WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:13 pm GMT

|		
PDB ID	:	4BPQ
EMDB ID	:	EMD-2387
Title	:	Structure and substrate induced conformational changes of the secondary citrate-sodium symporter CitS revealed by electron crystallography
Authors	:	Kebbel, F.; Kurz, M.; Arheit, M.; Gruetter, M.G.; Stahlberg, H.
Deposited on	:	2013-05-27
Resolution	:	6.00 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 6.00 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	Percentile Ranks	Value
Clashscore		63

Worse   *Better*

▌ Percentile relative to all structures

◫ Percentile relative to all EM structures
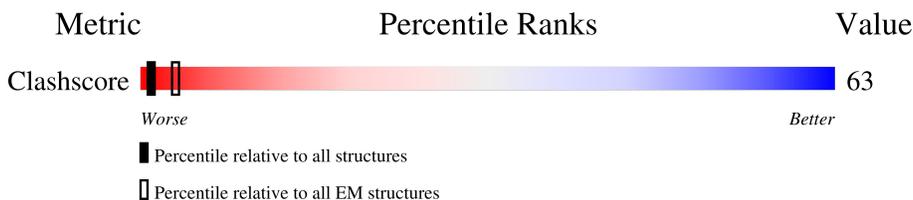
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297

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 <=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	318	37% / 66% / 26% / · / ·
1	B	318	37% / 67% / 29% / ·

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3110 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 CITRATE\:SODIUM SYMPORTER.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	304	Total 1520	C 912	N 304	O 304	0	0
1	B	318	Total 1590	C 954	N 318	O 318	0	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: CITRATE\:SODIUM SYMPORTER
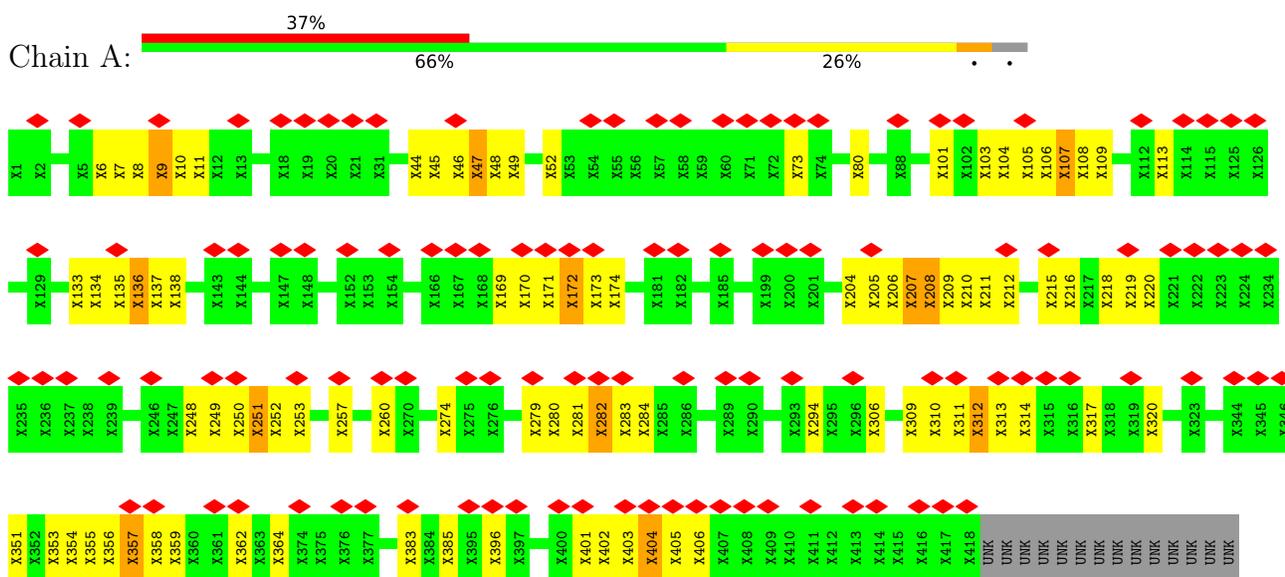
• Molecule 1: CITRATE\:SODIUM SYMPORTER
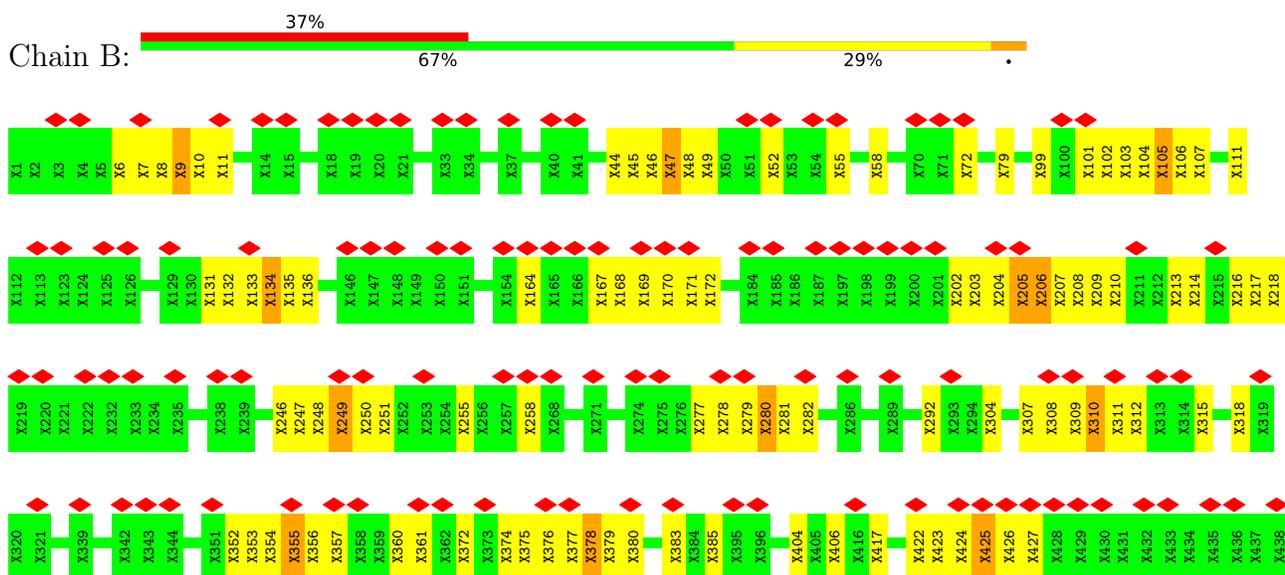
X439

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a=Not provided Å, b=Not provided Å, c=Not provided Å, γ=Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	OTHER	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	6	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	244.378	Depositor
Minimum map value	-151.810	Depositor
Average map value	0.381	Depositor
Map value standard deviation	19.640	Depositor
Recommended contour level	46.2	Depositor
Map size (Å)	100.0, 100.0, 100.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	22
1	B	0	24
All	All	0	46

