



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:18 PM UTC

PDB ID : 8XN1 / pdb_00008xn1
EMDB ID : EMD-38494
Title : Cryo-EM structure of human ZnT3, in the presence of zinc, determined in an inward-facing conformation
Authors : Zhu, Z.; Qu, Q.; Long, Y.; Zhou, Z.
Deposited on : 2023-12-28
Resolution : 3.14 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

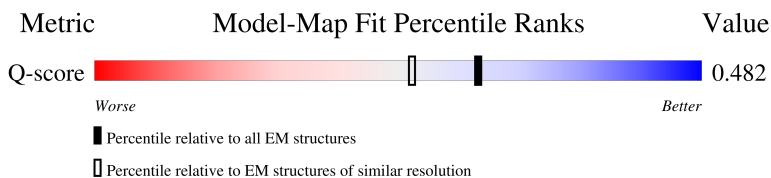
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 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	14483 (2.64 - 3.64)

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	391	 66% 16% 18%
1	B	391	 73% 11% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable proton-coupled zinc antiporter SLC30A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2314	1484	398	415	17		
1	B	327	Total	C	N	O	S	0	0
			2415	1563	409	425	18		

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	SER	-	expression tag	UNP Q99726
A	390	ASP	-	expression tag	UNP Q99726
A	391	LEU	-	expression tag	UNP Q99726
A	392	GLU	-	expression tag	UNP Q99726
A	393	VAL	-	expression tag	UNP Q99726
A	394	LEU	-	expression tag	UNP Q99726
A	395	PHE	-	expression tag	UNP Q99726
A	396	GLN	-	expression tag	UNP Q99726
A	397	GLY	-	expression tag	UNP Q99726
A	398	PRO	-	expression tag	UNP Q99726
A	399	GLU	-	expression tag	UNP Q99726
A	400	PHE	-	expression tag	UNP Q99726
A	401	TRP	-	expression tag	UNP Q99726
A	402	SER	-	expression tag	UNP Q99726
A	403	HIS	-	expression tag	UNP Q99726
A	404	PRO	-	expression tag	UNP Q99726
A	405	GLN	-	expression tag	UNP Q99726
A	406	PHE	-	expression tag	UNP Q99726
A	407	GLU	-	expression tag	UNP Q99726
A	408	LYS	-	expression tag	UNP Q99726
A	409	GLY	-	expression tag	UNP Q99726
A	410	GLY	-	expression tag	UNP Q99726
A	411	GLY	-	expression tag	UNP Q99726
A	412	SER	-	expression tag	UNP Q99726
A	413	GLY	-	expression tag	UNP Q99726
A	414	GLY	-	expression tag	UNP Q99726

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	GLY	-	expression tag	UNP Q99726
A	416	SER	-	expression tag	UNP Q99726
A	417	GLY	-	expression tag	UNP Q99726
A	418	GLY	-	expression tag	UNP Q99726
A	419	SER	-	expression tag	UNP Q99726
A	420	ALA	-	expression tag	UNP Q99726
A	421	TRP	-	expression tag	UNP Q99726
A	422	SER	-	expression tag	UNP Q99726
A	423	HIS	-	expression tag	UNP Q99726
A	424	PRO	-	expression tag	UNP Q99726
A	425	GLN	-	expression tag	UNP Q99726
A	426	PHE	-	expression tag	UNP Q99726
A	427	GLU	-	expression tag	UNP Q99726
A	428	LYS	-	expression tag	UNP Q99726
A	429	GLU	-	expression tag	UNP Q99726
A	430	PHE	-	expression tag	UNP Q99726
A	431	ASP	-	expression tag	UNP Q99726
A	432	ILE	-	expression tag	UNP Q99726
A	433	ASP	-	expression tag	UNP Q99726
A	434	TYR	-	expression tag	UNP Q99726
A	435	LYS	-	expression tag	UNP Q99726
A	436	ASP	-	expression tag	UNP Q99726
A	437	ASP	-	expression tag	UNP Q99726
A	438	ASP	-	expression tag	UNP Q99726
A	439	ASP	-	expression tag	UNP Q99726
A	440	LYS	-	expression tag	UNP Q99726
B	389	SER	-	expression tag	UNP Q99726
B	390	ASP	-	expression tag	UNP Q99726
B	391	LEU	-	expression tag	UNP Q99726
B	392	GLU	-	expression tag	UNP Q99726
B	393	VAL	-	expression tag	UNP Q99726
B	394	LEU	-	expression tag	UNP Q99726
B	395	PHE	-	expression tag	UNP Q99726
B	396	GLN	-	expression tag	UNP Q99726
B	397	GLY	-	expression tag	UNP Q99726
B	398	PRO	-	expression tag	UNP Q99726
B	399	GLU	-	expression tag	UNP Q99726
B	400	PHE	-	expression tag	UNP Q99726
B	401	TRP	-	expression tag	UNP Q99726
B	402	SER	-	expression tag	UNP Q99726
B	403	HIS	-	expression tag	UNP Q99726
B	404	PRO	-	expression tag	UNP Q99726

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	405	GLN	-	expression tag	UNP Q99726
B	406	PHE	-	expression tag	UNP Q99726
B	407	GLU	-	expression tag	UNP Q99726
B	408	LYS	-	expression tag	UNP Q99726
B	409	GLY	-	expression tag	UNP Q99726
B	410	GLY	-	expression tag	UNP Q99726
B	411	GLY	-	expression tag	UNP Q99726
B	412	SER	-	expression tag	UNP Q99726
B	413	GLY	-	expression tag	UNP Q99726
B	414	GLY	-	expression tag	UNP Q99726
B	415	GLY	-	expression tag	UNP Q99726
B	416	SER	-	expression tag	UNP Q99726
B	417	GLY	-	expression tag	UNP Q99726
B	418	GLY	-	expression tag	UNP Q99726
B	419	SER	-	expression tag	UNP Q99726
B	420	ALA	-	expression tag	UNP Q99726
B	421	TRP	-	expression tag	UNP Q99726
B	422	SER	-	expression tag	UNP Q99726
B	423	HIS	-	expression tag	UNP Q99726
B	424	PRO	-	expression tag	UNP Q99726
B	425	GLN	-	expression tag	UNP Q99726
B	426	PHE	-	expression tag	UNP Q99726
B	427	GLU	-	expression tag	UNP Q99726
B	428	LYS	-	expression tag	UNP Q99726
B	429	GLU	-	expression tag	UNP Q99726
B	430	PHE	-	expression tag	UNP Q99726
B	431	ASP	-	expression tag	UNP Q99726
B	432	ILE	-	expression tag	UNP Q99726
B	433	ASP	-	expression tag	UNP Q99726
B	434	TYR	-	expression tag	UNP Q99726
B	435	LYS	-	expression tag	UNP Q99726
B	436	ASP	-	expression tag	UNP Q99726
B	437	ASP	-	expression tag	UNP Q99726
B	438	ASP	-	expression tag	UNP Q99726
B	439	ASP	-	expression tag	UNP Q99726
B	440	LYS	-	expression tag	UNP Q99726

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

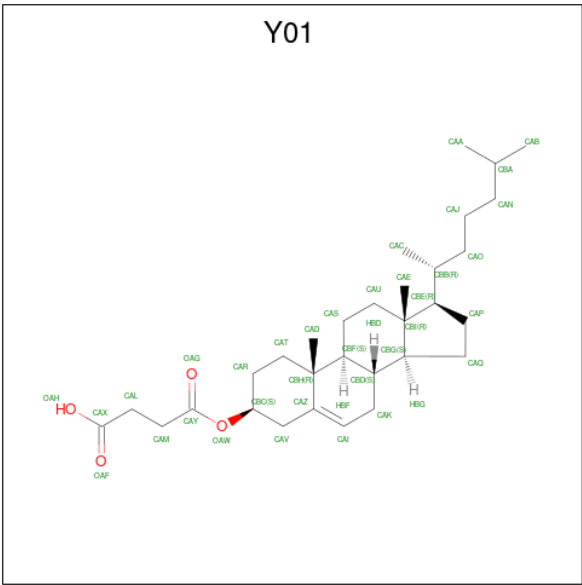
Mol	Chain	Residues	Atoms	AltConf
2	A	3	Total Zn 3 3	0

Continued on next page...

Continued from previous page...

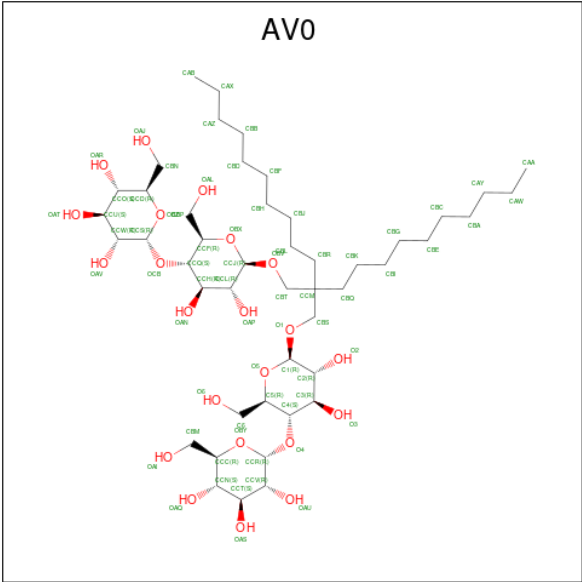
Mol	Chain	Residues	Atoms		AltConf
2	B	3	Total	Zn	0
			3	3	

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄) (labeled as "Ligand of Interest" by depositor).



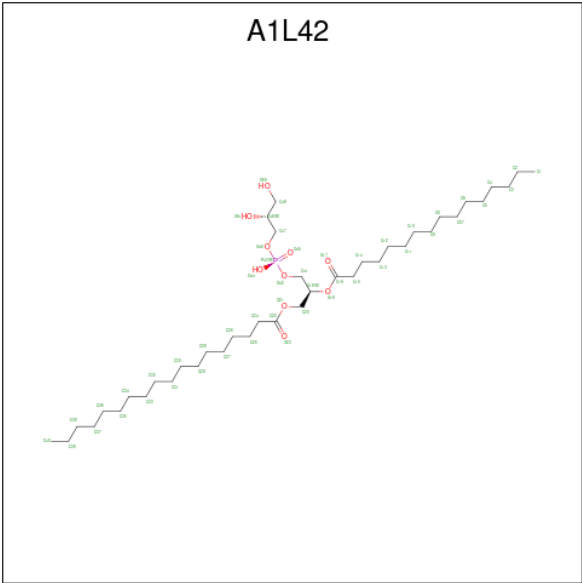
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	

- Molecule 4 is Lauryl Maltose Neopentyl Glycol (CCD ID: AV0) (formula: C₄₇H₈₈O₂₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			69	47	22	
4	B	1	Total	C	O	0
			69	47	22	

- Molecule 5 is (1S)-2-[[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: A1L42) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).

