-O24
4	B	1002	6OU	C21-O22-P23-O25
4	B	1002	6OU	C21-O22-P23-O26
4	B	1002	6OU	O26-C27-C28-N29
4	A	902	6OU	C27-O26-P23-O22
4	A	902	6OU	C27-O26-P23-O25
4	A	902	6OU	O26-C27-C28-N29
4	A	902	6OU	C33-C31-O30-C20
4	A	904	6OU	O30-C20-C21-O22
4	A	904	6OU	C21-O22-P23-O24
4	A	904	6OU	C21-O22-P23-O26
4	A	904	6OU	O26-C27-C28-N29
4	A	904	6OU	C33-C31-O30-C20
4	D	1001	6OU	C27-O26-P23-O25
4	D	1002	6OU	C21-O22-P23-O24
4	D	1002	6OU	C21-O22-P23-O25
4	D	1002	6OU	C21-O22-P23-O26
4	D	1002	6OU	O26-C27-C28-N29
4	C	902	6OU	C27-O26-P23-O22
4	C	902	6OU	C27-O26-P23-O25

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Mol	Chain	Res	Type	Atoms
4	C	902	6OU	O26-C27-C28-N29
4	C	902	6OU	C33-C31-O30-C20
4	C	904	6OU	O30-C20-C21-O22
4	C	904	6OU	C21-O22-P23-O24
4	C	904	6OU	C21-O22-P23-O26
4	C	904	6OU	O26-C27-C28-N29
4	C	904	6OU	C33-C31-O30-C20
5	B	1003	LBN	C1-O1-P1-O2
5	B	1003	LBN	C1-O1-P1-O3
5	B	1003	LBN	N1-C6-C9-O2
5	D	1003	LBN	C1-O1-P1-O2
5	D	1003	LBN	C1-O1-P1-O3
5	D	1003	LBN	N1-C6-C9-O2
6	A	901	A1B32	O32-C33-C35-C37
6	A	901	A1B32	O38-C39-C41-C42
6	A	901	A1B32	O40-C39-C41-C42
6	C	901	A1B32	O32-C33-C35-C37
6	C	901	A1B32	O38-C39-C41-C42
6	C	901	A1B32	O40-C39-C41-C42
7	A	903	D39	N-C-C1-O
7	A	903	D39	C39-C-C1-O
7	A	903	D39	C1-O-P-O3
7	A	903	D39	C1-O-P-O2
7	C	903	D39	N-C-C1-O
7	C	903	D39	C39-C-C1-O
7	C	903	D39	C1-O-P-O3
7	C	903	D39	C1-O-P-O2
7	A	903	D39	O5-C5-O4-C4
7	C	903	D39	O5-C5-O4-C4
7	A	903	D39	C6-C5-O4-C4
7	C	903	D39	C6-C5-O4-C4
4	B	1002	6OU	O32-C31-O30-C20
4	A	904	6OU	O32-C31-O30-C20
4	D	1002	6OU	O32-C31-O30-C20
4	C	904	6OU	O32-C31-O30-C20
5	B	1003	LBN	C26-C25-O5-C3
5	D	1003	LBN	C26-C25-O5-C3
4	B	1002	6OU	C33-C31-O30-C20
4	D	1002	6OU	C33-C31-O30-C20
4	A	902	6OU	O32-C31-O30-C20
4	C	902	6OU	O32-C31-O30-C20
5	B	1003	LBN	O6-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
5	D	1003	LBN	O6-C25-O5-C3
6	A	901	A1B32	C41-C39-O38-C05
6	C	901	A1B32	C41-C39-O38-C05
4	A	902	6OU	C15-C16-O18-C19
4	A	904	6OU	C15-C16-O18-C19
4	C	902	6OU	C15-C16-O18-C19
4	C	904	6OU	C15-C16-O18-C19
4	A	904	6OU	C31-C33-C34-C35
4	C	904	6OU	C31-C33-C34-C35
5	B	1003	LBN	C25-C26-C27-C28
5	D	1003	LBN	C25-C26-C27-C28
6	A	901	A1B32	O40-C39-O38-C05
6	C	901	A1B32	O40-C39-O38-C05
4	A	904	6OU	O17-C16-O18-C19
4	C	904	6OU	O17-C16-O18-C19
4	A	902	6OU	O17-C16-O18-C19
4	C	902	6OU	O17-C16-O18-C19
4	A	904	6OU	C13-C14-C15-C16
4	C	904	6OU	C13-C14-C15-C16
4	B	1001	6OU	C15-C16-O18-C19
4	D	1001	6OU	C15-C16-O18-C19
7	A	903	D39	C21-C22-C23-C24
7	C	903	D39	C21-C22-C23-C24
4	B	1001	6OU	C45-C46-C47-C48
4	A	902	6OU	C06-C07-C08-C09
4	D	1001	6OU	C45-C46-C47-C48
4	C	902	6OU	C06-C07-C08-C09
5	B	1003	LBN	C38-C39-C40-C41
5	D	1003	LBN	C38-C39-C40-C41
4	A	904	6OU	C35-C36-C37-C38
4	C	904	6OU	C35-C36-C37-C38
4	A	902	6OU	C05-C06-C07-C08
4	C	902	6OU	C05-C06-C07-C08
4	B	1001	6OU	O17-C16-O18-C19
4	D	1001	6OU	O17-C16-O18-C19
4	A	904	6OU	C36-C37-C38-C39
4	C	904	6OU	C36-C37-C38-C39
4	D	1001	6OU	C43-C44-C45-C46
4	B	1001	6OU	C43-C44-C45-C46
4	D	1002	6OU	C07-C08-C09-C10
4	B	1002	6OU	C07-C08-C09-C10
4	B	1002	6OU	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
4	D	1002	6OU	C42-C43-C44-C45
7	A	903	D39	C25-C26-C27-C28
7	C	903	D39	C25-C26-C27-C28
5	B	1003	LBN	C35-C34-O7-C2
5	D	1003	LBN	C35-C34-O7-C2
7	A	903	D39	C22-C21-O6-C3
7	C	903	D39	C22-C21-O6-C3
5	B	1003	LBN	O8-C34-O7-C2
5	D	1003	LBN	O8-C34-O7-C2
7	A	903	D39	O7-C21-O6-C3
7	C	903	D39	O7-C21-O6-C3
4	B	1001	6OU	C37-C38-C39-C40
4	B	1002	6OU	C37-C38-C39-C40
4	D	1001	6OU	C37-C38-C39-C40
4	D	1002	6OU	C37-C38-C39-C40
4	B	1002	6OU	C12-C13-C14-C15
4	D	1002	6OU	C12-C13-C14-C15
4	B	1002	6OU	O30-C20-C21-O22
4	D	1002	6OU	O30-C20-C21-O22
5	B	1003	LBN	C39-C40-C41-C42
5	D	1003	LBN	C39-C40-C41-C42
4	D	1002	6OU	C13-C14-C15-C16
4	D	1002	6OU	C33-C34-C35-C36
4	B	1002	6OU	C33-C34-C35-C36
4	B	1002	6OU	C13-C14-C15-C16
5	B	1003	LBN	C26-C27-C28-C29
5	D	1003	LBN	C26-C27-C28-C29
4	B	1001	6OU	C31-C33-C34-C35
4	D	1001	6OU	C31-C33-C34-C35
4	A	904	6OU	C09-C10-C11-C12
4	C	904	6OU	C09-C10-C11-C12
4	B	1001	6OU	O18-C19-C20-C21
4	D	1001	6OU	O18-C19-C20-C21
4	A	904	6OU	C04-C05-C06-C07
4	C	904	6OU	C04-C05-C06-C07
4	B	1002	6OU	C41-C42-C43-C44
4	D	1002	6OU	C41-C42-C43-C44
4	A	902	6OU	C03-C04-C05-C06
4	C	902	6OU	C03-C04-C05-C06
6	A	901	A1B32	O32-C33-C35-C36
6	C	901	A1B32	O32-C33-C35-C36
4	A	902	6OU	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	C	902	6OU	C35-C36-C37-C38
4	A	902	6OU	O18-C19-C20-O30
4	C	902	6OU	O18-C19-C20-O30
4	D	1002	6OU	C35-C36-C37-C38
4	B	1002	6OU	C35-C36-C37-C38
4	A	904	6OU	C08-C09-C10-C11
4	C	904	6OU	C08-C09-C10-C11
7	C	903	D39	C23-C24-C25-C26
7	A	903	D39	C23-C24-C25-C26
4	B	1002	6OU	C19-C20-C21-O22
4	A	904	6OU	C19-C20-C21-O22
4	D	1002	6OU	C19-C20-C21-O22
4	C	904	6OU	C19-C20-C21-O22
7	A	903	D39	O3-C2-C3-C4
7	C	903	D39	O3-C2-C3-C4
4	B	1001	6OU	C41-C42-C43-C44
4	D	1001	6OU	C41-C42-C43-C44
4	D	1002	6OU	C02-C03-C04-C05
4	B	1002	6OU	C02-C03-C04-C05
4	A	902	6OU	C19-C20-C21-O22
4	C	902	6OU	C19-C20-C21-O22
5	B	1003	LBN	C3-C2-O7-C34
5	D	1003	LBN	C3-C2-O7-C34
4	A	902	6OU	O18-C19-C20-C21
4	A	904	6OU	O18-C19-C20-C21
4	C	902	6OU	O18-C19-C20-C21
4	C	904	6OU	O18-C19-C20-C21
4	B	1001	6OU	O18-C19-C20-O30
4	D	1001	6OU	O18-C19-C20-O30
6	A	901	A1B32	O34-C33-C35-C37
6	C	901	A1B32	O34-C33-C35-C37
7	A	903	D39	C-C1-O-P
7	C	903	D39	C-C1-O-P
6	A	901	A1B32	C30-C06-C31-O32
6	C	901	A1B32	C30-C06-C31-O32
4	A	902	6OU	O30-C20-C21-O22
4	C	902	6OU	O30-C20-C21-O22
7	A	903	D39	O3-C2-C3-O6
7	C	903	D39	O3-C2-C3-O6
4	A	904	6OU	O18-C19-C20-O30
4	C	904	6OU	O18-C19-C20-O30
4	B	1002	6OU	C27-O26-P23-O22

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Mol	Chain	Res	Type	Atoms
4	B	1002	6OU	C27-O26-P23-O25
4	A	902	6OU	C27-O26-P23-O24
4	D	1002	6OU	C27-O26-P23-O22
4	D	1002	6OU	C27-O26-P23-O25
4	C	902	6OU	C27-O26-P23-O24
7	A	903	D39	C1-O-P-O1
7	C	903	D39	C1-O-P-O1
4	B	1002	6OU	C20-C21-O22-P23
4	D	1002	6OU	C20-C21-O22-P23
4	A	904	6OU	C01-C02-C03-C04
4	C	904	6OU	C01-C02-C03-C04
4	C	904	6OU	C06-C07-C08-C09
4	A	904	6OU	C06-C07-C08-C09
4	B	1002	6OU	C04-C05-C06-C07
4	D	1002	6OU	C04-C05-C06-C07
4	B	1001	6OU	C36-C37-C38-C39
4	A	902	6OU	C12-C13-C14-C15
4	D	1001	6OU	C36-C37-C38-C39
4	C	902	6OU	C12-C13-C14-C15
4	A	904	6OU	C05-C06-C07-C08
4	C	904	6OU	C05-C06-C07-C08
4	B	1002	6OU	C40-C41-C42-C43
4	A	902	6OU	C38-C39-C40-C41
4	D	1002	6OU	C40-C41-C42-C43
4	C	902	6OU	C38-C39-C40-C41
4	B	1001	6OU	C19-C20-O30-C31
4	B	1001	6OU	C21-C20-O30-C31
4	D	1001	6OU	C19-C20-O30-C31
4	D	1001	6OU	C21-C20-O30-C31
7	A	903	D39	C27-C28-C29-C30
7	C	903	D39	C27-C28-C29-C30
5	B	1003	LBN	O1-C1-C2-O7
5	D	1003	LBN	O1-C1-C2-O7
5	B	1003	LBN	O1-C1-C2-C3
5	D	1003	LBN	O1-C1-C2-C3
4	B	1001	6OU	C40-C41-C42-C43
4	D	1001	6OU	C40-C41-C42-C43
4	A	902	6OU	C07-C08-C09-C10
4	C	902	6OU	C07-C08-C09-C10
4	A	904	6OU	C38-C39-C40-C41
4	C	904	6OU	C38-C39-C40-C41
7	A	903	D39	O6-C21-C22-C23