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	UNK	Mainchain
1	A	107	UNK	Mainchain
1	A	135	UNK	Mainchain
1	A	136	UNK	Mainchain
1	A	171	UNK	Mainchain
1	A	172	UNK	Mainchain
1	A	207	UNK	Mainchain
1	A	208	UNK	Mainchain
1	A	250	UNK	Mainchain
1	A	251	UNK	Mainchain
1	A	281	UNK	Mainchain
1	A	282	UNK	Mainchain
1	A	311	UNK	Mainchain
1	A	312	UNK	Mainchain
1	A	356	UNK	Mainchain
1	A	357	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	A	402	UNK	Mainchain
1	A	404	UNK	Mainchain
1	A	46	UNK	Mainchain
1	A	47	UNK	Mainchain
1	A	8	UNK	Mainchain
1	A	9	UNK	Mainchain
1	B	104	UNK	Mainchain
1	B	105	UNK	Mainchain
1	B	133	UNK	Mainchain
1	B	134	UNK	Mainchain
1	B	169	UNK	Mainchain
1	B	170	UNK	Mainchain
1	B	205	UNK	Mainchain
1	B	206	UNK	Mainchain
1	B	248	UNK	Mainchain
1	B	249	UNK	Mainchain
1	B	279	UNK	Mainchain
1	B	280	UNK	Mainchain
1	B	309	UNK	Mainchain
1	B	310	UNK	Mainchain
1	B	354	UNK	Mainchain
1	B	355	UNK	Mainchain
1	B	377	UNK	Mainchain
1	B	378	UNK	Mainchain
1	B	423	UNK	Mainchain
1	B	425	UNK	Mainchain
1	B	46	UNK	Mainchain
1	B	47	UNK	Mainchain
1	B	8	UNK	Mainchain
1	B	9	UNK	Mainchain

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	1520	0	327	126	0
1	B	1590	0	342	135	0
All	All	3110	0	669	237	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 63.

