



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:01 AM UTC

PDB ID : 5FN5 / pdb_00005fn5
EMDB ID : EMD-3240
Title : Cryo-EM structure of gamma secretase in class 3 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 : 4.30 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:

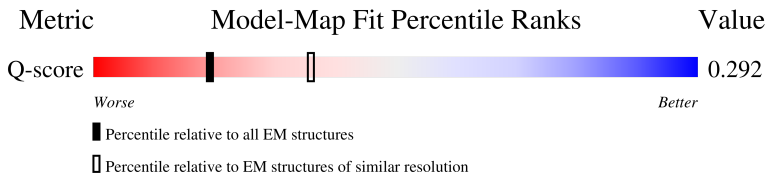
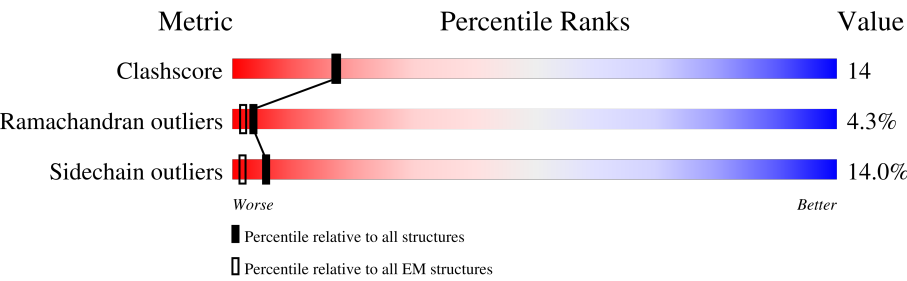
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.30 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	4585 (3.80 - 4.80)

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	 10% 62% 26% 5% • 6%
2	B	467	 23% 19% 6% 52%
3	C	265	 13% 54% 31% 6% • 8%
4	D	101	 14% 67% 25% • • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9645 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.

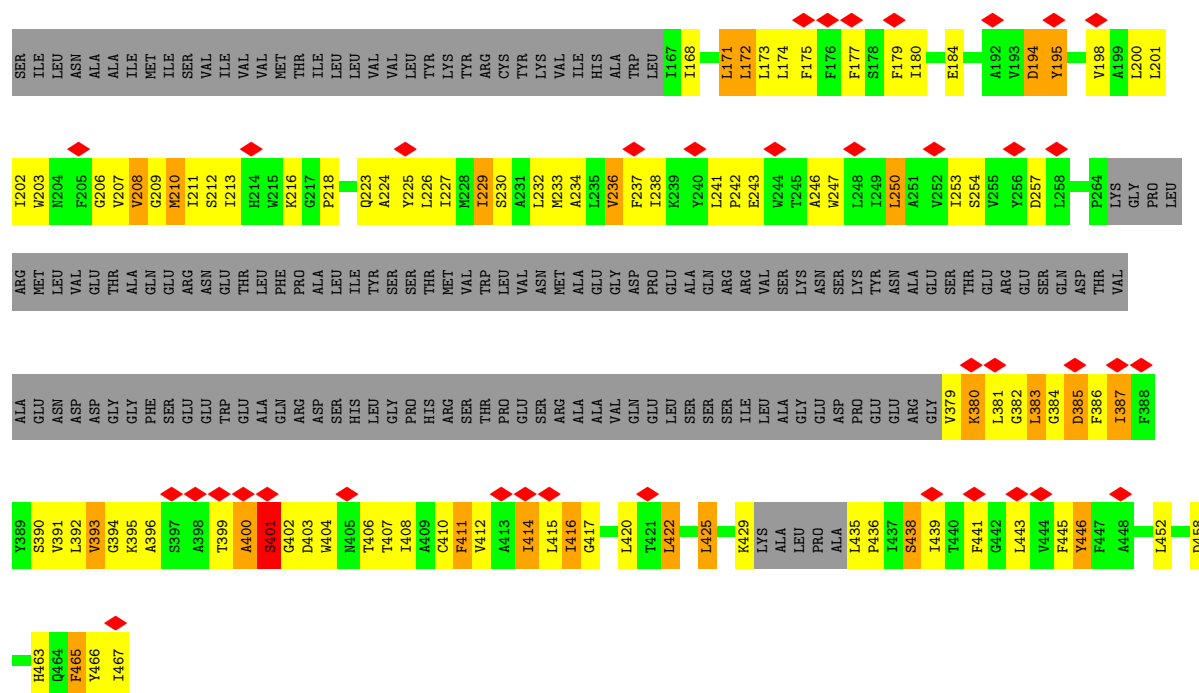
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	223	Total	C	N	O	S	0	0
			1735	1189	256	280	10		

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

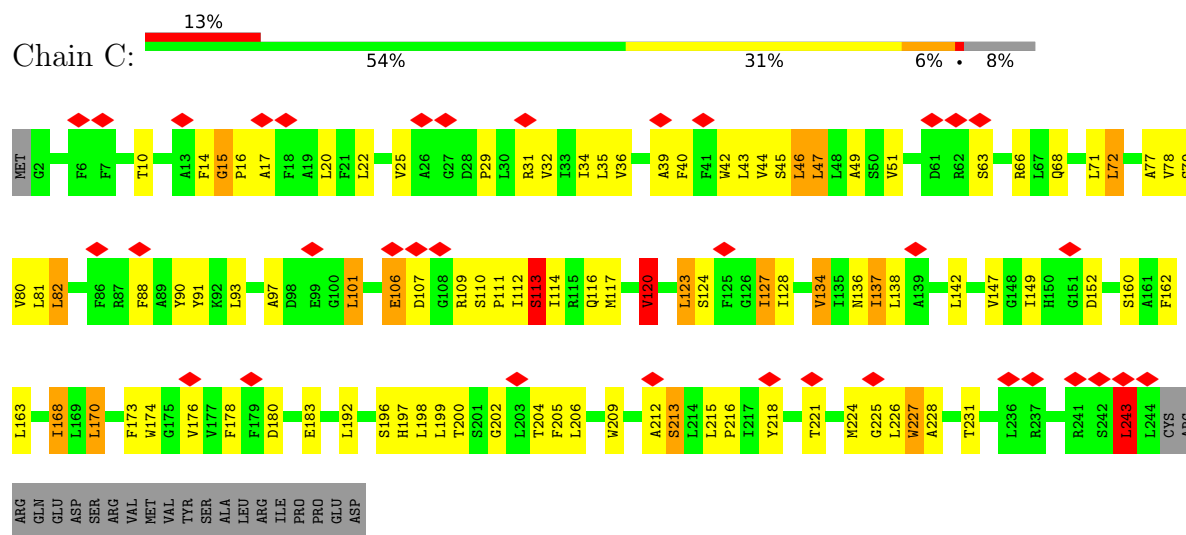
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1868	1252	299	313	4		

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

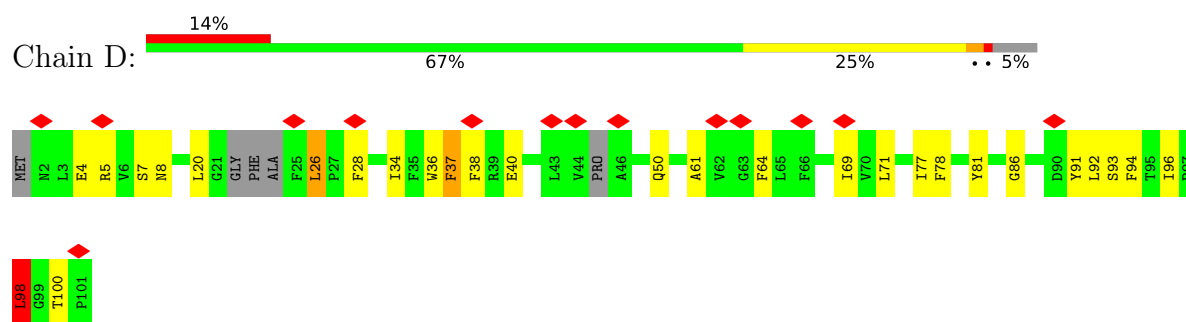
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			820	560	129	130	1		



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



• Molecule 4: Gamma-secretase subunit PEN-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66720	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	0.116	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	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	0.70	1/5345 (0.0%)	1.13	14/7284 (0.2%)
2	B	0.94	1/1780 (0.1%)	1.47	6/2430 (0.2%)
3	C	0.83	1/1920 (0.1%)	1.41	7/2619 (0.3%)
4	D	0.85	0/849	1.21	1/1155 (0.1%)
All	All	0.79	3/9894 (0.0%)	1.26	28/13488 (0.2%)

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	8
2	B	0	5
3	C	0	2
4	D	0	1
All	All	0	16