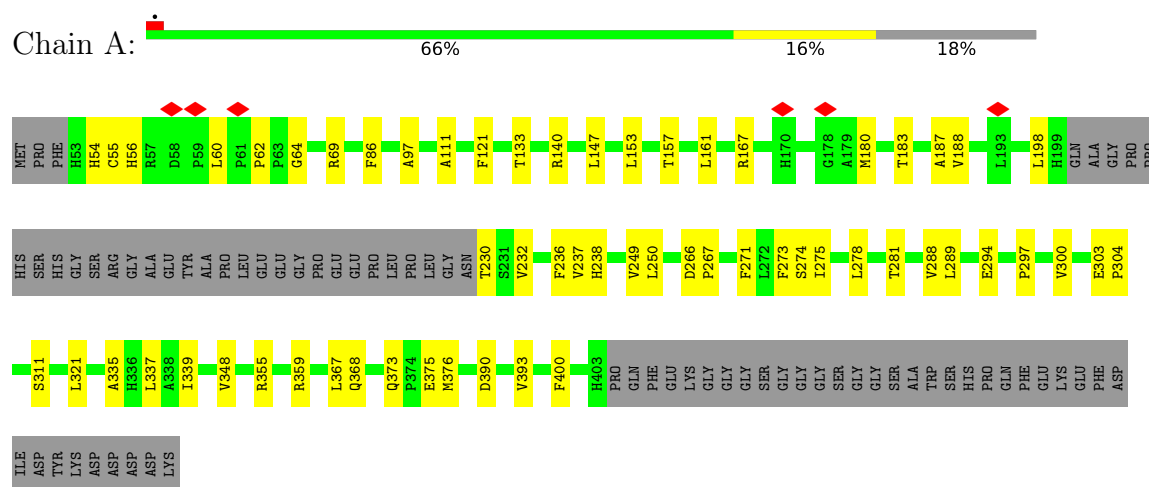


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	O	P	0
			41	30	10	1	

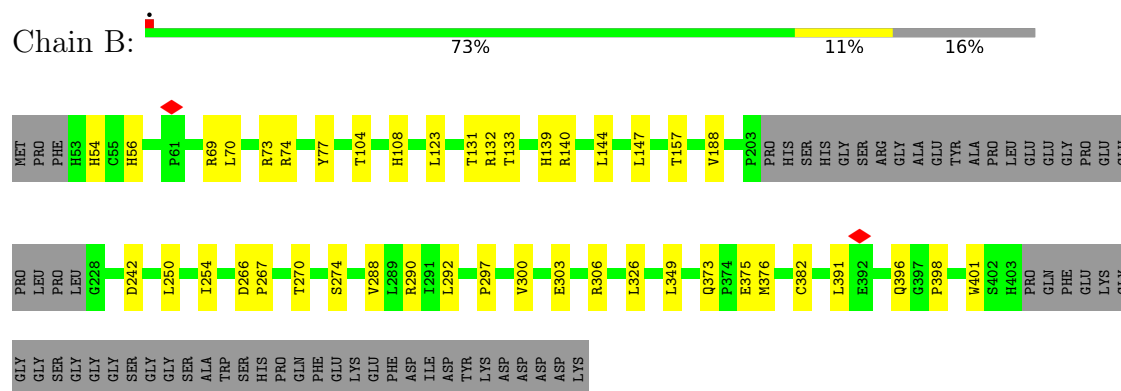
3 Residue-property plots

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: Probable proton-coupled zinc antiporter SLC30A3



- Molecule 1: Probable proton-coupled zinc antiporter SLC30A3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	341267	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.544	Depositor
Minimum map value	-2.152	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	216.32, 216.32, 216.32	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AV0, Y01, A1L42, ZN

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	0.14	0/2367	0.33	0/3241
1	B	0.13	0/2479	0.31	0/3392
All	All	0.14	0/4846	0.32	0/6633

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	2314	0	2228	47	0
1	B	2415	0	2347	34	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	70	0	98	3	0
4	A	69	0	0	2	0
4	B	69	0	0	0	0
5	B	41	0	0	0	0
All	All	4984	0	4673	70	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 7.

All (70) 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:56:HIS:HE1	1:B:382:CYS:SG	2.21	0.63
1:A:157:THR:HG21	1:A:278:LEU:HD21	1.83	0.61
1:B:157:THR:HG23	1:B:274:SER:HB2	1.83	0.60
1:B:74:ARG:HA	1:B:77:TYR:CE1	2.37	0.59
1:A:337:LEU:HD12	1:A:367:LEU:HD13	1.85	0.59
1:A:303:GLU:OE1	1:B:132:ARG:NH1	2.37	0.58
1:A:230:THR:HG23	1:A:232:VAL:H	1.68	0.57
1:B:104:THR:OG1	1:B:270:THR:OG1	2.20	0.56
1:A:294:GLU:OE2	1:B:140:ARG:NH2	2.37	0.55
1:A:321:LEU:HD13	1:A:335:ALA:HB2	1.89	0.55
1:A:289:LEU:HB3	3:A:505:Y01:HAT2	1.89	0.53
1:A:121:PHE:HD2	3:A:504:Y01:HAU2	1.75	0.52
1:B:297:PRO:HG2	1:B:300:VAL:HB	1.91	0.52
1:B:373:GLN:O	1:B:375:GLU:N	2.44	0.51
1:B:139:HIS:HB2	1:B:326:LEU:HD23	1.93	0.50
1:A:147:LEU:HB2	1:A:288:VAL:HG11	1.94	0.50
1:A:86:PHE:HE1	1:A:187:ALA:HA	1.77	0.49
1:B:398:PRO:HA	1:B:401:TRP:HB2	1.94	0.48
1:A:368:GLN:HE21	1:B:349:LEU:HD21	1.78	0.48
1:B:69:ARG:HG3	1:B:123:LEU:HD11	1.95	0.48
1:A:180:MET:HA	1:A:183:THR:HG22	1.95	0.48
1:A:198:LEU:HB3	1:A:236:PHE:HD2	1.79	0.48
1:A:373:GLN:O	1:A:375:GLU:N	2.46	0.48
1:A:393:VAL:HG11	1:B:131:THR:HG21	1.94	0.48
1:B:250:LEU:O	1:B:254:ILE:HG12	2.14	0.48
1:B:396:GLN:OE1	1:B:396:GLN:N	2.47	0.47
1:A:121:PHE:CD2	3:A:504:Y01:HAC1	2.49	0.47
1:A:97:ALA:HB1	1:A:180:MET:HB2	1.95	0.47
1:A:161:LEU:HD21	1:A:274:SER:OG	2.15	0.47
1:B:70:LEU:HA	1:B:73:ARG:HG2	1.96	0.46
1:A:140:ARG:HD2	1:B:292:LEU:O	2.14	0.46
1:A:133:THR:HB	1:B:290:ARG:HH22	1.81	0.46
1:B:108:HIS:NE2	1:B:242:ASP:OD1	2.49	0.46
1:B:267:PRO:HA	1:B:270:THR:HG22	1.98	0.46
1:A:373:GLN:HB3	1:A:376:MET:HE3	1.99	0.45
1:B:147:LEU:HB2	1:B:288:VAL:HG11	1.97	0.45
1:A:271:PHE:O	1:A:275:ILE:HG12	2.17	0.44
1:A:54:HIS:CD2	1:A:55:CYS:H	2.35	0.44
1:A:54:HIS:CE1	1:B:376:MET:HG2	2.52	0.44
1:B:104:THR:HG1	1:B:270:THR:HG1	1.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:O	1:A:161:LEU:HD23	2.18	0.44
1:A:278:LEU:HA	1:A:281:THR:HG22	2.00	0.43
1:B:188:VAL:HG21	1:B:250:LEU:HD22	2.00	0.43
1:A:60:LEU:O	1:A:62:PRO:HD3	2.18	0.43
1:A:359:ARG:HE	1:A:359:ARG:HB2	1.72	0.43
1:A:198:LEU:HB3	1:A:236:PHE:CD2	2.53	0.43
1:A:337:LEU:N	1:A:368:GLN:O	2.51	0.43
1:A:167:ARG:HE	1:A:167:ARG:HB2	1.72	0.43
1:A:249:VAL:HG22	1:A:273:PHE:HE1	1.84	0.43
1:A:368:GLN:HE21	1:B:349:LEU:HD11	1.83	0.43
1:A:64:GLY:O	1:A:69:ARG:NH1	2.51	0.43
1:B:54:HIS:C	1:B:56:HIS:H	2.26	0.43
1:A:390:ASP:OD1	1:B:133:THR:OG1	2.37	0.42
1:A:297:PRO:HG2	1:A:300:VAL:HB	2.02	0.42
1:B:54:HIS:CD2	1:B:56:HIS:ND1	2.88	0.42
1:A:339:ILE:HG21	1:A:348:VAL:HG11	2.02	0.42
1:A:238:HIS:ND1	4:A:506:AV0:OAN	2.53	0.42
1:A:266:ASP:HB3	1:A:267:PRO:HD3	2.00	0.42
1:A:311:SER:OG	1:A:355:ARG:NH2	2.53	0.42
1:A:86:PHE:CE1	1:A:187:ALA:HA	2.55	0.42
1:A:400:PHE:CZ	1:B:73:ARG:HD2	2.55	0.42
1:B:266:ASP:HB3	1:B:267:PRO:HD3	2.01	0.41
1:B:391:LEU:HD12	1:B:391:LEU:HA	1.91	0.41
1:A:111:ALA:HB2	1:A:153:LEU:HD12	2.02	0.41
1:A:188:VAL:HG21	1:A:250:LEU:HD12	2.02	0.41
1:A:303:GLU:HB2	1:A:304:PRO:HD3	2.03	0.41
1:A:237:VAL:HG23	4:A:506:AV0:OAL	2.21	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.83	0.40
1:B:398:PRO:HA	1:B:401:TRP:HD1	1.86	0.40
1:B:303:GLU:OE2	1:B:306:ARG:NH2	2.54	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	317/391 (81%)	306 (96%)	11 (4%)	0	100	100
1	B	323/391 (83%)	311 (96%)	12 (4%)	0	100	100
All	All	640/782 (82%)	617 (96%)	23 (4%)	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	228/317 (72%)	228 (100%)	0	100	100
1	B	244/317 (77%)	244 (100%)	0	100	100
All	All	472/634 (74%)	472 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	HIS
1	B	174	HIS
1	B	322	HIS