All (237) 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:73:UNK:CB	1:B:417:UNK:HA	1.08	1.51
1:A:396:UNK:CA	1:B:72:UNK:CB	1.84	1.51
1:A:396:UNK:HA	1:B:72:UNK:CB	1.05	1.49
1:A:73:UNK:CB	1:B:417:UNK:CA	1.93	1.47
1:A:101:UNK:CB	1:A:257:UNK:C	1.95	1.44
1:B:99:UNK:CB	1:B:255:UNK:C	1.95	1.43
1:A:101:UNK:CA	1:A:257:UNK:O	1.74	1.35
1:B:99:UNK:CA	1:B:255:UNK:O	1.74	1.34
1:B:203:UNK:O	1:B:207:UNK:CB	1.77	1.33
1:A:133:UNK:O	1:A:137:UNK:CB	1.76	1.32
1:B:131:UNK:O	1:B:135:UNK:CB	1.76	1.32
1:A:205:UNK:O	1:A:209:UNK:CB	1.77	1.32
1:B:375:UNK:O	1:B:379:UNK:CB	1.83	1.26
1:B:352:UNK:O	1:B:356:UNK:CB	1.83	1.26
1:A:354:UNK:O	1:A:358:UNK:CB	1.83	1.24
1:A:309:UNK:O	1:A:313:UNK:CB	1.86	1.23
1:B:307:UNK:O	1:B:311:UNK:CB	1.86	1.22
1:A:134:UNK:O	1:A:138:UNK:CB	1.89	1.20
1:B:132:UNK:O	1:B:136:UNK:CB	1.89	1.19
1:B:44:UNK:O	1:B:48:UNK:CB	1.91	1.19
1:A:44:UNK:O	1:A:48:UNK:CB	1.91	1.17
1:B:216:UNK:CB	1:B:318:UNK:CB	2.22	1.17
1:A:218:UNK:CB	1:A:320:UNK:CB	2.22	1.16
1:A:113:UNK:HA	1:A:294:UNK:CB	1.76	1.16
1:A:208:UNK:N	1:A:306:UNK:CB	2.04	1.15
1:A:206:UNK:O	1:A:210:UNK:CB	1.95	1.14
1:B:111:UNK:HA	1:B:292:UNK:CB	1.76	1.14
1:B:204:UNK:O	1:B:208:UNK:CB	1.95	1.14
1:A:403:UNK:O	1:A:405:UNK:N	1.82	1.13
1:A:396:UNK:CB	1:B:72:UNK:CB	2.25	1.13
1:B:206:UNK:N	1:B:304:UNK:CB	2.04	1.12
1:B:424:UNK:O	1:B:426:UNK:N	1.82	1.12
1:A:6:UNK:O	1:A:10:UNK:CB	2.01	1.09
1:B:6:UNK:O	1:B:10:UNK:CB	2.01	1.08
1:A:208:UNK:C	1:A:309:UNK:CB	2.33	1.07
1:B:206:UNK:C	1:B:307:UNK:CB	2.33	1.06
1:A:101:UNK:CB	1:A:257:UNK:O	0.75	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:UNK:CB	1:A:306:UNK:CB	2.35	1.05
1:B:205:UNK:CB	1:B:304:UNK:CB	2.35	1.05
1:A:310:UNK:O	1:A:314:UNK:CB	2.05	1.05
1:B:99:UNK:CB	1:B:255:UNK:O	0.76	1.05
1:B:308:UNK:O	1:B:312:UNK:CB	2.05	1.04
1:A:104:UNK:O	1:A:108:UNK:CB	2.08	1.02
1:B:102:UNK:O	1:B:106:UNK:CB	2.08	1.01
1:B:376:UNK:O	1:B:380:UNK:CB	2.11	0.99
1:A:355:UNK:O	1:A:359:UNK:CB	2.11	0.99
1:B:353:UNK:O	1:B:357:UNK:CB	2.11	0.98
1:B:277:UNK:O	1:B:281:UNK:CB	2.12	0.97
1:A:279:UNK:O	1:A:283:UNK:CB	2.12	0.96
1:A:113:UNK:CA	1:A:294:UNK:CB	2.43	0.95
1:B:111:UNK:CA	1:B:292:UNK:CB	2.43	0.95
1:A:73:UNK:CB	1:B:417:UNK:CB	2.44	0.93
1:B:246:UNK:O	1:B:250:UNK:CB	2.17	0.93
1:A:80:UNK:CA	1:B:426:UNK:CB	2.47	0.93
1:A:248:UNK:O	1:A:252:UNK:CB	2.17	0.93
1:B:48:UNK:CB	1:B:378:UNK:CB	2.48	0.92
1:A:48:UNK:CB	1:A:357:UNK:CB	2.48	0.92
1:A:80:UNK:CB	1:B:426:UNK:CB	2.49	0.90
1:B:55:UNK:CB	1:B:360:UNK:CB	2.49	0.90
1:A:218:UNK:C	1:A:320:UNK:CB	2.51	0.89
1:B:216:UNK:C	1:B:318:UNK:CB	2.51	0.88
1:B:45:UNK:O	1:B:49:UNK:CB	2.21	0.88
1:A:45:UNK:O	1:A:49:UNK:CB	2.21	0.87
1:A:396:UNK:CB	1:B:72:UNK:N	2.37	0.87
1:A:216:UNK:HA	1:A:351:UNK:C	2.06	0.86
1:B:214:UNK:HA	1:B:372:UNK:C	2.06	0.85
1:A:216:UNK:HA	1:A:351:UNK:CA	2.06	0.85
1:A:216:UNK:HA	1:A:351:UNK:O	1.77	0.85
1:B:214:UNK:HA	1:B:372:UNK:CA	2.07	0.84
1:B:214:UNK:HA	1:B:372:UNK:O	1.77	0.84
1:A:80:UNK:HA	1:B:426:UNK:CB	2.09	0.82
1:B:202:UNK:O	1:B:304:UNK:CB	2.28	0.81
1:A:204:UNK:O	1:A:306:UNK:CB	2.28	0.80
1:A:113:UNK:CB	1:A:294:UNK:CB	2.61	0.79
1:A:403:UNK:O	1:A:404:UNK:C	2.31	0.79
1:B:111:UNK:CB	1:B:292:UNK:CB	2.61	0.79
1:A:73:UNK:N	1:B:417:UNK:CB	2.47	0.78
1:A:7:UNK:O	1:A:11:UNK:CB	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:UNK:O	1:B:11:UNK:CB	2.33	0.77
1:B:424:UNK:O	1:B:425:UNK:C	2.31	0.77
1:A:396:UNK:CB	1:B:72:UNK:CA	2.63	0.75
1:A:133:UNK:C	1:A:137:UNK:CB	2.66	0.74
1:B:131:UNK:C	1:B:135:UNK:CB	2.66	0.72
1:A:405:UNK:CB	1:B:79:UNK:CA	2.68	0.70
1:B:422:UNK:C	1:B:424:UNK:H2	2.05	0.69
1:B:103:UNK:O	1:B:107:UNK:CB	2.41	0.69
1:B:424:UNK:C	1:B:426:UNK:N	2.56	0.69
1:A:401:UNK:C	1:A:403:UNK:H2	2.05	0.68
1:A:105:UNK:O	1:A:109:UNK:CB	2.41	0.68
1:A:403:UNK:O	1:A:406:UNK:N	2.27	0.68
1:B:203:UNK:C	1:B:207:UNK:CB	2.69	0.68
1:B:424:UNK:O	1:B:427:UNK:N	2.27	0.68
1:A:205:UNK:C	1:A:209:UNK:CB	2.69	0.67
1:B:307:UNK:O	1:B:311:UNK:N	2.27	0.67
1:A:309:UNK:O	1:A:313:UNK:CA	2.43	0.67
1:A:309:UNK:O	1:A:313:UNK:N	2.27	0.67
1:A:405:UNK:CB	1:B:79:UNK:CB	2.73	0.67
1:B:307:UNK:O	1:B:311:UNK:CA	2.43	0.67
1:A:101:UNK:HA	1:A:257:UNK:O	1.91	0.66
1:A:52:UNK:CB	1:A:353:UNK:CB	2.74	0.66
1:B:52:UNK:CB	1:B:374:UNK:CB	2.74	0.66
1:B:131:UNK:O	1:B:135:UNK:CA	2.44	0.66
1:A:216:UNK:HA	1:A:351:UNK:HA	1.78	0.66
1:A:403:UNK:C	1:A:405:UNK:N	2.56	0.65
1:B:218:UNK:N	1:B:372:UNK:CB	2.59	0.65
1:B:278:UNK:O	1:B:282:UNK:CB	2.45	0.65
1:A:280:UNK:O	1:A:284:UNK:CB	2.45	0.65
1:A:216:UNK:CA	1:A:351:UNK:O	2.44	0.64
1:B:203:UNK:O	1:B:207:UNK:CA	2.45	0.64
1:A:133:UNK:O	1:A:137:UNK:CA	2.44	0.64
1:B:214:UNK:CA	1:B:372:UNK:O	2.44	0.64
1:A:220:UNK:N	1:A:351:UNK:CB	2.59	0.64
1:A:80:UNK:C	1:B:426:UNK:CB	2.76	0.64
1:A:212:UNK:HA	1:A:313:UNK:CB	2.27	0.64
1:B:210:UNK:HA	1:B:311:UNK:CB	2.27	0.64
1:B:134:UNK:O	1:B:135:UNK:C	2.46	0.63
1:B:214:UNK:HA	1:B:372:UNK:HA	1.78	0.63
1:A:205:UNK:O	1:A:209:UNK:CA	2.46	0.63
1:A:136:UNK:O	1:A:137:UNK:C	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:UNK:CA	1:A:351:UNK:C	2.78	0.62
1:A:216:UNK:CB	1:A:351:UNK:O	2.48	0.62
1:B:214:UNK:CB	1:B:372:UNK:O	2.48	0.62
1:A:103:UNK:N	1:A:260:UNK:CB	2.63	0.61
1:B:214:UNK:CA	1:B:372:UNK:C	2.78	0.61
1:A:208:UNK:O	1:A:209:UNK:C	2.48	0.61
1:A:309:UNK:C	1:A:313:UNK:CB	2.76	0.61
1:B:206:UNK:O	1:B:207:UNK:C	2.48	0.61
1:A:208:UNK:CA	1:A:309:UNK:CB	2.79	0.61
1:A:405:UNK:CB	1:B:79:UNK:HA	2.29	0.61
1:B:247:UNK:O	1:B:251:UNK:CB	2.49	0.61
1:A:396:UNK:CA	1:B:72:UNK:CA	2.74	0.61
1:B:101:UNK:N	1:B:258:UNK:CB	2.63	0.60
1:B:206:UNK:CA	1:B:307:UNK:CB	2.79	0.60
1:A:249:UNK:O	1:A:253:UNK:CB	2.49	0.60
1:A:208:UNK:O	1:A:309:UNK:CB	2.51	0.59
1:A:211:UNK:CB	1:A:310:UNK:HA	2.33	0.59
1:B:167:UNK:O	1:B:171:UNK:CB	2.50	0.59
1:B:99:UNK:HA	1:B:255:UNK:O	1.91	0.59
1:B:307:UNK:C	1:B:311:UNK:CB	2.76	0.58
1:B:209:UNK:CB	1:B:308:UNK:HA	2.33	0.58
1:A:169:UNK:O	1:A:173:UNK:CB	2.51	0.58
1:B:217:UNK:N	1:B:372:UNK:CB	2.67	0.58
1:B:206:UNK:O	1:B:307:UNK:CB	2.51	0.57
1:A:215:UNK:HA	1:A:317:UNK:HA	1.87	0.57
1:A:219:UNK:N	1:A:351:UNK:CB	2.67	0.57
1:A:354:UNK:O	1:A:358:UNK:CA	2.52	0.56
1:B:213:UNK:HA	1:B:315:UNK:HA	1.86	0.56
1:A:73:UNK:CA	1:B:417:UNK:CB	2.83	0.56
1:B:352:UNK:O	1:B:356:UNK:CA	2.52	0.55
1:A:405:UNK:CB	1:B:79:UNK:O	2.55	0.55
1:B:217:UNK:CA	1:B:372:UNK:CB	2.82	0.55
1:B:6:UNK:O	1:B:10:UNK:N	2.40	0.55
1:B:355:UNK:O	1:B:356:UNK:C	2.53	0.55
1:A:104:UNK:O	1:A:108:UNK:N	2.40	0.55
1:B:58:UNK:O	1:B:361:UNK:O	2.24	0.55
1:A:80:UNK:O	1:B:426:UNK:CB	2.54	0.55
1:A:6:UNK:O	1:A:10:UNK:N	2.40	0.55
1:B:102:UNK:O	1:B:106:UNK:N	2.40	0.55
1:B:277:UNK:O	1:B:281:UNK:N	2.40	0.55
1:B:375:UNK:O	1:B:379:UNK:CA	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:UNK:CA	1:A:351:UNK:CB	2.82	0.54
1:A:44:UNK:O	1:A:48:UNK:N	2.40	0.54
1:B:213:UNK:HA	1:B:315:UNK:CA	2.38	0.54
1:A:248:UNK:O	1:A:252:UNK:N	2.41	0.54
1:A:279:UNK:O	1:A:283:UNK:N	2.40	0.54
1:B:44:UNK:O	1:B:48:UNK:N	2.40	0.54
1:A:357:UNK:O	1:A:358:UNK:C	2.53	0.53
1:A:364:UNK:C	1:A:383:UNK:O	2.56	0.53
1:B:378:UNK:O	1:B:379:UNK:C	2.53	0.53
1:A:354:UNK:O	1:A:358:UNK:N	2.42	0.53
1:B:246:UNK:O	1:B:250:UNK:N	2.41	0.53
1:A:215:UNK:HA	1:A:317:UNK:CA	2.38	0.53
1:B:375:UNK:O	1:B:379:UNK:N	2.42	0.53
1:B:385:UNK:C	1:B:404:UNK:O	2.56	0.53
1:A:405:UNK:CB	1:B:79:UNK:C	2.87	0.52
1:B:352:UNK:O	1:B:356:UNK:N	2.42	0.52
1:B:55:UNK:CA	1:B:360:UNK:CB	2.87	0.52
1:A:218:UNK:CA	1:A:320:UNK:CB	2.88	0.51
1:A:47:UNK:O	1:A:48:UNK:C	2.56	0.51
1:A:401:UNK:C	1:A:403:UNK:N	2.68	0.50
1:B:47:UNK:O	1:B:48:UNK:C	2.56	0.50
1:B:216:UNK:CA	1:B:318:UNK:CB	2.88	0.50
1:A:7:UNK:O	1:A:11:UNK:N	2.45	0.50
1:B:7:UNK:O	1:B:11:UNK:N	2.45	0.50
1:A:105:UNK:O	1:A:109:UNK:N	2.45	0.49
1:B:9:UNK:O	1:B:10:UNK:C	2.59	0.49
1:B:103:UNK:O	1:B:107:UNK:N	2.45	0.49
1:A:9:UNK:O	1:A:10:UNK:C	2.59	0.49
1:B:247:UNK:O	1:B:251:UNK:N	2.46	0.49
1:B:278:UNK:O	1:B:282:UNK:N	2.45	0.49
1:B:352:UNK:C	1:B:356:UNK:CB	2.82	0.49
1:A:280:UNK:O	1:A:284:UNK:N	2.45	0.49
1:A:107:UNK:O	1:A:108:UNK:C	2.61	0.49
1:A:274:UNK:CB	1:B:164:UNK:H2	2.26	0.49
1:A:45:UNK:O	1:A:49:UNK:N	2.46	0.48
1:B:45:UNK:O	1:B:49:UNK:N	2.46	0.48
1:B:105:UNK:O	1:B:106:UNK:C	2.61	0.48
1:A:249:UNK:O	1:A:253:UNK:N	2.46	0.48
1:B:310:UNK:O	1:B:311:UNK:C	2.61	0.48
1:B:280:UNK:O	1:B:281:UNK:C	2.62	0.48
1:A:44:UNK:O	1:A:48:UNK:CA	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:UNK:O	1:B:171:UNK:N	2.47	0.47
1:B:203:UNK:O	1:B:207:UNK:N	2.47	0.47
1:A:362:UNK:O	1:A:385:UNK:C	2.60	0.47
1:B:44:UNK:O	1:B:48:UNK:CA	2.58	0.47
1:A:169:UNK:O	1:A:173:UNK:N	2.47	0.47
1:B:249:UNK:O	1:B:250:UNK:C	2.63	0.47
1:B:353:UNK:O	1:B:357:UNK:N	2.48	0.47
1:B:376:UNK:O	1:B:380:UNK:N	2.48	0.47
1:A:205:UNK:O	1:A:209:UNK:N	2.47	0.47
1:A:355:UNK:O	1:A:359:UNK:N	2.48	0.47
1:A:251:UNK:O	1:A:252:UNK:C	2.63	0.47
1:A:282:UNK:O	1:A:283:UNK:C	2.62	0.47
1:A:312:UNK:O	1:A:313:UNK:C	2.61	0.47
1:B:375:UNK:C	1:B:379:UNK:CB	2.82	0.47
1:A:354:UNK:C	1:A:358:UNK:CB	2.82	0.46
1:B:422:UNK:C	1:B:424:UNK:N	2.68	0.46
1:B:58:UNK:C	1:B:361:UNK:O	2.64	0.46
1:B:383:UNK:O	1:B:406:UNK:C	2.60	0.46
1:A:73:UNK:CA	1:B:417:UNK:CA	2.84	0.44
1:A:133:UNK:O	1:A:137:UNK:N	2.50	0.44
1:B:131:UNK:O	1:B:135:UNK:N	2.50	0.44
1:A:212:UNK:CA	1:A:313:UNK:CB	2.96	0.43
1:A:403:UNK:O	1:A:405:UNK:CA	2.64	0.43
1:B:206:UNK:CB	1:B:307:UNK:CB	2.96	0.43
1:A:170:UNK:O	1:A:174:UNK:N	2.52	0.43
1:A:208:UNK:CB	1:A:309:UNK:CB	2.96	0.43
1:B:168:UNK:O	1:B:172:UNK:N	2.51	0.43
1:B:204:UNK:O	1:B:208:UNK:N	2.53	0.42
1:B:210:UNK:CA	1:B:311:UNK:CB	2.96	0.42
1:A:206:UNK:O	1:A:210:UNK:N	2.53	0.42
1:B:308:UNK:O	1:B:312:UNK:N	2.53	0.42
1:A:310:UNK:O	1:A:314:UNK:N	2.53	0.41
1:B:424:UNK:O	1:B:426:UNK:CA	2.64	0.41
1:A:73:UNK:CB	1:B:417:UNK:C	2.88	0.41
1:A:401:UNK:O	1:A:403:UNK:N	2.54	0.40
1:A:172:UNK:O	1:A:173:UNK:C	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	14
1	A	13