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SER	CA-C	6.30	1.61	1.52
3	C	243	LEU	N-CA	5.46	1.53	1.46
1	A	579	VAL	CA-C	5.43	1.58	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	120	VAL	N-CA-CB	7.66	119.51	110.55
1	A	547	GLY	N-CA-C	-7.44	102.37	112.57
2	B	400	ALA	N-CA-C	7.42	121.49	109.40
2	B	387	ILE	CB-CA-C	-7.11	102.87	111.97
1	A	92	PRO	N-CA-C	7.08	119.34	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	ILE	CB-CA-C	-6.65	103.46	111.97
1	A	91	ASN	CA-C-N	6.12	126.68	120.38
1	A	91	ASN	C-N-CA	6.12	126.68	120.38
1	A	239	THR	N-CA-C	6.04	123.67	110.80
1	A	644	GLU	N-CA-C	6.04	119.96	112.47
3	C	110	SER	N-CA-C	5.99	113.61	108.22
2	B	380	LYS	N-CA-C	5.80	118.36	108.90
3	C	199	LEU	CA-C-O	-5.77	114.43	120.55
1	A	302	PHE	N-CA-CB	5.73	118.64	110.16
1	A	218	PHE	N-CA-CB	5.67	120.07	110.49
1	A	199	HIS	N-CA-C	5.62	121.56	114.31
4	D	5	ARG	N-CA-C	-5.58	105.11	111.14
3	C	88	PHE	CA-C-O	5.53	126.63	120.82
1	A	210	PHE	N-CA-C	5.42	121.79	109.81
1	A	573	ASN	N-CA-CB	5.40	117.84	110.01
3	C	106	GLU	N-CA-C	5.37	116.99	111.03
1	A	162	ILE	N-CA-C	5.26	116.33	111.81
3	C	101	LEU	N-CA-C	5.22	117.38	111.11
1	A	436	ILE	N-CA-C	5.17	120.09	109.34
2	B	414	ILE	CB-CA-C	-5.10	105.44	111.97
2	B	208	VAL	CB-CA-C	5.09	120.51	112.26
3	C	43	LEU	CB-CA-C	-5.08	102.90	110.88
1	A	519	THR	N-CA-CB	5.03	117.30	110.01

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	VAL	Peptide
1	A	290	ASN	Peptide
1	A	472	SER	Peptide
1	A	49	PRO	Peptide
1	A	546	LEU	Peptide
1	A	612	ASN	Peptide
1	A	62	CYS	Peptide
1	A	646	SER	Peptide
2	B	106	TYR	Peptide
2	B	400	ALA	Peptide
2	B	401	SER	Peptide
2	B	402	GLY	Peptide
2	B	465	PHE	Peptide
3	C	113	SER	Peptide

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Mol	Chain	Res	Type	Group
3	C	213	SER	Peptide
4	D	4	GLU	Peptide

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	109	0
2	B	1735	0	1790	99	0
3	C	1868	0	1907	69	0
4	D	820	0	810	15	0
All	All	9645	0	9627	265	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 14.

