



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:24 PM UTC

PDB ID : 8TZ2 / pdb_00008tz2
EMDB ID : EMD-41731
Title : Cryo-EM structure of bovine concentrative nucleoside transporter 3 in MSP2N2 nanodiscs, apo state
Authors : Wright, N.J.; Lee, S.-Y.
Deposited on : 2023-08-26
Resolution : 2.80 Å(reported)
Based on initial model : 3TIJ

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

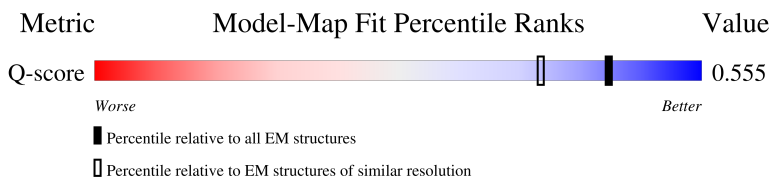
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	715	
1	B	715	
1	C	715	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24828 atoms, of which 12402 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 Sodium/nucleoside cotransporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	533	Total	C	H	N	O	S	0	0
			8129	2706	4055	642	697	29		
1	C	533	Total	C	H	N	O	S	0	0
			8129	2706	4055	642	697	29		
1	B	533	Total	C	H	N	O	S	0	0
			8129	2706	4055	642	697	29		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP F1MGR1
A	-13	ASP	-	expression tag	UNP F1MGR1
A	-12	TYR	-	expression tag	UNP F1MGR1
A	-11	LYS	-	expression tag	UNP F1MGR1
A	-10	ASP	-	expression tag	UNP F1MGR1
A	-9	ASP	-	expression tag	UNP F1MGR1
A	-8	ASP	-	expression tag	UNP F1MGR1
A	-7	ASP	-	expression tag	UNP F1MGR1
A	-6	LYS	-	expression tag	UNP F1MGR1
A	-5	LEU	-	expression tag	UNP F1MGR1
A	-4	GLU	-	expression tag	UNP F1MGR1
A	-3	ALA	-	expression tag	UNP F1MGR1
A	-2	THR	-	expression tag	UNP F1MGR1
A	-1	MET	-	expression tag	UNP F1MGR1
A	0	ALA	-	expression tag	UNP F1MGR1
A	698	SER	-	expression tag	UNP F1MGR1
A	699	ASN	-	expression tag	UNP F1MGR1
A	700	SER	-	expression tag	UNP F1MGR1
C	-14	MET	-	initiating methionine	UNP F1MGR1
C	-13	ASP	-	expression tag	UNP F1MGR1
C	-12	TYR	-	expression tag	UNP F1MGR1
C	-11	LYS	-	expression tag	UNP F1MGR1
C	-10	ASP	-	expression tag	UNP F1MGR1
C	-9	ASP	-	expression tag	UNP F1MGR1

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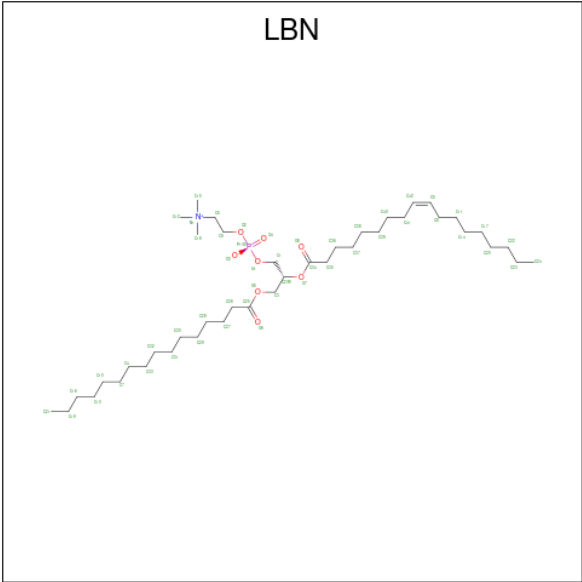
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	ASP	-	expression tag	UNP F1MGR1
C	-7	ASP	-	expression tag	UNP F1MGR1
C	-6	LYS	-	expression tag	UNP F1MGR1
C	-5	LEU	-	expression tag	UNP F1MGR1
C	-4	GLU	-	expression tag	UNP F1MGR1
C	-3	ALA	-	expression tag	UNP F1MGR1
C	-2	THR	-	expression tag	UNP F1MGR1
C	-1	MET	-	expression tag	UNP F1MGR1
C	0	ALA	-	expression tag	UNP F1MGR1
C	698	SER	-	expression tag	UNP F1MGR1
C	699	ASN	-	expression tag	UNP F1MGR1
C	700	SER	-	expression tag	UNP F1MGR1
B	-14	MET	-	initiating methionine	UNP F1MGR1
B	-13	ASP	-	expression tag	UNP F1MGR1
B	-12	TYR	-	expression tag	UNP F1MGR1
B	-11	LYS	-	expression tag	UNP F1MGR1
B	-10	ASP	-	expression tag	UNP F1MGR1
B	-9	ASP	-	expression tag	UNP F1MGR1
B	-8	ASP	-	expression tag	UNP F1MGR1
B	-7	ASP	-	expression tag	UNP F1MGR1
B	-6	LYS	-	expression tag	UNP F1MGR1
B	-5	LEU	-	expression tag	UNP F1MGR1
B	-4	GLU	-	expression tag	UNP F1MGR1
B	-3	ALA	-	expression tag	UNP F1MGR1
B	-2	THR	-	expression tag	UNP F1MGR1
B	-1	MET	-	expression tag	UNP F1MGR1
B	0	ALA	-	expression tag	UNP F1MGR1
B	698	SER	-	expression tag	UNP F1MGR1
B	699	ASN	-	expression tag	UNP F1MGR1
B	700	SER	-	expression tag	UNP F1MGR1

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Na 2 2	0
2	C	2	Total Na 2 2	0
2	B	2	Total Na 2 2	0

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			87	28	50	8	1	
3	A	1	Total	C	H	O	P	0
			56	18	29	8	1	
3	C	1	Total	C	H	O	P	0
			87	28	50	8	1	
3	C	1	Total	C	H	O	P	0
			56	18	29	8	1	
3	B	1	Total	C	H	O	P	0
			87	28	50	8	1	
3	B	1	Total	C	H	O	P	0
			56	18	29	8	1	

- Molecule 4 is water.

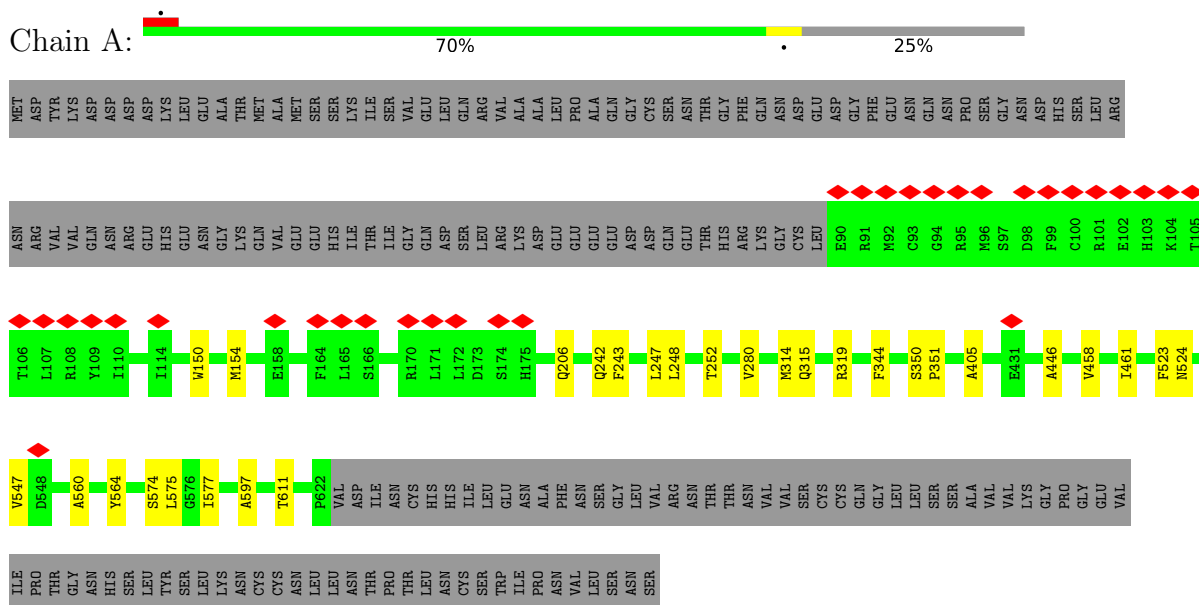
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	O	0
			2	2	
4	C	2	Total	O	0
			2	2	
4	B	2	Total	O	0
			2	2	

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.

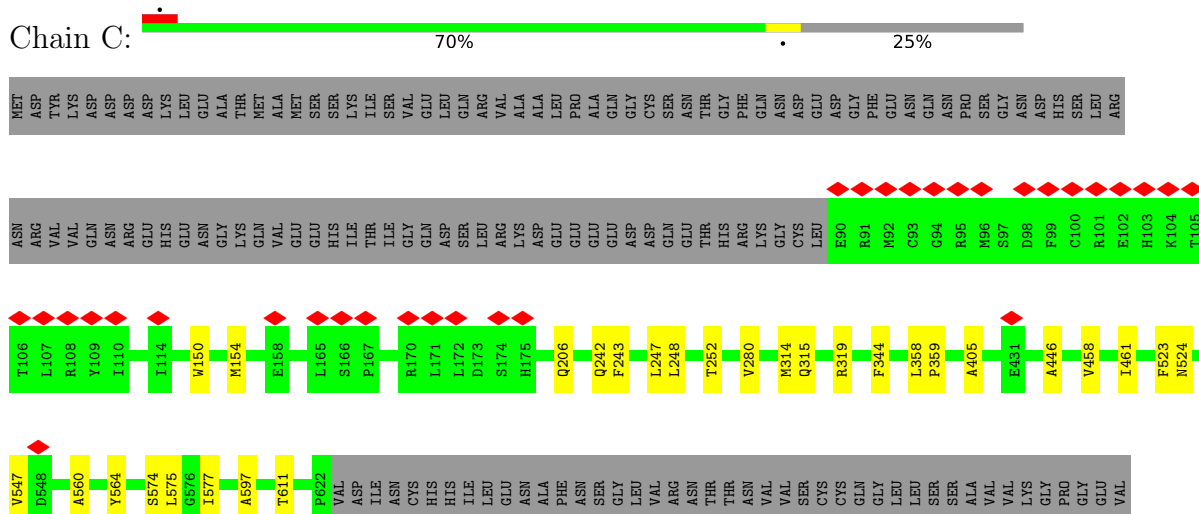
• Molecule 1: Sodium/nucleoside cotransporter