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	224:UNK	C	234:UNK	N	58.60
1	B	222:UNK	C	232:UNK	N	58.60
1	A	323:UNK	C	333:UNK	N	51.51
1	B	321:UNK	C	331:UNK	N	51.51
1	A	115:UNK	C	125:UNK	N	43.69
1	B	113:UNK	C	123:UNK	N	43.69
1	A	156:UNK	C	166:UNK	N	42.33
1	B	154:UNK	C	164:UNK	N	42.33
1	A	385:UNK	C	395:UNK	N	36.48
1	B	406:UNK	C	416:UNK	N	36.48
1	A	60:UNK	C	71:UNK	N	36.18
1	B	60:UNK	C	70:UNK	N	36.18
1	A	21:UNK	C	31:UNK	N	34.68
1	B	21:UNK	C	31:UNK	N	34.68
1	B	89:UNK	C	99:UNK	N	34.00
1	A	90:UNK	C	101:UNK	N	33.99
1	A	296:UNK	C	306:UNK	N	31.32
1	B	294:UNK	C	304:UNK	N	31.31
1	A	189:UNK	C	199:UNK	N	28.67
1	B	187:UNK	C	197:UNK	N	28.67
1	A	346:UNK	C	351:UNK	N	24.04
1	A	260:UNK	C	270:UNK	N	21.04
1	B	258:UNK	C	268:UNK	N	21.04
1	A	364:UNK	C	374:UNK	N	17.86
1	B	385:UNK	C	395:UNK	N	17.86
1	B	362:UNK	C	372:UNK	N	14.67
1	B	344:UNK	C	349:UNK	N	10.12