All (265) 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)
2:B:452:LEU:HD13	3:C:51:VAL:HG22	1.43	0.97
2:B:441:PHE:O	2:B:445:PHE:HB3	1.67	0.95
2:B:241:LEU:HD23	2:B:246:ALA:HB3	1.51	0.89
1:A:529:ALA:HB1	1:A:546:LEU:HD22	1.54	0.87
1:A:73:ILE:HG21	1:A:660:ILE:HD11	1.60	0.80
3:C:170:LEU:HD22	3:C:221:THR:HG23	1.67	0.76
2:B:100:ILE:HD13	2:B:394:GLY:HA2	1.67	0.75
2:B:417:GLY:HA3	2:B:438:SER:HA	1.68	0.74
4:D:34:ILE:O	4:D:38:PHE:HB3	1.87	0.73
2:B:237:PHE:CD2	2:B:246:ALA:HB1	2.23	0.73
2:B:207:VAL:HG21	4:D:26:LEU:HD11	1.71	0.73
2:B:247:TRP:O	2:B:250:LEU:HG	1.89	0.73
2:B:416:ILE:HG12	3:C:40:PHE:HB2	1.70	0.71
3:C:34:ILE:O	3:C:90:TYR:OH	2.07	0.71
2:B:250:LEU:O	2:B:253:ILE:HG22	1.91	0.70
3:C:20:LEU:HD12	3:C:123:LEU:HD23	1.74	0.70
1:A:303:VAL:HG21	1:A:522:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:ILE:HA	3:C:117:MET:HE2	1.75	0.69
2:B:175:PHE:CE1	2:B:206:GLY:HA3	2.28	0.68
1:A:303:VAL:HG21	1:A:522:LEU:CD1	2.22	0.68
2:B:417:GLY:HA3	2:B:438:SER:CA	2.25	0.67
2:B:234:ALA:HA	2:B:391:VAL:HG22	1.77	0.67
2:B:168:ILE:HG23	2:B:171:LEU:HD13	1.78	0.66
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.77	0.65
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.79	0.65
2:B:233:MET:O	2:B:236:VAL:HG12	1.97	0.65
2:B:466:TYR:HB2	3:C:204:THR:HG21	1.77	0.64
3:C:47:LEU:O	3:C:51:VAL:HG23	1.97	0.64
1:A:303:VAL:HG11	1:A:522:LEU:HD13	1.80	0.64
1:A:182:LEU:HB2	1:A:288:PHE:CD2	2.33	0.64
2:B:411:PHE:HA	2:B:414:ILE:HD12	1.81	0.63
4:D:34:ILE:HD11	4:D:61:ALA:HA	1.80	0.63
3:C:20:LEU:HD12	3:C:123:LEU:CD2	2.28	0.63
1:A:121:LEU:HD21	1:A:178:PHE:CE1	2.34	0.63
2:B:387:ILE:O	2:B:391:VAL:HG23	1.99	0.63
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.80	0.62
2:B:210:MET:SD	2:B:210:MET:N	2.72	0.62
2:B:198:VAL:HG21	4:D:94:PHE:CD2	2.35	0.62
2:B:425:LEU:O	2:B:429:LYS:N	2.33	0.62
1:A:401:LEU:HD13	1:A:439:VAL:HG11	1.81	0.62
2:B:89:VAL:HA	2:B:386:PHE:CE1	2.35	0.61
3:C:116:GLN:O	3:C:120:VAL:HG13	2.00	0.61
1:A:299:VAL:O	1:A:303:VAL:HG23	2.00	0.61
2:B:226:LEU:HD13	2:B:380:LYS:HG3	1.82	0.61
1:A:36:VAL:HG21	3:C:137:ILE:HG22	1.83	0.61
2:B:91:LEU:HD12	2:B:92:CYS:N	2.16	0.60
1:A:223:ALA:HB2	1:A:247:VAL:HG22	1.82	0.60
2:B:237:PHE:O	2:B:241:LEU:HG	2.01	0.60
2:B:383:LEU:O	2:B:387:ILE:HG13	2.01	0.60
1:A:96:VAL:HG13	1:A:118:ILE:HD11	1.84	0.60
3:C:40:PHE:O	3:C:44:VAL:HG23	2.01	0.60
2:B:208:VAL:HG11	4:D:28:PHE:CD1	2.37	0.59
1:A:260:LEU:HD13	1:A:312:LEU:CD1	2.33	0.59
1:A:299:VAL:HA	1:A:302:PHE:CE2	2.36	0.59
1:A:368:VAL:HG11	1:A:490:VAL:HG11	1.84	0.59
2:B:436:PRO:HA	2:B:439:ILE:HD12	1.83	0.59
1:A:162:ILE:HD11	1:A:164:TRP:CD2	2.38	0.59
2:B:210:MET:HA	2:B:210:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:PHE:O	1:A:429:ARG:NH2	2.35	0.58
3:C:16:PRO:O	3:C:20:LEU:HG	2.04	0.58
1:A:375:GLU:HA	1:A:412:ILE:HG23	1.86	0.58
1:A:680:LEU:HD13	3:C:15:GLY:HA2	1.86	0.58
2:B:257:ASP:HB3	2:B:435:LEU:HD23	1.85	0.58
2:B:404:TRP:O	2:B:407:THR:HG22	2.04	0.58
2:B:84:MET:O	2:B:88:PRO:HD2	2.05	0.57
2:B:466:TYR:CE2	3:C:163:LEU:HB3	2.40	0.57
2:B:416:ILE:CG1	3:C:40:PHE:HB2	2.34	0.56
4:D:92:LEU:HD12	4:D:93:SER:N	2.21	0.56
2:B:441:PHE:O	2:B:445:PHE:CB	2.46	0.56
3:C:35:LEU:HA	3:C:124:SER:HB2	1.86	0.56
1:A:62:CYS:SG	1:A:180:ILE:HD12	2.46	0.56
2:B:177:PHE:HA	2:B:180:ILE:HD12	1.86	0.56
3:C:176:VAL:HG11	3:C:228:ALA:HB1	1.88	0.56
2:B:171:LEU:HD12	2:B:210:MET:CG	2.35	0.55
1:A:634:ALA:O	1:A:638:SER:N	2.40	0.55
2:B:171:LEU:HD12	2:B:210:MET:HG3	1.87	0.55
2:B:208:VAL:HG23	2:B:225:TYR:CZ	2.42	0.55
3:C:113:SER:OG	3:C:116:GLN:N	2.39	0.55
1:A:662:LEU:HD13	3:C:149:ILE:HB	1.89	0.55
2:B:92:CYS:HB3	2:B:386:PHE:CE1	2.41	0.55
2:B:403:ASP:O	2:B:404:TRP:C	2.50	0.55
2:B:96:VAL:O	2:B:100:ILE:HD12	2.07	0.55
1:A:40:ILE:CG1	3:C:147:VAL:HG22	2.37	0.54
2:B:175:PHE:CE2	2:B:203:TRP:HA	2.42	0.54
3:C:134:VAL:HG22	3:C:138:LEU:HB2	1.88	0.54
1:A:275:VAL:HG12	1:A:324:ASN:HB3	1.90	0.54
1:A:183:LEU:HD12	1:A:189:THR:HG22	1.88	0.54
2:B:218:PRO:HB3	4:D:36:TRP:CE2	2.42	0.54
3:C:174:TRP:O	3:C:178:PHE:N	2.41	0.54
2:B:466:TYR:CD1	3:C:163:LEU:HD23	2.41	0.54
3:C:173:PHE:CG	3:C:225:GLY:HA2	2.43	0.54
3:C:31:ARG:HA	3:C:34:ILE:HD12	1.90	0.54
1:A:480:VAL:HG12	1:A:519:THR:HG21	1.89	0.53
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.90	0.53
1:A:260:LEU:HD22	1:A:312:LEU:HD13	1.90	0.53
2:B:395:LYS:O	2:B:399:THR:HG23	2.09	0.53
3:C:42:TRP:CH2	3:C:46:LEU:HD13	2.44	0.53
3:C:17:ALA:HB1	3:C:127:ILE:HD11	1.90	0.53
1:A:257:TRP:CD1	1:A:326:MET:HE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:LEU:C	2:B:171:LEU:HD23	2.34	0.53
2:B:174:LEU:C	2:B:174:LEU:HD23	2.34	0.53
2:B:417:GLY:HA3	2:B:438:SER:CB	2.39	0.52
1:A:95:MET:HE1	1:A:217:LEU:HB2	1.91	0.52
2:B:82:VAL:HG11	2:B:422:LEU:HG	1.90	0.52
1:A:247:VAL:O	1:A:248:CYS:HB2	2.08	0.52
2:B:224:ALA:O	2:B:227:ILE:HG12	2.09	0.52
3:C:174:TRP:CH2	3:C:197:HIS:HA	2.44	0.52
2:B:390:SER:O	2:B:393:VAL:HG12	2.10	0.51
1:A:49:PRO:HB3	1:A:181:PHE:CZ	2.45	0.51
2:B:223:GLN:HA	2:B:226:LEU:HD12	1.91	0.51
3:C:127:ILE:HG22	3:C:128:ILE:N	2.25	0.51
1:A:385:GLN:O	1:A:391:ARG:HB2	2.10	0.51
1:A:280:THR:OG1	1:A:305:GLN:NE2	2.44	0.51
1:A:656:ILE:HD12	1:A:657:ARG:HA	1.92	0.51
2:B:241:LEU:HB2	2:B:242:PRO:C	2.36	0.51
3:C:35:LEU:O	3:C:124:SER:OG	2.26	0.51
1:A:425:SER:O	1:A:426:SER:C	2.54	0.50
3:C:173:PHE:CD1	3:C:225:GLY:HA2	2.47	0.50
1:A:456:ILE:HD12	1:A:456:ILE:N	2.26	0.50
3:C:227:TRP:O	3:C:231:THR:HG23	2.11	0.50
3:C:200:THR:O	3:C:204:THR:HG23	2.12	0.50
2:B:195:TYR:HA	4:D:94:PHE:HB2	1.93	0.49
3:C:39:ALA:N	3:C:124:SER:OG	2.45	0.49
1:A:338:ILE:HD12	1:A:339:GLY:N	2.27	0.49
3:C:106:GLU:N	3:C:107:ASP:HA	2.27	0.49
1:A:635:PHE:CZ	1:A:649:THR:HG23	2.47	0.49
2:B:385:ASP:OD1	2:B:385:ASP:N	2.46	0.49
2:B:207:VAL:HG11	4:D:26:LEU:HD21	1.94	0.49
2:B:225:TYR:O	2:B:229:ILE:HG12	2.13	0.49
3:C:176:VAL:CG1	3:C:228:ALA:HB1	2.43	0.49
1:A:200:ASN:O	1:A:201:LEU:HD13	2.13	0.49
1:A:282:LEU:HD12	1:A:302:PHE:CD2	2.48	0.49
2:B:173:LEU:HD23	2:B:173:LEU:C	2.38	0.48
2:B:381:LEU:H	2:B:382:GLY:HA3	1.76	0.48
2:B:241:LEU:HD22	2:B:243:GLU:O	2.13	0.48
1:A:108:MET:HE1	1:A:121:LEU:HD11	1.96	0.48
3:C:42:TRP:CE3	3:C:128:ILE:HG23	2.49	0.48
3:C:78:VAL:HG12	3:C:82:LEU:HD22	1.96	0.48
3:C:25:VAL:HG12	3:C:32:VAL:HG22	1.96	0.48
1:A:450:ASN:C	1:A:450:ASN:HD22	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:PHE:O	3:C:15:GLY:C	2.56	0.48
2:B:194:ASP:HB3	4:D:78:PHE:CZ	2.48	0.48
1:A:111:LEU:HD21	1:A:118:ILE:HD13	1.96	0.48
1:A:40:ILE:HG13	3:C:147:VAL:HG22	1.97	0.47
1:A:227:THR:HG21	1:A:647:THR:HB	1.95	0.47
2:B:89:VAL:HA	2:B:386:PHE:CZ	2.50	0.47
2:B:207:VAL:HG11	4:D:26:LEU:CD2	2.43	0.47
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.49	0.47
1:A:183:LEU:CD1	1:A:189:THR:HG22	2.45	0.47
1:A:555:ILE:HG22	1:A:555:ILE:O	2.15	0.47
3:C:170:LEU:HD22	3:C:221:THR:CG2	2.40	0.47
1:A:120:GLY:C	1:A:121:LEU:HD23	2.38	0.47
1:A:690:ILE:O	1:A:694:ALA:N	2.47	0.47
3:C:17:ALA:HB1	3:C:127:ILE:CD1	2.44	0.47
1:A:335:PHE:O	1:A:338:ILE:HG23	2.15	0.47
1:A:223:ALA:HB3	1:A:651:SER:HB2	1.97	0.47
2:B:103:VAL:HG11	2:B:106:TYR:CD2	2.49	0.47
1:A:86:LEU:O	1:A:117:ARG:NE	2.48	0.46
2:B:467:ILE:HD11	3:C:79:SER:OG	2.14	0.46
1:A:338:ILE:HG22	1:A:646:SER:OG	2.15	0.46
2:B:92:CYS:SG	2:B:230:SER:OG	2.69	0.46
2:B:465:PHE:CZ	3:C:72:LEU:HD22	2.50	0.46
3:C:136:ASN:N	3:C:136:ASN:HD22	2.14	0.46
3:C:215:LEU:N	3:C:216:PRO:CD	2.79	0.46
2:B:383:LEU:HD22	2:B:384:GLY:N	2.31	0.45
1:A:421:PRO:O	1:A:422:LEU:HB2	2.16	0.45
3:C:170:LEU:HD12	3:C:174:TRP:CE2	2.51	0.45
3:C:209:TRP:O	3:C:212:ALA:HB3	2.17	0.45
2:B:226:LEU:CD1	2:B:380:LYS:HG3	2.46	0.45
1:A:626:ARG:O	1:A:627:LEU:HD23	2.17	0.45
4:D:34:ILE:O	4:D:38:PHE:CB	2.62	0.45
1:A:84:TRP:CD1	1:A:85:VAL:N	2.85	0.45
1:A:182:LEU:HD22	1:A:288:PHE:CG	2.51	0.45
2:B:200:LEU:HD23	2:B:201:LEU:HD12	1.99	0.45
2:B:177:PHE:CE1	2:B:236:VAL:HG23	2.51	0.45
3:C:127:ILE:CG2	3:C:128:ILE:N	2.79	0.45
3:C:170:LEU:HD12	3:C:174:TRP:CZ2	2.51	0.44
1:A:212:LEU:O	1:A:662:LEU:HA	2.17	0.44
3:C:196:SER:O	3:C:200:THR:HG23	2.17	0.44
1:A:396:ASP:O	1:A:400:THR:HG23	2.17	0.44
1:A:260:LEU:HD13	1:A:312:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ILE:HD12	1:A:656:ILE:C	2.43	0.44
2:B:241:LEU:HD13	2:B:243:GLU:HA	2.00	0.44
1:A:363:VAL:HA	1:A:439:VAL:O	2.18	0.44
1:A:164:TRP:CZ2	1:A:423:PRO:HA	2.52	0.44
1:A:541:ASP:OD1	1:A:541:ASP:N	2.51	0.44
2:B:211:ILE:HD12	2:B:212:SER:N	2.32	0.44
2:B:224:ALA:HA	2:B:227:ILE:HG12	1.99	0.44
1:A:50:CYS:SG	1:A:180:ILE:HD12	2.58	0.44
1:A:280:THR:HG22	1:A:281:ARG:O	2.18	0.44
2:B:200:LEU:CD2	2:B:201:LEU:HD12	2.48	0.44
3:C:80:VAL:HG11	3:C:198:LEU:HG	1.99	0.44
1:A:631:LEU:HD23	1:A:635:PHE:HB2	1.99	0.43
4:D:98:LEU:O	4:D:100:THR:N	2.49	0.43
1:A:633:PRO:HG2	1:A:645:TYR:CD1	2.53	0.43
1:A:147:VAL:HG11	1:A:431:LEU:HB3	2.01	0.43
2:B:410:CYS:SG	2:B:446:TYR:HB2	2.59	0.43
1:A:182:LEU:HD22	1:A:288:PHE:CB	2.48	0.43
1:A:280:THR:HG21	1:A:302:PHE:HA	2.01	0.43
1:A:374:LEU:N	1:A:374:LEU:HD23	2.33	0.43
1:A:49:PRO:HB2	1:A:50:CYS:O	2.19	0.43
2:B:208:VAL:HA	2:B:211:ILE:HG13	2.00	0.43
2:B:254:SER:HB2	2:B:439:ILE:CD1	2.49	0.43
1:A:121:LEU:HD23	1:A:121:LEU:N	2.34	0.43
1:A:197:GLN:O	1:A:201:LEU:HD21	2.18	0.43
2:B:209:GLY:O	2:B:213:ILE:HG12	2.19	0.43
2:B:88:PRO:HA	2:B:91:LEU:HG	2.00	0.43
1:A:497:ALA:O	1:A:501:LEU:HD23	2.19	0.43
2:B:171:LEU:HD23	2:B:172:LEU:N	2.33	0.43
2:B:465:PHE:CG	3:C:205:PHE:HD1	2.37	0.43
4:D:77:ILE:O	4:D:81:TYR:N	2.46	0.43
1:A:223:ALA:HB2	1:A:247:VAL:CG2	2.48	0.43
1:A:247:VAL:HA	1:A:652:ARG:HG2	2.00	0.43
1:A:152:TYR:CE2	1:A:383:VAL:HG11	2.54	0.42
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.84	0.42
1:A:50:CYS:SG	1:A:62:CYS:N	2.91	0.42
1:A:422:LEU:C	1:A:422:LEU:HD23	2.43	0.42
1:A:258:SER:CB	1:A:571:LEU:HD21	2.49	0.42
2:B:416:ILE:CG1	3:C:40:PHE:CB	2.97	0.42
3:C:77:ALA:O	3:C:81:LEU:HG	2.19	0.42
2:B:403:ASP:O	2:B:406:THR:N	2.53	0.42
1:A:162:ILE:HD12	1:A:163:GLN:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:SER:O	1:A:595:GLU:C	2.63	0.42
2:B:80:LYS:O	2:B:83:ILE:HG22	2.19	0.42
1:A:200:ASN:C	1:A:201:LEU:HD22	2.45	0.42
1:A:578:VAL:HG22	1:A:579:VAL:H	1.85	0.42
3:C:80:VAL:HG13	3:C:197:HIS:CE1	2.54	0.42
1:A:299:VAL:HA	1:A:302:PHE:CZ	2.54	0.42
2:B:241:LEU:CD2	2:B:246:ALA:HB3	2.36	0.42
1:A:86:LEU:O	1:A:117:ARG:CD	2.68	0.41
1:A:323:ARG:HB2	1:A:502:ALA:HA	2.01	0.41
4:D:37:PHE:CD1	4:D:37:PHE:N	2.88	0.41
1:A:279:ALA:HA	1:A:328:VAL:HG13	2.00	0.41
1:A:282:LEU:HD22	1:A:329:PHE:CB	2.50	0.41
1:A:300:ALA:O	1:A:304:THR:HG23	2.20	0.41
1:A:397:LEU:O	1:A:400:THR:OG1	2.25	0.41
2:B:234:ALA:O	2:B:238:ILE:HD12	2.20	0.41
1:A:599:LEU:O	1:A:600:TYR:CD2	2.74	0.41
1:A:210:PHE:CG	1:A:665:SER:HB3	2.55	0.41
1:A:217:LEU:HD12	1:A:658:ALA:CB	2.51	0.41
1:A:264:ASN:HA	1:A:599:LEU:HG	2.01	0.41
2:B:247:TRP:CZ2	2:B:443:LEU:HD11	2.55	0.41
2:B:465:PHE:CE1	3:C:72:LEU:HD22	2.54	0.41
1:A:53:LEU:N	1:A:53:LEU:HD12	2.35	0.41
2:B:83:ILE:HG12	3:C:29:PRO:HB2	2.03	0.41
3:C:170:LEU:HG	3:C:174:TRP:CH2	2.56	0.41
1:A:415:ARG:HB3	1:A:416:PRO:HD2	2.02	0.41
2:B:92:CYS:HG	2:B:230:SER:HG	1.66	0.41
2:B:203:TRP:O	2:B:207:VAL:HG23	2.20	0.41
3:C:49:ALA:HB2	3:C:79:SER:HA	2.02	0.41
1:A:301:SER:O	1:A:304:THR:OG1	2.29	0.41
1:A:421:PRO:O	1:A:422:LEU:CB	2.69	0.40
1:A:426:SER:O	1:A:427:LEU:C	2.65	0.40
1:A:457:TYR:O	1:A:459:THR:N	2.54	0.40
2:B:396:ALA:O	2:B:399:THR:OG1	2.22	0.40
3:C:97:ALA:O	3:C:101:LEU:N	2.35	0.40
1:A:246:ILE:HG22	1:A:246:ILE:O	2.21	0.40
1:A:282:LEU:HD12	1:A:302:PHE:CG	2.56	0.40
1:A:480:VAL:HG12	1:A:519:THR:CG2	2.50	0.40
2:B:233:MET:HB3	2:B:387:ILE:HG21	2.03	0.40
2:B:463:HIS:CE1	3:C:72:LEU:HD11	2.56	0.40
3:C:10:THR:HB	3:C:138:LEU:HD21	2.02	0.40
2:B:379:VAL:HG12	2:B:380:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:TYR:CE1	3:C:163:LEU:HD23	2.56	0.40
3:C:202:GLY:HA2	3:C:205:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/709 (94%)	527 (80%)	96 (14%)	40 (6%)	1	13
2	B	215/467 (46%)	195 (91%)	17 (8%)	3 (1%)	9	39
3	C	241/265 (91%)	219 (91%)	17 (7%)	5 (2%)	5	30
4	D	90/101 (89%)	78 (87%)	8 (9%)	4 (4%)	2	17
All	All	1209/1542 (78%)	1019 (84%)	138 (11%)	52 (4%)	3	17