Chain A:



• Molecule 1: Sodium/nucleoside cotransporter

Chain C:



ILE	PRO	THR	GLY	ASN	HIS	SER	LEU	TYR	SER	LEU	LEU	LYS	ASN	CYS	CYS	ASN	LEU	SER	LEU	ASN	THR	THR	THR	LEU	ASN	CYS	SER	TRP	ILE	PRO	ASN	VAL	LEU	SER	ASN	SER
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● Molecule 1: Sodium/nucleoside cotransporter



MET	ASP	TYR	LYS	ASP	ASP	ASP	LYS	LEU	GLU	ALA	THR	MET	ALA	MET	ASN	SER	SER	LYS	ILE	SER	VAL	GLN	LEU	GLN	ASP	SER	GLN	ARG	VAL	ALA	ALA	LEU	PRO	ALA	GLN	GLY	CYS	SER	ASN	THR	GLY	PHE	GLN	ASN	ASP	GLU	ASP	GLY	PHE	GLU	ASN	GLN	ASN	PRO	SER	GLY	ASN	ASP	HIS	SER	LEU	ARG
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ASN	ARG	VAL	GLN	ASN	ARG	GLU	HIS	GLU	GLY	ASN	GLN	VAL	GLU	GLU	HIS	ILE	THR	ILE	GLY	ASP	LEU	ARG	LYS	ASP	GLU	GLU	GLU	ASP	GLN	THR	HIS	ARG	LYS	GLY	CYS	LEU	E90	R91	M92	C93	G94	R95	M96	S97	D98	F99	C100	R101	E102	H103	K104	T105
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T106	L107	R108	Y109	I110	I114	W150	M154	E158	S166	R170	L171	D172	S174	H175	Q206	Q242	F243	L247	L248	T252	V280	N314	Q315	R319	F344	L388	P359	A405	E431	A446	V458	T461	F523	N524	V547	D548
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A560	Y564	S574	L575	G576	I577	A597	G608	T611	F622	VAL	ASP	ILE	ASN	CYS	HIS	ASN	ILE	LEU	GLU	ASN	ALA	PHE	ASN	ASN	SER	GLY	VAL	ARG	ASN	THR	THR	ASN	VAL	SER	CYS	CYS	GLN	GLY	LEU	LEU	SER	ALA	VAL	LYS	PRO	GLY	GLU	VAL
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ILE	PRO	THR	GLY	ASN	HIS	SER	LEU	TYR	SER	LEU	LEU	LYS	ASN	CYS	ASN	LEU	LEU	ASN	THR	PRO	THR	LEU	ASN	CYS	SER	TRP	ILE	PRO	ASN	VAL	LEU	SER	ASN	SER
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	102248	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.889	Depositor
Minimum map value	-2.409	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LBN, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/4186	0.31	0/5699
1	B	0.18	0/4186	0.31	0/5699
1	C	0.18	0/4186	0.31	0/5699
All	All	0.18	0/12558	0.31	0/17097

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	4055	4072	19	0
1	B	4074	4055	4072	20	0
1	C	4074	4055	4072	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	64	79	0	0	0
3	B	64	79	0	0	0
3	C	64	79	0	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	2	0	0	0	0
All	All	12426	12402	12216	52	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 2.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:O	1:A:252:THR:OG1	2.11	0.69
1:C:248:LEU:O	1:C:252:THR:OG1	2.11	0.69
1:B:248:LEU:O	1:B:252:THR:OG1	2.11	0.66
1:B:206:GLN:N	1:B:206:GLN:OE1	2.31	0.64
1:C:206:GLN:OE1	1:C:206:GLN:N	2.31	0.63
1:C:458:VAL:HG12	1:B:446:ALA:HB1	1.83	0.60
1:A:206:GLN:N	1:A:206:GLN:OE1	2.31	0.59
1:A:461:ILE:HG13	1:C:280:VAL:HG21	1.85	0.58
1:B:242:GLN:OE1	1:B:611:THR:HG22	2.07	0.55
1:A:242:GLN:OE1	1:A:611:THR:HG22	2.07	0.55
1:C:242:GLN:OE1	1:C:611:THR:HG22	2.07	0.55
1:A:243:PHE:CE2	1:A:247:LEU:HD11	2.46	0.51
1:C:243:PHE:CE2	1:C:247:LEU:HD11	2.46	0.51
1:B:243:PHE:CE2	1:B:247:LEU:HD11	2.46	0.50
1:C:314:MET:HE2	1:C:344:PHE:CD2	2.47	0.49
1:A:446:ALA:HB1	1:B:458:VAL:HG12	1.93	0.49
1:A:575:LEU:HD11	1:A:597:ALA:HB1	1.95	0.49
1:C:461:ILE:HG13	1:B:280:VAL:HG21	1.94	0.49
1:B:575:LEU:HD11	1:B:597:ALA:HB1	1.95	0.49
1:A:314:MET:HE2	1:A:344:PHE:CD2	2.47	0.49
1:B:314:MET:HE2	1:B:344:PHE:CD2	2.47	0.49
1:B:547:VAL:O	1:B:547:VAL:HG23	2.14	0.48
1:C:547:VAL:HG23	1:C:547:VAL:O	2.14	0.48
1:C:575:LEU:HD11	1:C:597:ALA:HB1	1.95	0.48
1:A:280:VAL:HG21	1:B:461:ILE:HG13	1.97	0.47
1:A:560:ALA:O	1:A:564:TYR:HD1	1.98	0.47
1:C:560:ALA:O	1:C:564:TYR:HD1	1.98	0.47
1:A:547:VAL:O	1:A:547:VAL:HG23	2.14	0.46
1:C:150:TRP:O	1:C:154:MET:HG2	2.16	0.46
1:B:560:ALA:O	1:B:564:TYR:HD1	1.98	0.46
1:B:150:TRP:O	1:B:154:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:O	1:A:154:MET:HG2	2.16	0.45
1:A:458:VAL:HG12	1:C:446:ALA:HB1	1.99	0.43
1:B:523:PHE:O	1:B:524:ASN:HB3	2.19	0.43
1:A:523:PHE:O	1:A:524:ASN:HB3	2.19	0.43
1:C:523:PHE:O	1:C:524:ASN:HB3	2.19	0.43
1:A:242:GLN:CD	1:A:405:ALA:HB2	2.45	0.42
1:C:574:SER:O	1:C:577:ILE:HG13	2.20	0.42
1:A:574:SER:O	1:A:577:ILE:HG13	2.19	0.42
1:C:242:GLN:CD	1:C:405:ALA:HB2	2.45	0.42
1:B:574:SER:O	1:B:577:ILE:HG13	2.19	0.42
1:B:242:GLN:CD	1:B:405:ALA:HB2	2.45	0.42
1:C:314:MET:HE2	1:C:344:PHE:CG	2.55	0.41
1:A:314:MET:HE2	1:A:344:PHE:CG	2.56	0.41
1:B:315:GLN:O	1:B:319:ARG:HG3	2.21	0.41
1:B:314:MET:HE2	1:B:344:PHE:CG	2.56	0.41
1:B:608:CYS:O	1:B:611:THR:OG1	2.37	0.41
1:A:315:GLN:O	1:A:319:ARG:HG3	2.21	0.41
1:A:350:SER:N	1:A:351:PRO:CD	2.84	0.40
1:C:315:GLN:O	1:C:319:ARG:HG3	2.21	0.40
1:C:358:LEU:N	1:C:359:PRO:CD	2.85	0.40
1:B:358:LEU:N	1:B:359:PRO:CD	2.85	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	A	531/715 (74%)	525 (99%)	6 (1%)	0	100	100
1	B	531/715 (74%)	525 (99%)	6 (1%)	0	100	100
1	C	531/715 (74%)	525 (99%)	6 (1%)	0	100	100
All	All	1593/2145 (74%)	1575 (99%)	18 (1%)	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	A	421/608 (69%)	421 (100%)	0	100	100
1	B	421/608 (69%)	421 (100%)	0	100	100
1	C	421/608 (69%)	421 (100%)	0	100	100
All	All	1263/1824 (69%)	1263 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	A	367	HIS
1	A	423	ASN
1	C	265	GLN
1	C	367	HIS
1	C	423	ASN
1	B	265	GLN
1	B	347	GLN
1	B	367	HIS
1	B	423	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	LBN	C	803	-	36,36,51	1.38	5 (13%)	39,41,59	1.06	2 (5%)
3	LBN	A	804	-	26,26,51	1.61	6 (23%)	29,31,59	1.14	2 (6%)
3	LBN	B	803	-	36,36,51	1.38	5 (13%)	39,41,59	1.06	2 (5%)
3	LBN	B	804	-	26,26,51	1.61	6 (23%)	29,31,59	1.14	2 (6%)
3	LBN	A	803	-	36,36,51	1.37	5 (13%)	39,41,59	1.06	2 (5%)
3	LBN	C	804	-	26,26,51	1.61	6 (23%)	29,31,59	1.14	2 (6%)