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-2387. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1　Orthogonal projections ⓘ

6.1.1　Primary map

| X | Y | Z |
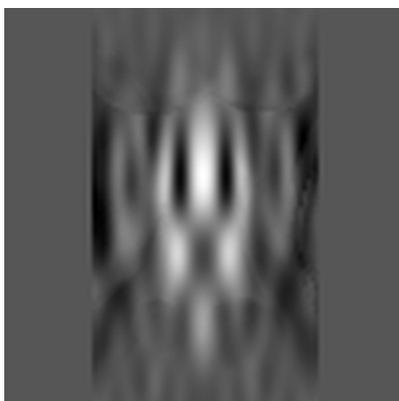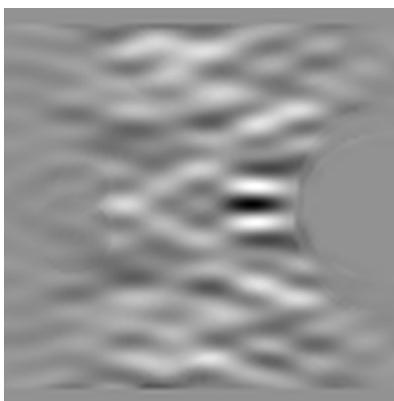
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ
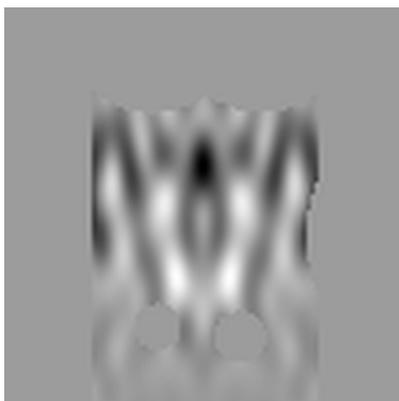
6.2.1　Primary map
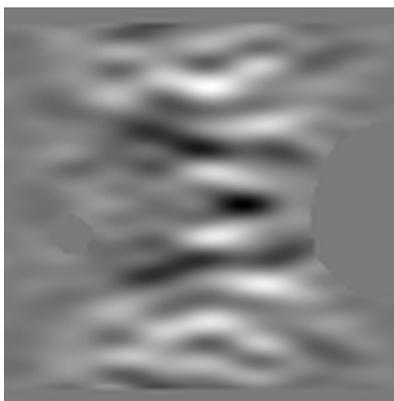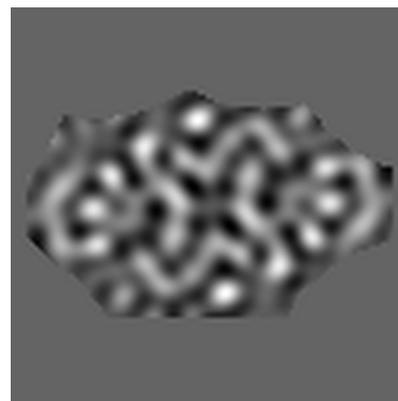
| X Index: 50 | Y Index: 50 | Z Index: 50 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
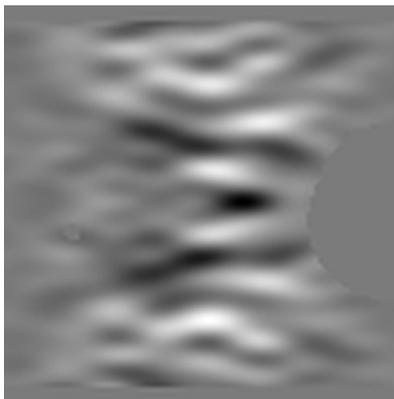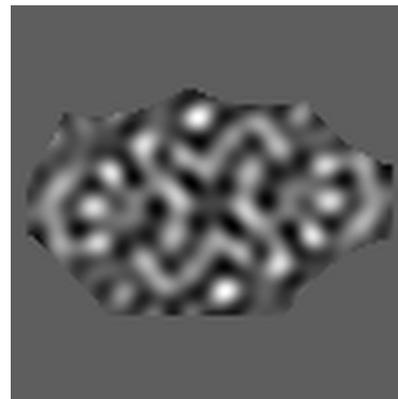
X Index: 47   Y Index: 49   Z Index: 51

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 46.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation (i)