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	A	333	GLU
1	A	336	ASP
1	A	422	LEU
1	A	472	SER
1	A	632	SER
1	A	655	ASP
3	C	243	LEU
1	A	89	GLY
1	A	103	PHE
1	A	268	THR
1	A	289	TRP
1	A	436	ILE

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Mol	Chain	Res	Type
1	A	446	GLY
1	A	458	ASP
1	A	460	ALA
1	A	530	ASN
2	B	401	SER
3	C	15	GLY
3	C	111	PRO
1	A	239	THR
1	A	473	PRO
1	A	594	SER
1	A	631	LEU
2	B	216	LYS
3	C	213	SER
1	A	243	ASN
1	A	358	ASN
1	A	371	ARG
1	A	561	THR
1	A	646	SER
3	C	113	SER
4	D	20	LEU
4	D	86	GLY
1	A	225	ILE
1	A	316	PRO
1	A	559	SER
1	A	580	ASN
1	A	589	PRO
4	D	7	SER
1	A	257	TRP
1	A	421	PRO
1	A	451	LYS
2	B	102	SER
4	D	98	LEU
1	A	210	PHE
1	A	503	GLY
1	A	244	PRO
1	A	332	GLY
1	A	66	ILE
1	A	267	GLY
1	A	412	ILE