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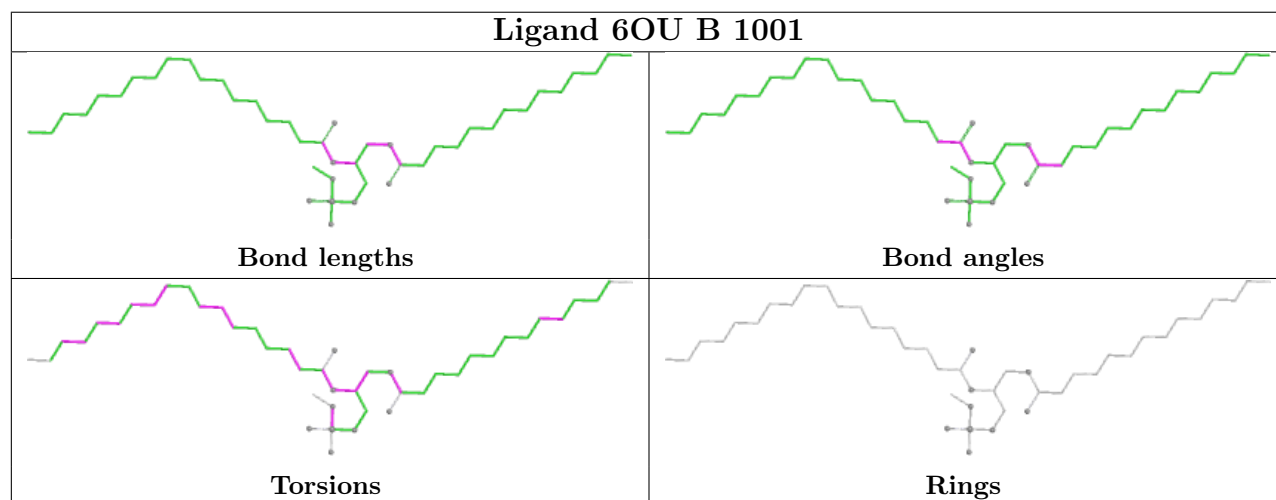
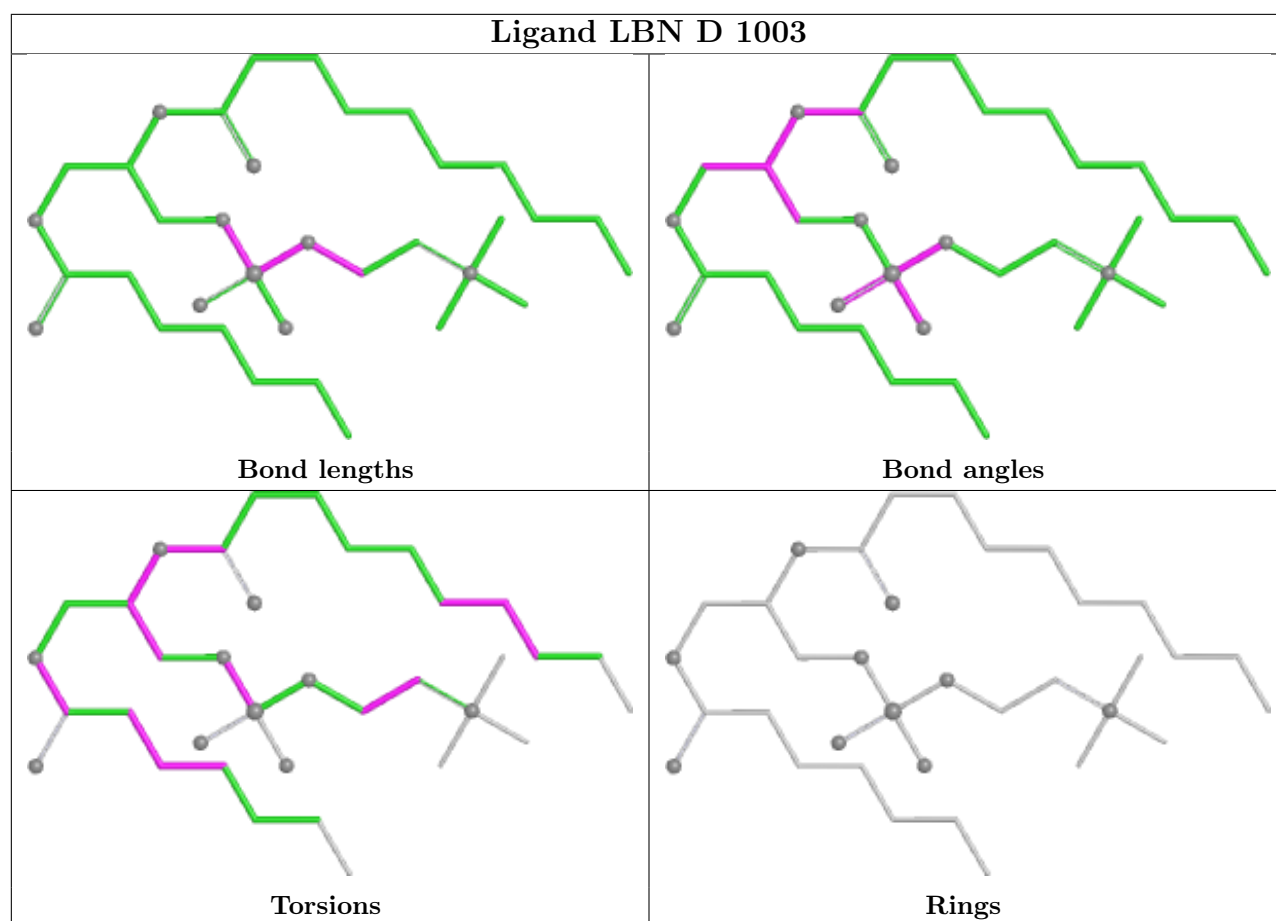
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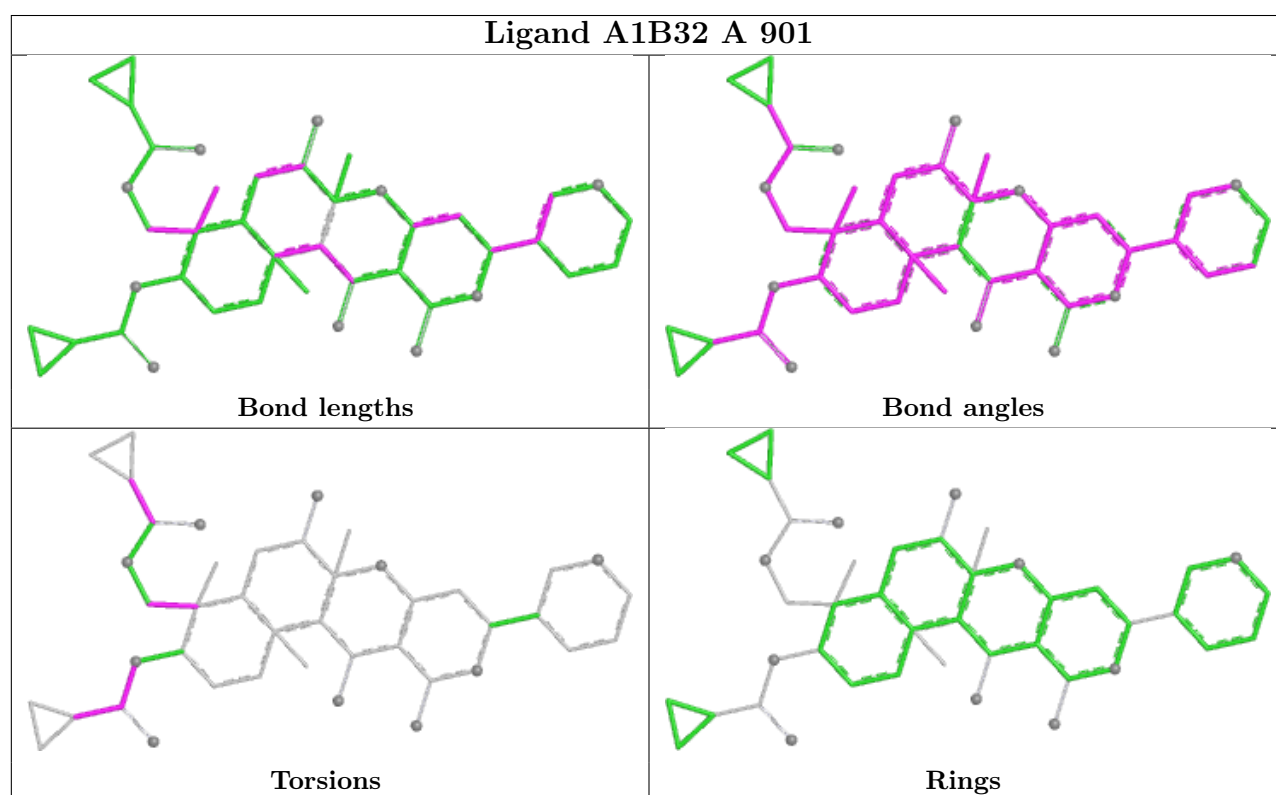
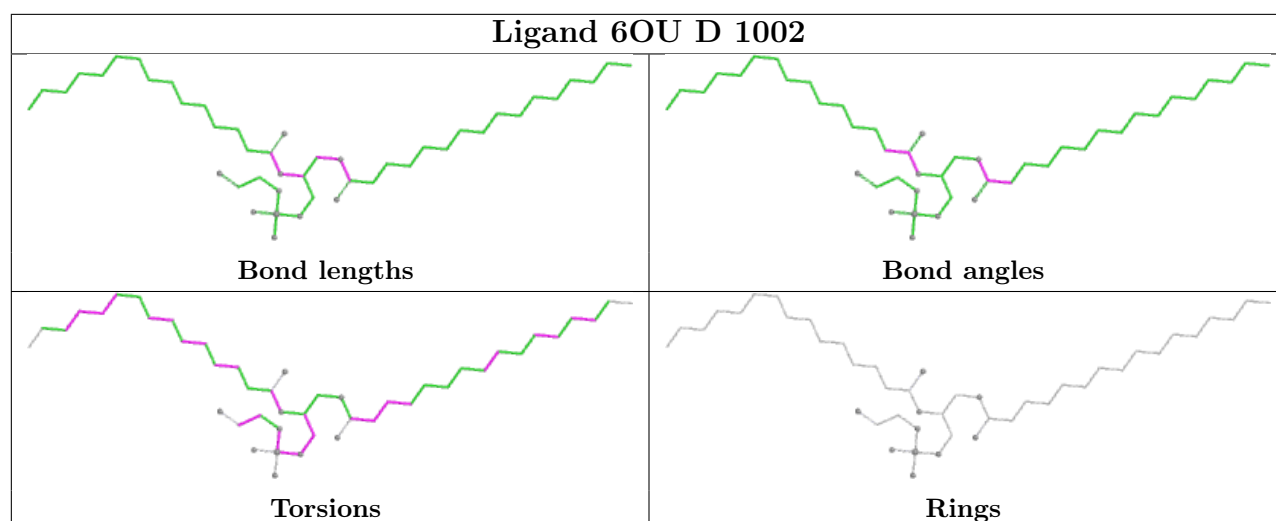
Mol	Chain	Res	Type	Atoms
7	C	903	D39	O6-C21-C22-C23
4	A	904	6OU	C07-C08-C09-C10
4	C	904	6OU	C07-C08-C09-C10
4	B	1002	6OU	C14-C15-C16-O18
4	D	1002	6OU	C14-C15-C16-O18
4	D	1001	6OU	O32-C31-O30-C20
6	A	901	A1B32	O40-C39-C41-C43
6	C	901	A1B32	O40-C39-C41-C43
4	B	1001	6OU	O32-C31-O30-C20
4	C	904	6OU	C12-C13-C14-C15
4	A	904	6OU	C12-C13-C14-C15
4	A	904	6OU	C14-C15-C16-O18
4	C	904	6OU	C14-C15-C16-O18
4	B	1001	6OU	C06-C07-C08-C09
4	D	1001	6OU	C06-C07-C08-C09
4	D	1002	6OU	C14-C15-C16-O17
4	B	1002	6OU	C14-C15-C16-O17
7	C	903	D39	O7-C21-C22-C23
7	A	903	D39	O7-C21-C22-C23
4	A	904	6OU	C14-C15-C16-O17
4	C	904	6OU	C14-C15-C16-O17
5	B	1003	LBN	C37-C38-C39-C40