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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	Y01	A	504	-	38,38,38	0.72	2 (5%)	57,57,57	0.82	3 (5%)
4	AV0	A	506	-	72,72,72	1.15	5 (6%)	92,98,98	1.57	18 (19%)
4	AV0	B	505	-	72,72,72	1.09	7 (9%)	92,98,98	1.39	9 (9%)
3	Y01	A	505	-	38,38,38	0.75	2 (5%)	57,57,57	1.05	5 (8%)
5	A1L42	B	504	-	40,40,50	1.16	4 (10%)	43,46,56	0.97	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
3	Y01	A	504	-	-	8/19/77/77	0/4/4/4
4	AV0	A	506	-	-	27/50/130/130	0/4/4/4
4	AV0	B	505	-	-	35/50/130/130	0/4/4/4
3	Y01	A	505	-	-	5/19/77/77	0/4/4/4
5	A1L42	B	504	-	-	30/45/45/55	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	A1L42	C31-C32	-3.75	1.33	1.51
3	A	505	Y01	OAF-CAX	3.10	1.32	1.22
4	A	506	AV0	OBZ-CCS	2.98	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	Y01	OAH-CAX	-2.94	1.21	1.30
3	A	505	Y01	OAH-CAX	-2.80	1.21	1.30
3	A	504	Y01	OAF-CAX	2.77	1.31	1.22
4	B	505	AV0	OBZ-CCS	2.73	1.48	1.41
5	B	504	A1L42	O18-C19	-2.60	1.40	1.46
4	A	506	AV0	CBS-CCM	2.54	1.59	1.53
5	B	504	A1L42	O21-C22	2.53	1.40	1.33
4	A	506	AV0	O5-C5	2.33	1.50	1.44
4	B	505	AV0	CCH-CCQ	-2.29	1.46	1.52
4	A	506	AV0	CCH-CCQ	-2.23	1.46	1.52
4	A	506	AV0	CCV-CCT	-2.22	1.46	1.52
5	B	504	A1L42	O18-C16	2.19	1.40	1.34
4	B	505	AV0	CCV-CCT	-2.15	1.46	1.52
4	B	505	AV0	CCL-CCH	-2.14	1.46	1.52
4	B	505	AV0	OBY-CCR	2.06	1.47	1.41
4	B	505	AV0	OAS-CCT	2.02	1.48	1.43
4	B	505	AV0	OAN-CCH	2.01	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	AV0	CCS-OCB-CCQ	-5.22	105.60	117.98
4	A	506	AV0	O1-C1-C2	4.16	114.59	108.27
4	B	505	AV0	CCT-CCN-CCC	4.06	117.60	110.23
5	B	504	A1L42	O18-C16-C15	3.94	120.00	111.48
4	A	506	AV0	O5-C5-C4	3.83	117.64	109.72
4	A	506	AV0	CBL-CBR-CCM	-3.59	106.31	117.19
4	B	505	AV0	CBK-CBQ-CCM	-3.55	106.43	117.19
4	A	506	AV0	CBS-O1-C1	3.32	121.74	113.31
4	B	505	AV0	O4-CCR-CCV	3.28	116.15	108.09
4	A	506	AV0	OBZ-CCD-CCO	3.20	115.47	109.70
4	B	505	AV0	OBY-CCC-CCN	3.19	115.44	109.70
4	B	505	AV0	CBP-CCF-CCQ	-3.07	104.75	113.38
4	A	506	AV0	C2-C3-C4	3.01	116.51	109.68
4	A	506	AV0	CCS-OCB-CCQ	-2.97	110.93	117.98
4	A	506	AV0	C3-C4-C5	2.95	117.47	110.93
4	A	506	AV0	CCR-O4-C4	-2.91	111.08	117.98
3	A	505	Y01	CBC-CAV-CAZ	2.80	115.59	111.45
5	B	504	A1L42	O21-C22-C24	2.77	120.29	111.83
3	A	505	Y01	OAW-CBC-CAR	-2.77	101.83	108.37
4	A	506	AV0	CCL-CCH-CCQ	2.72	115.84	109.68
4	A	506	AV0	C1-C2-C3	2.65	115.58	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	Y01	OAW-CBC-CAV	-2.63	102.63	108.04
4	A	506	AV0	OAN-CCH-CCQ	-2.57	103.34	109.94
3	A	504	Y01	OAH-CAX-CAL	2.57	122.13	114.00
4	A	506	AV0	CBK-CBQ-CCM	-2.57	109.40	117.19
4	A	506	AV0	CCU-CCO-CCD	2.55	114.86	110.23
3	A	505	Y01	OAH-CAX-CAL	2.49	121.86	114.00
4	B	505	AV0	CBR-CCM-CBQ	-2.31	105.67	109.96
3	A	504	Y01	OAF-CAX-CAL	-2.26	115.92	123.09
4	A	506	AV0	CCS-OBZ-CCD	2.20	118.01	113.72
4	B	505	AV0	CCW-CCU-CCO	2.19	114.67	110.83
4	A	506	AV0	CCJ-OBX-CCF	-2.16	109.51	113.72
3	A	505	Y01	OAF-CAX-CAL	-2.15	116.27	123.09
4	B	505	AV0	CBL-CBR-CCM	-2.12	110.74	117.19
4	A	506	AV0	CBP-CCF-CCQ	-2.09	107.49	113.38
3	A	505	Y01	CAU-CBI-CBG	-2.08	104.14	107.25
4	A	506	AV0	OAN-CCH-CCL	-2.01	105.64	110.38

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	Y01	OAG-CAY-OAW-CBC
3	A	504	Y01	CAM-CAY-OAW-CBC
4	A	506	AV0	C2-C1-O1-CBS
4	A	506	AV0	O5-C1-O1-CBS
4	A	506	AV0	CBK-CBQ-CCM-CBR
4	A	506	AV0	O1-CBS-CCM-CBQ
4	A	506	AV0	O1-CBS-CCM-CBR
4	B	505	AV0	O5-C1-O1-CBS
4	B	505	AV0	CCV-CCR-O4-C4
4	B	505	AV0	CBL-CBR-CCM-CBQ
4	B	505	AV0	CBL-CBR-CCM-CBS
4	B	505	AV0	CBL-CBR-CCM-CBT
4	B	505	AV0	O1-CBS-CCM-CBQ
5	B	504	A1L42	C15-C16-O18-C19
5	B	504	A1L42	C41-O42-P43-O44
5	B	504	A1L42	C41-O42-P43-O45
5	B	504	A1L42	C41-O42-P43-O46
5	B	504	A1L42	C47-O46-P43-O42
5	B	504	A1L42	C47-O46-P43-O44
5	B	504	A1L42	C47-O46-P43-O45
4	A	506	AV0	OBZ-CCS-OCB-CCQ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	505	AV0	OAL-CBP-CCF-CCQ
4	A	506	AV0	O1-CBS-CCM-CBT
5	B	504	A1L42	O17-C16-O18-C19
4	B	505	AV0	OAL-CBP-CCF-OBX
5	B	504	A1L42	O46-C47-C48-O51
4	B	505	AV0	O5-C5-C6-O6
4	A	506	AV0	OAI-CBM-CCC-OBX
4	B	505	AV0	OAI-CBM-CCC-OBX
3	A	505	Y01	CAJ-CAO-CBB-CAC
4	A	506	AV0	OBX-CCJ-OBV-CBT
4	B	505	AV0	CBD-CBF-CBH-CBJ
3	A	505	Y01	CAJ-CAO-CBB-CBE
4	A	506	AV0	CCV-CCR-O4-C4
4	B	505	AV0	OAI-CBM-CCC-CCN
4	A	506	AV0	OAI-CBM-CCC-CCN
4	B	505	AV0	C4-C5-C6-O6
4	A	506	AV0	CAZ-CBB-CBD-CBF
4	B	505	AV0	C2-C1-O1-CBS
3	A	504	Y01	CAJ-CAO-CBB-CBE
5	B	504	A1L42	C24-C22-O21-C20
3	A	504	Y01	CAN-CAJ-CAO-CBB
4	A	506	AV0	OBX-CCR-O4-C4
3	A	504	Y01	CAJ-CAO-CBB-CAC
4	B	505	AV0	CAZ-CBB-CBD-CBF
4	B	505	AV0	CBJ-CBL-CBR-CCM
5	B	504	A1L42	C47-C48-C49-O50
5	B	504	A1L42	O23-C22-O21-C20
4	B	505	AV0	OBZ-CCS-OCB-CCQ
4	A	506	AV0	CAY-CBA-CBC-CBE
4	A	506	AV0	CBG-CBI-CBK-CBQ
4	A	506	AV0	C4-C5-C6-O6
4	B	505	AV0	CBA-CBC-CBE-CBG
5	B	504	A1L42	C35-C36-C37-C38
5	B	504	A1L42	C33-C34-C35-C36
4	A	506	AV0	CBD-CBF-CBH-CBJ
4	B	505	AV0	CAX-CAZ-CBB-CBD
5	B	504	A1L42	C25-C26-C27-C28
4	B	505	AV0	CBC-CBE-CBG-CBI
5	B	504	A1L42	C12-C13-C14-C15
4	B	505	AV0	CCH-CCQ-OCB-CCS
5	B	504	A1L42	C22-C24-C25-C26
4	A	506	AV0	CBC-CBE-CBG-CBI

Continued on next page...

Continued from previous page...