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%)	517 (89%)	66 (11%)	5	21
2	B	183/408 (45%)	149 (81%)	34 (19%)	1	10
3	C	192/214 (90%)	157 (82%)	35 (18%)	2	10
4	D	85/89 (96%)	74 (87%)	11 (13%)	4	17
All	All	1043/1323 (79%)	897 (86%)	146 (14%)	5	15

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	50	CYS
1	A	64	SER
1	A	69	ASP
1	A	70	THR
1	A	84	TRP
1	A	86	LEU
1	A	107	LEU
1	A	111	LEU
1	A	114	ARG
1	A	121	LEU
1	A	129	SER
1	A	139	GLN
1	A	177	SER
1	A	180	ILE
1	A	190	LYS
1	A	197	GLN
1	A	201	LEU
1	A	202	SER
1	A	231	MET
1	A	233	ARG
1	A	237	GLN
1	A	250	PRO
1	A	256	VAL

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Mol	Chain	Res	Type
1	A	264	ASN
1	A	269	LEU
1	A	296	GLU
1	A	333	GLU
1	A	343	MET
1	A	344	VAL
1	A	370	LEU
1	A	374	LEU
1	A	391	ARG
1	A	396	ASP
1	A	425	SER
1	A	437	SER
1	A	464	ASN
1	A	472	SER
1	A	487	LEU
1	A	512	GLN
1	A	520	ARG
1	A	522	LEU
1	A	537	ILE
1	A	539	ARG
1	A	541	ASP
1	A	551	LEU
1	A	561	THR
1	A	566	VAL
1	A	574	LEU
1	A	586	CYS
1	A	587	GLN
1	A	604	TRP
1	A	605	VAL
1	A	610	HIS
1	A	624	THR
1	A	631	LEU
1	A	636	GLU
1	A	637	LEU
1	A	638	SER
1	A	643	THR
1	A	644	GLU
1	A	649	THR
1	A	659	ARG
1	A	666	LYS
1	A	677	PHE
1	A	698	PHE

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Mol	Chain	Res	Type
2	B	81	HIS
2	B	83	ILE
2	B	89	VAL
2	B	91	LEU
2	B	93	MET
2	B	99	THR
2	B	101	LYS
2	B	105	PHE
2	B	171	LEU
2	B	172	LEU
2	B	179	PHE
2	B	184	GLU
2	B	194	ASP
2	B	195	TYR
2	B	202	ILE
2	B	210	MET
2	B	232	LEU
2	B	236	VAL
2	B	250	LEU
2	B	383	LEU
2	B	385	ASP
2	B	392	LEU
2	B	393	VAL
2	B	408	ILE
2	B	411	PHE
2	B	412	VAL
2	B	415	LEU
2	B	416	ILE
2	B	420	LEU
2	B	422	LEU
2	B	425	LEU
2	B	438	SER
2	B	446	TYR
2	B	458	ASP
3	C	22	LEU
3	C	36	VAL
3	C	45	SER
3	C	46	LEU
3	C	47	LEU
3	C	63	SER
3	C	66	ARG
3	C	68	GLN

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Mol	Chain	Res	Type
3	C	71	LEU
3	C	72	LEU
3	C	82	LEU
3	C	91	TYR
3	C	93	LEU
3	C	109	ARG
3	C	112	ILE
3	C	120	VAL
3	C	123	LEU
3	C	127	ILE
3	C	134	VAL
3	C	137	ILE
3	C	142	LEU
3	C	152	ASP
3	C	160	SER
3	C	162	PHE
3	C	168	ILE
3	C	170	LEU
3	C	180	ASP
3	C	183	GLU
3	C	192	LEU
3	C	206	LEU
3	C	218	TYR
3	C	224	MET
3	C	226	LEU
3	C	227	TRP
3	C	243	LEU
4	D	8	ASN
4	D	26	LEU
4	D	37	PHE
4	D	40	GLU
4	D	50	GLN
4	D	64	PHE
4	D	69	ILE
4	D	71	LEU
4	D	91	TYR
4	D	96	ILE
4	D	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	83	GLN
1	A	102	HIS
1	A	139	GLN
1	A	142	ASN
1	A	150	ASN
1	A	163	GLN
1	A	222	HIS
1	A	331	GLN
1	A	428	GLN
1	A	444	HIS
1	A	450	ASN
1	A	454	GLN
1	A	462	ASN
1	A	506	ASN
1	A	531	ASN
1	A	535	GLN
1	A	568	GLN
1	A	580	ASN
1	A	596	ASN
2	B	222	GLN
2	B	223	GLN
3	C	136	ASN
3	C	171	HIS
4	D	50	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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.

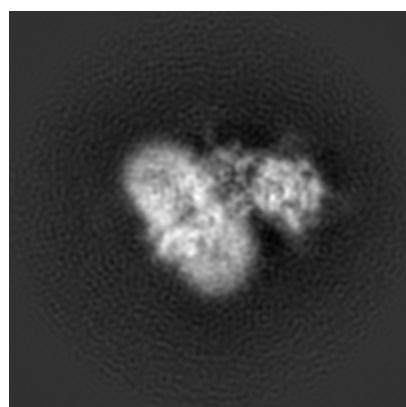
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3240. These allow visual inspection of the internal detail of the map and identification of artifacts.

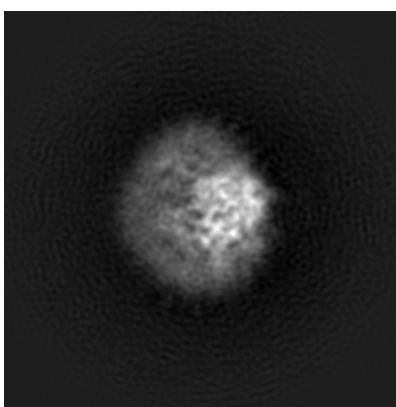
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

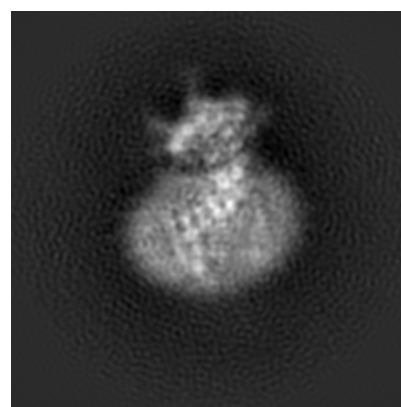
6.1.1 Primary map



X



Y

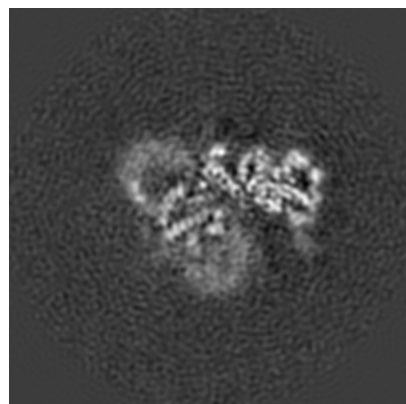


Z

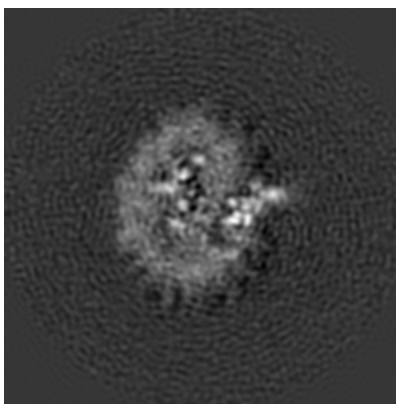
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