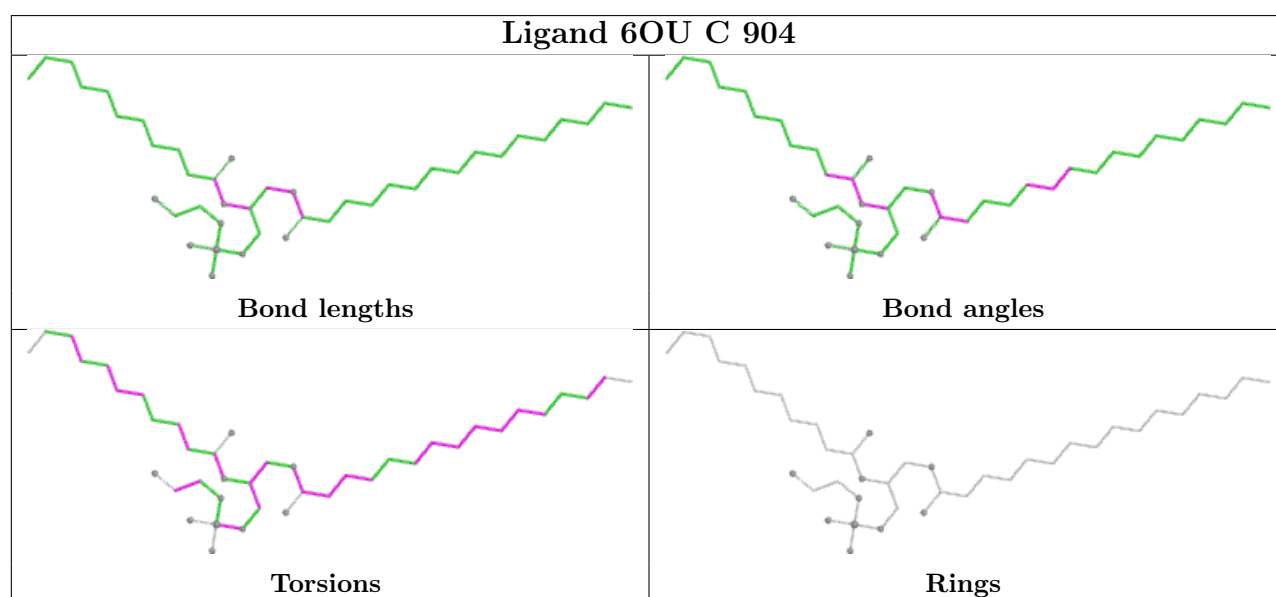
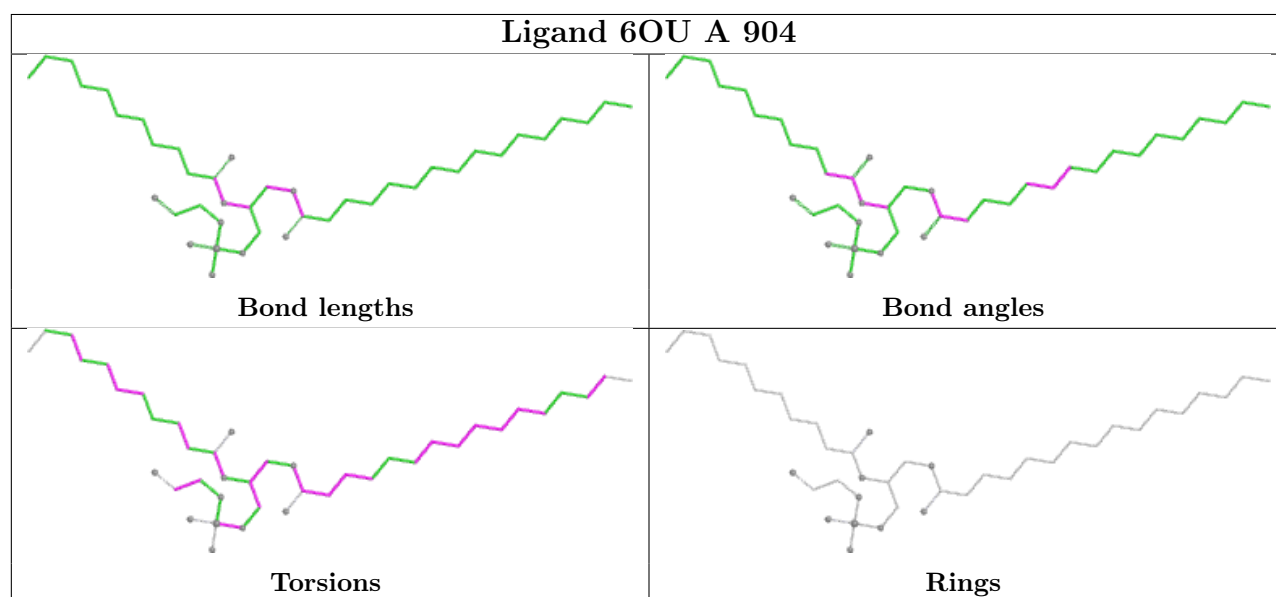
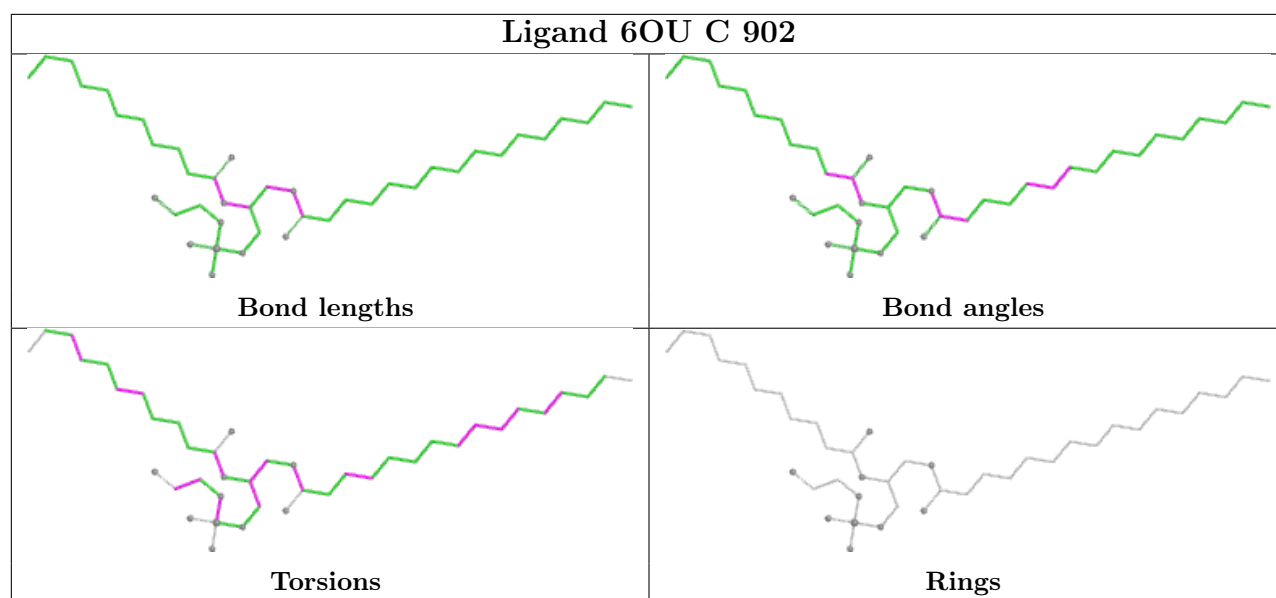
There are no ring outliers.

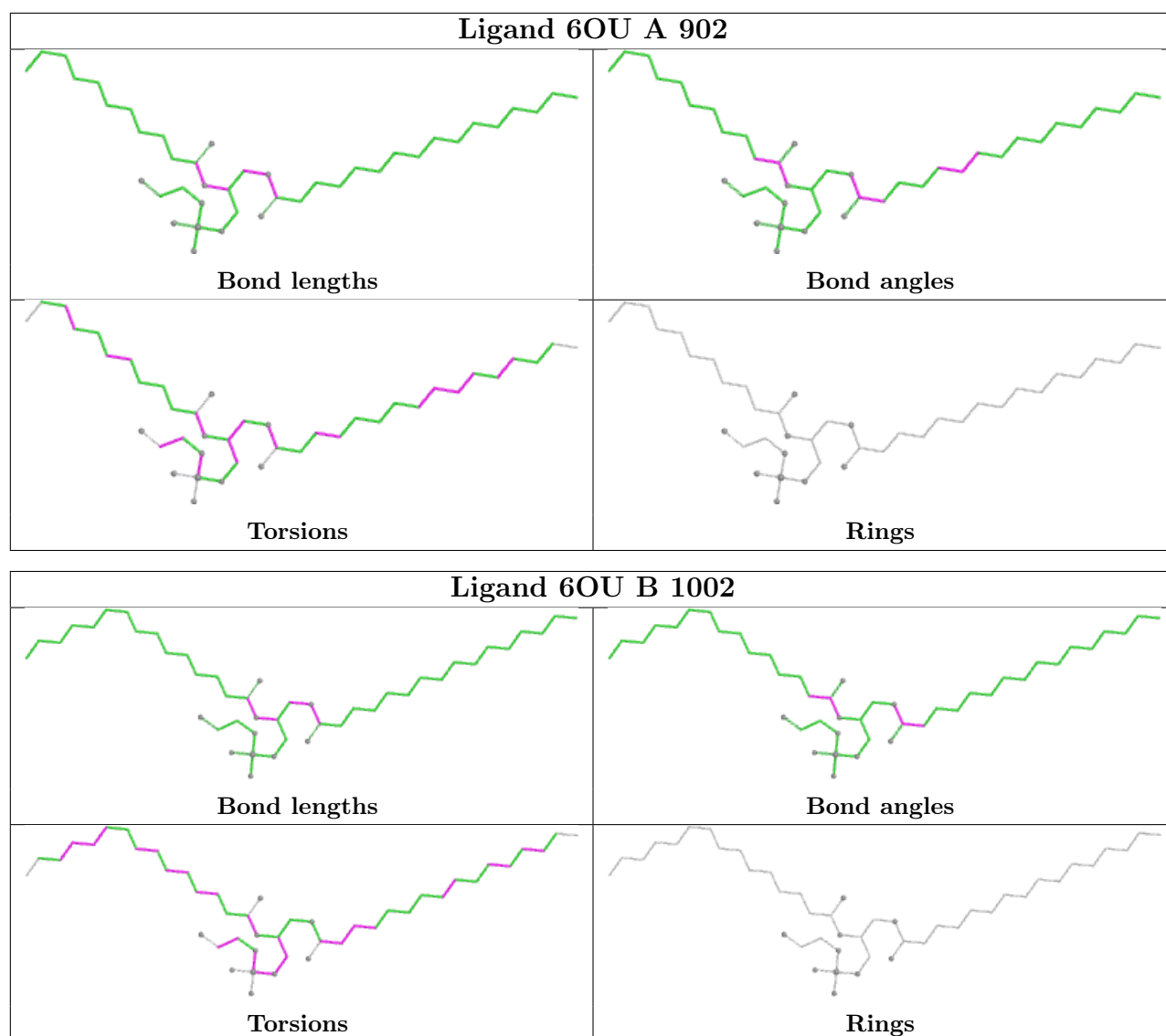
No monomer is involved in short contacts.

