



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:35 PM UTC

PDB ID : 5FN4 / pdb_00005fn4
EMDB ID : EMD-3239
Title : Cryo-EM structure of gamma secretase in class 2 of the apo- state ensemble
Authors : Bai, X.C.; Rajendra, E.; Yang, G.H.; Shi, Y.G.; Scheres, S.H.W.
Deposited on : 2015-11-10
Resolution : 4.00 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:

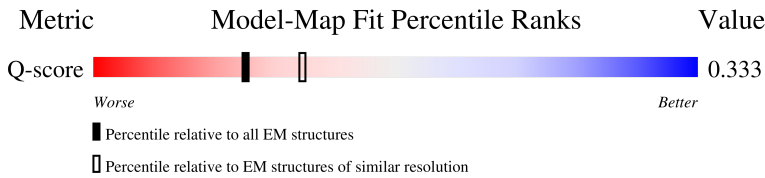
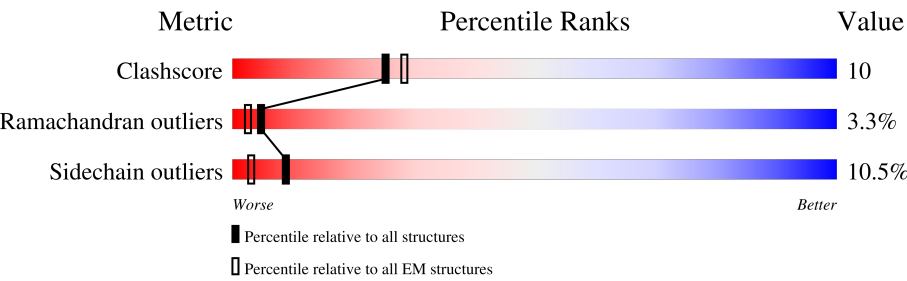
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 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	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	7587 (3.50 - 4.50)

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	709	66%25%6%
2	B	467	6%27%15%54%
3	C	265	5%65%23%8%
4	D	101	5%80%16%

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Mol	Chain	Length	Quality of chain
5	G	25	56% 84% 8% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9776 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 Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	665	Total	C	N	O	S	0	0
			5222	3312	888	1001	21		

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	217	Total	C	N	O	S	0	0
			1714	1180	251	274	9		

- Molecule 3 is a protein called Gamma-secretase subunit APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1868	1252	299	313	4		

- Molecule 4 is a protein called Gamma-secretase subunit PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			847	579	133	134	1		

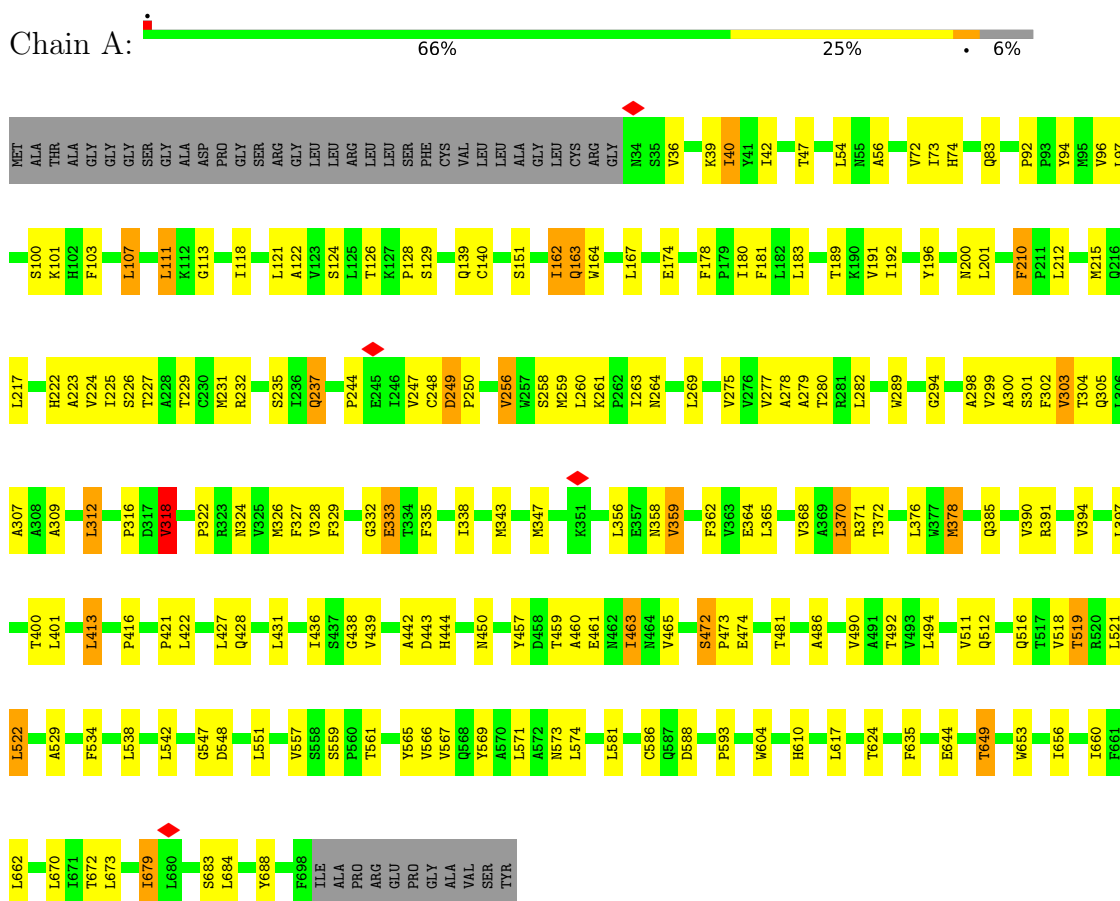
- Molecule 5 is a protein called POLY ALA CHAIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	25	Total	C	N	O	0	0
			125	75	25	25		