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
3	LBN	C	803	-	-	20/38/38/55	-
3	LBN	A	804	-	-	11/28/28/55	-
3	LBN	B	803	-	-	20/38/38/55	-
3	LBN	B	804	-	-	11/28/28/55	-
3	LBN	A	803	-	-	20/38/38/55	-
3	LBN	C	804	-	-	11/28/28/55	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	LBN	P1-O4	4.68	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	LBN	P1-O4	4.67	1.65	1.50
3	A	803	LBN	P1-O4	4.65	1.64	1.50
3	B	803	LBN	P1-O4	4.65	1.64	1.50
3	C	804	LBN	P1-O4	4.65	1.64	1.50
3	C	803	LBN	P1-O4	4.63	1.64	1.50
3	B	803	LBN	O7-C34	3.20	1.43	1.34
3	C	803	LBN	O7-C34	3.18	1.43	1.34
3	A	803	LBN	O7-C34	3.18	1.43	1.34
3	A	804	LBN	O7-C34	3.11	1.43	1.34
3	C	804	LBN	O7-C34	3.11	1.43	1.34
3	B	804	LBN	O7-C34	3.09	1.43	1.34
3	A	804	LBN	O5-C25	2.71	1.41	1.33
3	B	804	LBN	O5-C25	2.70	1.41	1.33
3	C	804	LBN	O5-C25	2.70	1.41	1.33
3	C	803	LBN	O5-C25	2.63	1.41	1.33
3	A	803	LBN	O5-C25	2.61	1.41	1.33
3	B	803	LBN	O5-C25	2.59	1.40	1.33
3	C	803	LBN	P1-O1	2.24	1.67	1.60
3	B	803	LBN	P1-O1	2.23	1.67	1.60
3	A	803	LBN	P1-O1	2.22	1.67	1.60
3	C	804	LBN	O7-C2	-2.12	1.41	1.46
3	A	804	LBN	O7-C2	-2.12	1.41	1.46
3	B	804	LBN	O7-C2	-2.12	1.41	1.46
3	A	804	LBN	P1-O1	2.10	1.66	1.60
3	B	804	LBN	P1-O1	2.10	1.66	1.60
3	C	804	LBN	P1-O1	2.09	1.66	1.60
3	B	803	LBN	O7-C2	-2.06	1.41	1.46
3	C	803	LBN	O7-C2	-2.06	1.41	1.46
3	C	804	LBN	O5-C3	-2.04	1.40	1.45
3	B	804	LBN	O5-C3	-2.03	1.40	1.45
3	A	803	LBN	O7-C2	-2.03	1.41	1.46
3	A	804	LBN	O5-C3	-2.01	1.40	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	LBN	O7-C34-C35	4.03	120.21	111.48
3	A	803	LBN	O7-C34-C35	4.01	120.16	111.48
3	C	803	LBN	O7-C34-C35	4.00	120.14	111.48
3	C	804	LBN	O7-C34-C35	3.78	119.65	111.48
3	A	804	LBN	O7-C34-C35	3.76	119.62	111.48
3	B	804	LBN	O7-C34-C35	3.76	119.61	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803	LBN	O5-C25-C26	2.49	119.42	111.83
3	C	804	LBN	O5-C25-C26	2.48	119.41	111.83
3	A	803	LBN	O5-C25-C26	2.48	119.40	111.83
3	B	803	LBN	O5-C25-C26	2.48	119.40	111.83
3	B	804	LBN	O5-C25-C26	2.48	119.40	111.83
3	A	804	LBN	O5-C25-C26	2.48	119.39	111.83

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	LBN	C2-C1-O1-P1
3	A	803	LBN	C35-C34-O7-C2
3	A	804	LBN	C35-C34-O7-C2
3	C	803	LBN	C2-C1-O1-P1
3	C	803	LBN	C35-C34-O7-C2
3	C	804	LBN	C35-C34-O7-C2
3	B	803	LBN	C2-C1-O1-P1
3	B	803	LBN	C35-C34-O7-C2
3	B	804	LBN	C35-C34-O7-C2
3	A	803	LBN	O8-C34-O7-C2
3	C	803	LBN	O8-C34-O7-C2
3	B	803	LBN	O8-C34-O7-C2
3	A	803	LBN	O6-C25-O5-C3
3	C	803	LBN	O6-C25-O5-C3
3	B	803	LBN	O6-C25-O5-C3
3	A	804	LBN	O8-C34-O7-C2
3	C	804	LBN	O8-C34-O7-C2
3	B	804	LBN	O8-C34-O7-C2
3	A	803	LBN	C26-C25-O5-C3
3	C	803	LBN	C26-C25-O5-C3
3	B	803	LBN	C26-C25-O5-C3
3	A	803	LBN	C34-C35-C36-C37
3	C	803	LBN	C34-C35-C36-C37
3	B	803	LBN	C34-C35-C36-C37
3	A	803	LBN	C20-C22-C23-C24
3	C	803	LBN	C20-C22-C23-C24
3	B	803	LBN	C20-C22-C23-C24
3	C	804	LBN	C35-C36-C37-C38
3	A	803	LBN	C37-C38-C39-C40
3	C	803	LBN	C37-C38-C39-C40
3	B	803	LBN	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
3	B	804	LBN	C35-C36-C37-C38
3	A	804	LBN	C35-C36-C37-C38
3	A	804	LBN	C39-C40-C41-C42
3	C	804	LBN	C39-C40-C41-C42
3	B	804	LBN	C39-C40-C41-C42
3	A	803	LBN	C1-C2-C3-O5
3	A	804	LBN	C1-C2-C3-O5
3	C	803	LBN	C1-C2-C3-O5
3	C	804	LBN	C1-C2-C3-O5
3	B	803	LBN	C1-C2-C3-O5
3	B	804	LBN	C1-C2-C3-O5
3	A	803	LBN	C27-C28-C29-C30
3	C	803	LBN	C27-C28-C29-C30
3	B	803	LBN	C27-C28-C29-C30
3	A	803	LBN	C1-O1-P1-O2
3	C	803	LBN	C1-O1-P1-O2
3	B	803	LBN	C1-O1-P1-O2
3	A	804	LBN	C38-C39-C40-C41
3	C	804	LBN	C38-C39-C40-C41
3	B	804	LBN	C38-C39-C40-C41
3	A	803	LBN	O7-C2-C3-O5
3	C	803	LBN	O7-C2-C3-O5
3	B	803	LBN	O7-C2-C3-O5
3	A	804	LBN	O7-C2-C3-O5
3	C	804	LBN	O7-C2-C3-O5
3	B	804	LBN	O7-C2-C3-O5
3	A	803	LBN	C14-C11-C8-C5
3	C	803	LBN	C14-C11-C8-C5
3	B	803	LBN	C14-C11-C8-C5
3	A	803	LBN	C1-O1-P1-O4
3	C	803	LBN	C1-O1-P1-O4
3	B	803	LBN	C1-O1-P1-O4
3	A	804	LBN	C34-C35-C36-C37
3	C	804	LBN	C34-C35-C36-C37
3	B	804	LBN	C34-C35-C36-C37
3	C	803	LBN	C26-C27-C28-C29
3	A	803	LBN	C26-C27-C28-C29
3	B	803	LBN	C26-C27-C28-C29
3	A	804	LBN	O1-C1-C2-O7
3	C	804	LBN	O1-C1-C2-O7
3	B	804	LBN	O1-C1-C2-O7
3	A	803	LBN	C8-C11-C14-C17