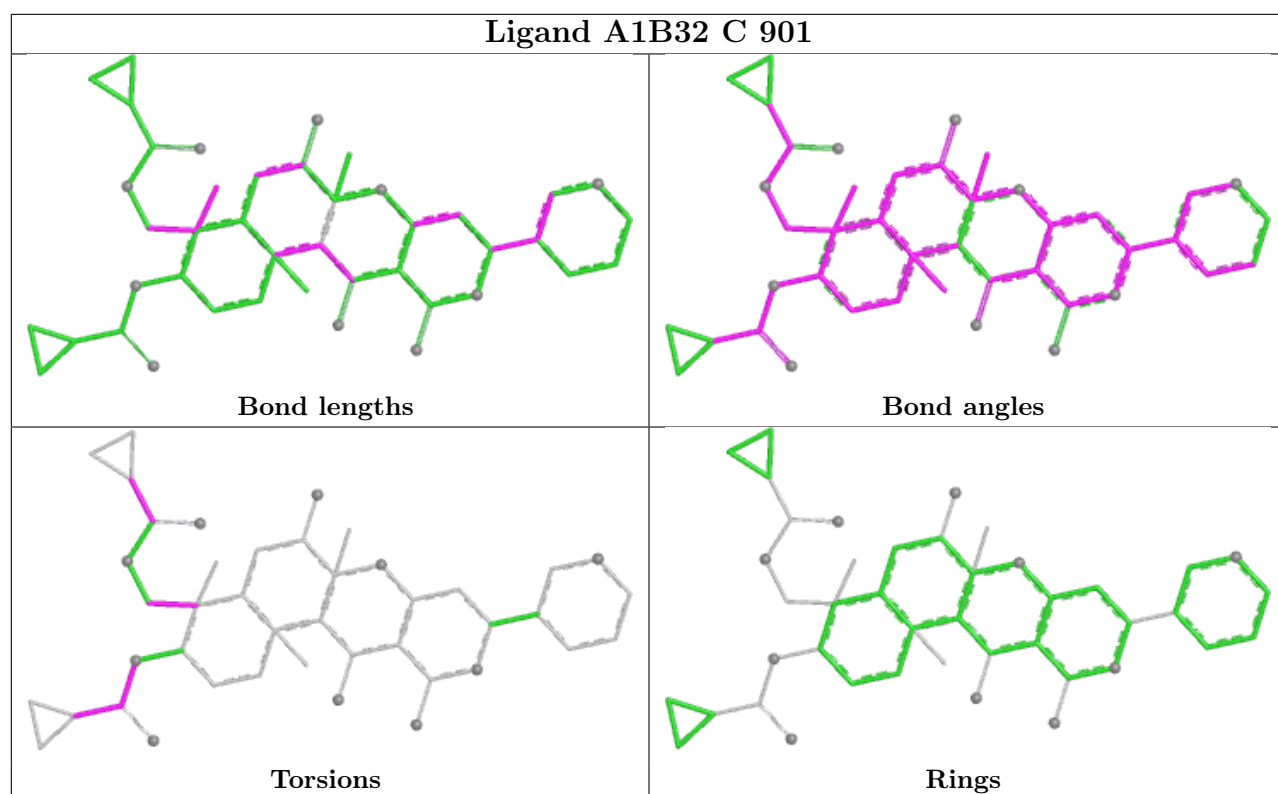
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