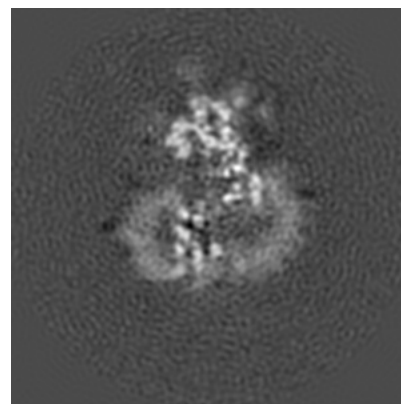
6.2.1 Primary map



X Index: 90



Y Index: 90

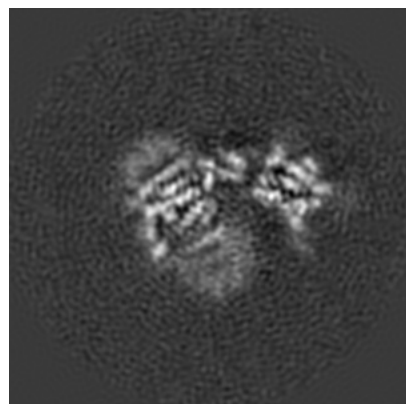


Z Index: 90

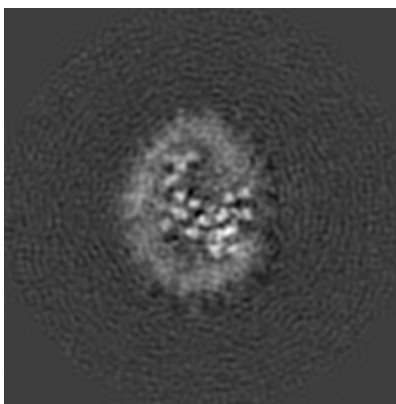
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

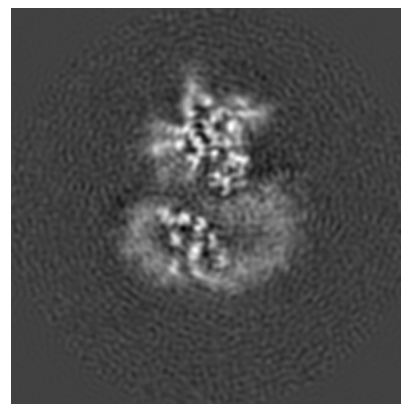
6.3.1 Primary map



X Index: 84



Y Index: 84

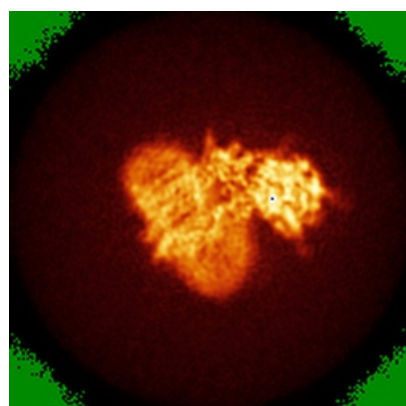


Z Index: 96

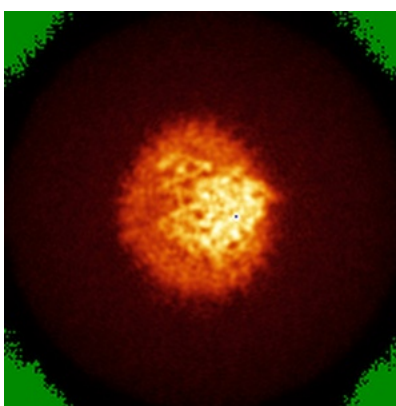
The images above show the largest variance slices of the map in three orthogonal directions.

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

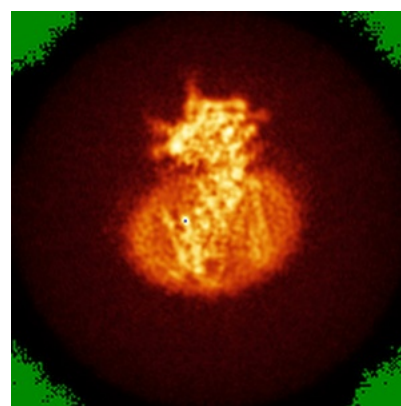
6.4.1 Primary map



X



Y

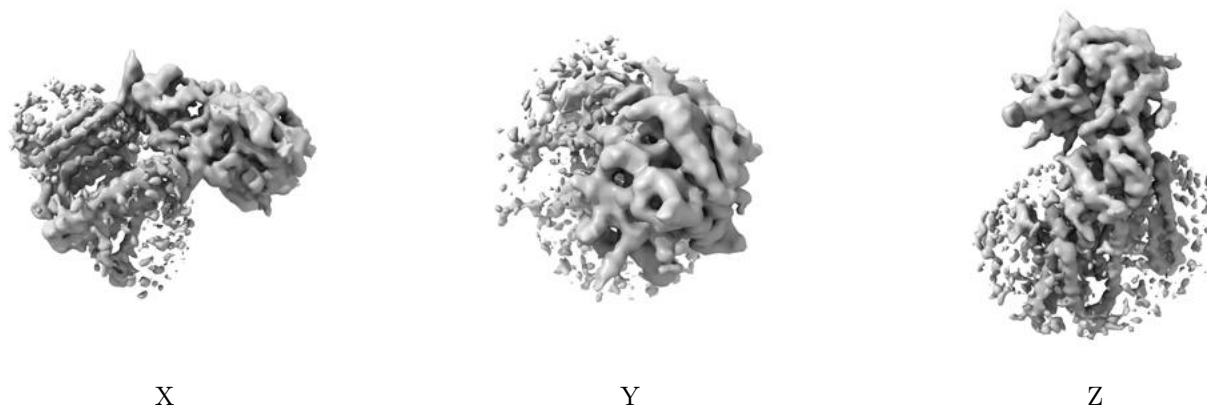


Z

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.

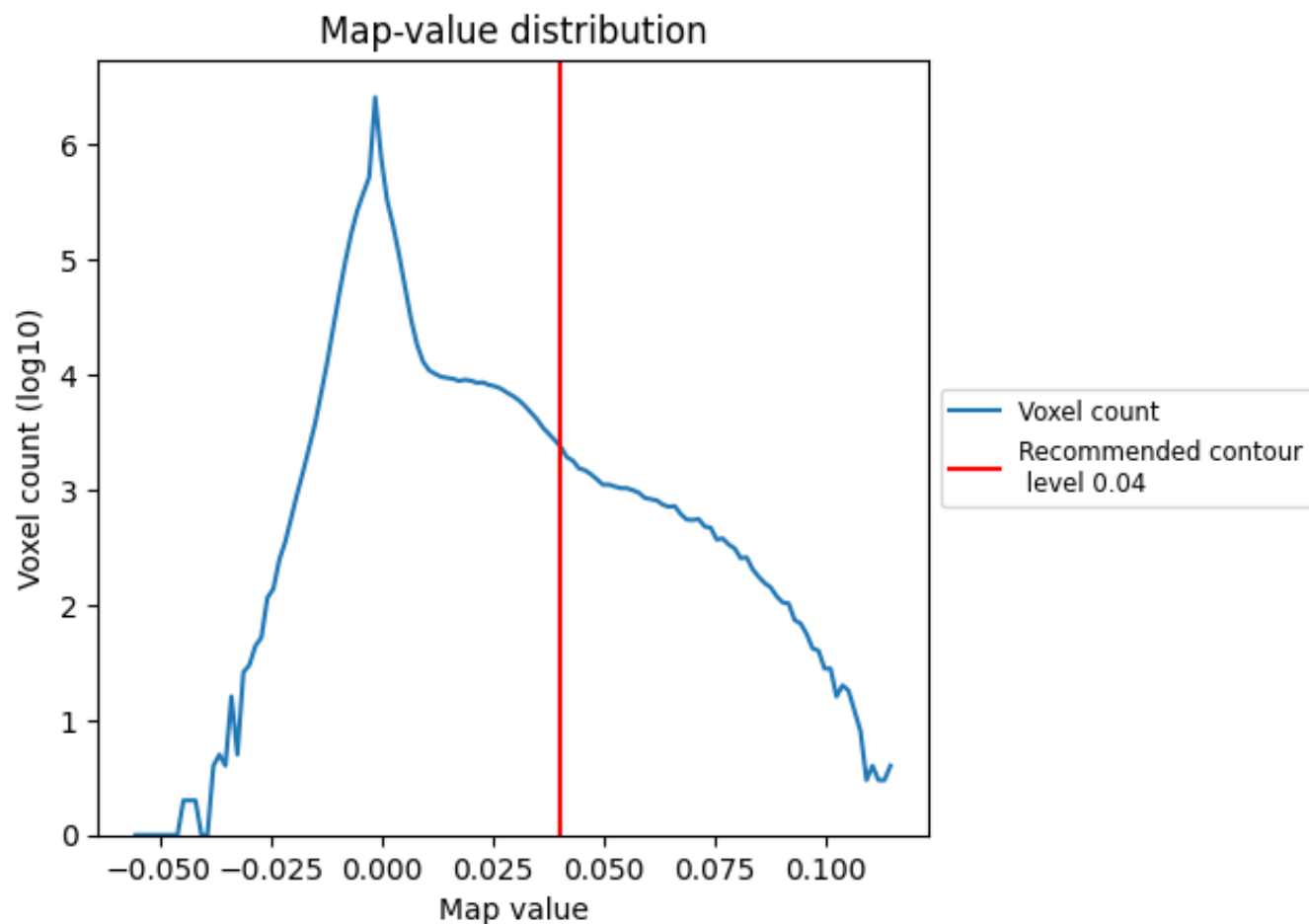
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