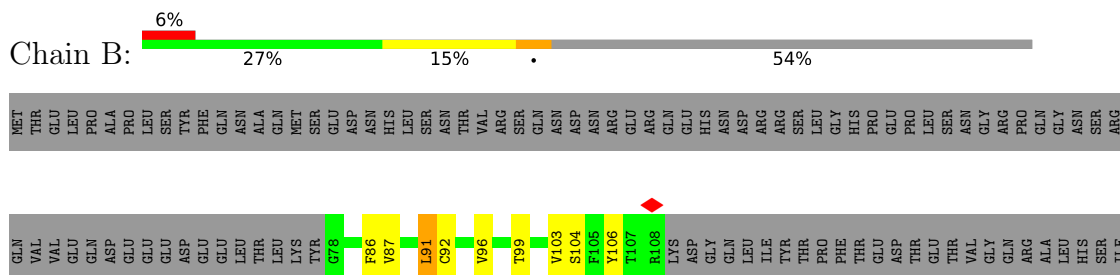
3 Residue-property plots

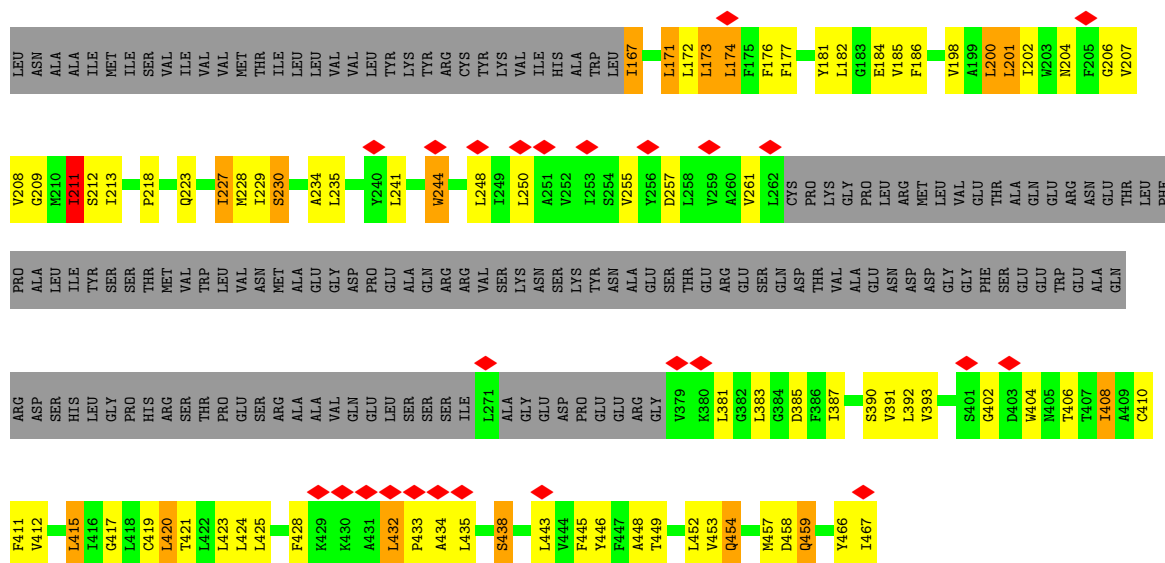
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

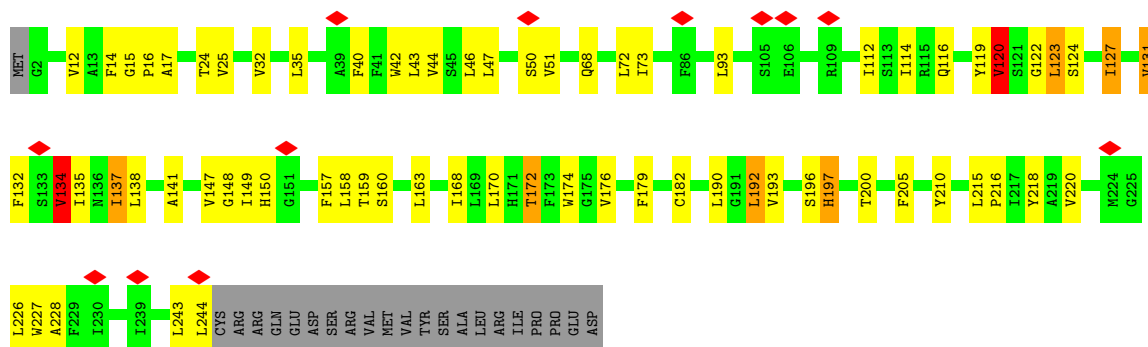


• Molecule 2: Presenilin-1

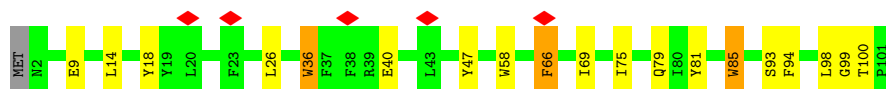
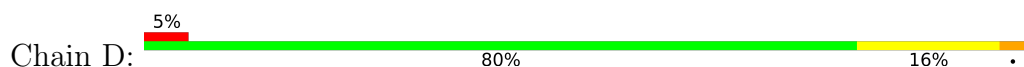




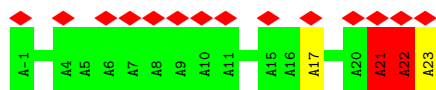
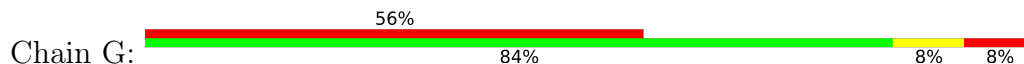
• Molecule 3: Gamma-secretase subunit APH-1A



• Molecule 4: Gamma-secretase subunit PEN-2



• Molecule 5: POLY ALA CHAIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	252.0, 252.0, 252.0	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.62	0/5345	1.06	4/7284 (0.1%)
2	B	0.69	0/1759	1.35	5/2399 (0.2%)
3	C	0.71	2/1920 (0.1%)	1.32	2/2619 (0.1%)
4	D	0.72	0/880	1.26	1/1201 (0.1%)
5	G	0.99	0/124	1.96	2/172 (1.2%)
All	All	0.66	2/10028 (0.0%)	1.20	14/13675 (0.1%)

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	1
2	B	0	1
5	G	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	244	LEU	C-O	7.44	1.38	1.23
3	C	197	HIS	C-O	5.85	1.30	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	22	ALA	O-C-N	-12.01	109.70	122.07
5	G	21	ALA	O-C-N	-11.98	109.73	122.07
1	A	162	ILE	N-CA-C	9.25	118.92	111.62
2	B	87	VAL	O-C-N	7.33	125.11	120.42
4	D	36	TRP	CB-CA-C	-6.76	100.17	110.92
2	B	211	ILE	N-CA-CB	6.32	117.95	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	PHE	CB-CA-C	-6.28	101.30	110.96
3	C	134	VAL	N-CA-C	6.09	116.80	111.56
3	C	120	VAL	N-CA-CB	6.04	118.75	110.54
2	B	227	ILE	N-CA-CB	5.65	117.16	110.55
1	A	200	ASN	N-CA-C	5.63	119.89	113.19
2	B	454	GLN	O-C-N	5.63	125.49	120.48
1	A	679	ILE	N-CA-CB	5.08	117.45	110.54
1	A	92	PRO	N-CA-C	5.06	116.88	110.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	PHE	Peptide
2	B	435	LEU	Peptide
5	G	21	ALA	Mainchain
5	G	22	ALA	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	5222	0	5120	106	0
2	B	1714	0	1810	64	0
3	C	1868	0	1907	48	0
4	D	847	0	836	8	0
5	G	125	0	127	5	0
All	All	9776	0	9800	204	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 10.