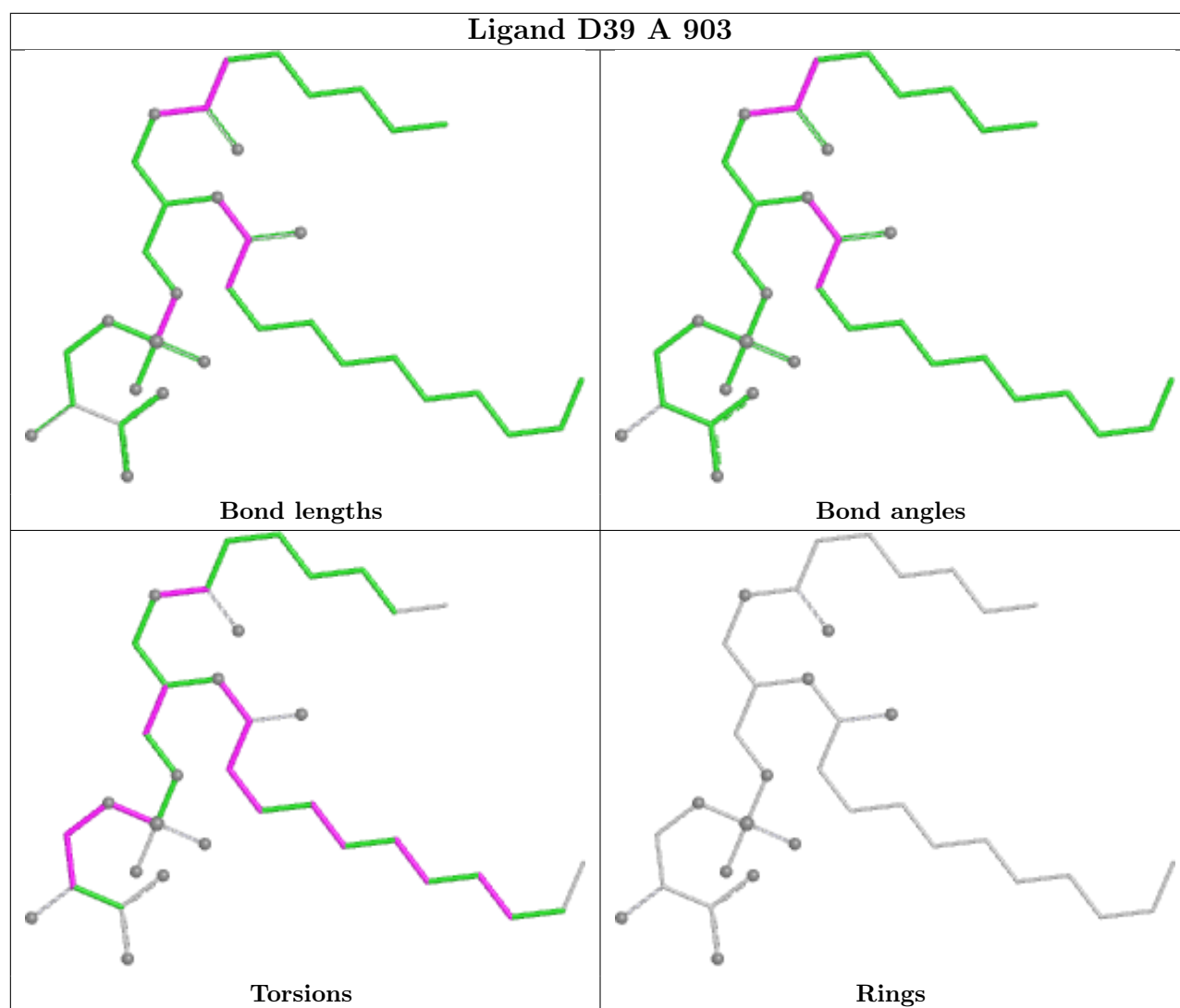


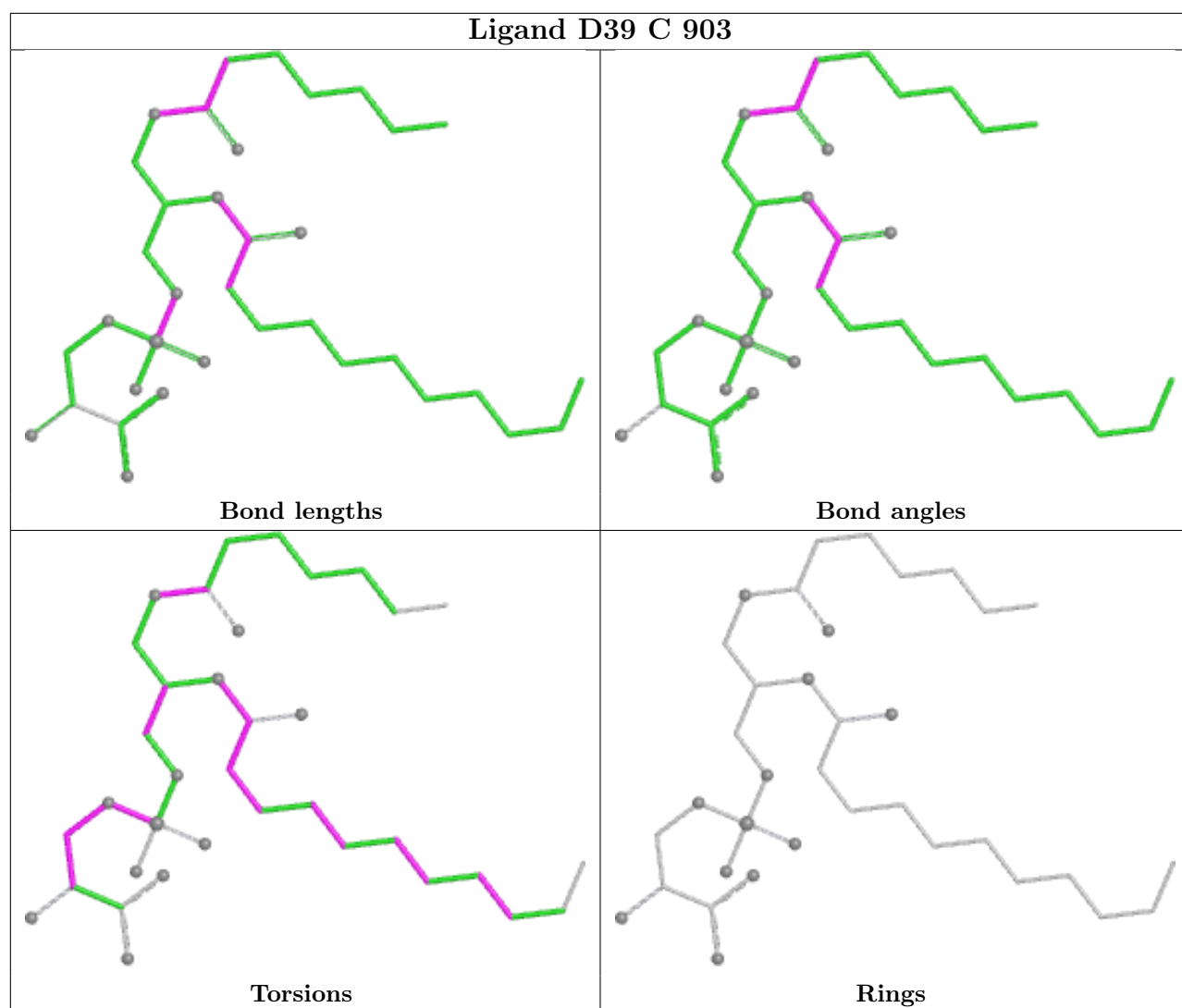


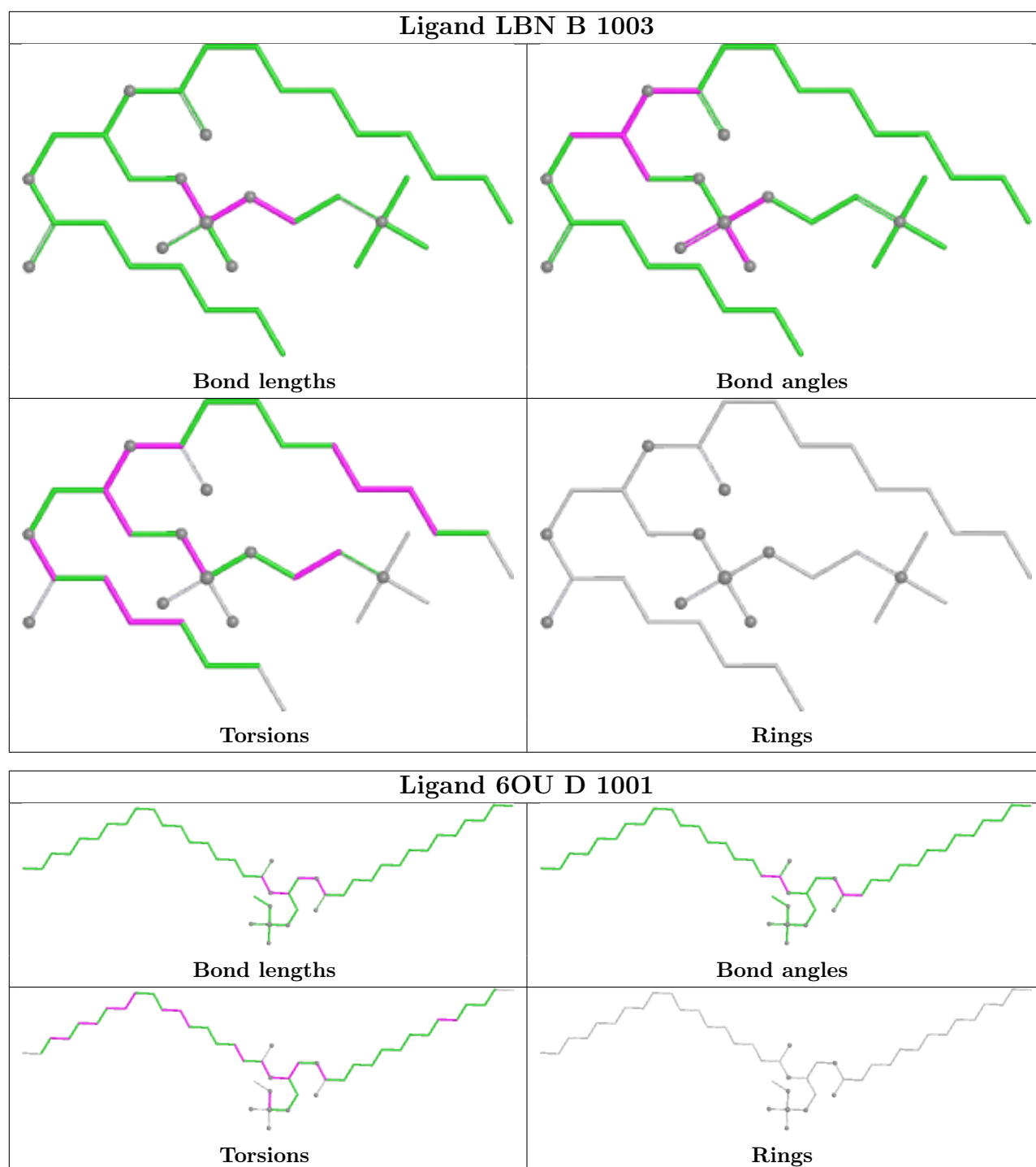












5.7 Other polymers [i](#)

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	14.98
1	D	16:UNK	C	31:CYS	N	14.98

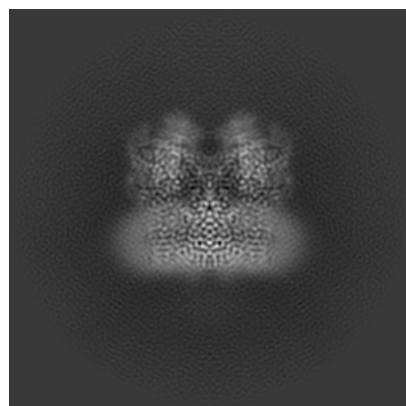
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49848. These allow visual inspection of the internal detail of the map and identification of artifacts.

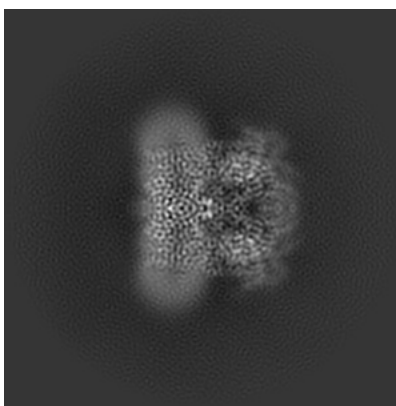
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

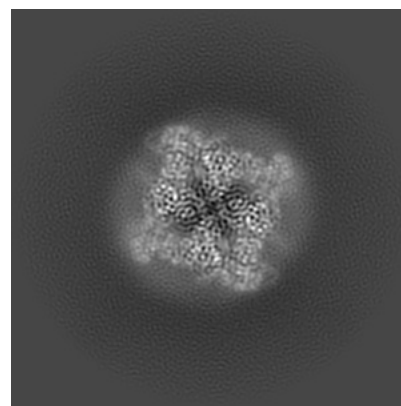
6.1.1 Primary map



X

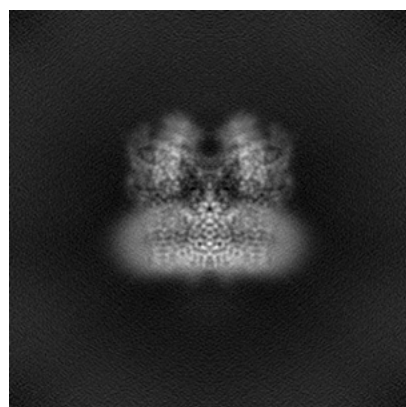


Y

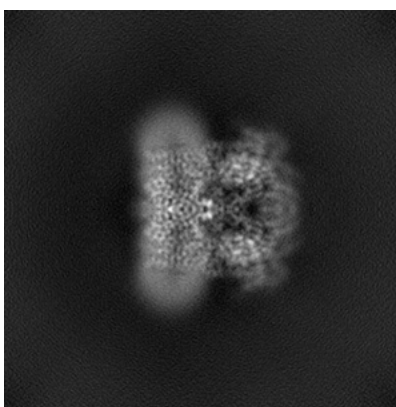


Z

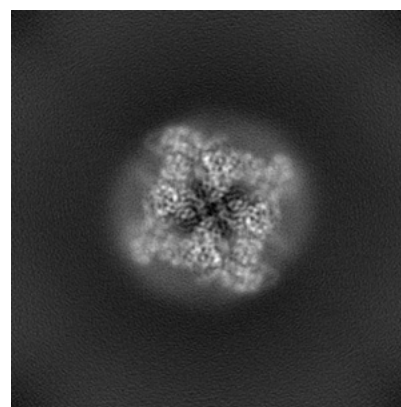
6.1.2 Raw map



X



Y

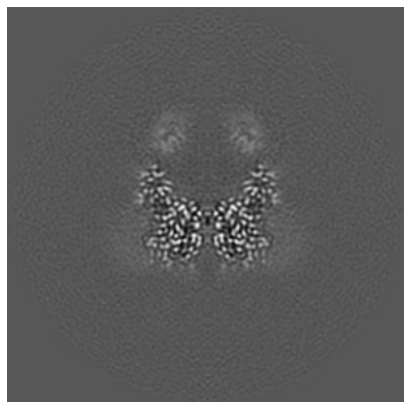


Z

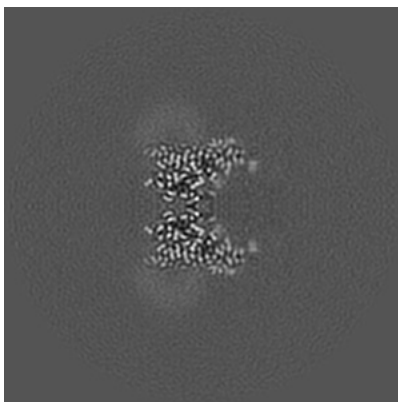
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

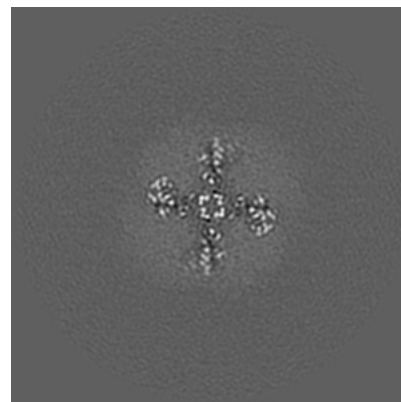
6.2.1 Primary map



X Index: 140

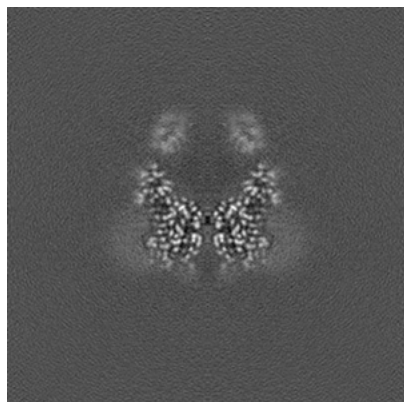


Y Index: 140

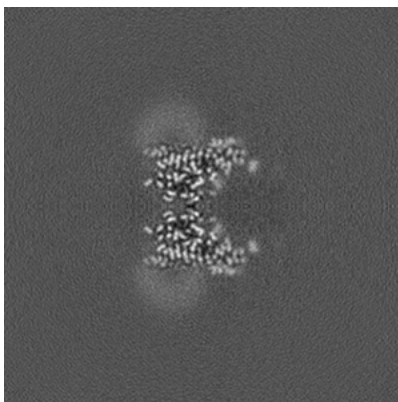


Z Index: 140

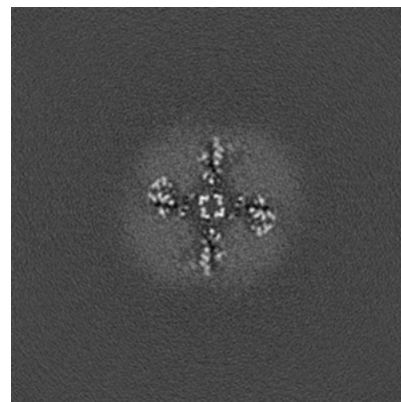
6.2.2 Raw map



X Index: 140



Y Index: 140

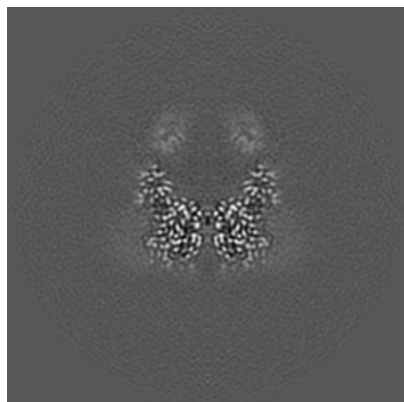


Z Index: 140

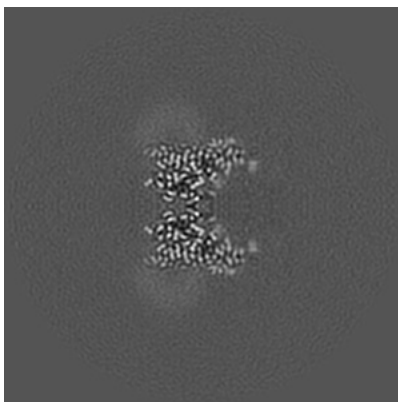
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