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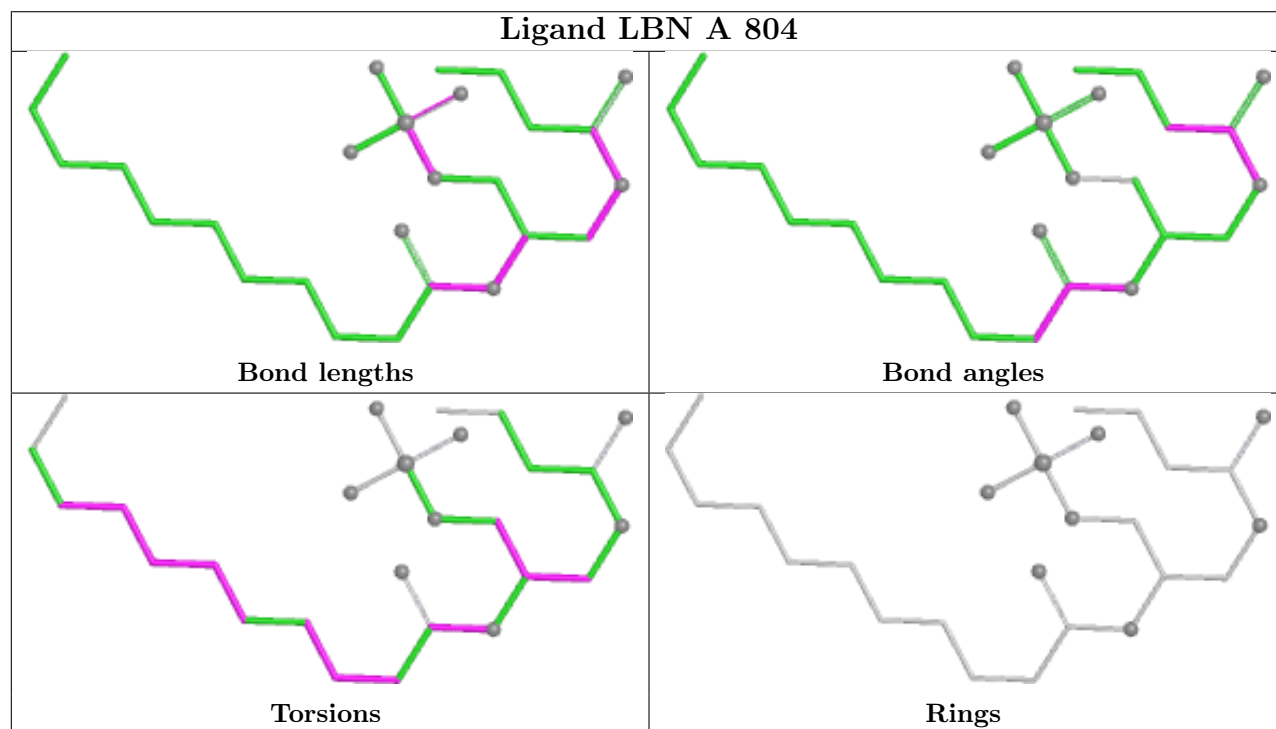
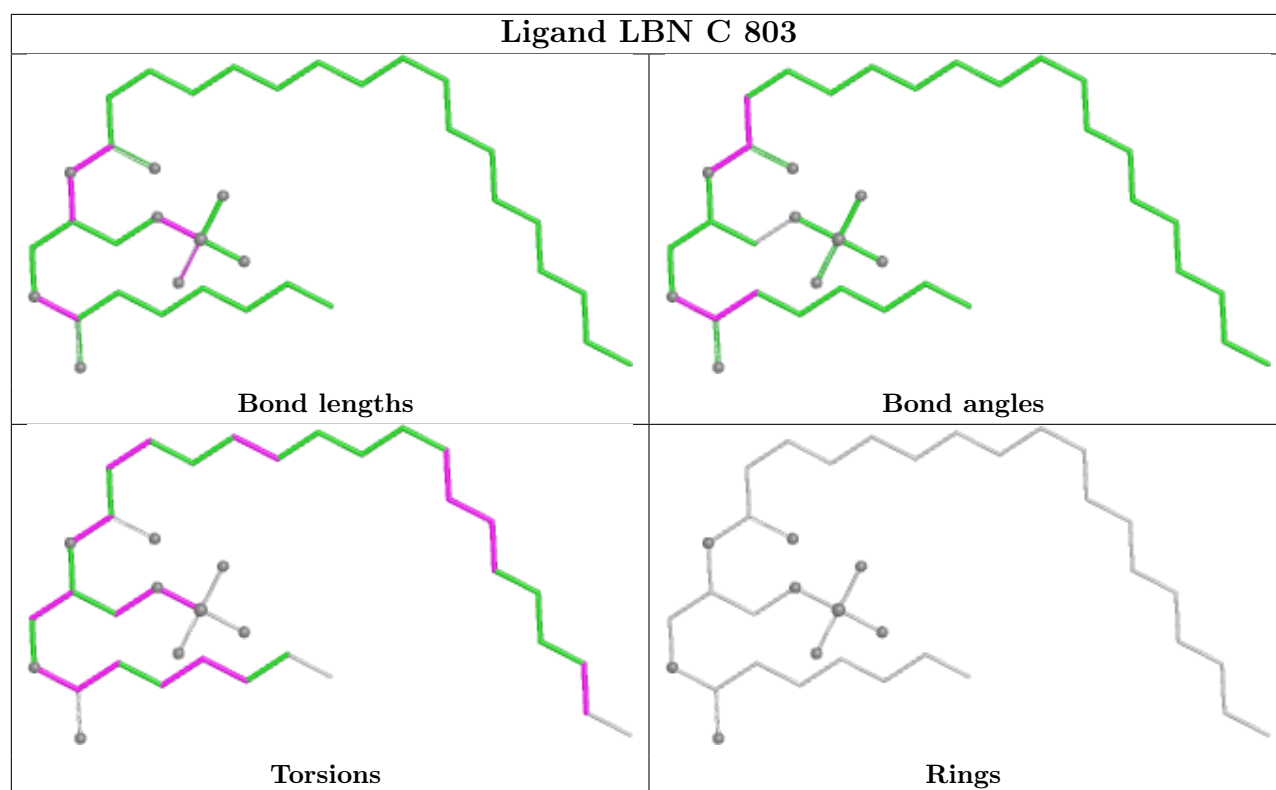
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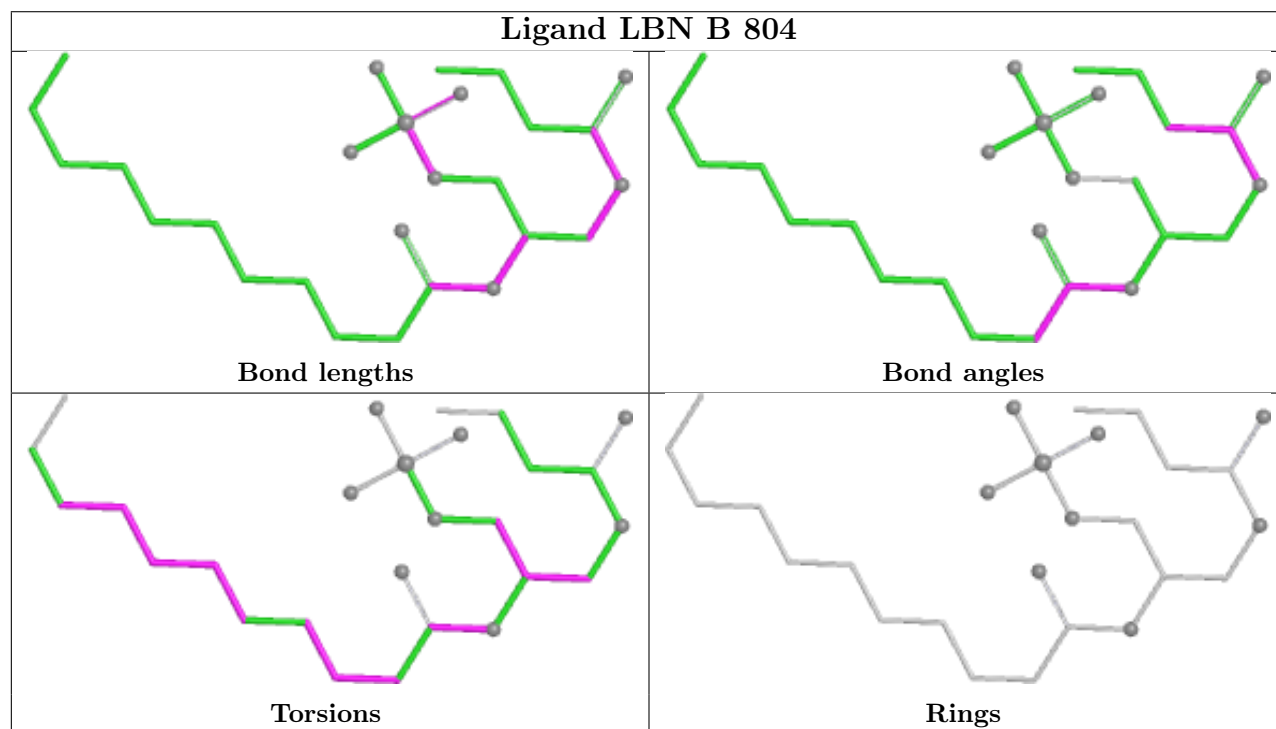
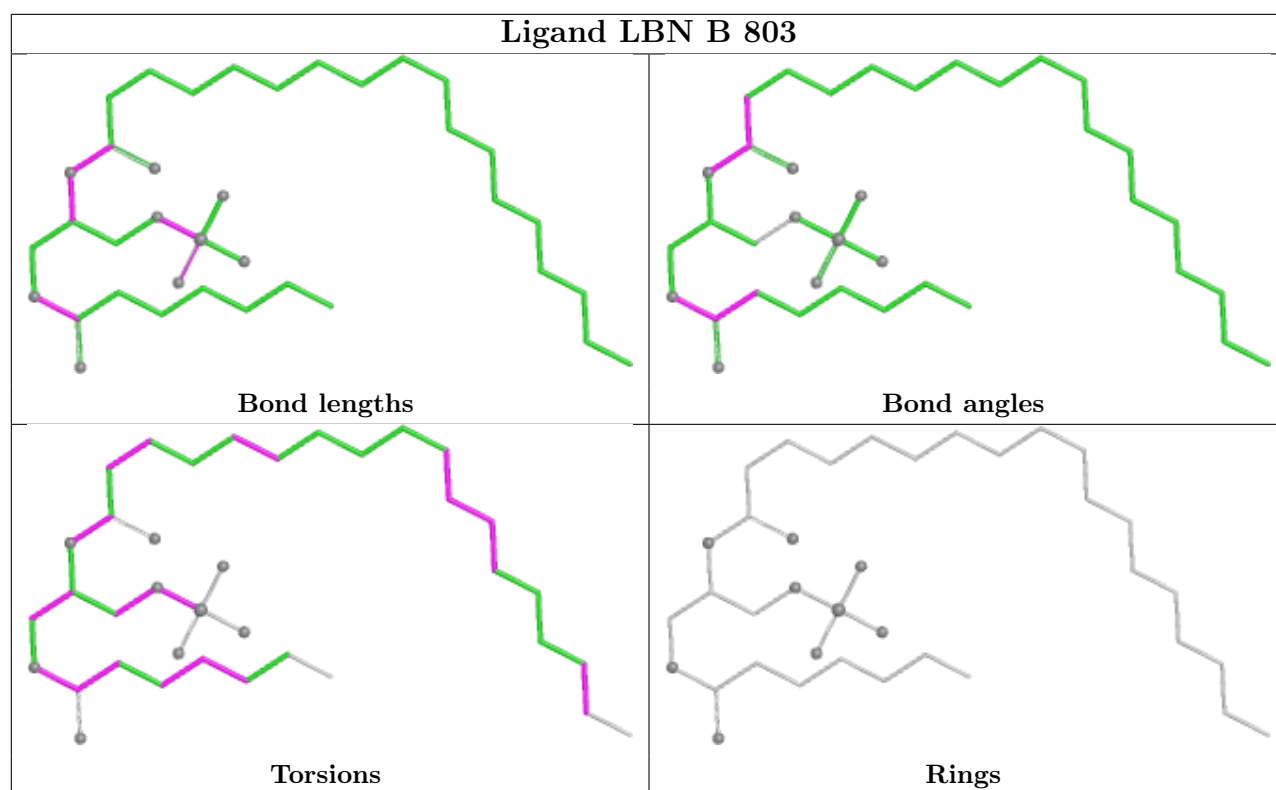
Mol	Chain	Res	Type	Atoms
3	C	803	LBN	C8-C11-C14-C17
3	B	803	LBN	C8-C11-C14-C17
3	A	803	LBN	C1-O1-P1-O3
3	C	803	LBN	C1-O1-P1-O3
3	B	803	LBN	C1-O1-P1-O3
3	A	803	LBN	C42-C5-C8-C11
3	C	803	LBN	C42-C5-C8-C11
3	B	803	LBN	C42-C5-C8-C11
3	C	804	LBN	C37-C38-C39-C40
3	B	804	LBN	C37-C38-C39-C40
3	A	804	LBN	C37-C38-C39-C40
3	A	803	LBN	O5-C25-C26-C27
3	C	803	LBN	O5-C25-C26-C27
3	B	803	LBN	O5-C25-C26-C27
3	A	803	LBN	O6-C25-C26-C27
3	C	803	LBN	O6-C25-C26-C27
3	B	803	LBN	O6-C25-C26-C27
3	A	804	LBN	C40-C41-C42-C5
3	C	804	LBN	C40-C41-C42-C5
3	B	804	LBN	C40-C41-C42-C5