All (204) 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:260:LEU:HD11	1:A:318:VAL:HG13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HG	2:B:229:ILE:HD11	1.65	0.78
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.65	0.77
1:A:672:THR:HG23	3:C:158:LEU:HD13	1.69	0.73
3:C:170:LEU:HD21	3:C:200:THR:HG21	1.71	0.69
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.73	0.68
2:B:406:THR:HA	2:B:449:THR:HG21	1.75	0.68
2:B:387:ILE:O	2:B:391:VAL:HG23	1.95	0.66
1:A:378:MET:HE3	1:A:413:LEU:HD22	1.76	0.66
1:A:162:ILE:HD11	1:A:164:TRP:CE2	2.30	0.66
1:A:122:ALA:HB2	1:A:215:MET:HE1	1.77	0.66
3:C:40:PHE:O	3:C:44:VAL:HG23	1.97	0.64
1:A:181:PHE:CD1	1:A:217:LEU:HD21	2.32	0.64
2:B:457:MET:HE2	3:C:132:PHE:HB3	1.79	0.64
4:D:98:LEU:O	4:D:100:THR:N	2.30	0.63
2:B:104:SER:O	2:B:106:TYR:N	2.32	0.62
1:A:401:LEU:HD11	1:A:439:VAL:HG21	1.82	0.62
2:B:176:PHE:CZ	5:G:17:ALA:HB1	2.36	0.61
2:B:234:ALA:HA	2:B:391:VAL:HG22	1.82	0.61
1:A:516:GLN:O	1:A:519:THR:HG22	2.00	0.61
2:B:208:VAL:O	2:B:211:ILE:HG13	2.01	0.61
1:A:225:ILE:HG21	1:A:229:THR:HG21	1.82	0.60
3:C:179:PHE:O	3:C:182:CYS:SG	2.60	0.60
2:B:176:PHE:CZ	5:G:17:ALA:CB	2.84	0.60
1:A:280:THR:HG21	1:A:302:PHE:HA	1.84	0.58
1:A:299:VAL:HA	1:A:302:PHE:CE2	2.38	0.58
1:A:121:LEU:HD23	1:A:178:PHE:CE1	2.38	0.58
3:C:24:THR:HG21	3:C:119:TYR:CE1	2.38	0.58
3:C:35:LEU:O	3:C:124:SER:OG	2.13	0.58
1:A:47:THR:HG22	1:A:183:LEU:HD22	1.86	0.58
1:A:683:SER:HB2	3:C:16:PRO:HA	1.86	0.58
1:A:249:ASP:HB3	1:A:557:VAL:HG11	1.86	0.58
2:B:408:ILE:HD13	3:C:131:VAL:HG11	1.86	0.58
1:A:73:ILE:HD13	1:A:660:ILE:HD11	1.85	0.57
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.39	0.57
1:A:36:VAL:HG21	3:C:137:ILE:HG22	1.85	0.57
1:A:362:PHE:CD1	1:A:427:LEU:HD13	2.39	0.57
1:A:111:LEU:HG	1:A:118:ILE:HD13	1.85	0.57
1:A:371:ARG:NH2	1:A:486:ALA:HB1	2.19	0.57
1:A:54:LEU:HD11	1:A:223:ALA:HB1	1.87	0.57
1:A:124:SER:OG	1:A:189:THR:HG21	2.05	0.57
1:A:256:VAL:HG21	1:A:567:VAL:HG12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HB2	1:A:247:VAL:HG23	1.87	0.56
1:A:260:LEU:HD13	1:A:312:LEU:CD1	2.35	0.56
2:B:198:VAL:HG21	4:D:94:PHE:CD2	2.41	0.56
2:B:223:GLN:O	2:B:227:ILE:HG23	2.06	0.56
4:D:81:TYR:O	4:D:85:TRP:N	2.38	0.56
3:C:25:VAL:HG12	3:C:32:VAL:HG22	1.87	0.55
1:A:534:PHE:CE2	1:A:566:VAL:HG11	2.40	0.55
1:A:683:SER:CB	3:C:16:PRO:HA	2.37	0.55
1:A:210:PHE:CE1	1:A:212:LEU:HD12	2.41	0.55
1:A:422:LEU:HD22	1:A:428:GLN:HB3	1.88	0.55
1:A:307:ALA:HB2	1:A:518:VAL:HG22	1.88	0.54
3:C:192:LEU:HD13	3:C:227:TRP:HH2	1.72	0.54
1:A:111:LEU:HD23	1:A:118:ILE:HG21	1.90	0.54
1:A:54:LEU:HD11	1:A:223:ALA:CB	2.38	0.53
3:C:159:THR:HG21	3:C:210:TYR:CE1	2.43	0.53
1:A:679:ILE:HG21	3:C:12:VAL:HA	1.91	0.53
2:B:406:THR:HG23	2:B:449:THR:HB	1.91	0.53
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.91	0.52
3:C:116:GLN:O	3:C:120:VAL:HG13	2.08	0.52
1:A:385:GLN:O	1:A:391:ARG:HB2	2.10	0.52
2:B:448:ALA:HB1	3:C:47:LEU:HD21	1.91	0.52
2:B:402:GLY:N	2:B:454:GLN:HG3	2.25	0.52
5:G:21:ALA:O	5:G:22:ALA:C	2.51	0.52
5:G:22:ALA:O	5:G:23:ALA:C	2.51	0.52
2:B:250:LEU:HB3	2:B:443:LEU:HD11	1.92	0.52
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.92	0.52
2:B:106:TYR:CE1	2:B:235:LEU:HB3	2.44	0.51
1:A:56:ALA:HA	1:A:227:THR:HG22	1.92	0.51
1:A:101:LYS:HG3	1:A:126:THR:HG21	1.92	0.51
1:A:370:LEU:N	1:A:443:ASP:OD2	2.44	0.51
2:B:207:VAL:HB	4:D:26:LEU:HD21	1.92	0.51
1:A:121:LEU:CB	1:A:180:ILE:HG23	2.42	0.50
1:A:258:SER:HB2	1:A:571:LEU:HD21	1.92	0.50
1:A:684:LEU:O	1:A:688:TYR:HB2	2.11	0.50
2:B:174:LEU:HD22	2:B:206:GLY:HA2	1.94	0.50
3:C:216:PRO:O	3:C:220:VAL:HG23	2.11	0.50
1:A:365:LEU:N	1:A:365:LEU:HD12	2.26	0.50
1:A:635:PHE:CZ	1:A:649:THR:HG23	2.47	0.50
3:C:215:LEU:HB3	3:C:216:PRO:HD3	1.94	0.50
1:A:192:ILE:HG12	1:A:660:ILE:HD13	1.94	0.50
2:B:92:CYS:O	2:B:96:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:LEU:HD13	2:B:227:ILE:HD13	1.94	0.49
1:A:121:LEU:HB3	1:A:180:ILE:HG23	1.95	0.49
1:A:376:LEU:HD22	1:A:490:VAL:HG13	1.95	0.49
2:B:244:TRP:CE3	2:B:244:TRP:HA	2.48	0.49
1:A:309:ALA:HA	1:A:327:PHE:CZ	2.47	0.48
1:A:390:VAL:O	1:A:394:VAL:HG23	2.12	0.48
1:A:277:VAL:HG23	1:A:359:VAL:HG13	1.94	0.48
1:A:73:ILE:HG21	1:A:660:ILE:HD11	1.96	0.48
1:A:376:LEU:CD2	1:A:490:VAL:HG13	2.44	0.48
2:B:250:LEU:HD13	2:B:443:LEU:HD21	1.94	0.48
3:C:123:LEU:HD22	3:C:127:ILE:CD1	2.44	0.48
2:B:459:GLN:HG2	3:C:72:LEU:HD11	1.95	0.48
3:C:176:VAL:HG11	3:C:228:ALA:HB1	1.96	0.48
2:B:106:TYR:CD2	2:B:235:LEU:HD22	2.49	0.48
3:C:174:TRP:CH2	3:C:197:HIS:HA	2.49	0.48
1:A:335:PHE:O	1:A:338:ILE:HG23	2.14	0.48
1:A:303:VAL:HG21	1:A:522:LEU:HD12	1.95	0.47
3:C:122:GLY:HA3	3:C:172:THR:HA	1.94	0.47
1:A:279:ALA:O	1:A:305:GLN:NE2	2.47	0.47
1:A:111:LEU:CG	1:A:118:ILE:HD13	2.43	0.47