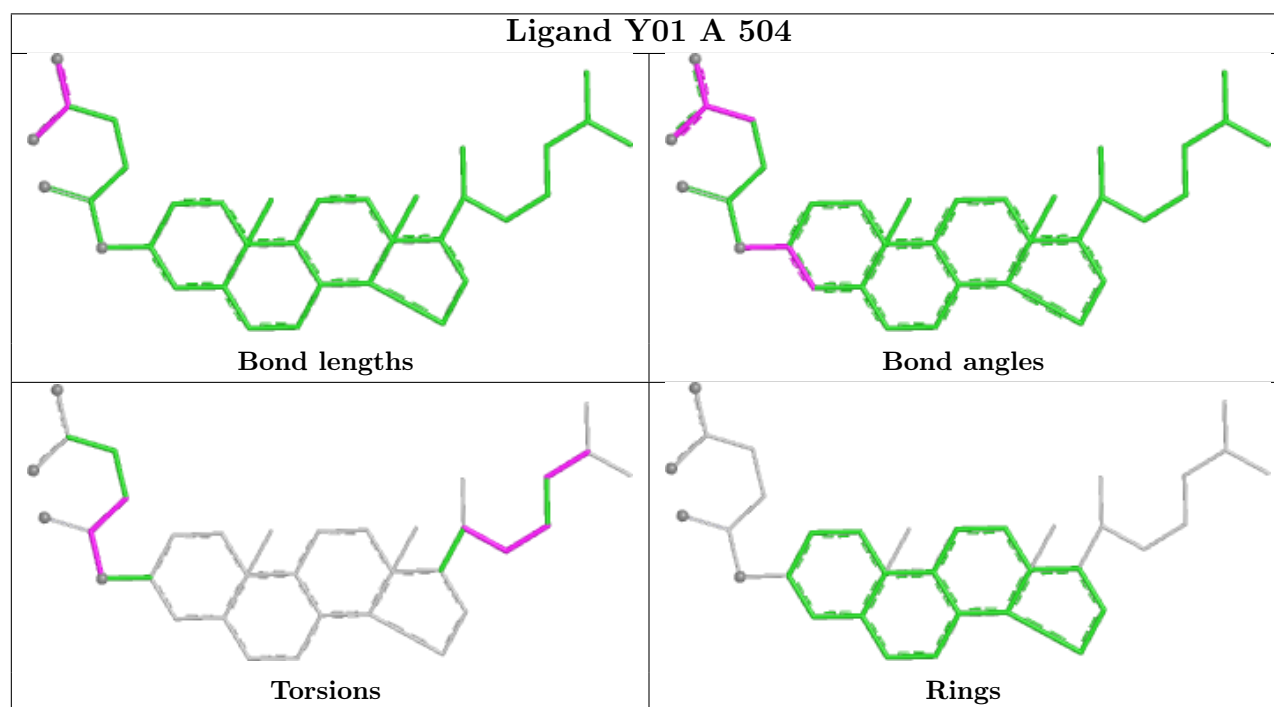
Mol	Chain	Res	Type	Atoms
4	B	505	AV0	CCF-CCQ-OCB-CCS
5	B	504	A1L42	O46-C47-C48-C49
4	B	505	AV0	CBH-CBJ-CBL-CBR
3	A	504	Y01	CAJ-CAN-CBA-CAB
4	A	506	AV0	CBF-CBH-CBJ-CBL
4	A	506	AV0	CAX-CAZ-CBB-CBD
5	B	504	A1L42	C34-C35-C36-C37
5	B	504	A1L42	O18-C19-C20-O21
5	B	504	A1L42	O51-C48-C49-O50
4	B	505	AV0	CAY-CBA-CBC-CBE
5	B	504	A1L42	C19-C41-O42-P43
4	B	505	AV0	CAA-CAW-CAY-CBA
3	A	504	Y01	CAJ-CAN-CBA-CAA
4	A	506	AV0	CBH-CBJ-CBL-CBR
4	A	506	AV0	CBK-CBQ-CCM-CBS
5	B	504	A1L42	O18-C19-C41-O42
5	B	504	A1L42	C36-C37-C38-C39
4	A	506	AV0	O5-C5-C6-O6
4	B	505	AV0	O1-CBS-CCM-CBR
4	A	506	AV0	CCM-CBS-O1-C1
5	B	504	A1L42	C41-C19-C20-O21
4	B	505	AV0	CBG-CBI-CBK-CBQ
5	B	504	A1L42	C20-C19-C41-O42
4	B	505	AV0	CCW-CCS-OCB-CCQ
3	A	505	Y01	CAN-CAJ-CAO-CBB
4	A	506	AV0	CBE-CBG-CBI-CBK
5	B	504	A1L42	C31-C32-C33-C34
4	B	505	AV0	C3-C4-O4-CCR
4	B	505	AV0	C5-C4-O4-CCR
4	A	506	AV0	CAB-CAX-CAZ-CBB
5	B	504	A1L42	C28-C29-C30-C31
4	B	505	AV0	CAW-CAY-CBA-CBC
5	B	504	A1L42	C26-C27-C28-C29
5	B	504	A1L42	C13-C14-C15-C16
4	B	505	AV0	CBB-CBD-CBF-CBH
4	B	505	AV0	OAJ-CBN-CCD-OBZ
4	A	506	AV0	CBB-CBD-CBF-CBH
3	A	505	Y01	CAM-CAL-CAX-OAF
4	B	505	AV0	O1-CBS-CCM-CBT
4	B	505	AV0	CCM-CBS-O1-C1
3	A	504	Y01	CAL-CAM-CAY-OAW
3	A	505	Y01	CAM-CAL-CAX-OAH

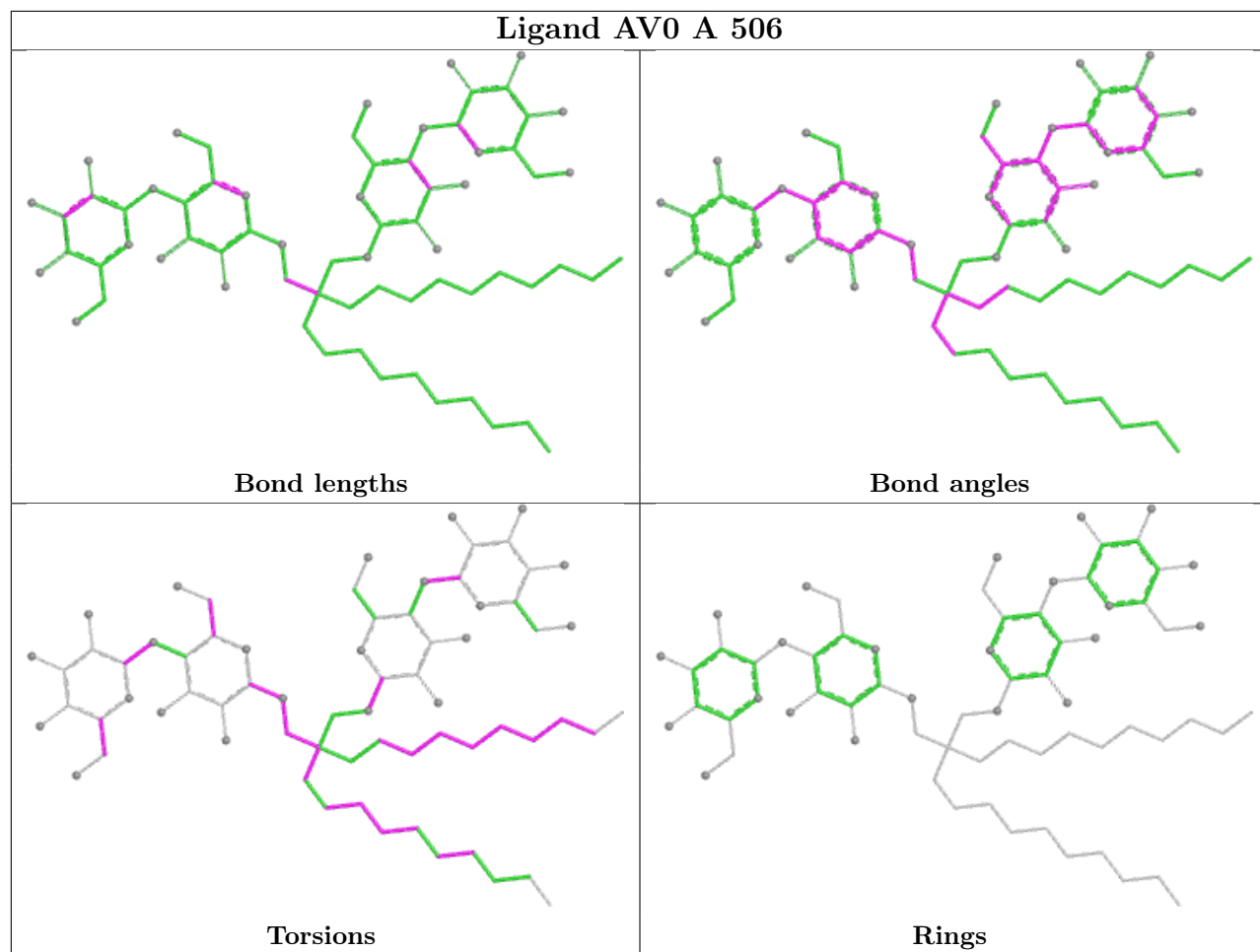
There are no ring outliers.

3 monomers are involved in 5 short contacts:

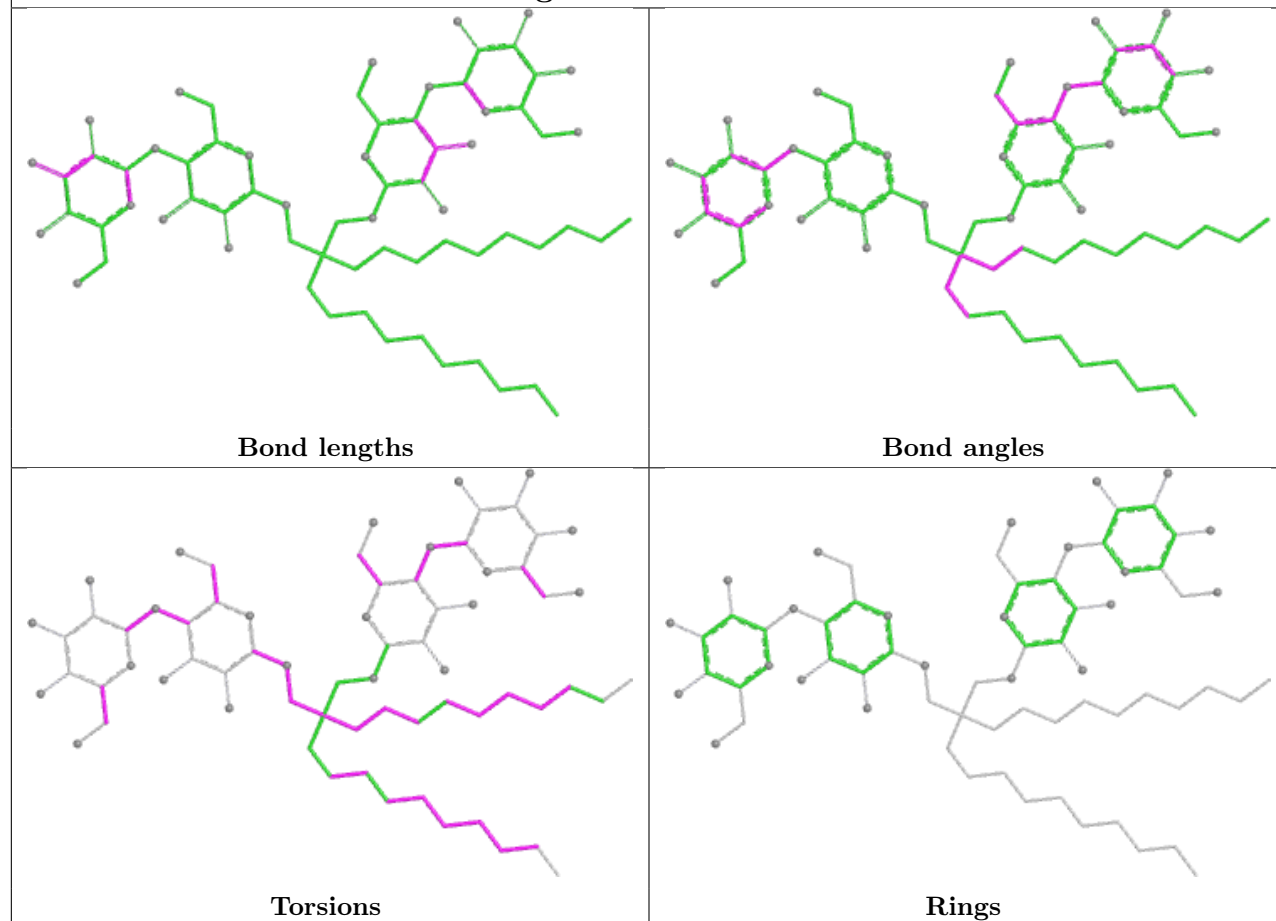
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	Y01	2	0
4	A	506	AV0	2	0
3	A	505	Y01	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