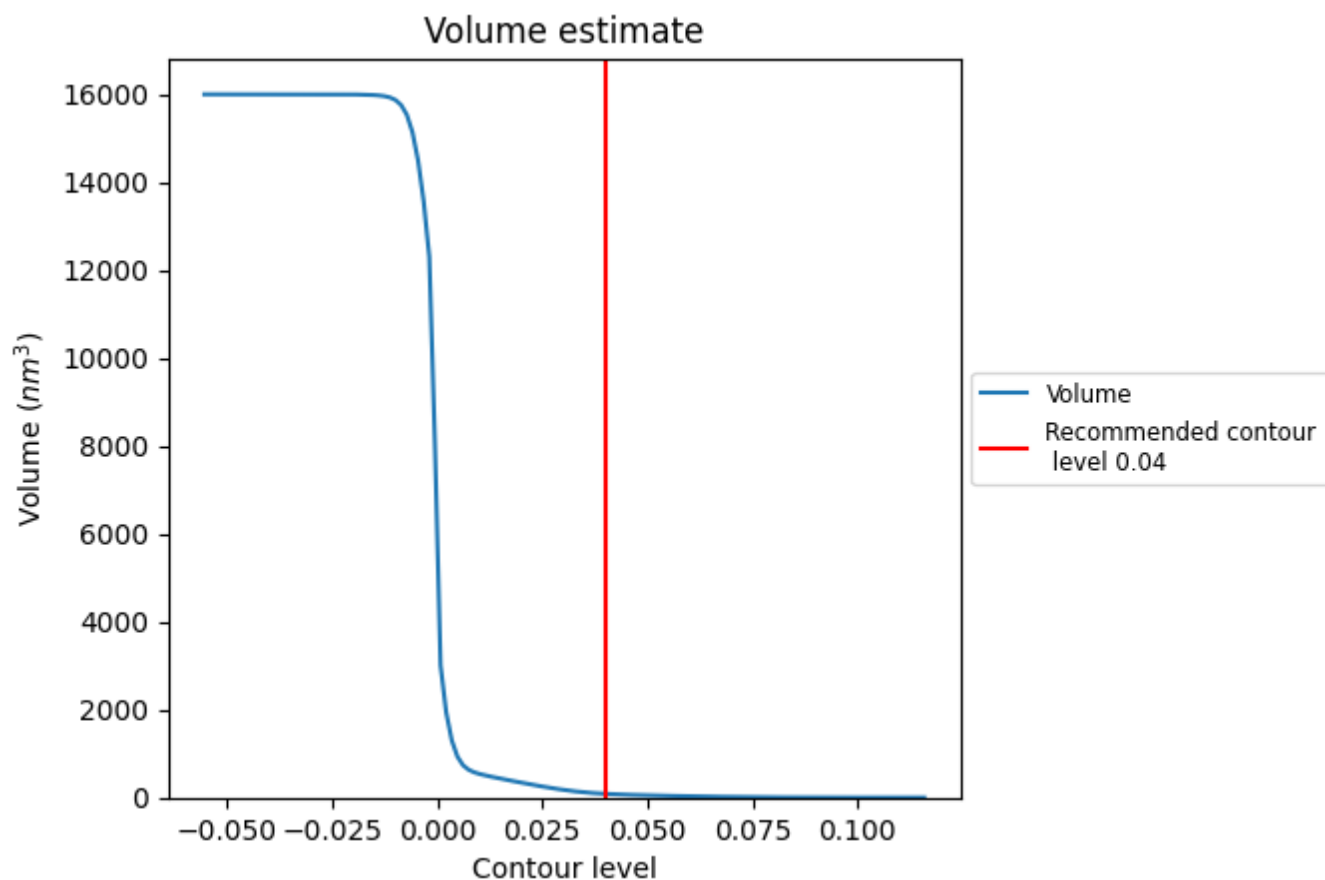
This section contains the results of statistical analysis of the map.

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.

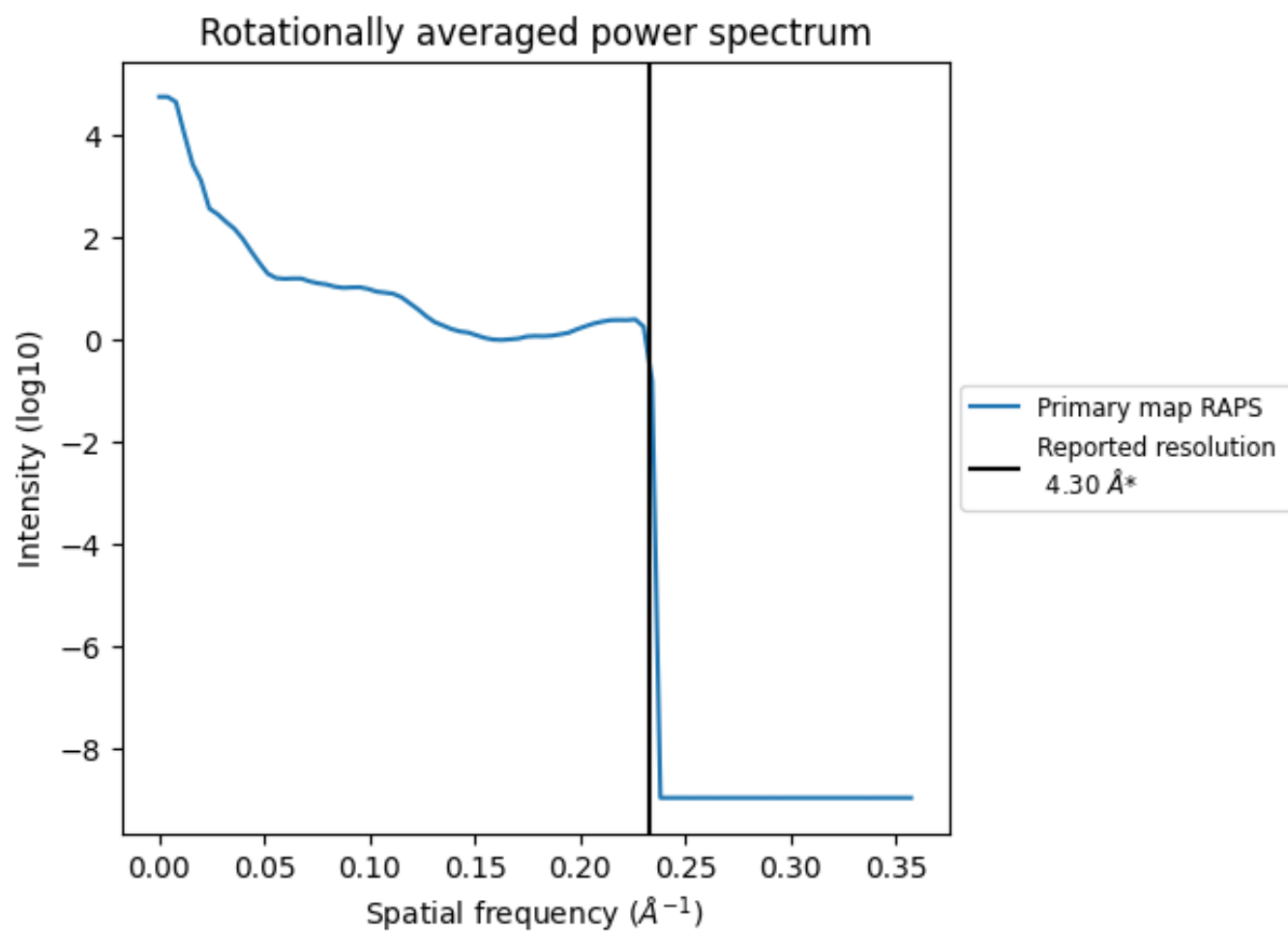
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm^3 ; this corresponds to an approximate mass of 77 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 0.233 Å⁻¹

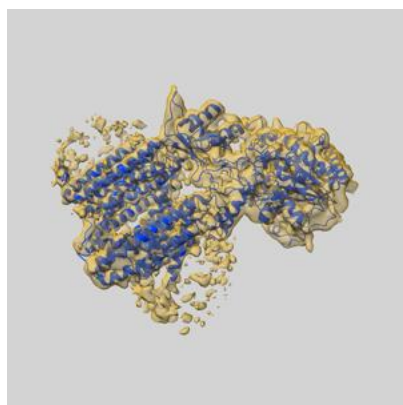
8 Fourier-Shell correlation ⓘ

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

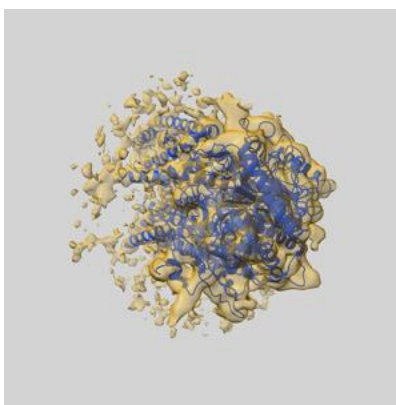
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3240 and PDB model 5FN5. Per-residue inclusion information can be found in section [3](#) on page [4](#).