2:B:421:THR:HG21	2:B:434:ALA:HA	1.96	0.47
2:B:466:TYR:CE2	3:C:163:LEU:HD23	2.49	0.47
1:A:378:MET:HE3	1:A:413:LEU:CD2	2.43	0.47
2:B:390:SER:O	2:B:393:VAL:HG12	2.15	0.47
2:B:218:PRO:HG3	4:D:36:TRP:CZ2	2.50	0.47
1:A:96:VAL:HG23	1:A:121:LEU:HD13	1.97	0.47
1:A:303:VAL:HG11	1:A:522:LEU:HD13	1.96	0.47
1:A:365:LEU:HD11	1:A:494:LEU:CD1	2.45	0.47
1:A:653:TRP:CD1	1:A:656:ILE:HG23	2.49	0.47
3:C:137:ILE:HD11	3:C:160:SER:HB3	1.95	0.47
1:A:111:LEU:CD2	1:A:118:ILE:HG21	2.44	0.47
1:A:126:THR:HG22	1:A:128:PRO:HD2	1.96	0.47
1:A:300:ALA:O	1:A:304:THR:HG23	2.15	0.47
2:B:411:PHE:O	2:B:415:LEU:HD13	2.14	0.47
1:A:72:VAL:HG13	1:A:94:TYR:CE1	2.49	0.47
1:A:673:LEU:C	1:A:673:LEU:HD23	2.41	0.47
2:B:452:LEU:HD13	3:C:51:VAL:HG22	1.97	0.46
2:B:181:TYR:O	2:B:185:VAL:HG23	2.14	0.46
1:A:368:VAL:HG13	1:A:376:LEU:HD13	1.97	0.46
3:C:196:SER:O	3:C:200:THR:HG23	2.15	0.46
1:A:42:ILE:HD11	3:C:150:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:GLY:O	2:B:404:TRP:N	2.48	0.46
2:B:410:CYS:SG	2:B:446:TYR:HB2	2.55	0.46
2:B:227:ILE:HG13	2:B:228:MET:N	2.29	0.46
2:B:445:PHE:O	2:B:449:THR:OG1	2.27	0.46
2:B:453:VAL:HA	3:C:50:SER:HB2	1.97	0.46
1:A:371:ARG:N	1:A:443:ASP:OD2	2.48	0.46
2:B:173:LEU:HA	2:B:177:PHE:CD2	2.51	0.46
2:B:417:GLY:HA3	2:B:438:SER:HA	1.98	0.46
1:A:328:VAL:C	1:A:329:PHE:CD1	2.94	0.46
2:B:432:LEU:N	2:B:433:PRO:CD	2.79	0.46
1:A:529:ALA:HB2	1:A:551:LEU:HG	1.98	0.45
1:A:365:LEU:HD11	1:A:494:LEU:HD11	1.98	0.45
2:B:408:ILE:O	2:B:412:VAL:HG23	2.15	0.45
1:A:36:VAL:HG21	3:C:137:ILE:CG2	2.47	0.45
2:B:420:LEU:O	2:B:424:LEU:HG	2.16	0.45
1:A:237:GLN:O	1:A:244:PRO:HB3	2.17	0.45
1:A:232:ARG:O	1:A:235:SER:OG	2.29	0.45
4:D:66:PHE:O	4:D:69:ILE:HG22	2.16	0.45
1:A:547:GLY:O	1:A:548:ASP:C	2.60	0.45
2:B:182:LEU:HD23	2:B:198:VAL:HG13	1.97	0.45
1:A:40:ILE:HD11	3:C:157:PHE:HZ	1.81	0.45
1:A:97:LEU:HA	1:A:122:ALA:HB3	1.98	0.45
2:B:466:TYR:CD2	3:C:163:LEU:HD23	2.52	0.45
3:C:197:HIS:O	3:C:200:THR:OG1	2.25	0.45
2:B:176:PHE:CZ	5:G:17:ALA:HB2	2.52	0.44
1:A:538:LEU:HD23	1:A:569:TYR:CG	2.52	0.44
1:A:492:THR:HG23	1:A:512:GLN:HA	2.00	0.44
3:C:147:VAL:HG12	3:C:148:GLY:N	2.33	0.44
1:A:107:LEU:C	1:A:107:LEU:HD12	2.42	0.44
1:A:275:VAL:HG12	1:A:324:ASN:HB3	1.99	0.44
1:A:427:LEU:HD11	1:A:438:GLY:HA3	2.00	0.44
2:B:103:VAL:O	2:B:104:SER:CB	2.66	0.44
3:C:134:VAL:O	3:C:137:ILE:N	2.47	0.44
1:A:74:HIS:HA	1:A:196:TYR:CE1	2.54	0.43
2:B:211:ILE:HD12	2:B:212:SER:N	2.34	0.43
2:B:244:TRP:HA	2:B:244:TRP:HE3	1.83	0.43
2:B:167:ILE:C	2:B:167:ILE:HD12	2.44	0.42
1:A:162:ILE:HD12	1:A:163:GLN:N	2.33	0.42
1:A:54:LEU:HD13	1:A:226:SER:O	2.20	0.42
1:A:542:LEU:HD21	1:A:565:TYR:CD1	2.54	0.42
1:A:282:LEU:HD11	1:A:567:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:VAL:HG22	3:C:138:LEU:CD1	2.49	0.42
3:C:192:LEU:HD13	3:C:227:TRP:CH2	2.53	0.42
1:A:231:MET:HE3	1:A:248:CYS:HB3	1.99	0.42
2:B:449:THR:HA	2:B:453:VAL:HB	2.00	0.42
3:C:73:ILE:HG23	3:C:205:PHE:CE2	2.54	0.42
2:B:230:SER:HA	2:B:387:ILE:HG12	2.01	0.42
2:B:200:LEU:C	2:B:200:LEU:HD23	2.45	0.42
2:B:200:LEU:HD23	2:B:201:LEU:N	2.35	0.42
1:A:42:ILE:HD12	3:C:149:ILE:HG12	2.02	0.42
3:C:42:TRP:CZ3	3:C:43:LEU:HD23	2.54	0.42
2:B:204:ASN:O	2:B:208:VAL:HG22	2.19	0.42
2:B:424:LEU:O	2:B:428:PHE:N	2.52	0.41
1:A:364:GLU:C	1:A:365:LEU:HD12	2.45	0.41
1:A:42:ILE:HG13	3:C:149:ILE:HG21	2.01	0.41
1:A:450:ASN:HD22	1:A:450:ASN:C	2.28	0.41
1:A:460:ALA:O	1:A:461:GLU:C	2.63	0.41
1:A:397:LEU:O	1:A:400:THR:OG1	2.32	0.41
2:B:209:GLY:O	2:B:213:ILE:HG12	2.20	0.41
2:B:182:LEU:HG	2:B:186:PHE:CE2	2.56	0.41
1:A:259:MET:SD	1:A:326:MET:HA	2.61	0.41
1:A:347:MET:HE3	1:A:356:LEU:HA	2.03	0.41
1:A:662:LEU:HD13	3:C:149:ILE:N	2.34	0.41
2:B:171:LEU:HD23	2:B:172:LEU:N	2.36	0.41
2:B:257:ASP:O	2:B:261:VAL:HG23	2.21	0.41
1:A:162:ILE:HD11	1:A:164:TRP:CD2	2.56	0.40
3:C:14:PHE:O	3:C:15:GLY:C	2.63	0.40
4:D:98:LEU:N	4:D:98:LEU:CD1	2.83	0.40
1:A:278:ALA:O	1:A:305:GLN:NE2	2.54	0.40
2:B:99:THR:CG2	2:B:235:LEU:HD21	2.51	0.40
2:B:211:ILE:HD13	4:D:18:TYR:OH	2.21	0.40
3:C:141:ALA:HB2	3:C:157:PHE:CE1	2.57	0.40
1:A:385:GLN:HE22	1:A:394:VAL:HB	1.87	0.40
1:A:534:PHE:CD2	1:A:566:VAL:HG11	2.56	0.40
2:B:96:VAL:O	2:B:99:THR:HG22	2.22	0.40
2:B:171:LEU:HD23	2:B:171:LEU:C	2.47	0.40
1:A:40:ILE:HD11	3:C:157:PHE:CZ	2.56	0.40
1:A:259:MET:HE3	1:A:263:ILE:CD1	2.52	0.40
1:A:261:LYS:HB2	1:A:324:ASN:HD21	1.87	0.40
1:A:442:ALA:HB1	1:A:444:HIS:CE1	2.57	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	513/709 (72%)	407 (79%)	83 (16%)	23 (4%)	2	20
2	B	100/467 (21%)	93 (93%)	6 (6%)	1 (1%)	12	45
3	C	80/265 (30%)	74 (92%)	6 (8%)	0	100	100
4	D	43/101 (43%)	37 (86%)	5 (12%)	1 (2%)	5	31
5	G	23/25 (92%)	23 (100%)	0	0	100	100
All	All	759/1567 (48%)	634 (84%)	100 (13%)	25 (3%)	5	24