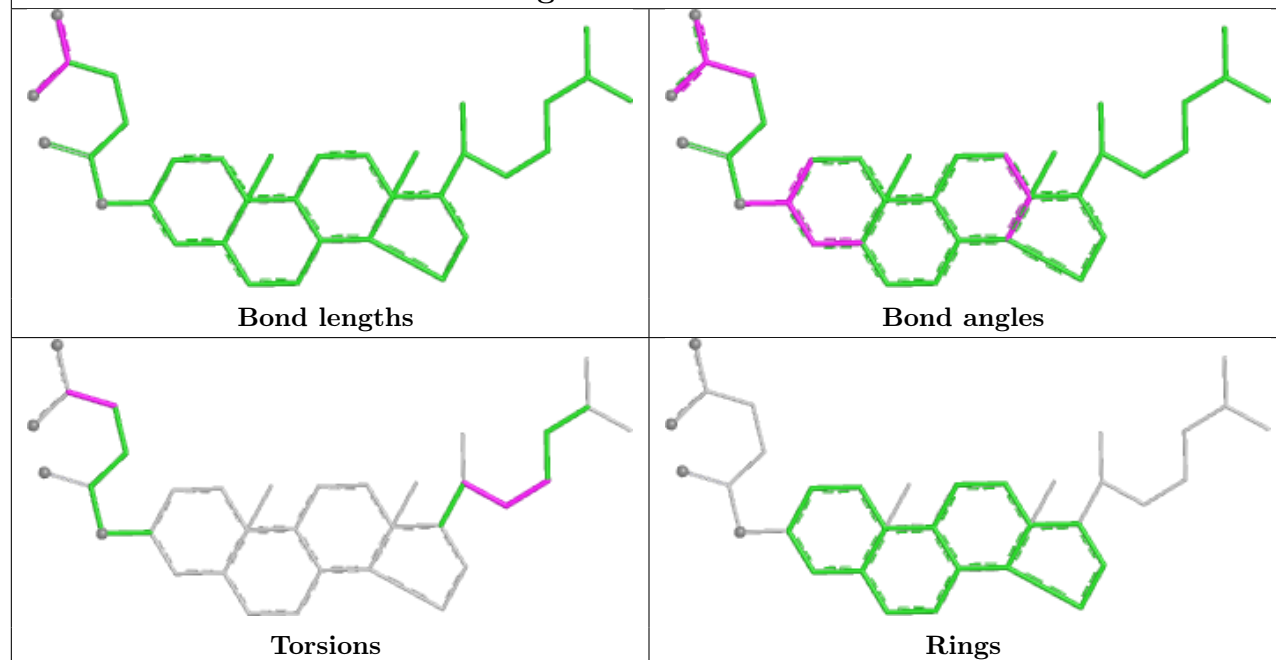


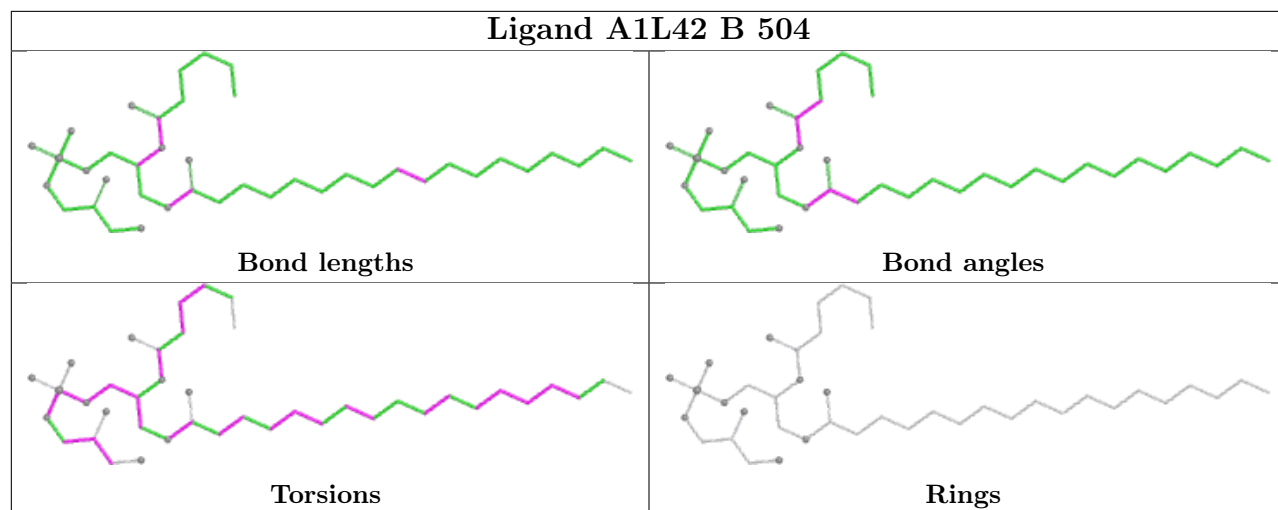


Ligand AV0 B 505



Ligand Y01 A 505





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

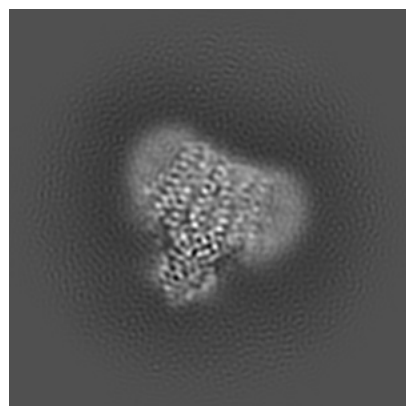
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38494. These allow visual inspection of the internal detail of the map and identification of artifacts.

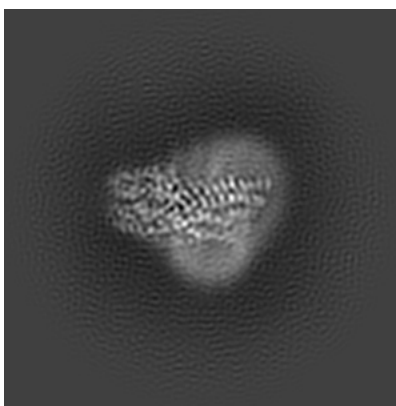
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

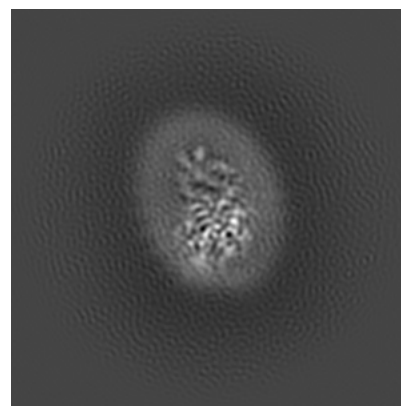
6.1.1 Primary map



X

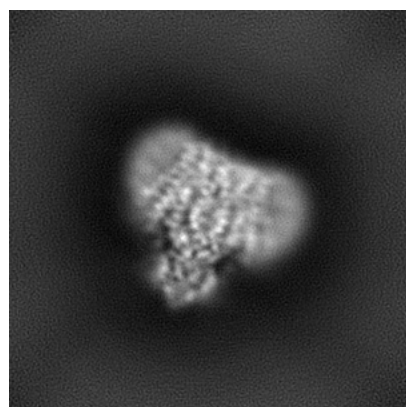


Y

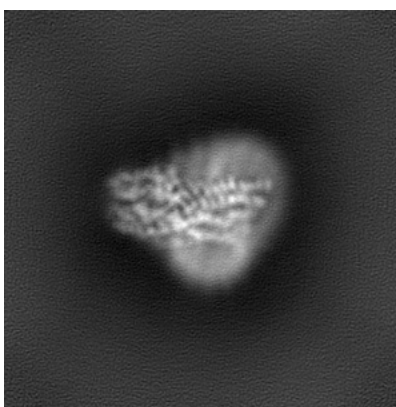


Z

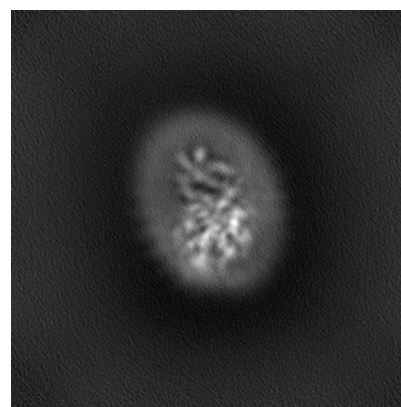
6.1.2 Raw map



X



Y

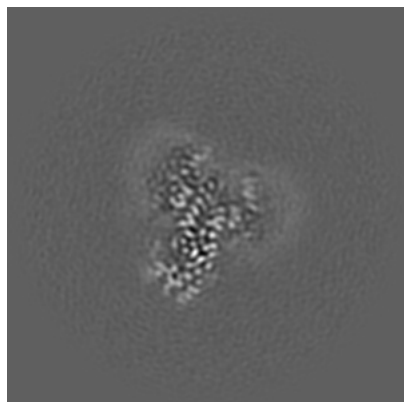


Z

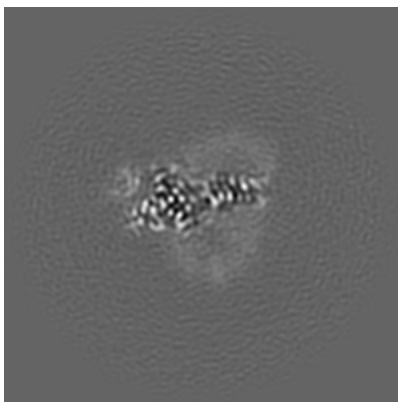
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