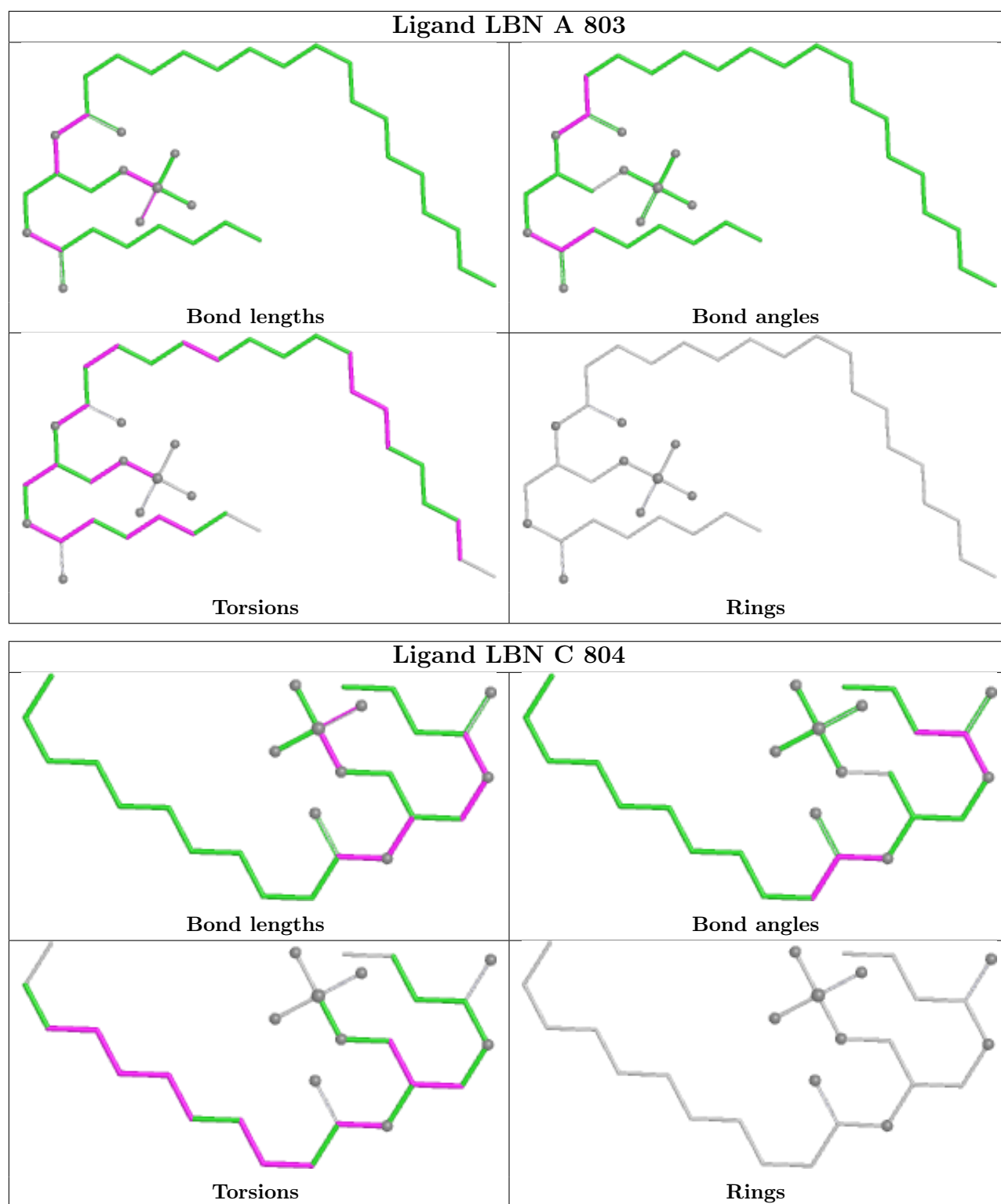
There are no ring outliers.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

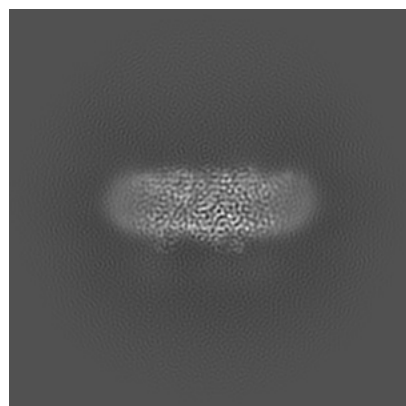
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41731. These allow visual inspection of the internal detail of the map and identification of artifacts.

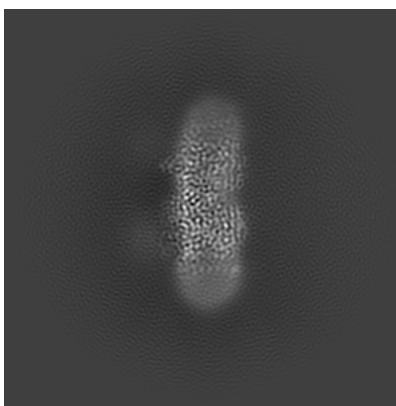
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

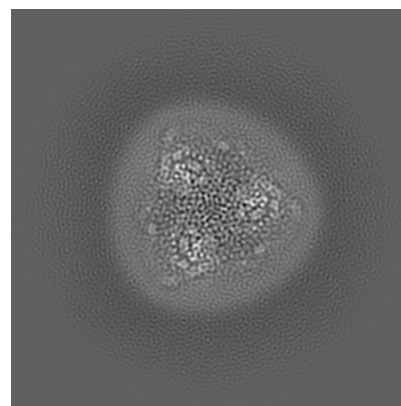
6.1.1 Primary map



X

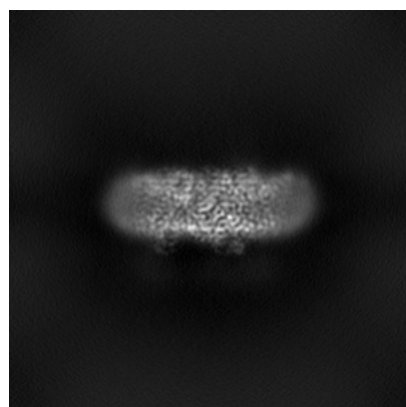


Y

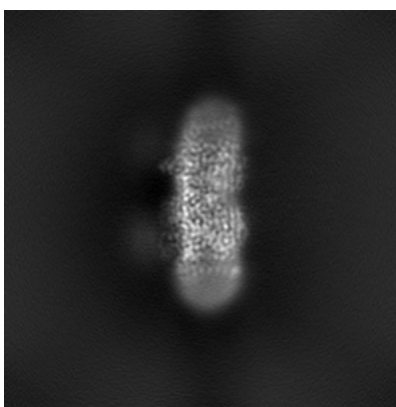


Z

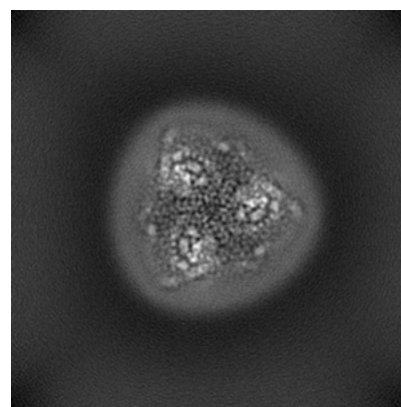
6.1.2 Raw map



X



Y

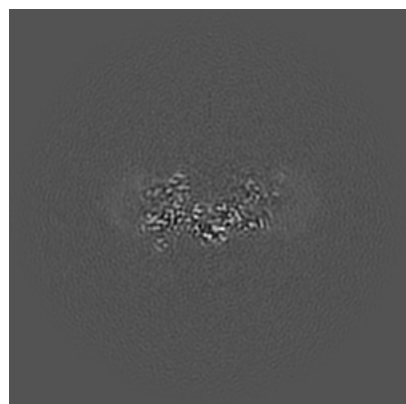


Z

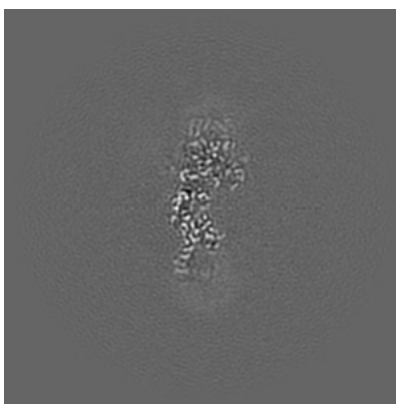
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

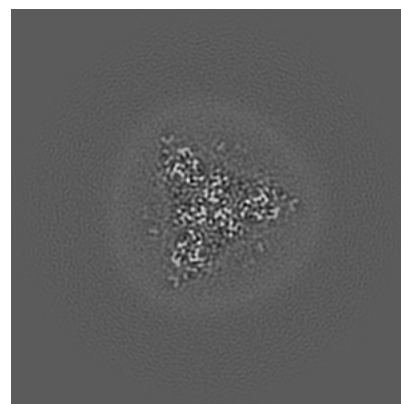
6.2.1 Primary map



X Index: 128

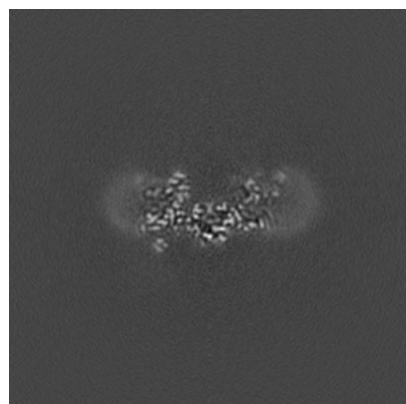


Y Index: 128

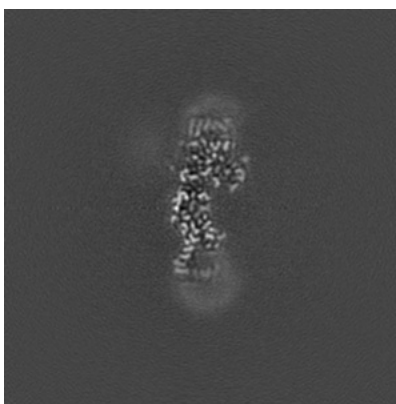


Z Index: 128

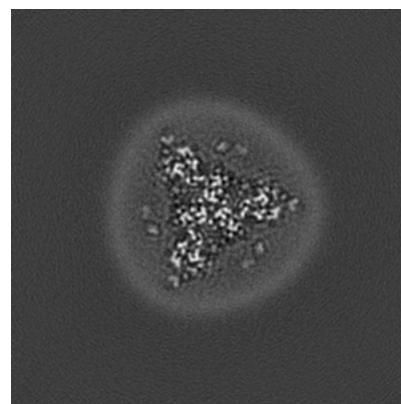
6.2.2 Raw map



X Index: 128



Y Index: 128

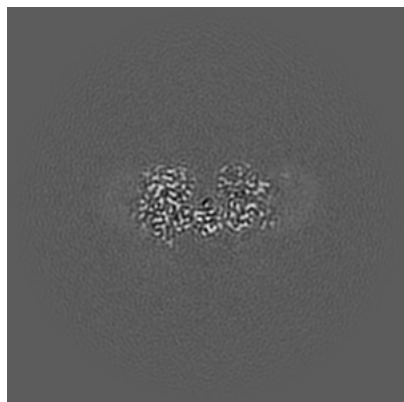


Z Index: 128

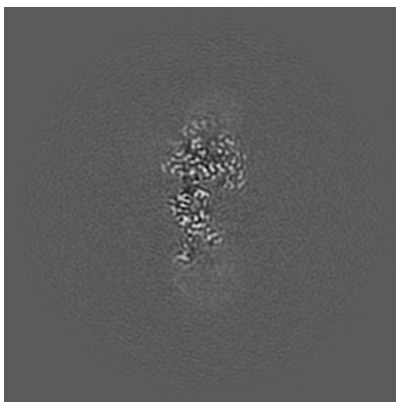
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