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	TRP
1	A	333	GLU
1	A	473	PRO
4	D	99	GLY
1	A	322	PRO
1	A	372	THR
1	A	421	PRO
1	A	472	SER
1	A	103	PHE
1	A	294	GLY
1	A	298	ALA
1	A	358	ASN
1	A	436	ILE
1	A	559	SER
1	A	332	GLY
1	A	129	SER
1	A	416	PRO
1	A	593	PRO
1	A	113	GLY
1	A	316	PRO
1	A	318	VAL

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Mol	Chain	Res	Type
1	A	359	VAL
1	A	511	VAL
1	A	40	ILE
2	B	432	LEU

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	583/612 (95%)	531 (91%)	52 (9%)	9	31
2	B	185/408 (45%)	156 (84%)	29 (16%)	2	15
3	C	192/214 (90%)	173 (90%)	19 (10%)	7	27
4	D	87/89 (98%)	77 (88%)	10 (12%)	5	22
All	All	1047/1323 (79%)	937 (90%)	110 (10%)	9	24

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	83	GLN
1	A	100	SER
1	A	107	LEU
1	A	111	LEU
1	A	139	GLN
1	A	140	CYS
1	A	151	SER
1	A	163	GLN
1	A	167	LEU
1	A	174	GLU
1	A	191	VAL
1	A	201	LEU
1	A	224	VAL
1	A	237	GLN
1	A	249	ASP
1	A	250	PRO

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Mol	Chain	Res	Type
1	A	256	VAL
1	A	264	ASN
1	A	269	LEU
1	A	301	SER
1	A	303	VAL
1	A	312	LEU
1	A	318	VAL
1	A	333	GLU
1	A	343	MET
1	A	370	LEU
1	A	378	MET
1	A	413	LEU
1	A	431	LEU
1	A	457	TYR
1	A	459	THR
1	A	463	ILE
1	A	472	SER
1	A	474	GLU
1	A	481	THR
1	A	519	THR
1	A	521	LEU
1	A	522	LEU
1	A	561	THR
1	A	573	ASN
1	A	574	LEU
1	A	581	LEU
1	A	586	CYS
1	A	588	ASP
1	A	604	TRP
1	A	610	HIS
1	A	617	LEU
1	A	624	THR
1	A	644	GLU
1	A	649	THR
1	A	670	LEU
2	B	91	LEU
2	B	167	ILE
2	B	171	LEU
2	B	173	LEU
2	B	174	LEU
2	B	184	GLU
2	B	200	LEU

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Mol	Chain	Res	Type
2	B	201	LEU
2	B	202	ILE
2	B	211	ILE
2	B	230	SER
2	B	241	LEU
2	B	244	TRP
2	B	248	LEU
2	B	255	VAL
2	B	381	LEU
2	B	383	LEU
2	B	385	ASP
2	B	392	LEU
2	B	408	ILE
2	B	415	LEU
2	B	419	CYS
2	B	420	LEU
2	B	423	LEU
2	B	425	LEU
2	B	438	SER
2	B	458	ASP
2	B	459	GLN
2	B	467	ILE
3	C	46	LEU
3	C	68	GLN
3	C	93	LEU
3	C	112	ILE
3	C	114	ILE
3	C	120	VAL
3	C	123	LEU
3	C	127	ILE
3	C	131	VAL
3	C	134	VAL
3	C	135	ILE
3	C	137	ILE
3	C	172	THR
3	C	190	LEU
3	C	192	LEU
3	C	193	VAL
3	C	218	TYR
3	C	226	LEU
3	C	243	LEU
4	D	9	GLU

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Mol	Chain	Res	Type
4	D	14	LEU
4	D	40	GLU
4	D	47	TYR
4	D	58	TRP
4	D	66	PHE
4	D	75	ILE
4	D	79	GLN
4	D	85	TRP
4	D	93	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	102	HIS
1	A	139	GLN
1	A	163	GLN
1	A	290	ASN
1	A	305	GLN
1	A	417	ASN
1	A	444	HIS
1	A	449	HIS
1	A	478	ASN
1	A	512	GLN
1	A	568	GLN
1	A	587	GLN
1	A	639	GLN
3	C	68	GLN
4	D	8	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](#)

There are no ligands in this entry.

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.

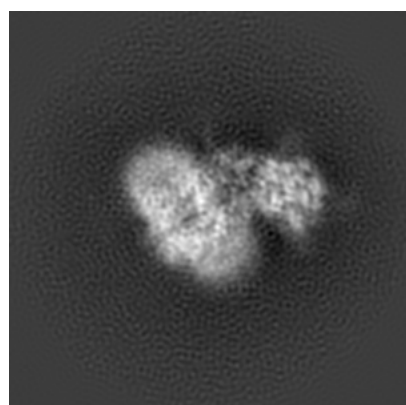
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3239. These allow visual inspection of the internal detail of the map and identification of artifacts.

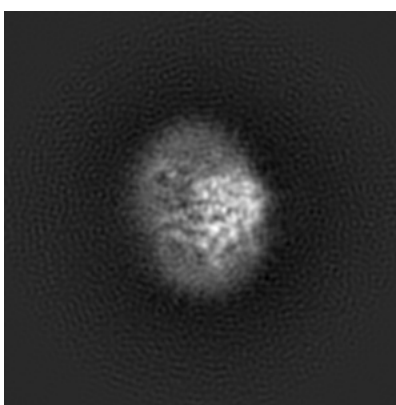
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

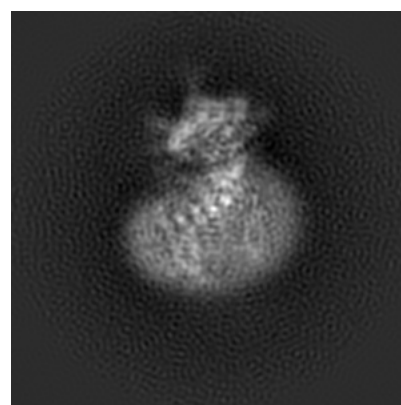
6.1.1 Primary map



X



Y

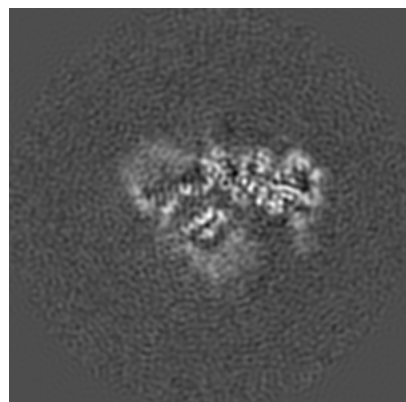


Z

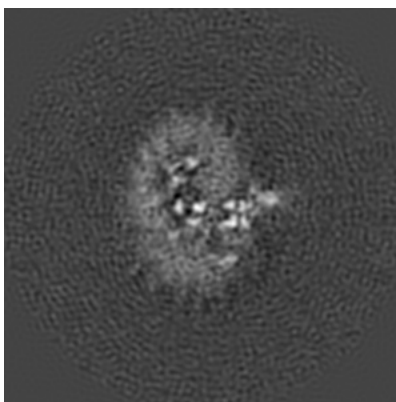
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