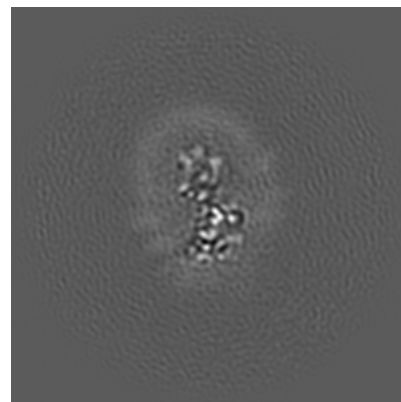
6.2.1 Primary map



X Index: 130

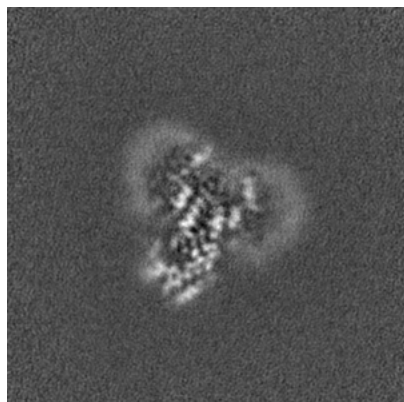


Y Index: 130

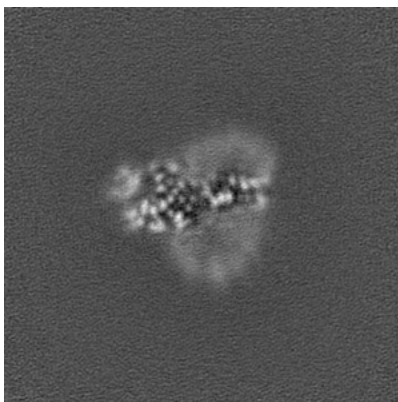


Z Index: 130

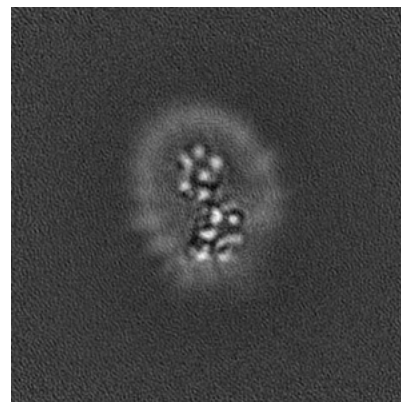
6.2.2 Raw map



X Index: 130



Y Index: 130

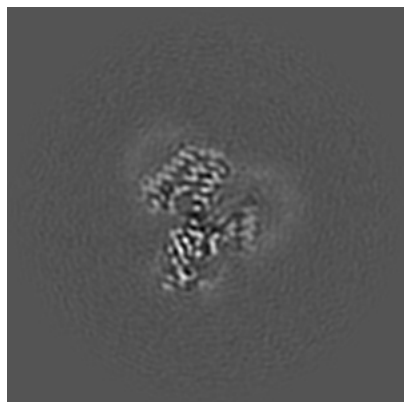


Z Index: 130

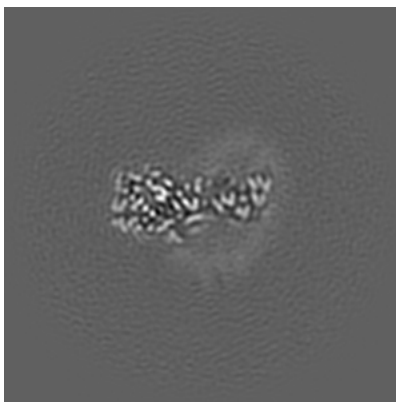
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

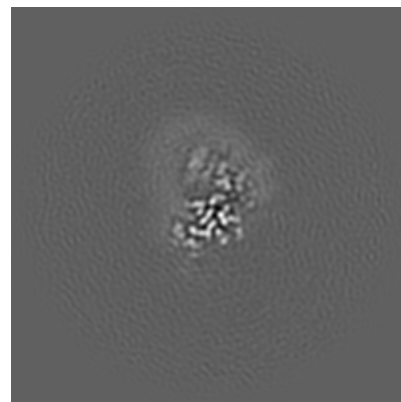
6.3.1 Primary map



X Index: 137

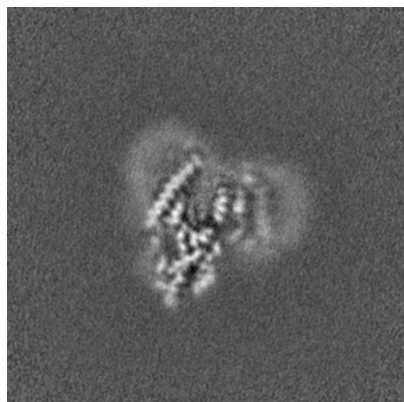


Y Index: 118

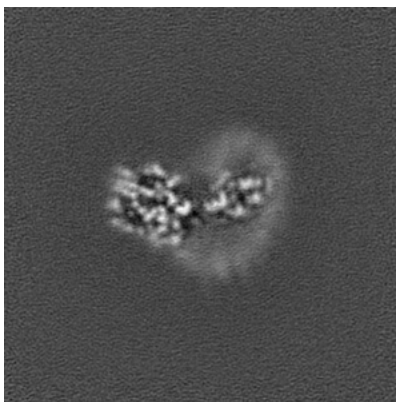


Z Index: 112

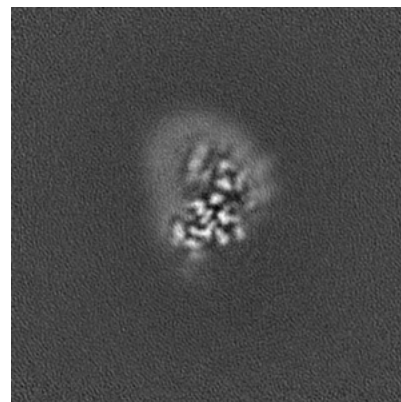
6.3.2 Raw map



X Index: 125



Y Index: 115

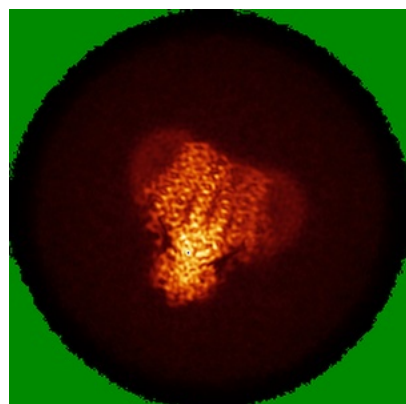


Z Index: 112

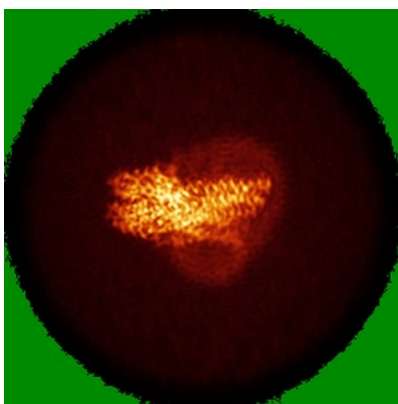
The images above show the largest variance slices of the map in three orthogonal directions.

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

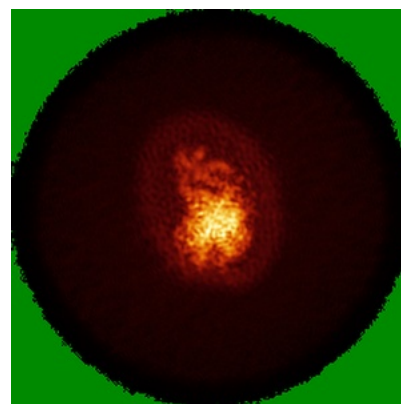
6.4.1 Primary map



X

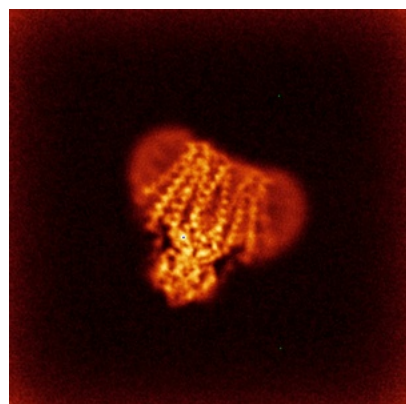


Y

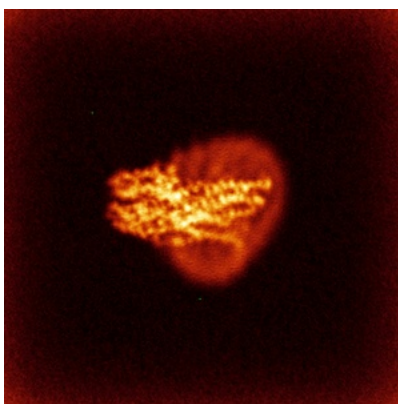


Z

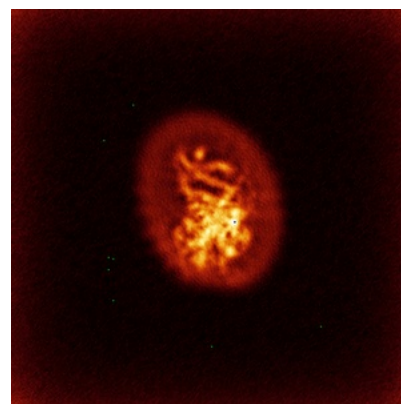
6.4.2 Raw map



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](#)

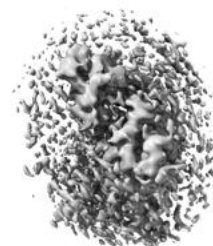
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.34. 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



X



Y



Z

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.