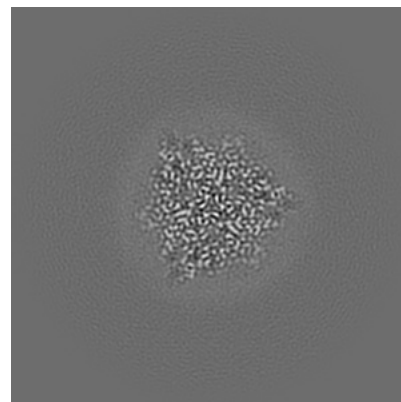
6.3.1 Primary map



X Index: 117

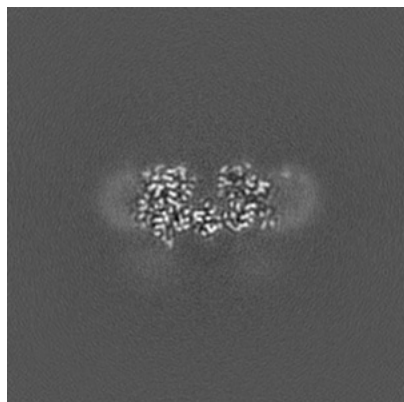


Y Index: 132

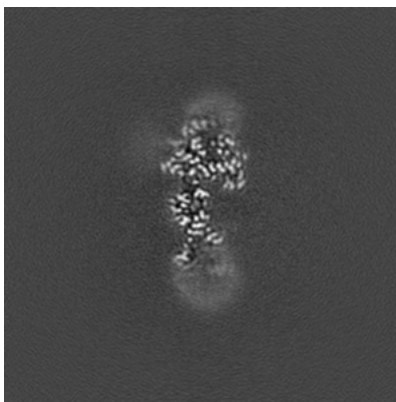


Z Index: 117

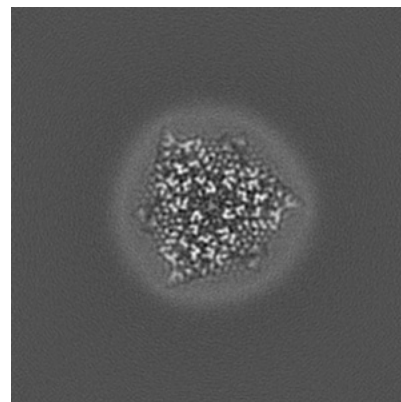
6.3.2 Raw map



X Index: 117



Y Index: 132

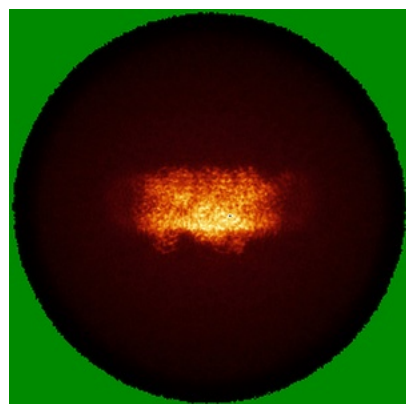


Z Index: 119

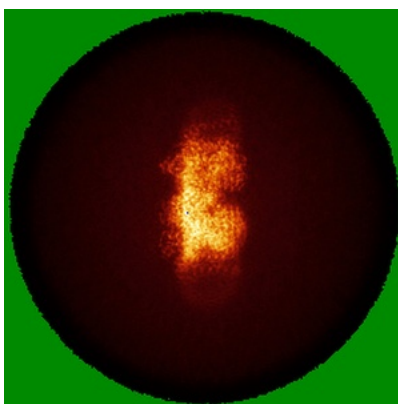
The images above show the largest variance slices of the map in three orthogonal directions.

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

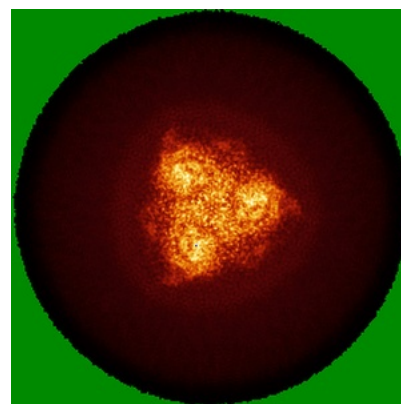
6.4.1 Primary map



X

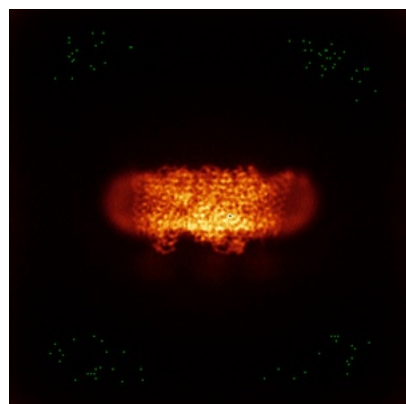


Y

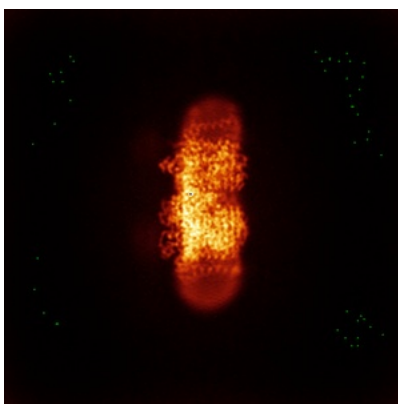


Z

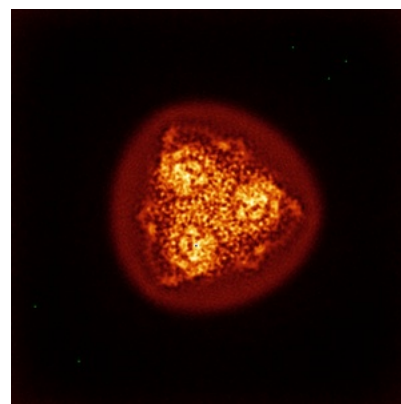
6.4.2 Raw map



X



Y

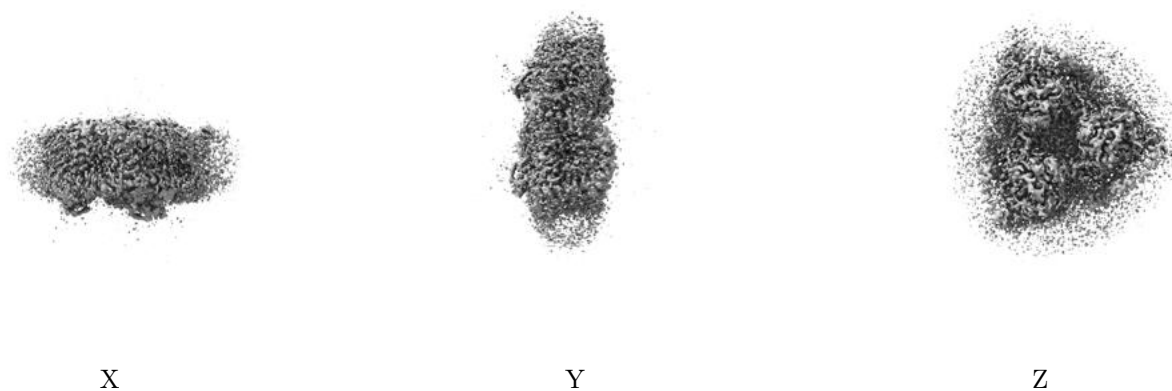


Z

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.

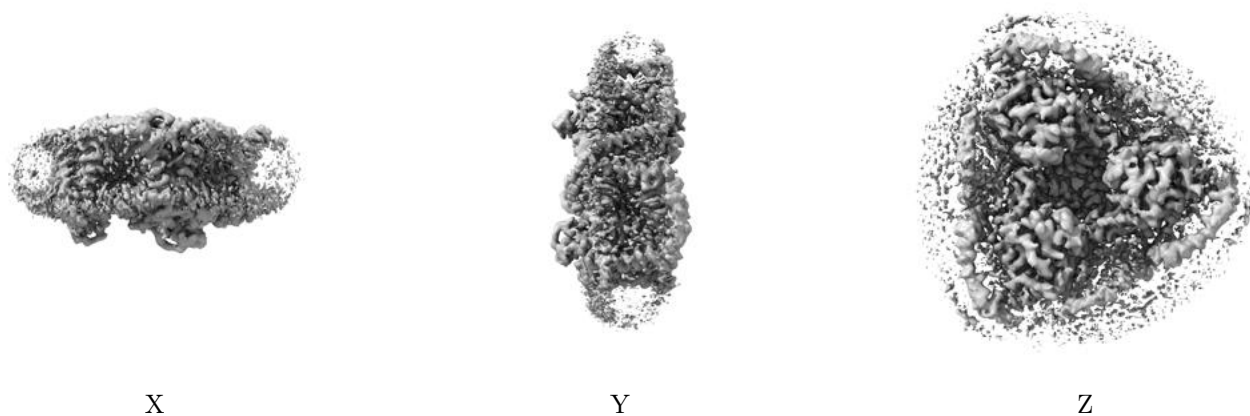
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