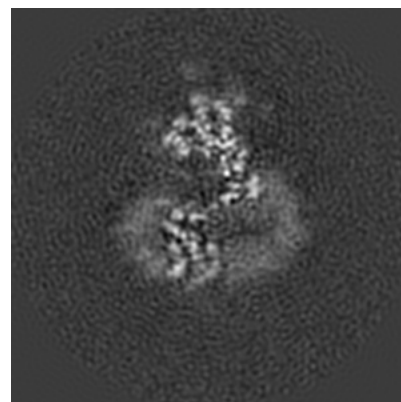
6.2.1 Primary map



X Index: 90



Y Index: 90

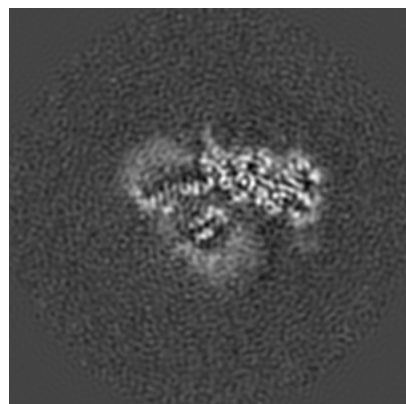


Z Index: 90

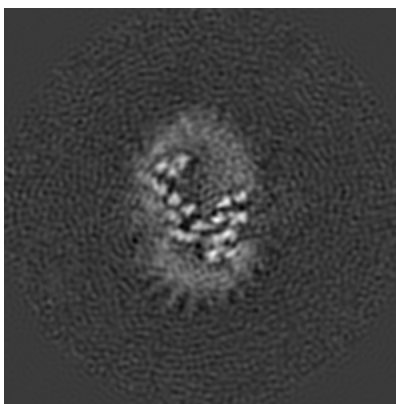
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

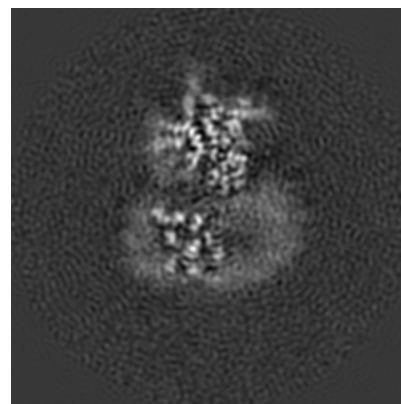
6.3.1 Primary map



X Index: 91



Y Index: 84

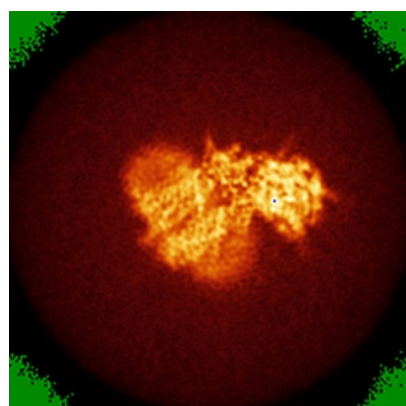


Z Index: 95

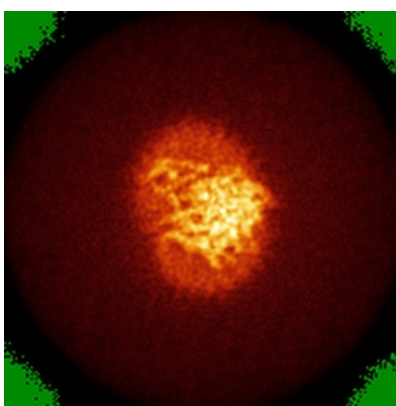
The images above show the largest variance slices of the map in three orthogonal directions.

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

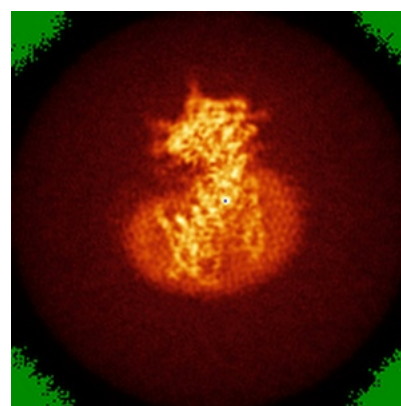
6.4.1 Primary map



X



Y



Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

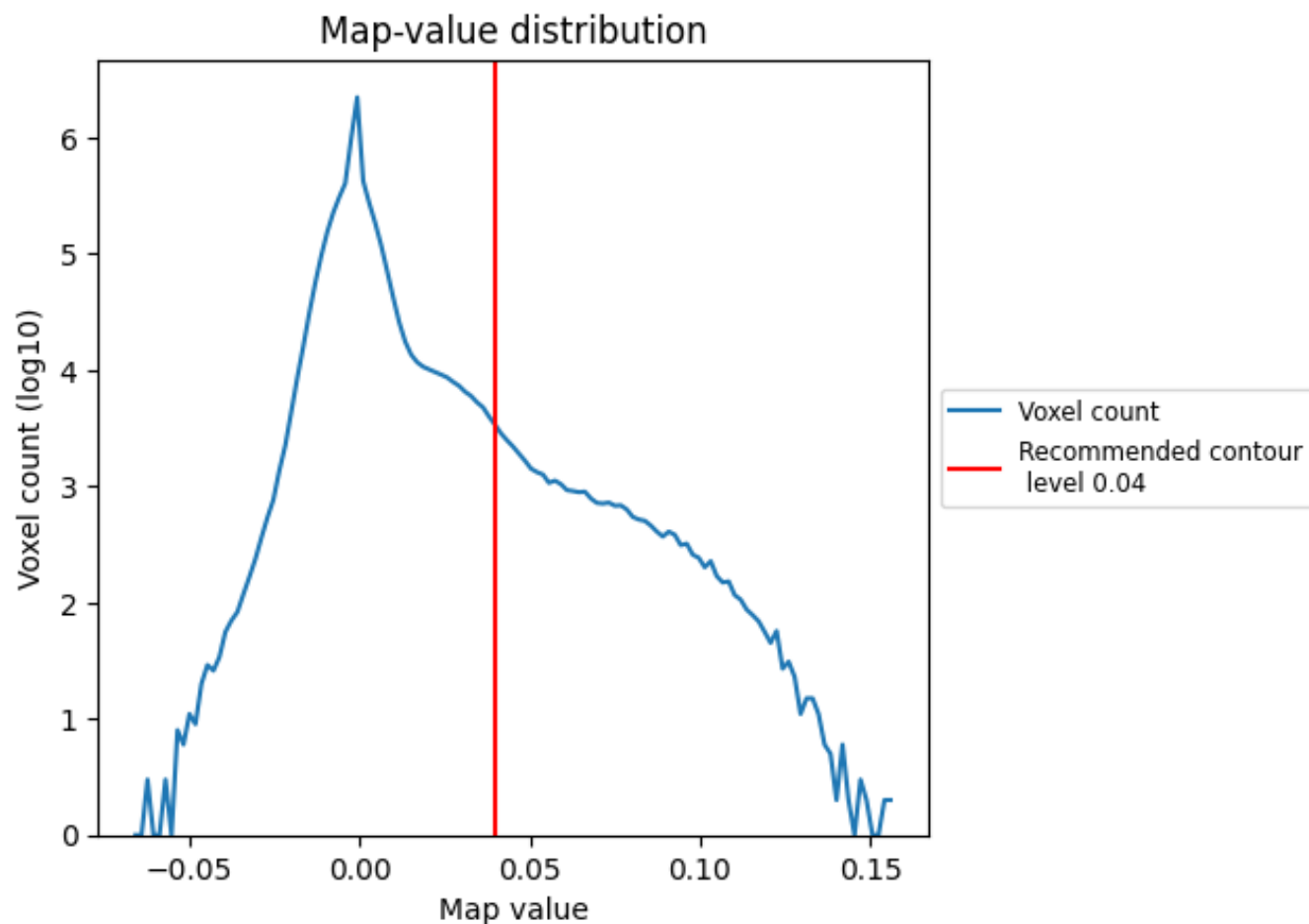
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