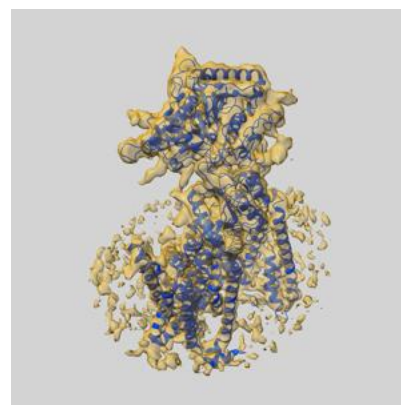
9.1 Map-model overlay [i](#)



X



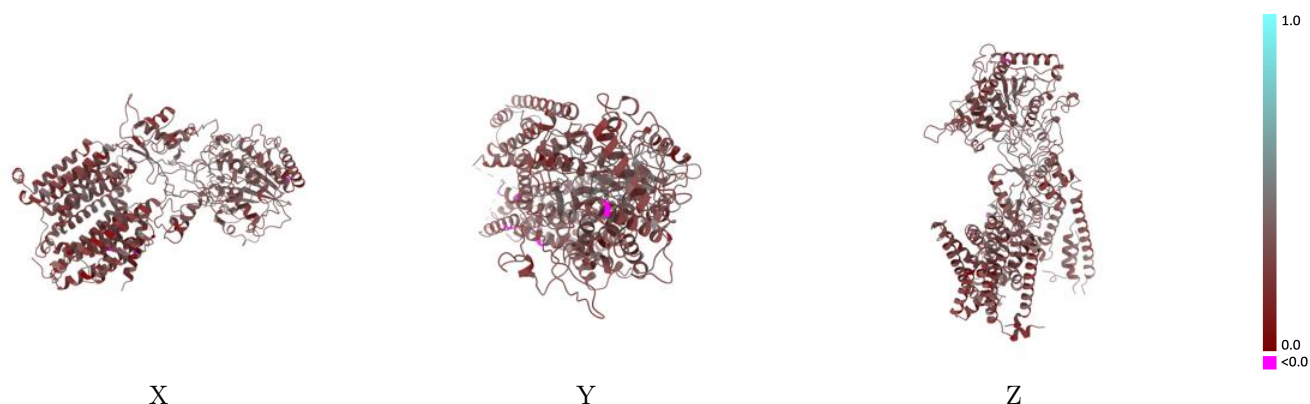
Y



Z

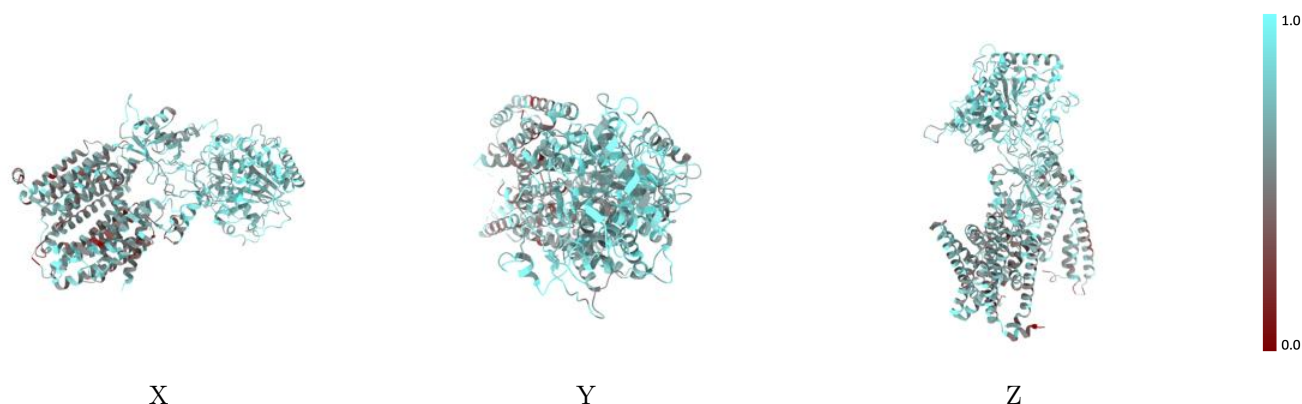
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



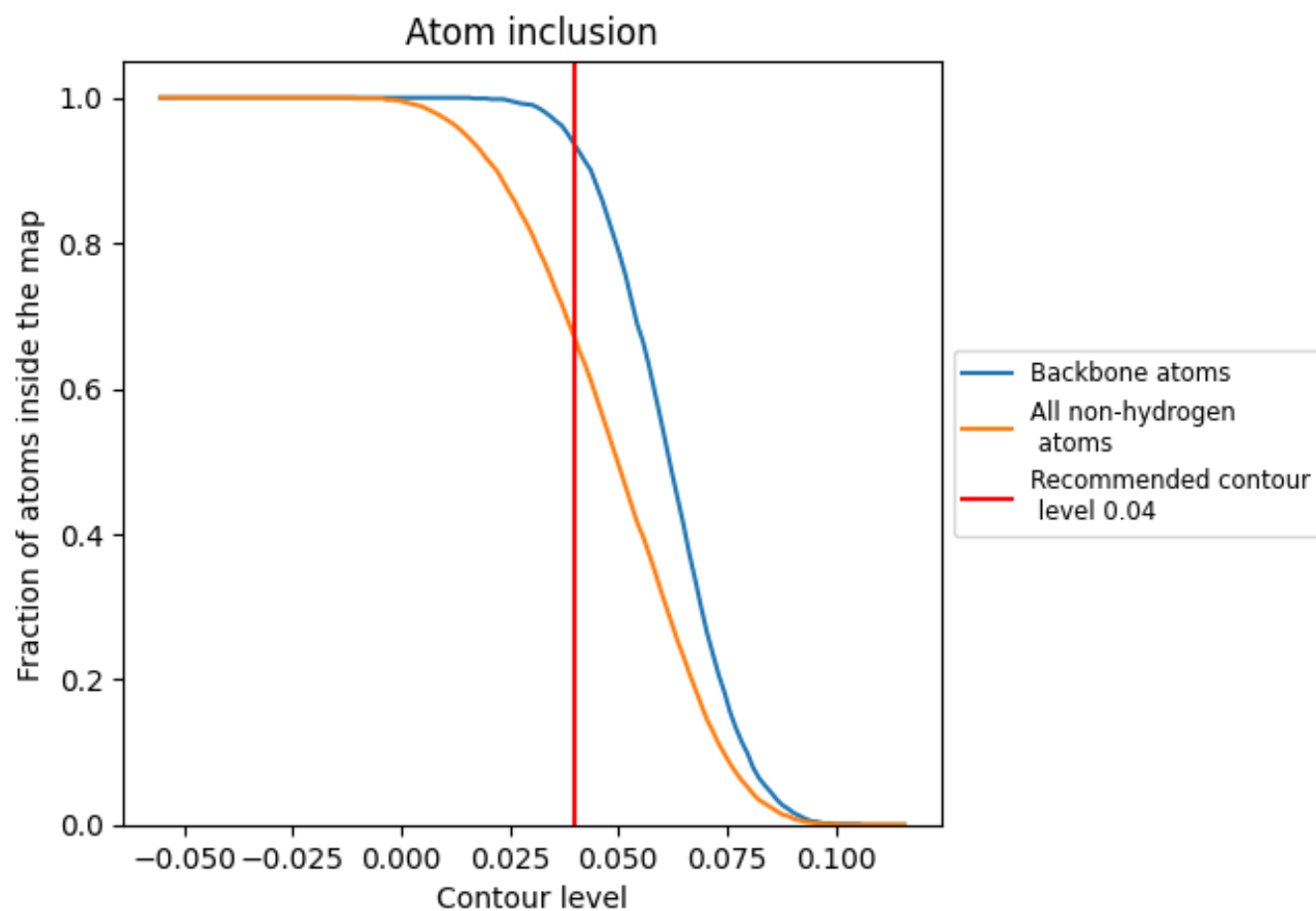
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 67% 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	0.6690	0.2920
A	0.7410	0.3170
B	0.5580	0.2600
C	0.5990	0.2610
D	0.6080	0.2740