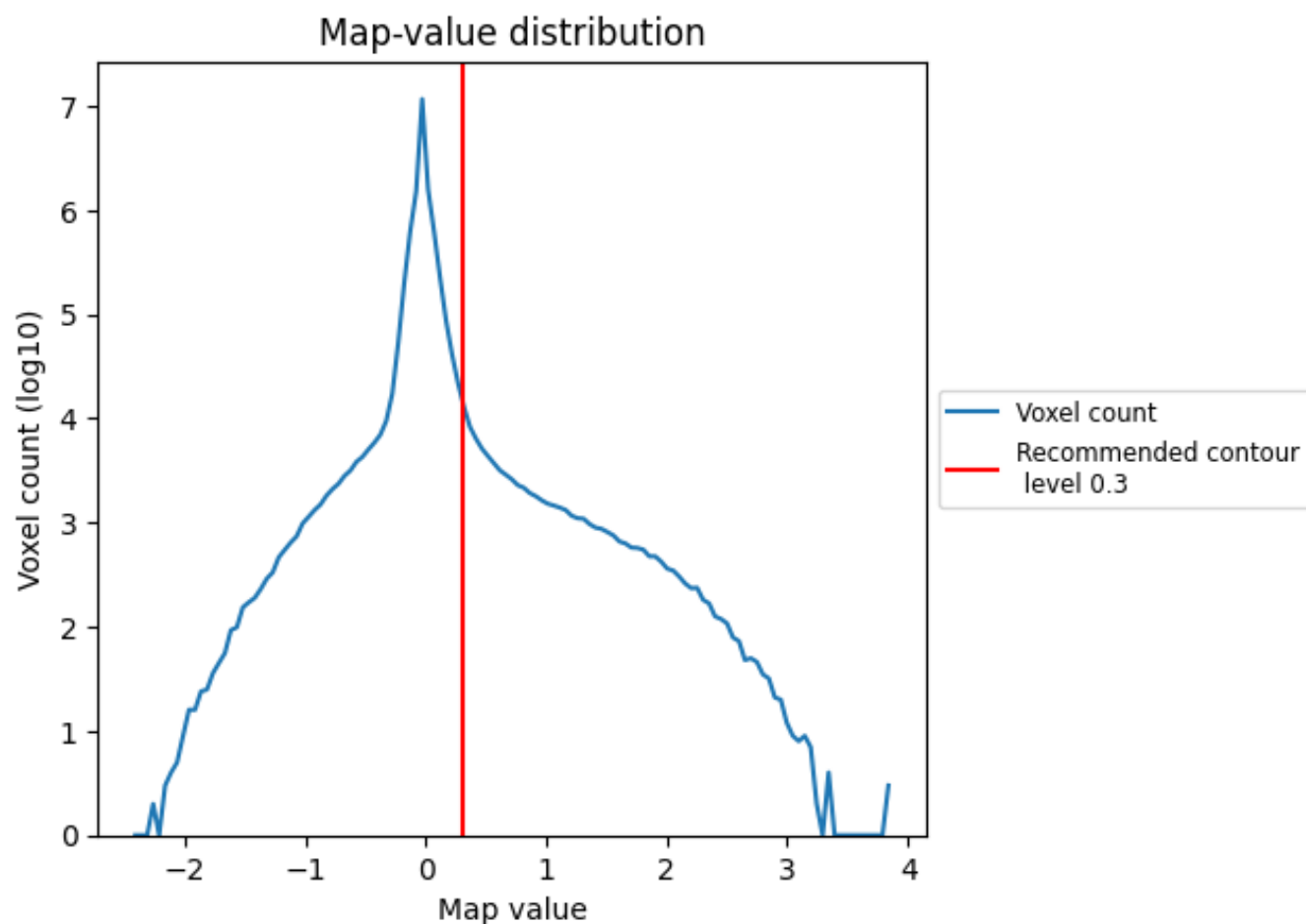
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

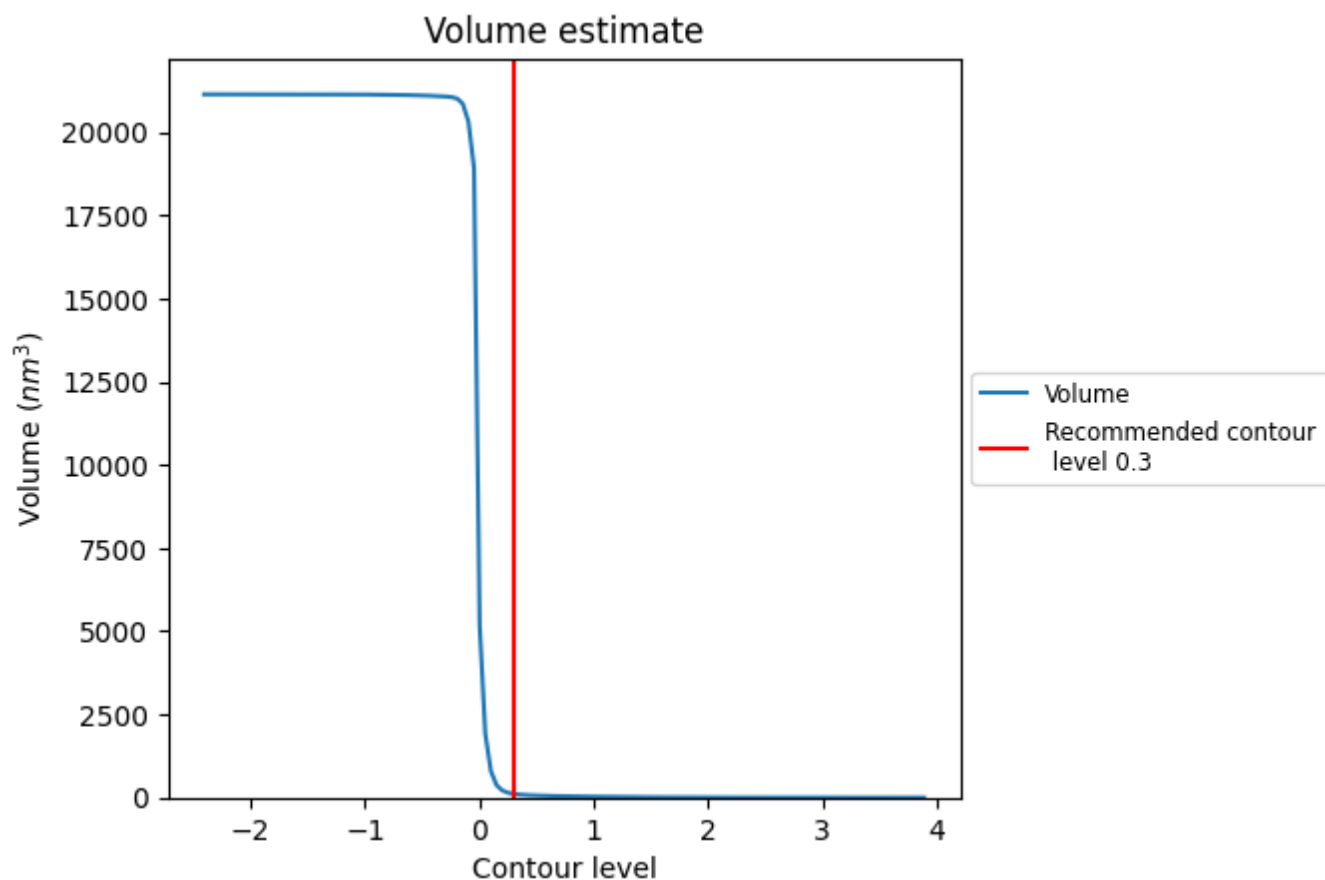
This section contains the results of statistical analysis of the map.

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.

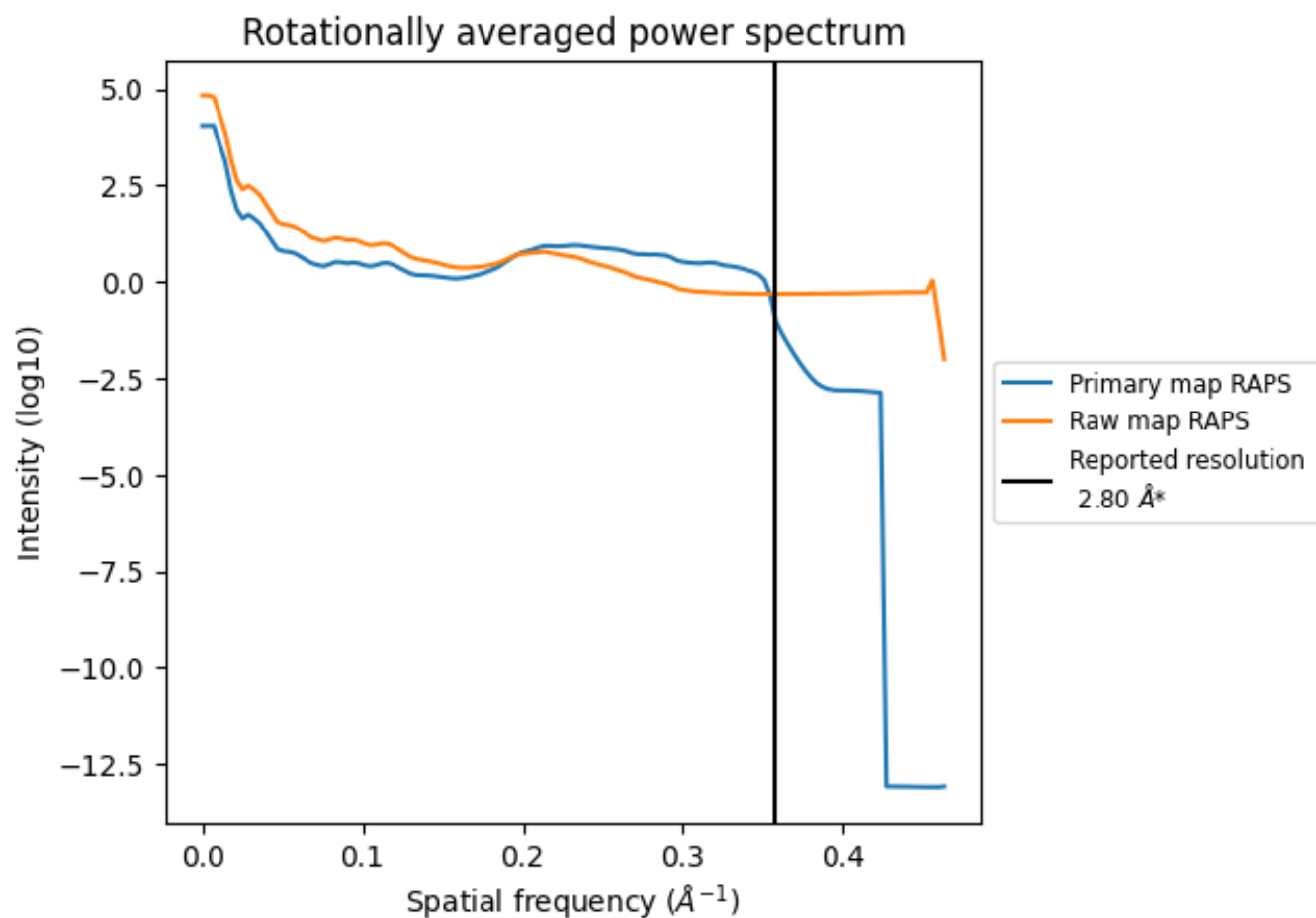
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm^3 ; this corresponds to an approximate mass of 99 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 ⓘ