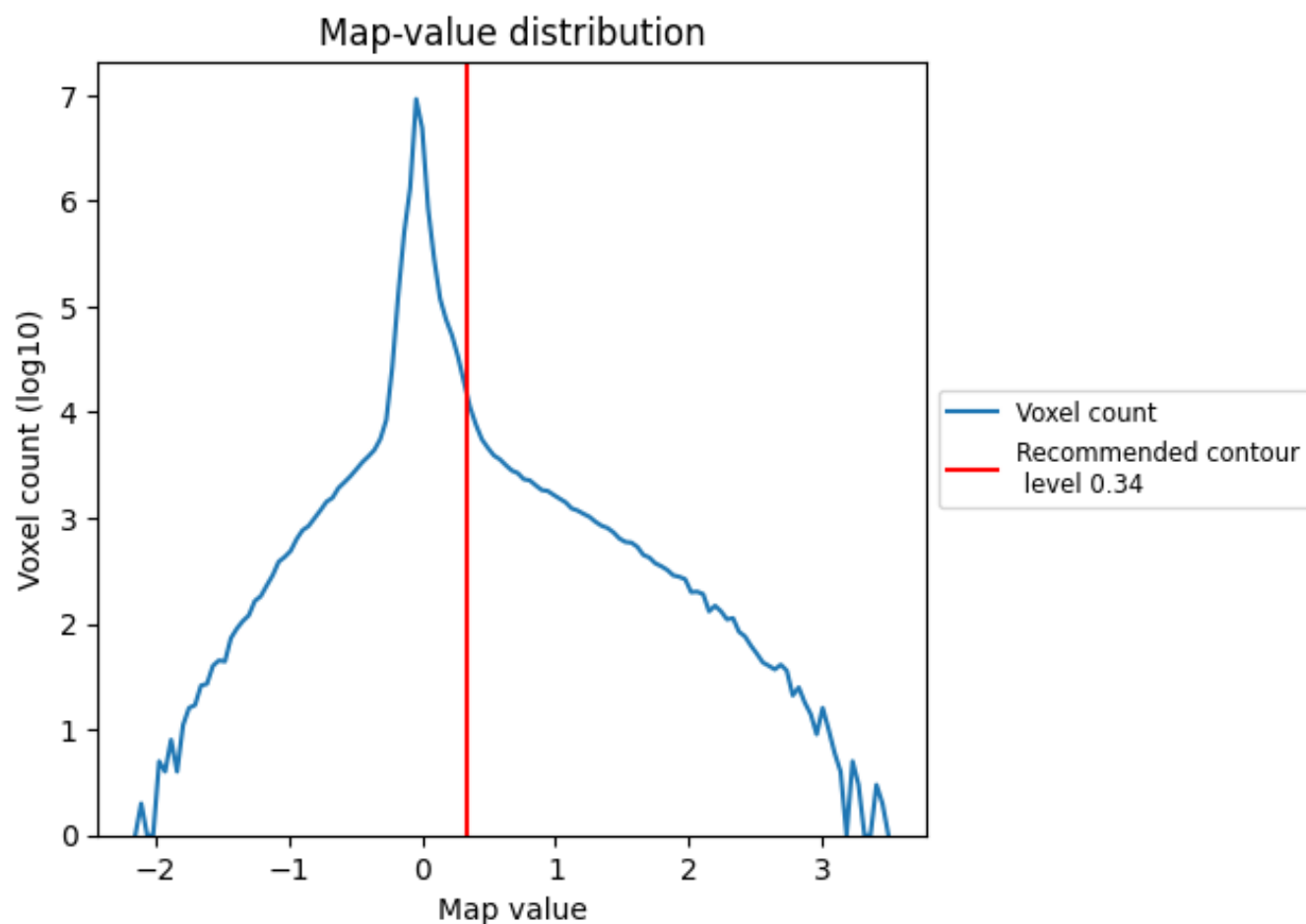
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

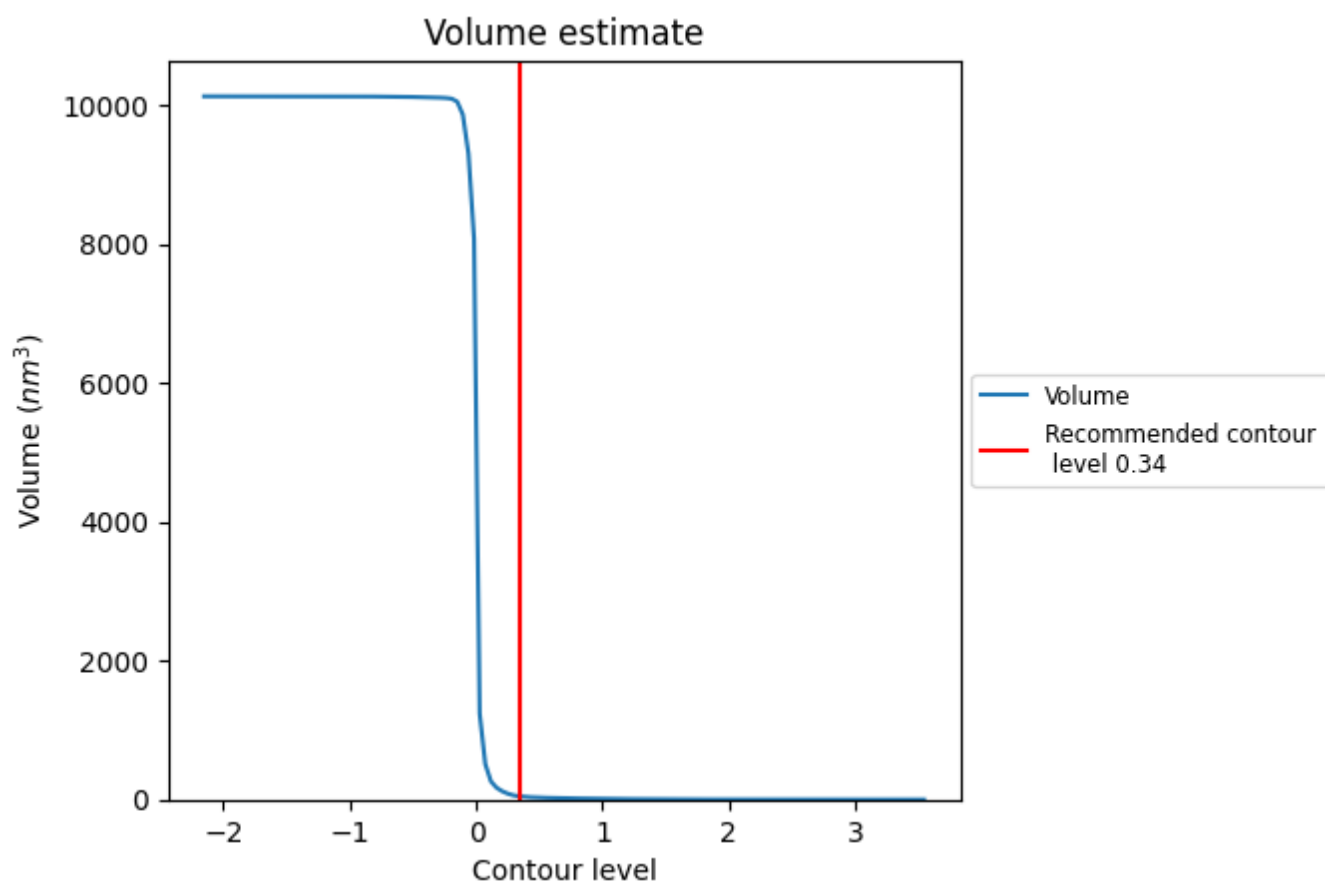
This section contains the results of statistical analysis of the map.

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.

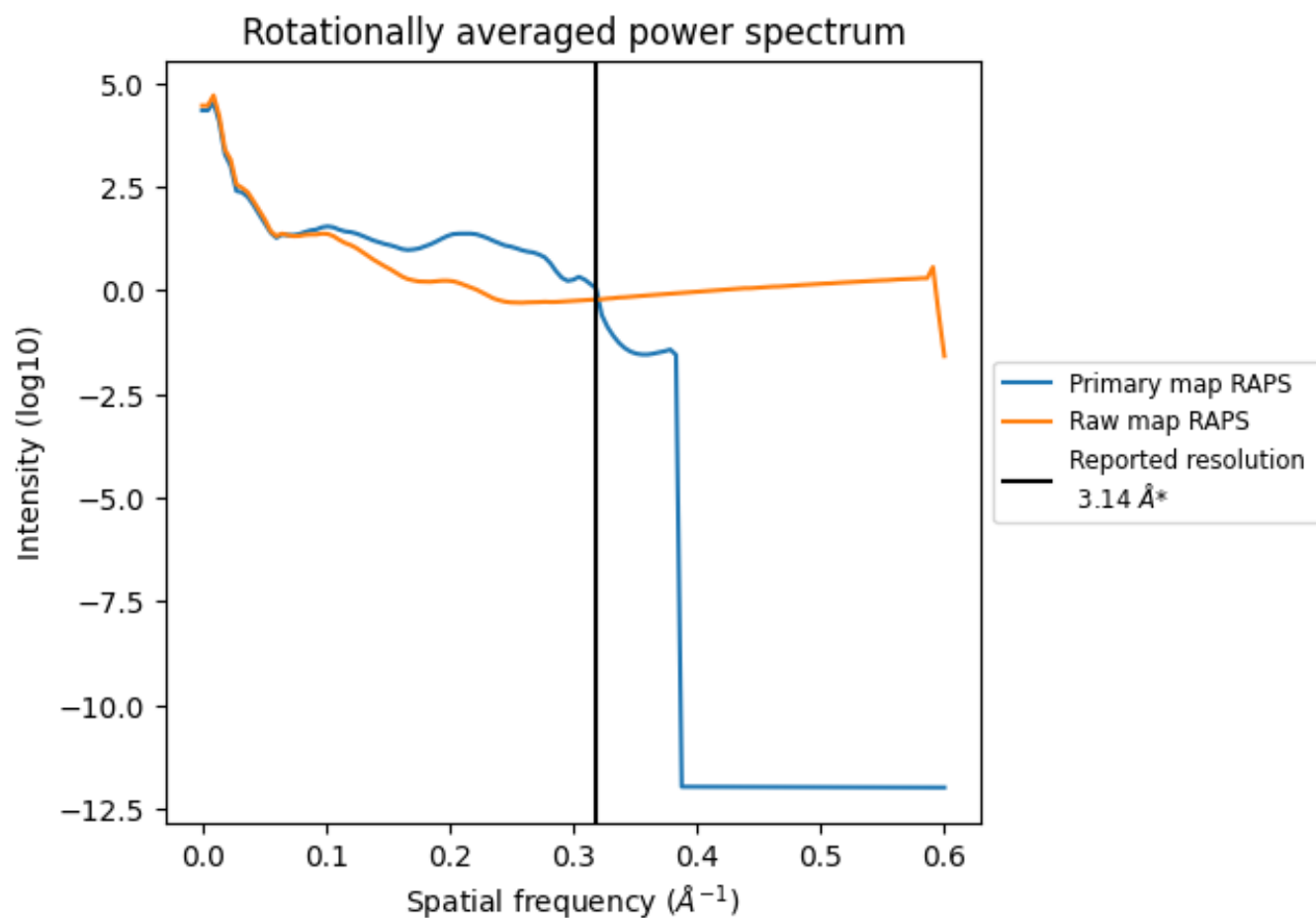
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm³; this corresponds to an approximate mass of 43 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 ⓘ