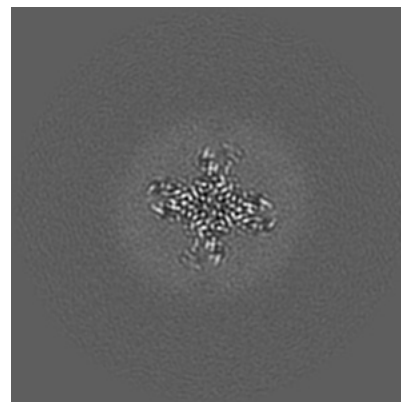
6.3.1 Primary map



X Index: 140

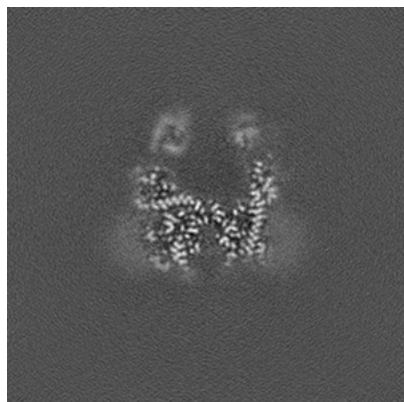


Y Index: 140

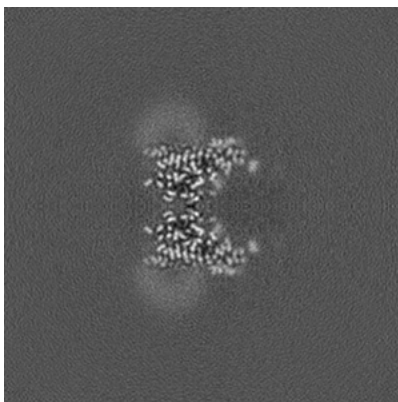


Z Index: 133

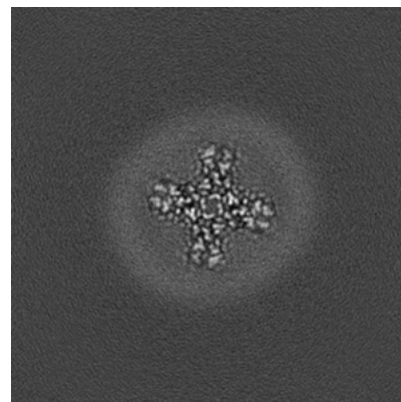
6.3.2 Raw map



X Index: 137



Y Index: 140

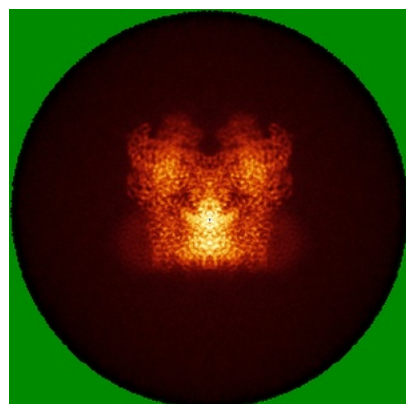


Z Index: 113

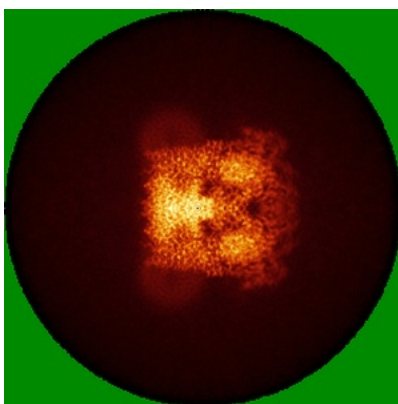
The images above show the largest variance slices of the map in three orthogonal directions.

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

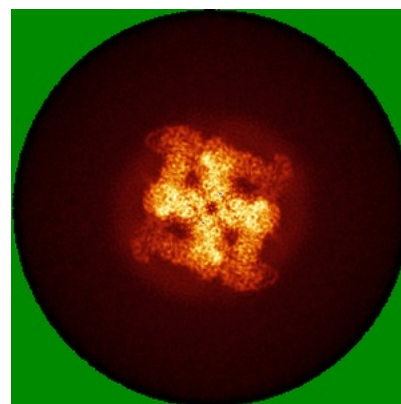
6.4.1 Primary map



X

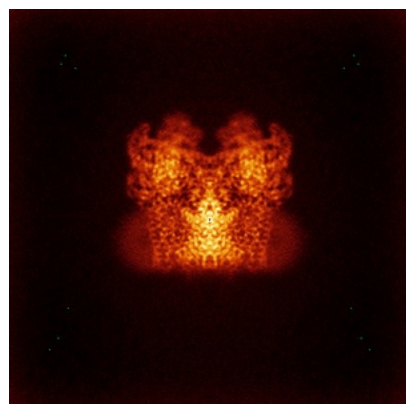


Y

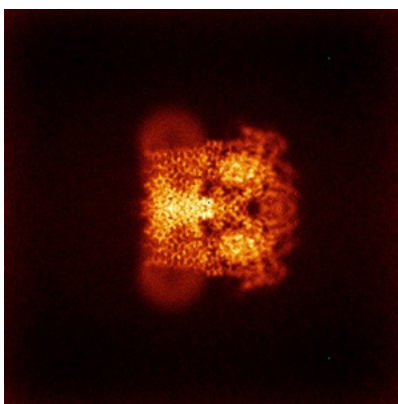


Z

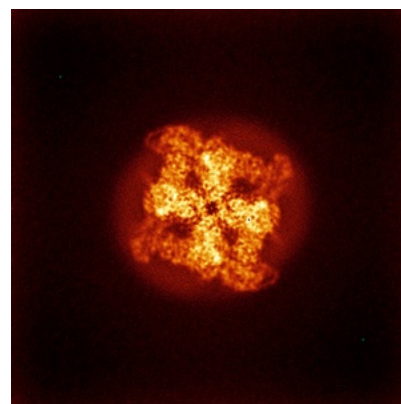
6.4.2 Raw map



X



Y

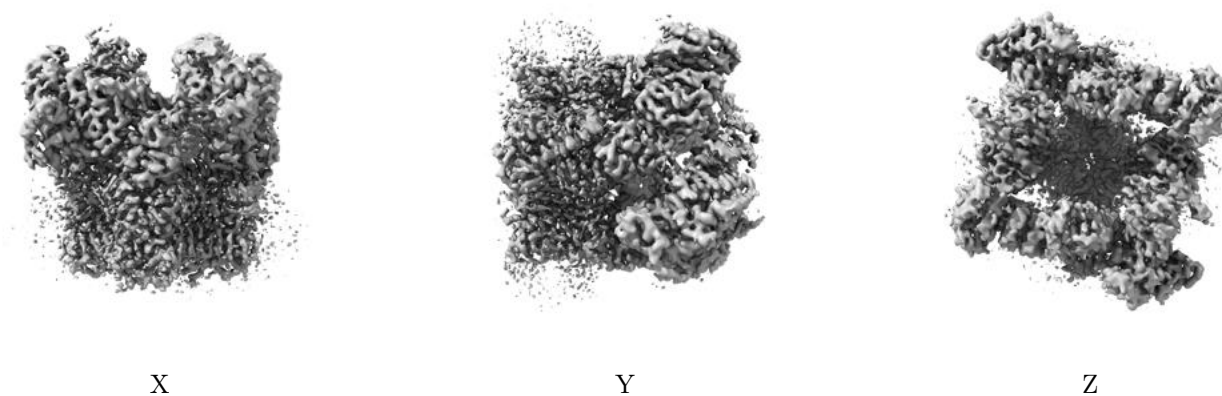


Z

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.

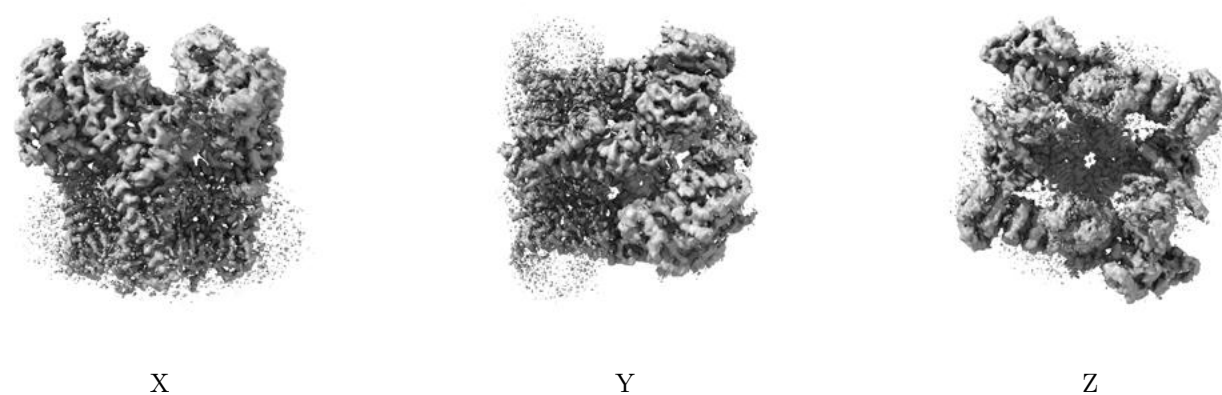
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