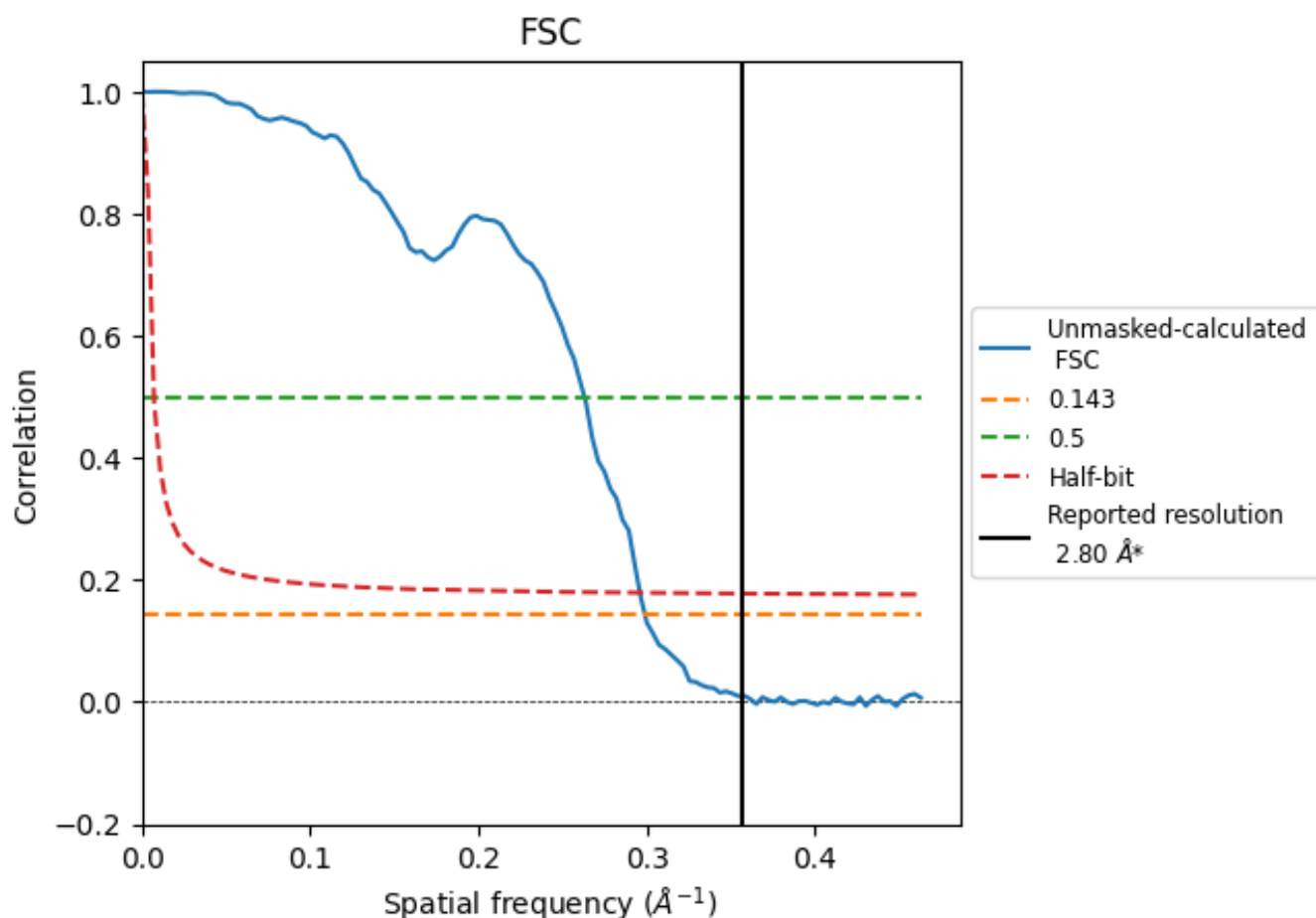


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	3.80	3.38

*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 3.34 differs from the reported value 2.8 by more than 10 %

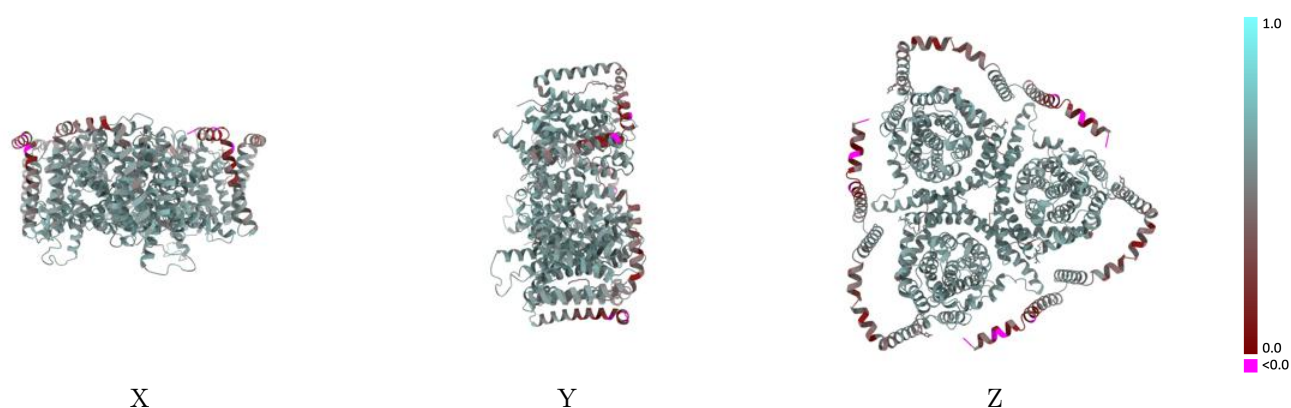
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41731 and PDB model 8TZ2. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

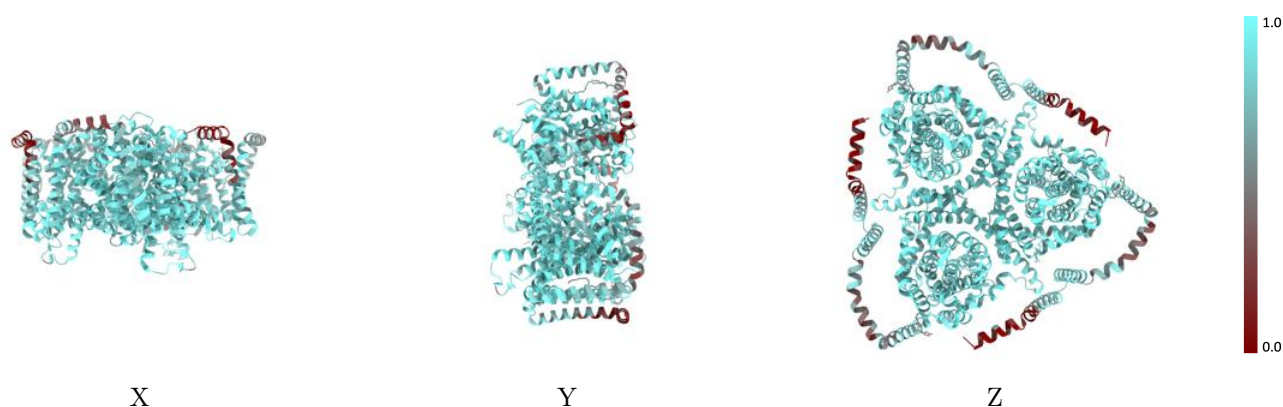
This section was not generated.

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



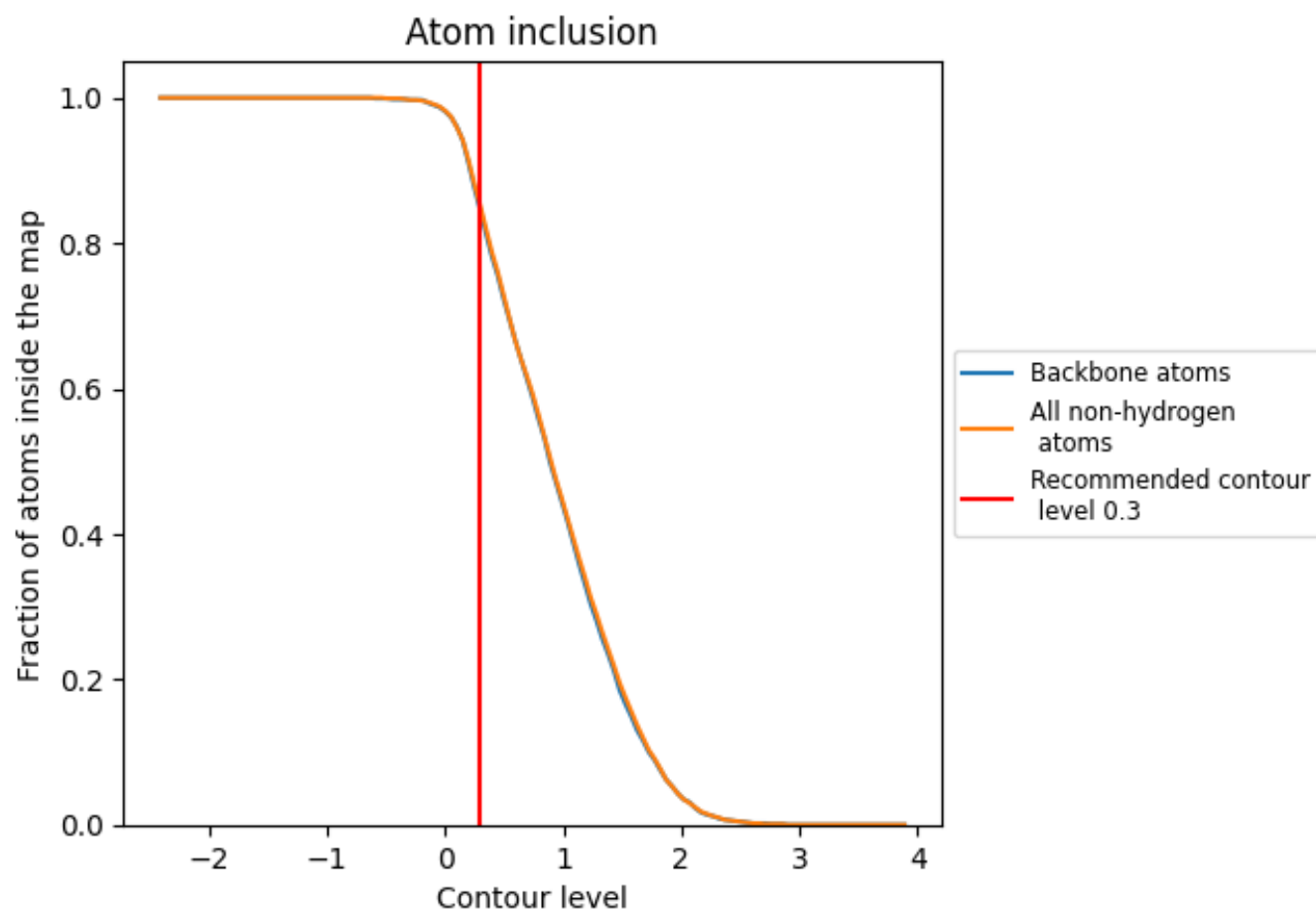
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 85% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.5550
A	0.8540	0.5550
B	0.8580	0.5560
C	0.8540	0.5550