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

7　Map analysis ⓘ

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

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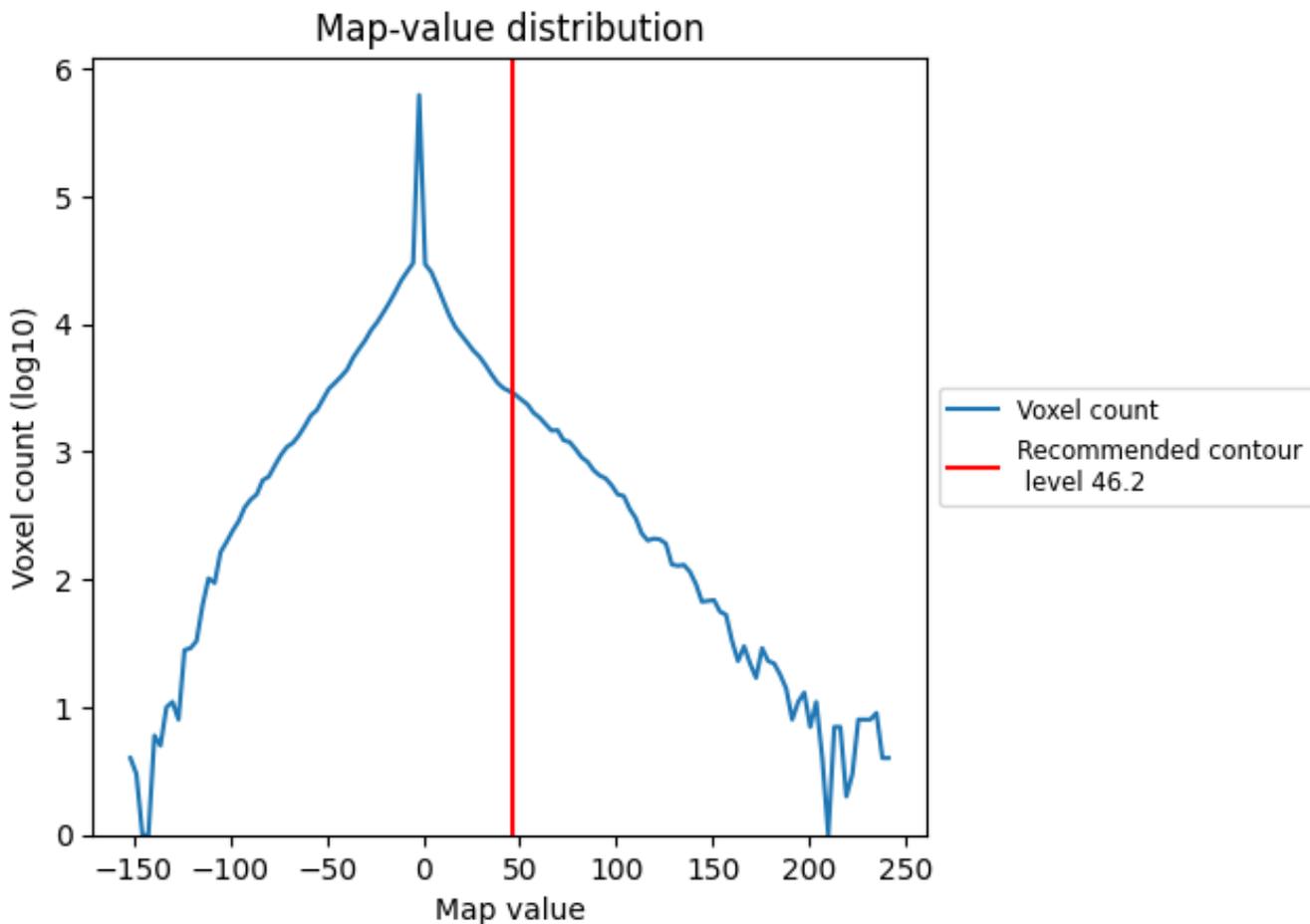
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
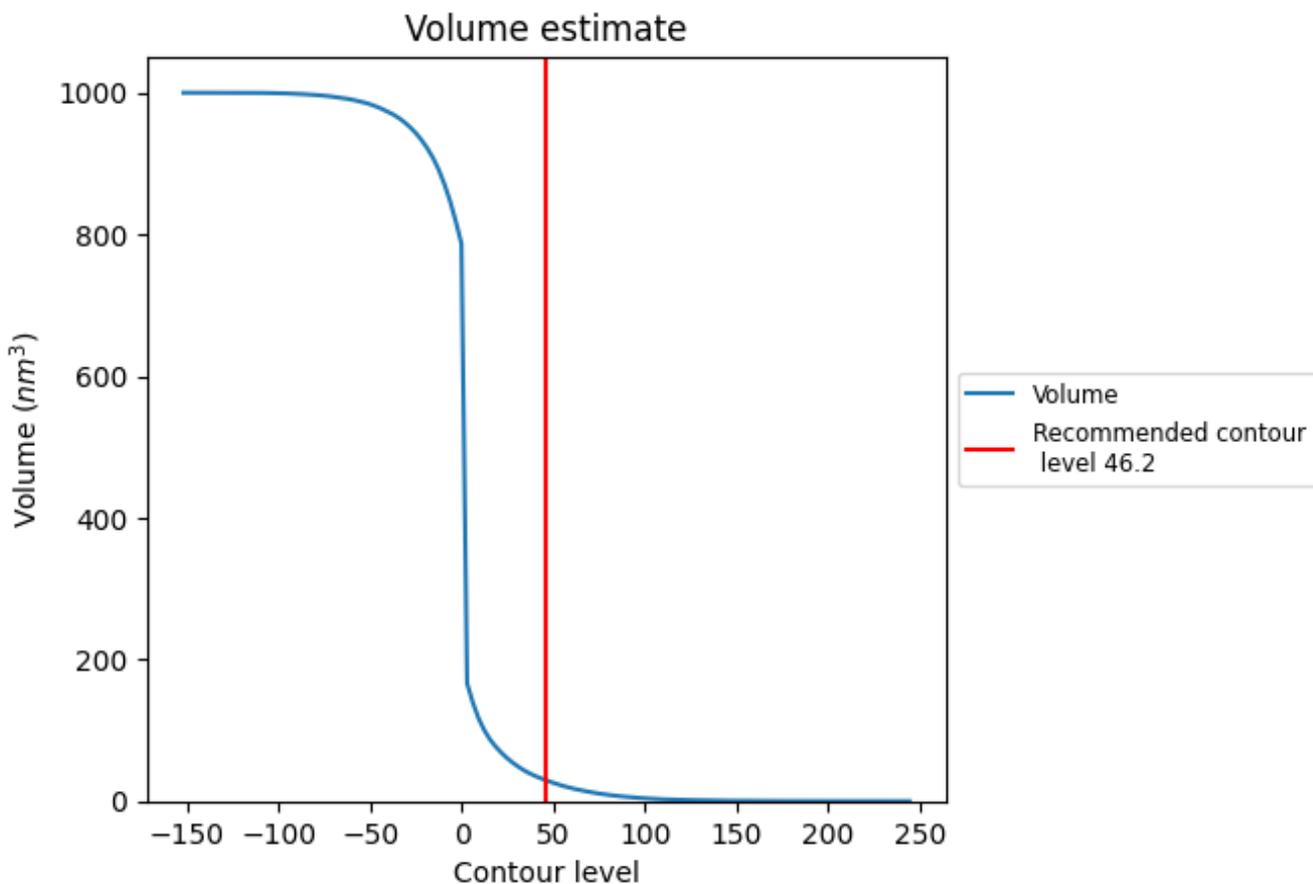
The volume at the recommended contour level is 29 nm^3; this corresponds to an approximate mass of 27 kDa.