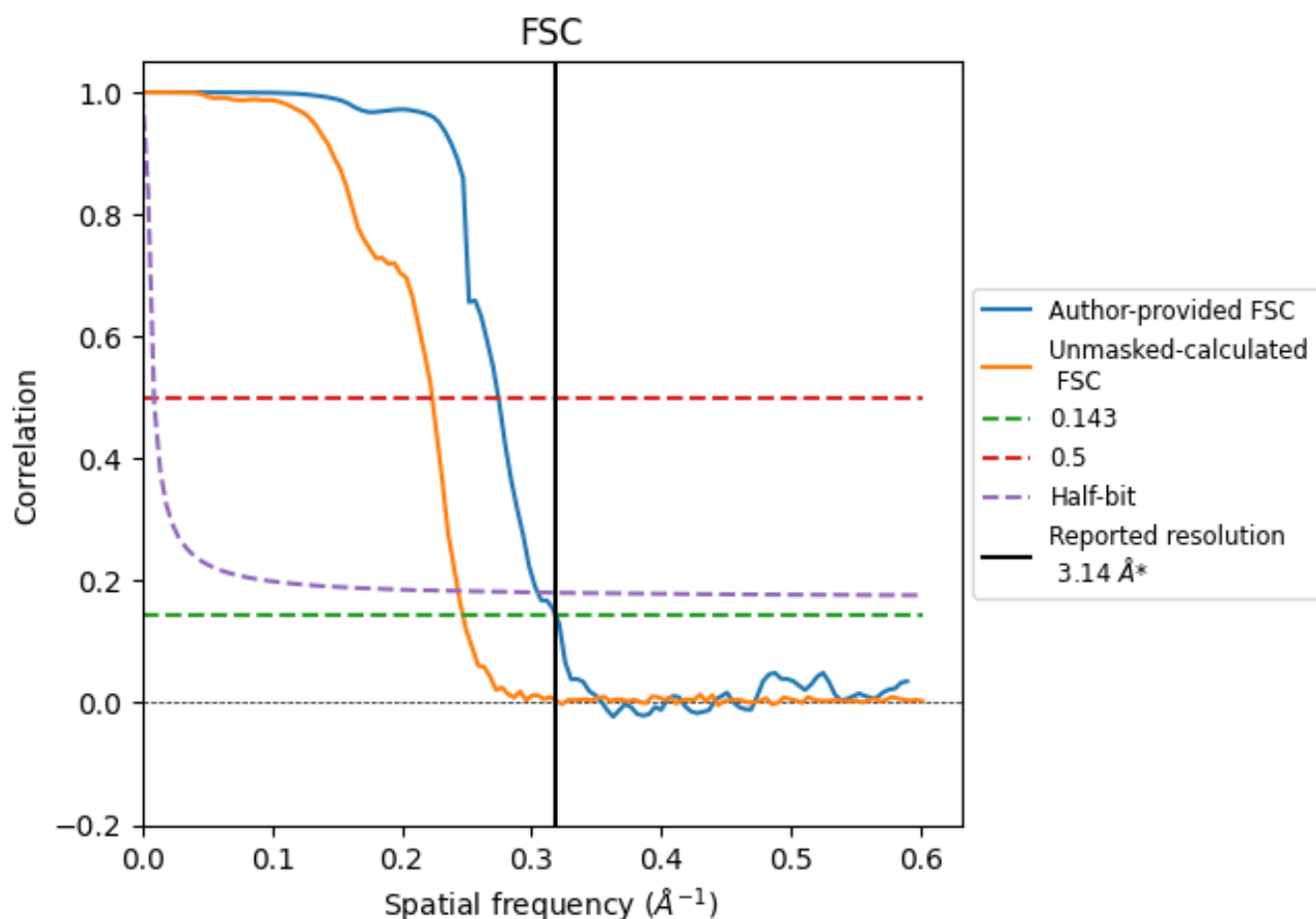


*Reported resolution corresponds to spatial frequency of $0.318 \text{ \AA}^{-1}$

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 0.318 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.64	3.28
Unmasked-calculated*	4.05	4.48	4.11

*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 4.05 differs from the reported value 3.14 by more than 10 %

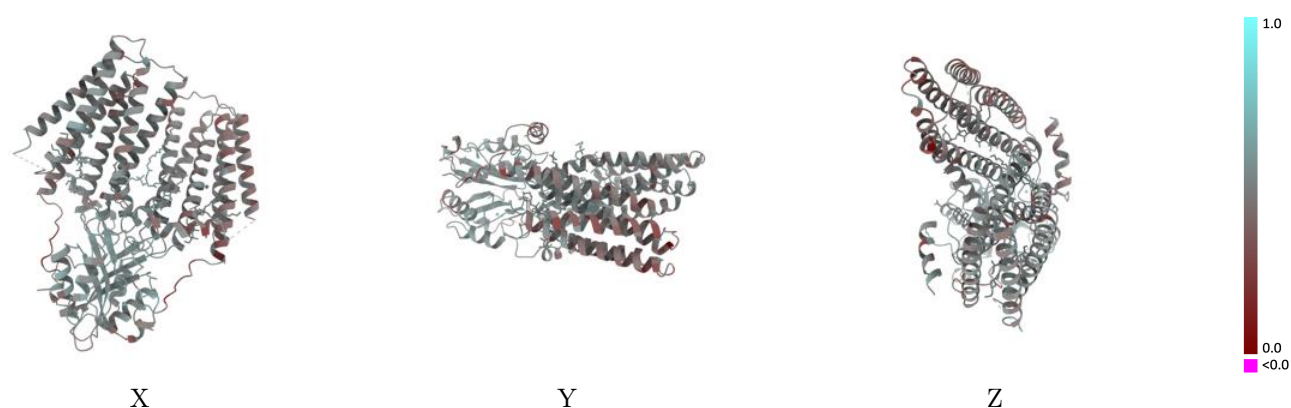
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38494 and PDB model 8XN1. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

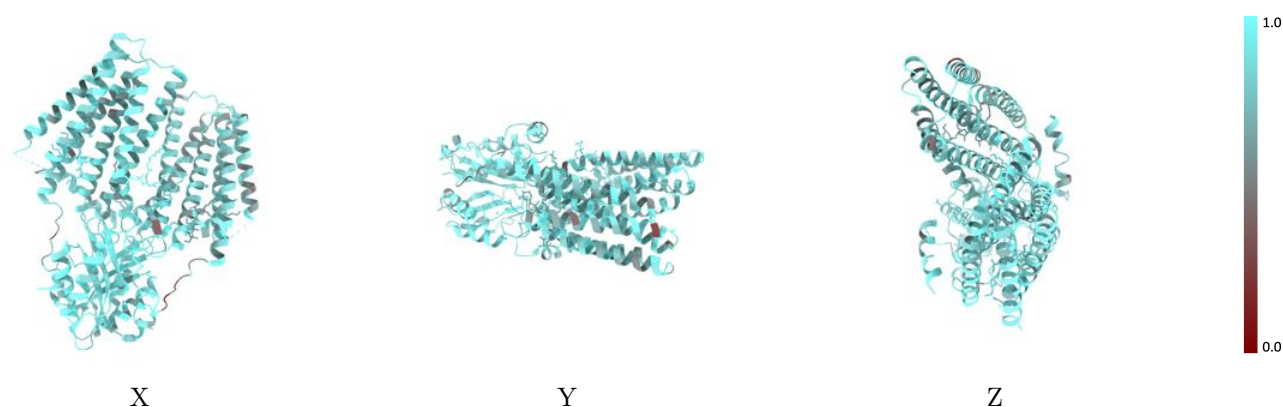
This section was not generated.

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



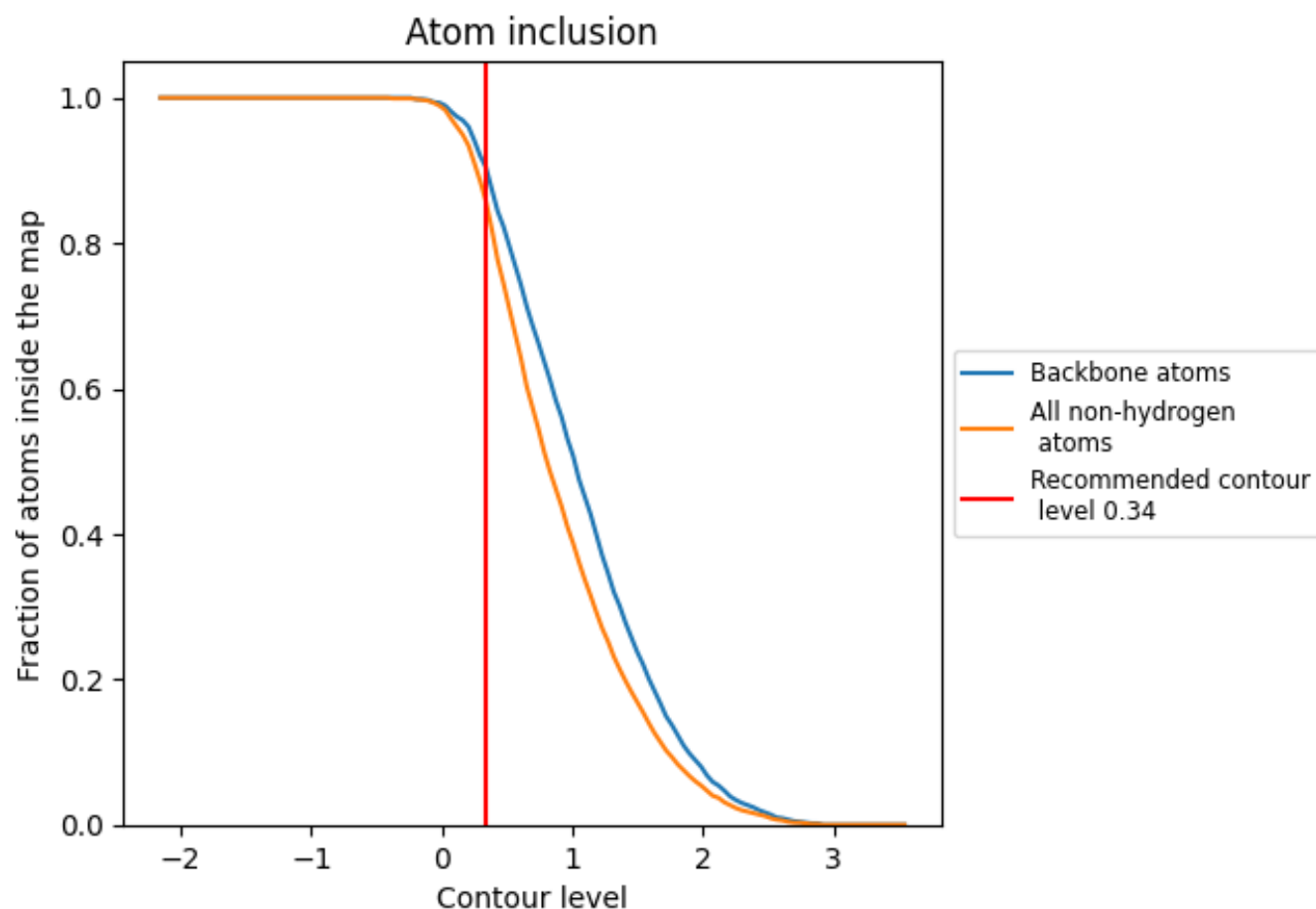
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.34).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8570	0.4820
A	0.8410	0.4720
B	0.8730	0.4920