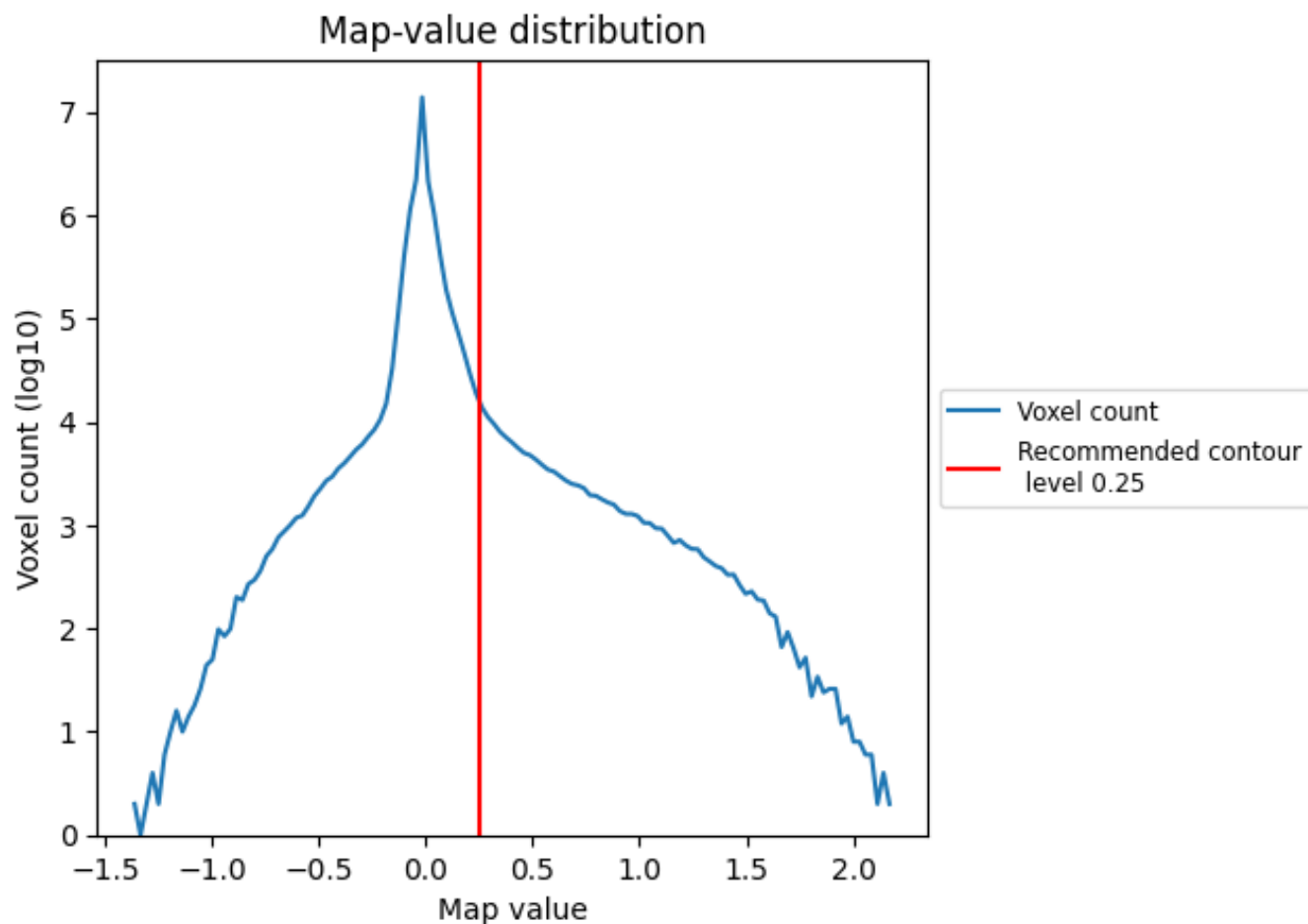
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

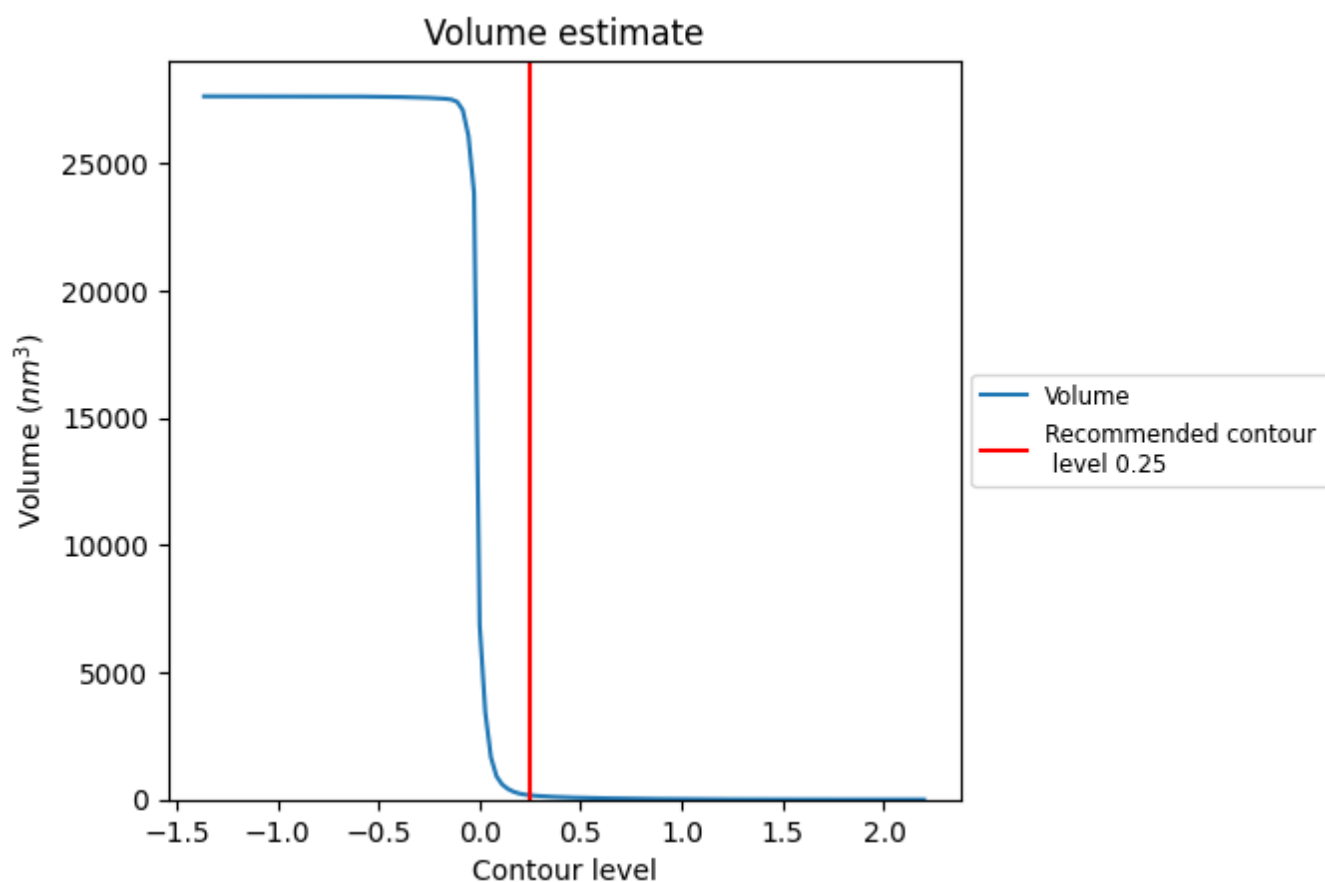
This section contains the results of statistical analysis of the map.

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.

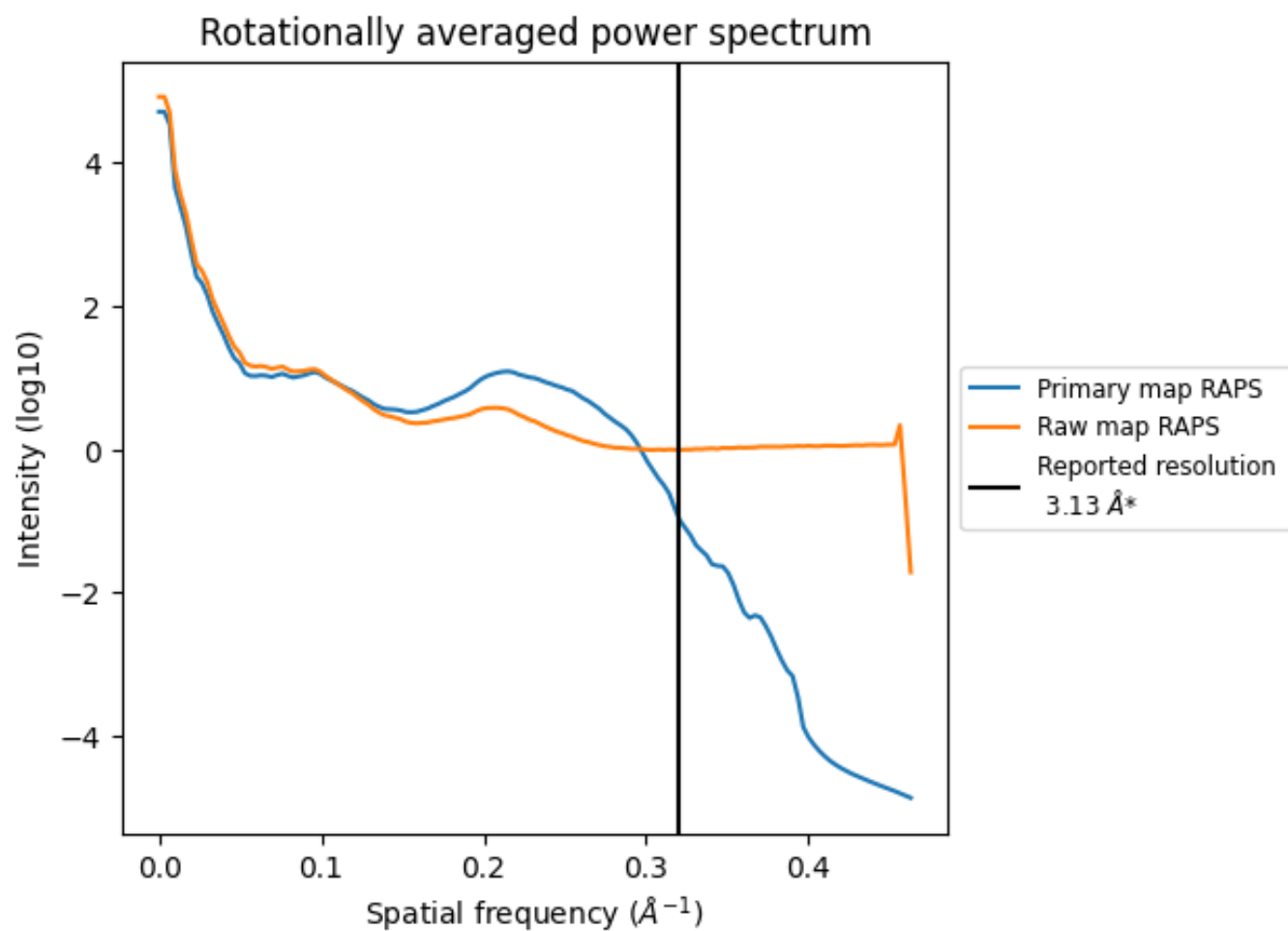
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 151 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 [i](#)