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　ⓘ
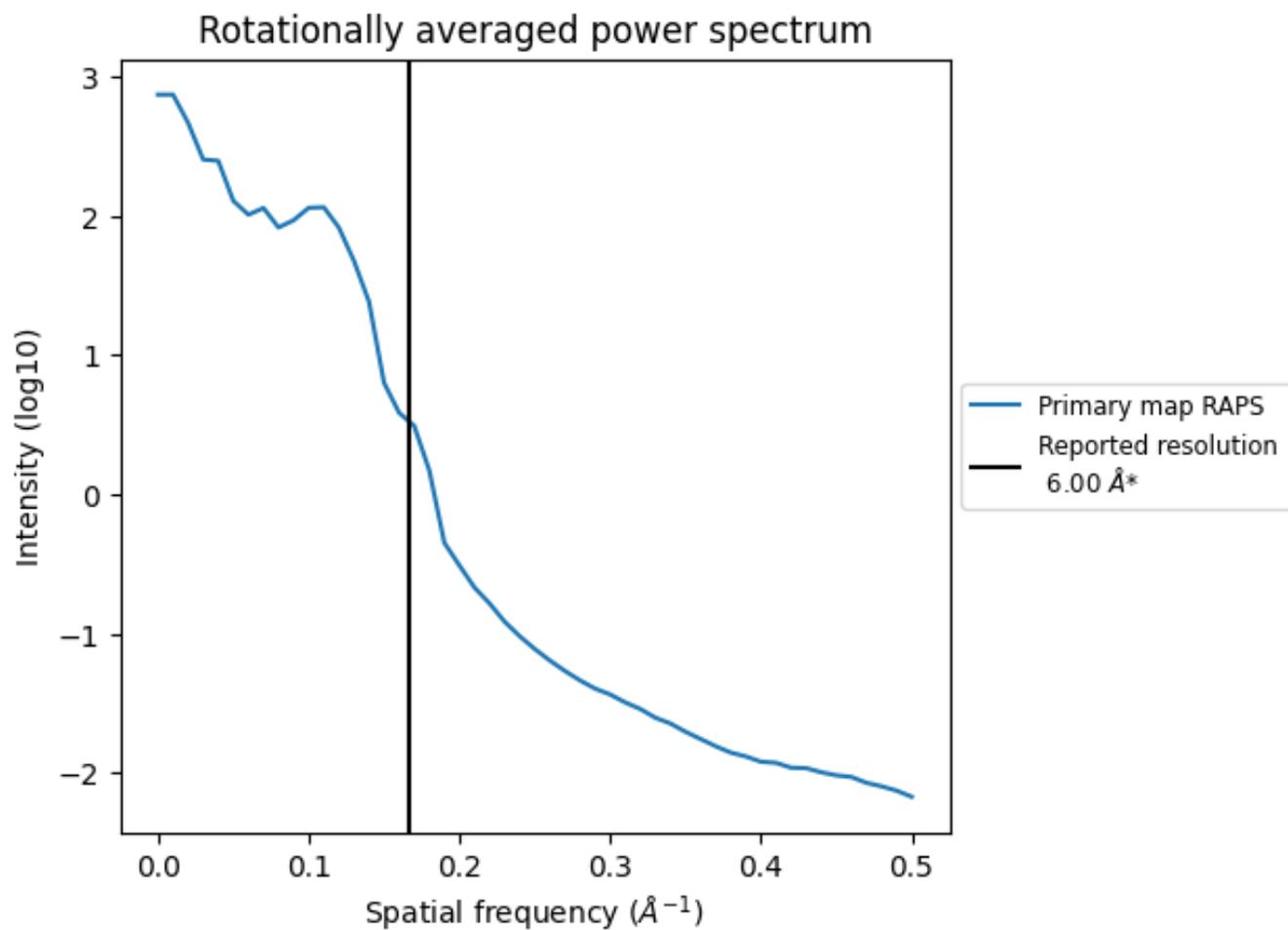
*Reported resolution corresponds to spatial frequency of 0.167 Å^{-1}