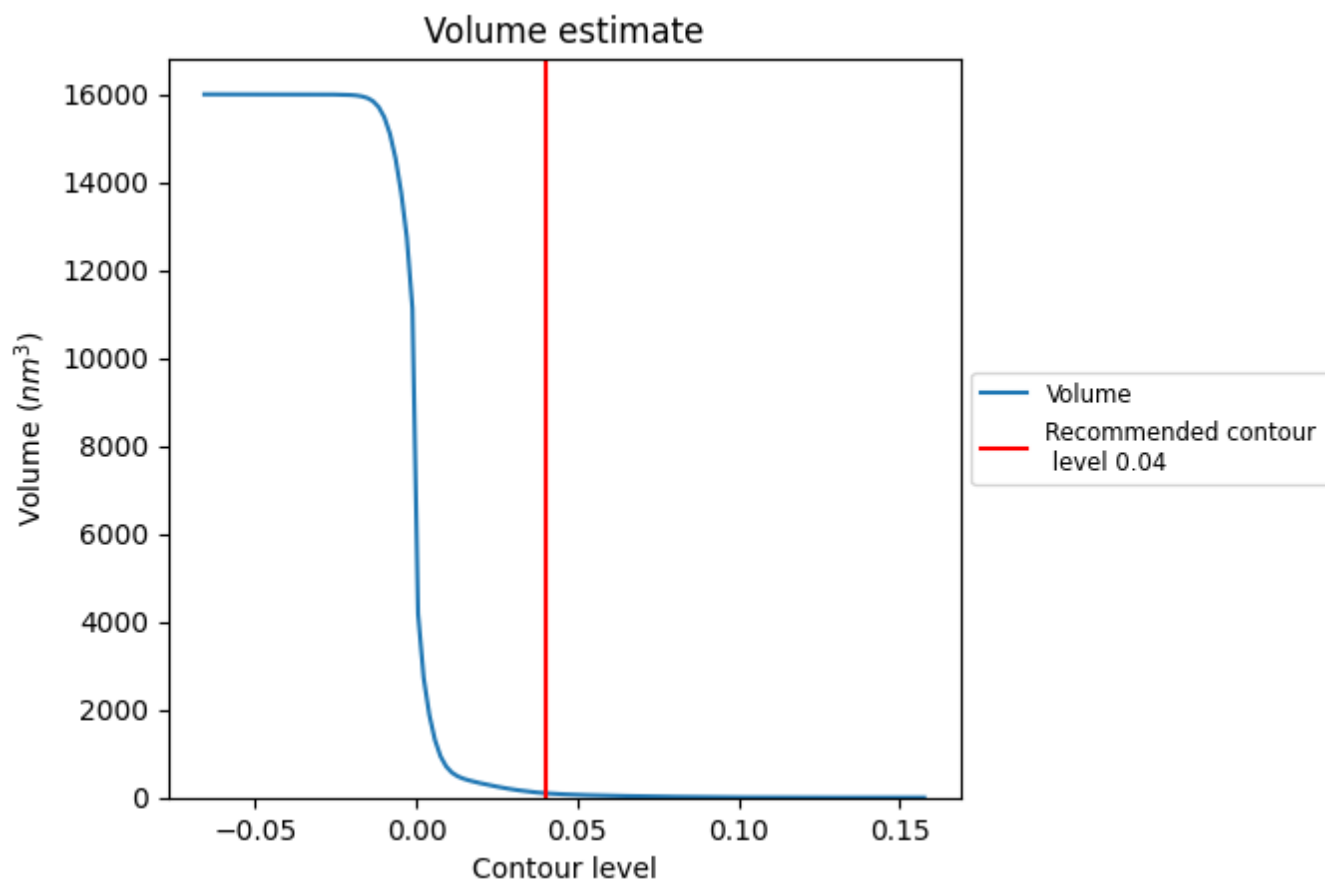
This section contains the results of statistical analysis of the map.

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.

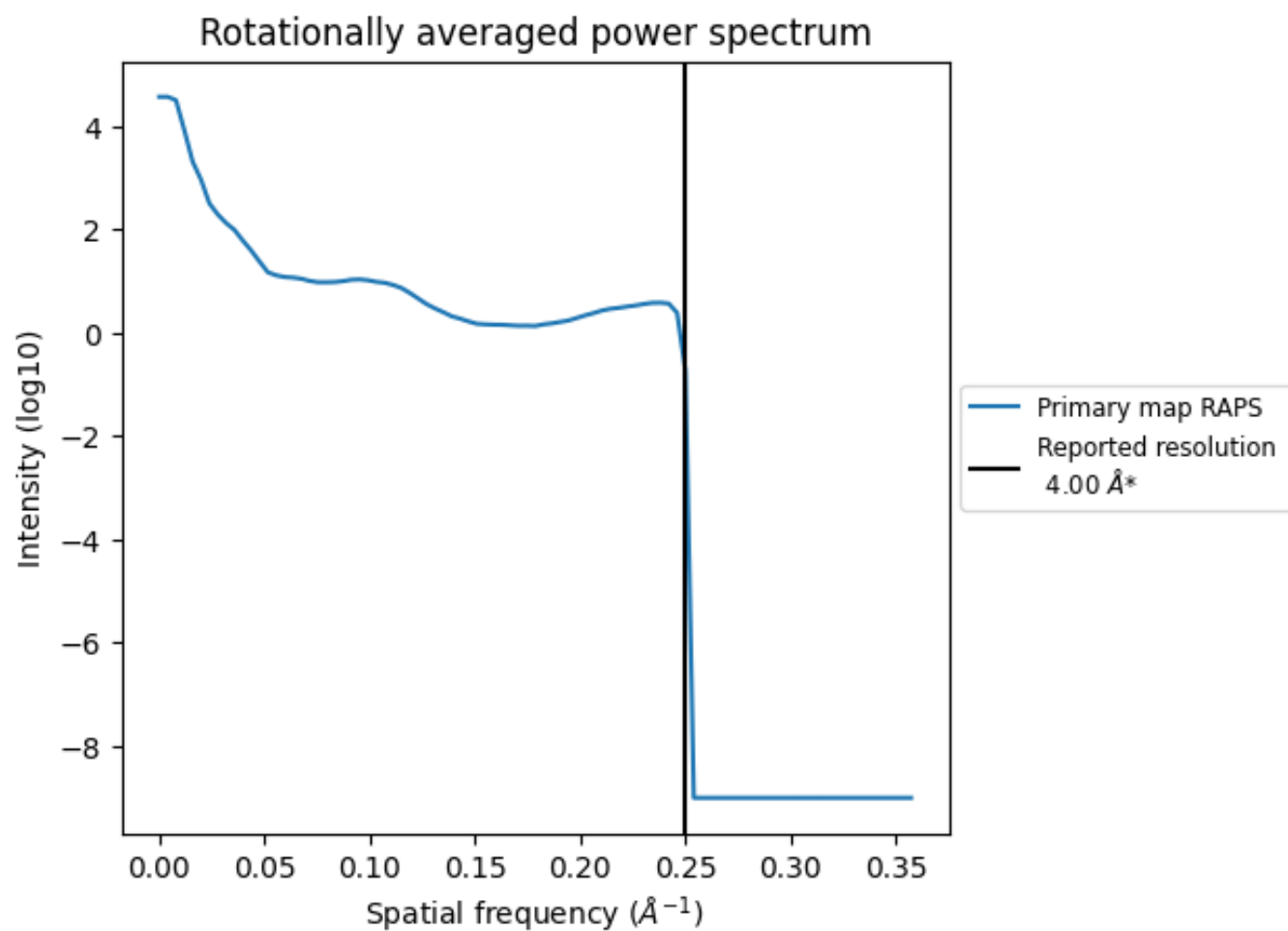
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 0.250 Å⁻¹