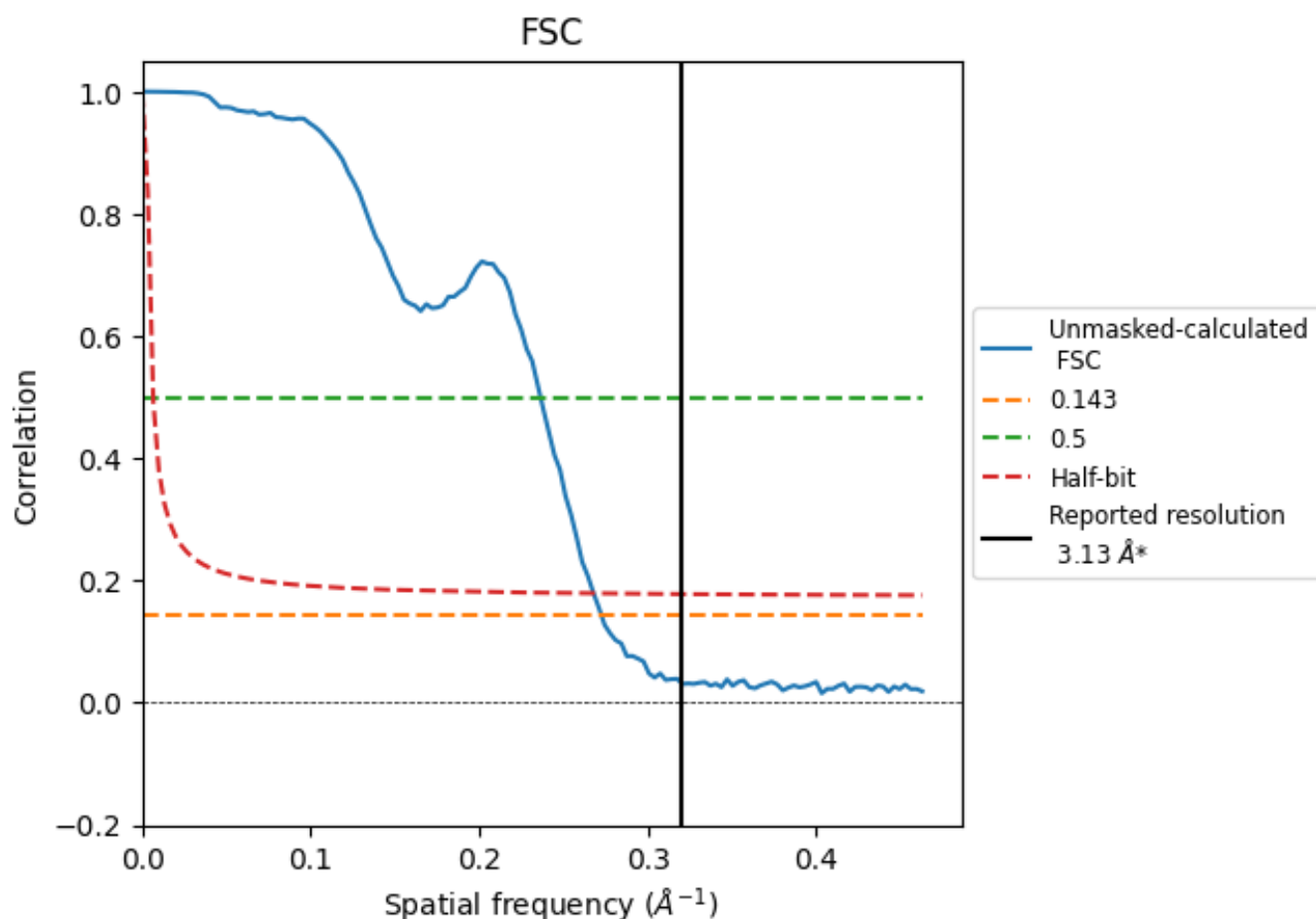


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

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 0.319 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

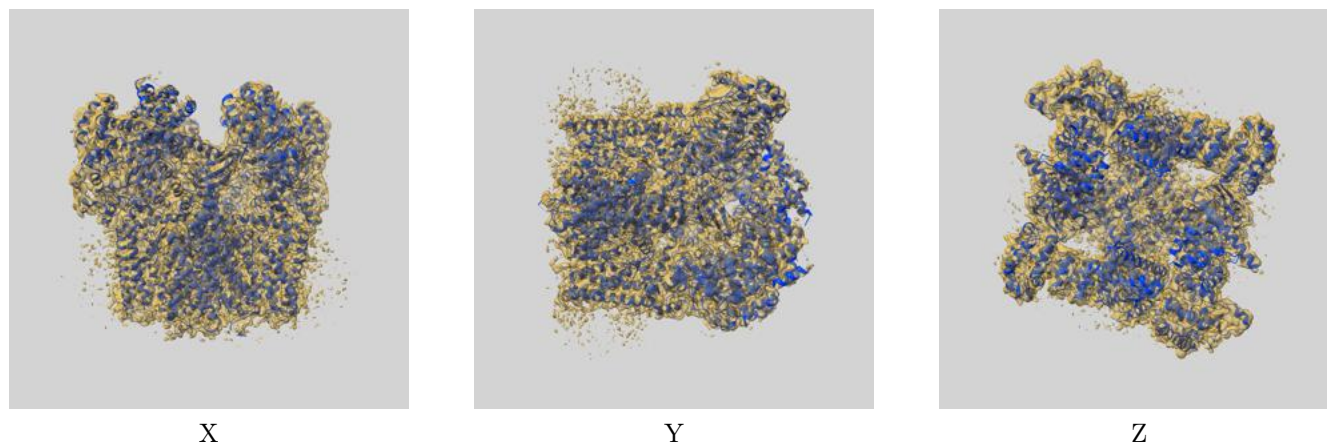
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.23	3.73

*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 3.67 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

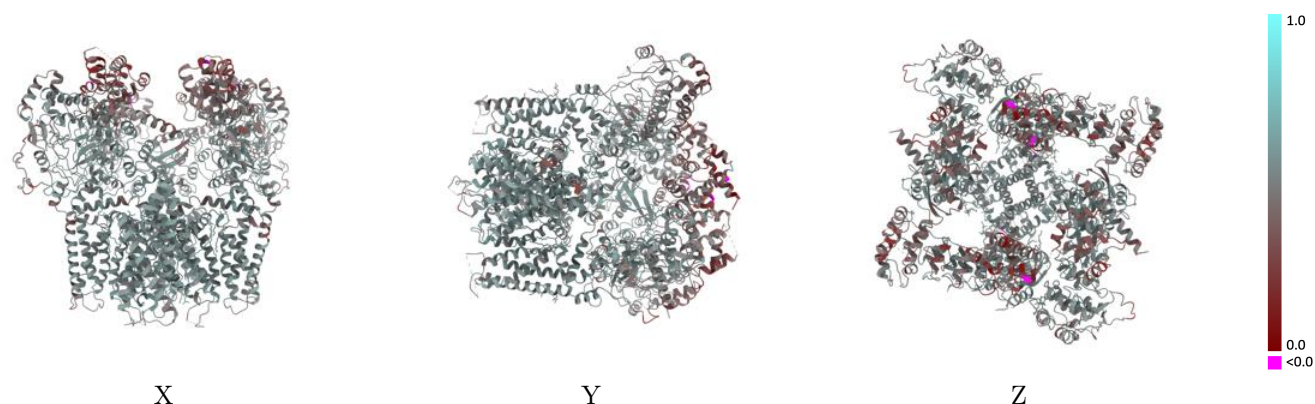
This section contains information regarding the fit between EMDB map EMD-49848 and PDB model 9NVR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



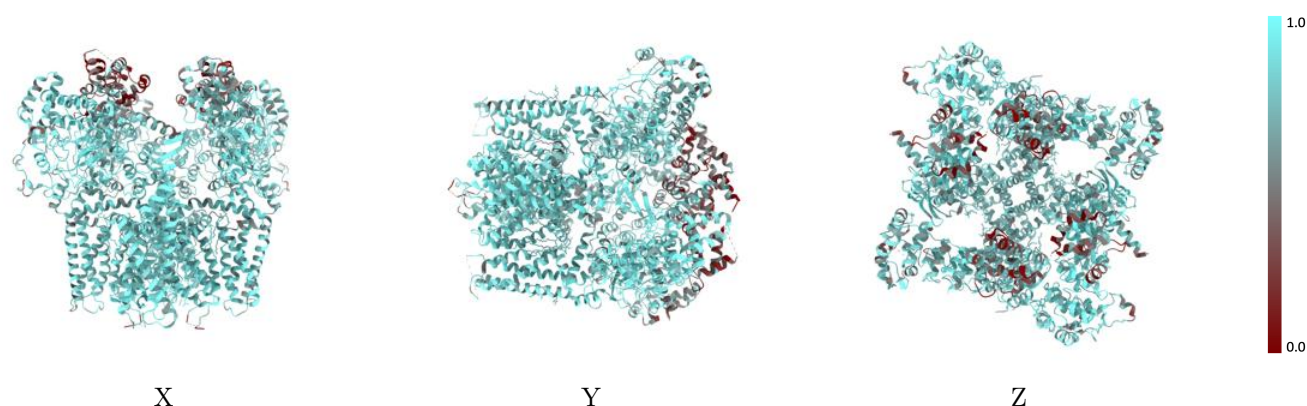
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



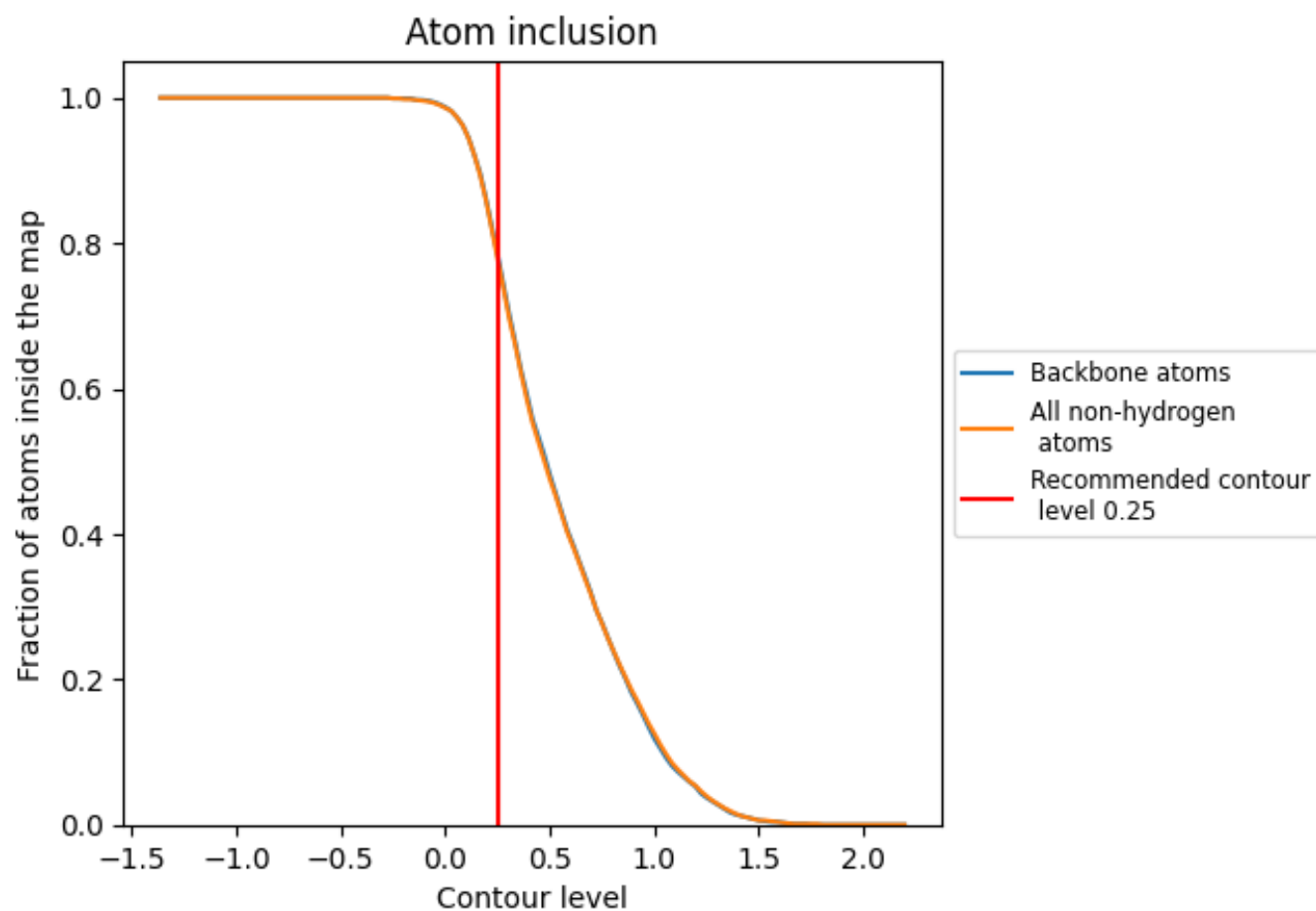
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.4970
A	0.8410	0.5240
B	0.8010	0.5010
C	0.8390	0.5230
D	0.8020	0.5000
E	0.3700	0.3210
F	0.3620	0.3190

1.0

0.0

<0.0