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-2387 and PDB model 4BPQ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ
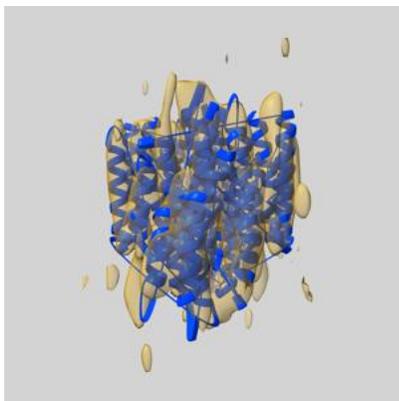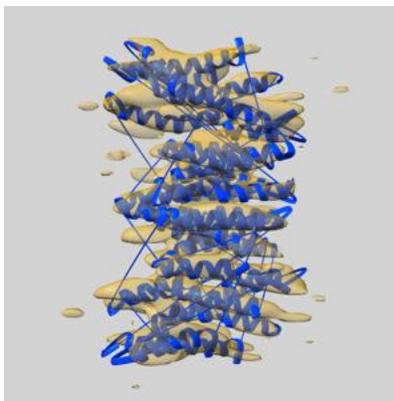
X   Y   Z
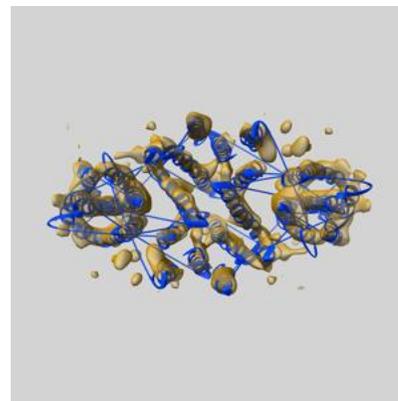
The images above show the 3D surface view of the map at the recommended contour level 46.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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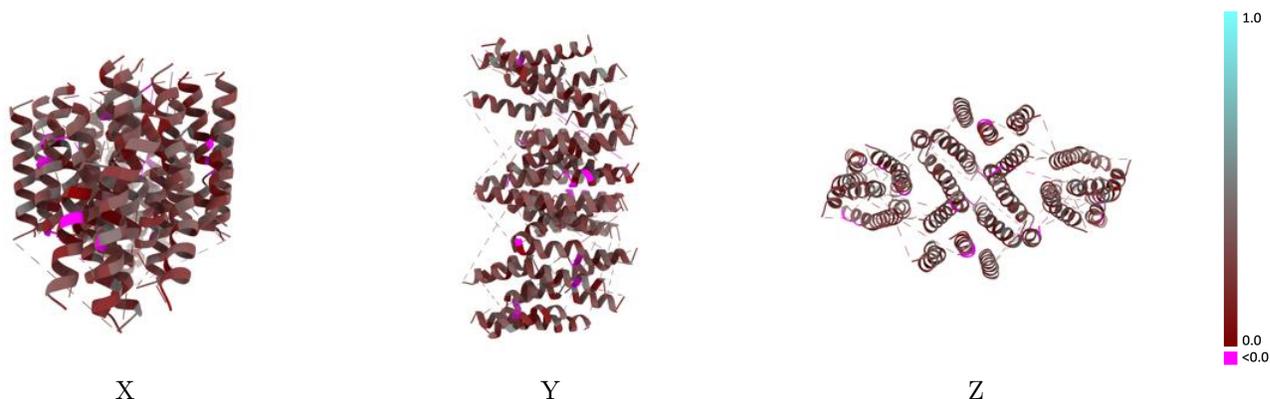
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
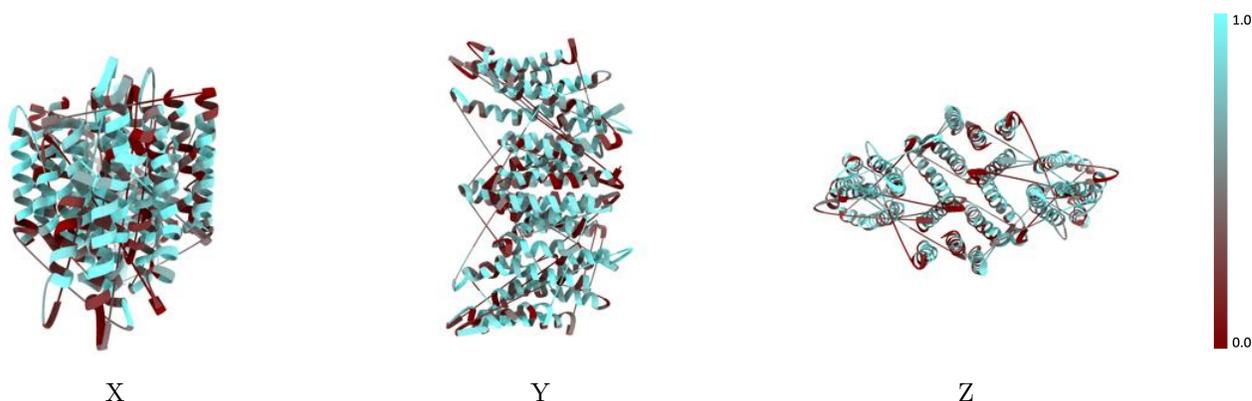
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (46.2).

9.4　Atom inclusion ⓘ
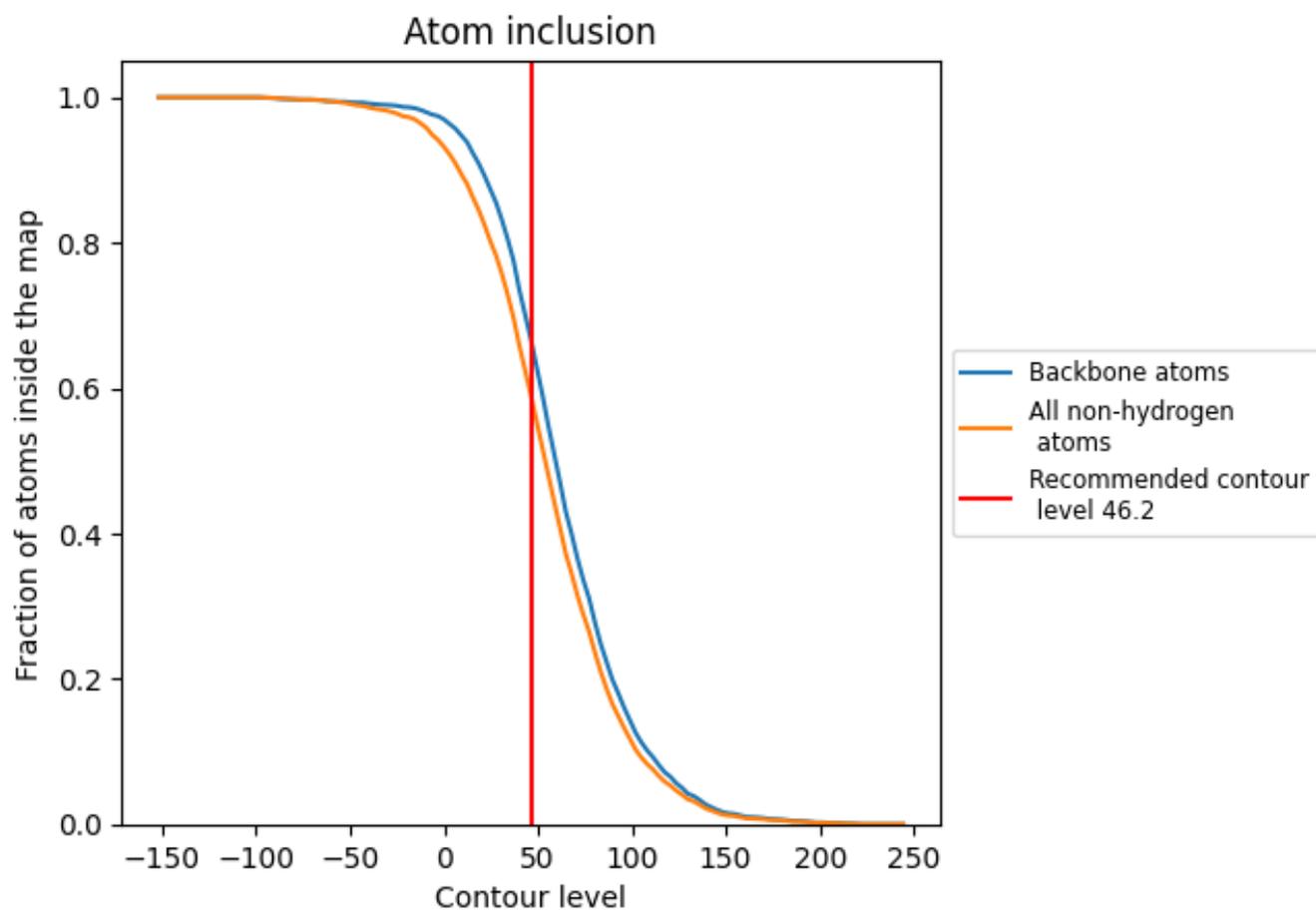
At the recommended contour level, 67% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (46.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5904	0.2420
A	0.5849	0.2410
B	0.5956	0.2430

1.0

0.0
<0.0