8 Fourier-Shell correlation

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

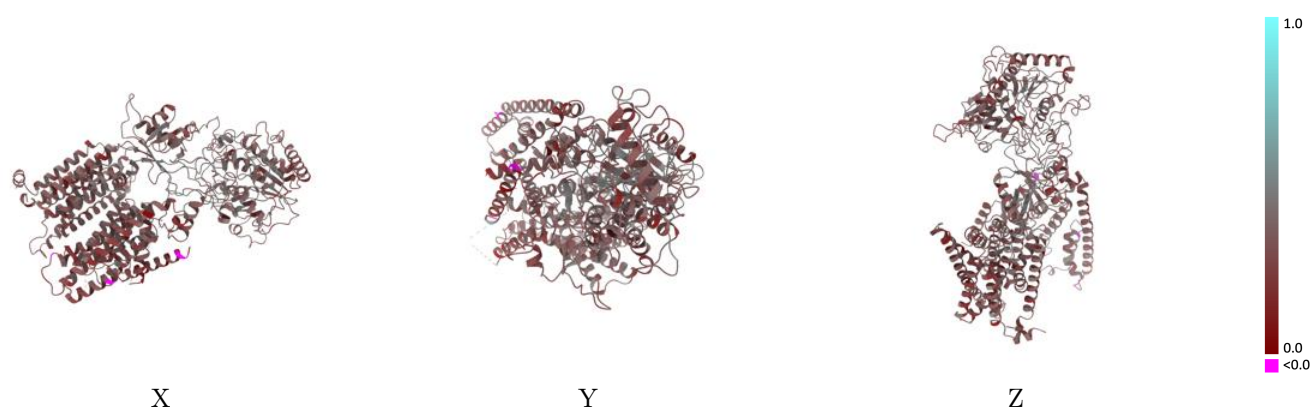
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3239 and PDB model 5FN4. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

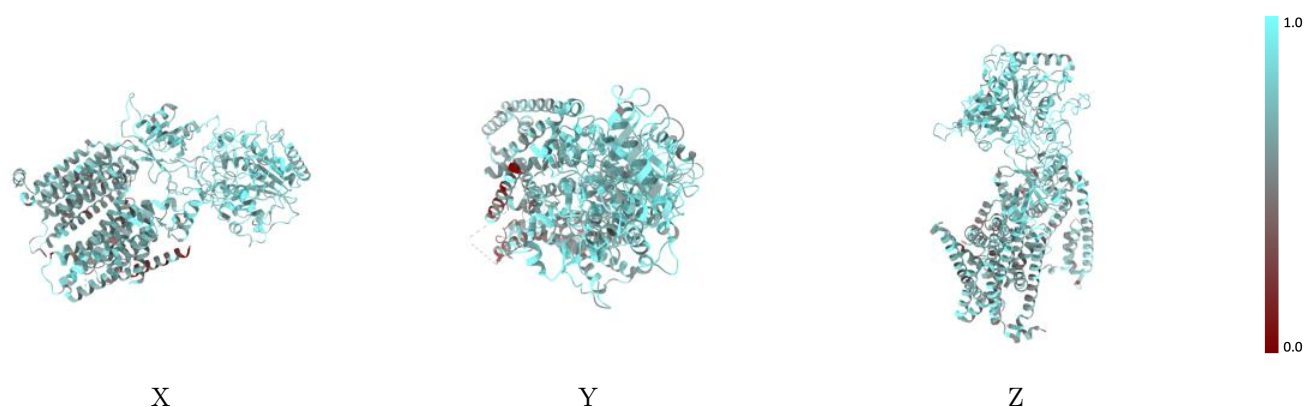
This section was not generated.

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



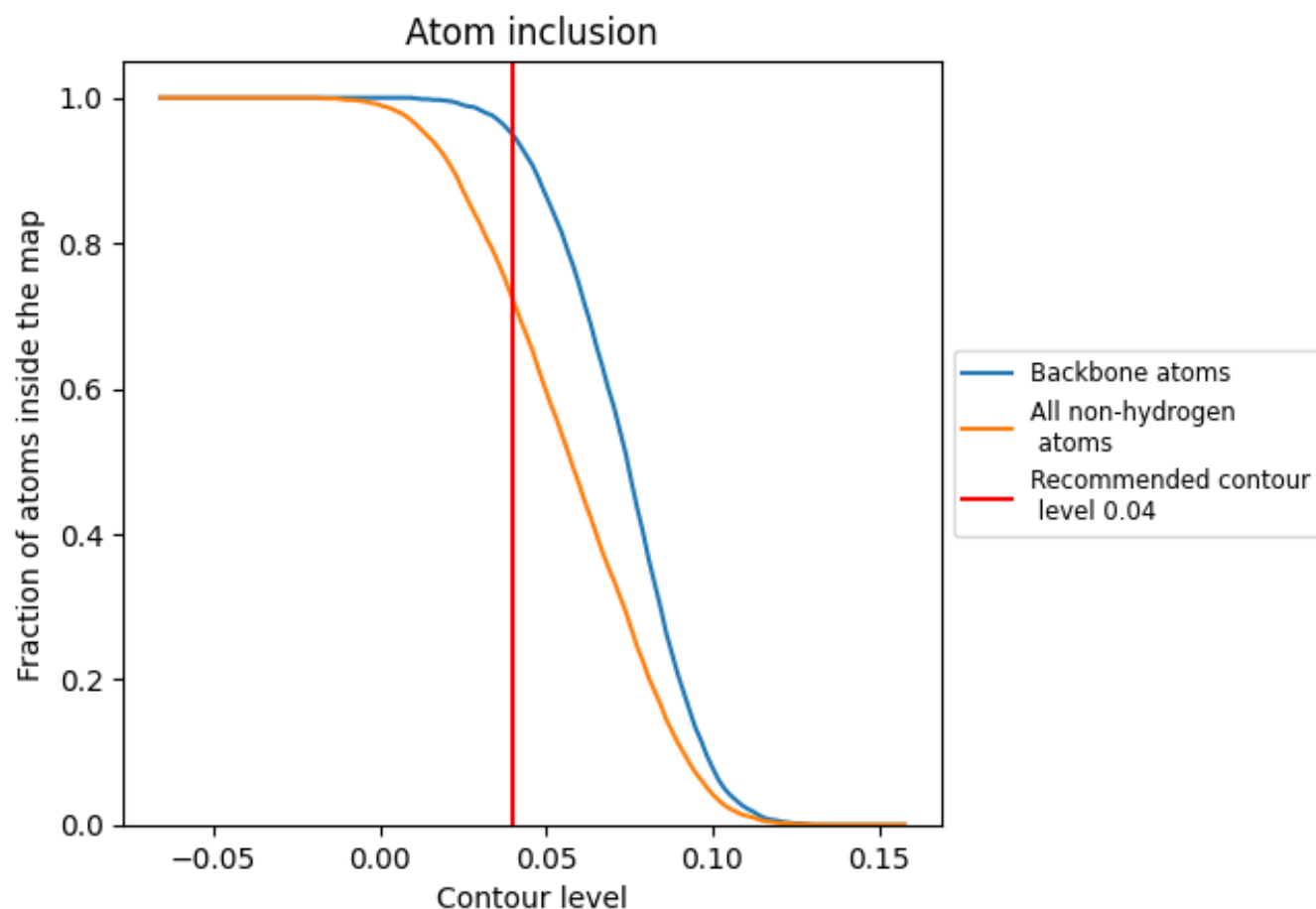
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 72% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.3330
A	0.7820	0.3630
B	0.6170	0.2990
C	0.6810	0.3080
D	0.6990	0.2930
G	0.4160	0.1890

