



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:13 AM UTC

PDB ID : 5FN3 / pdb_00005fn3
EMDB ID : EMD-3238
Title : Cryo-EM structure of gamma secretase in class 1 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 : 4.10 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:

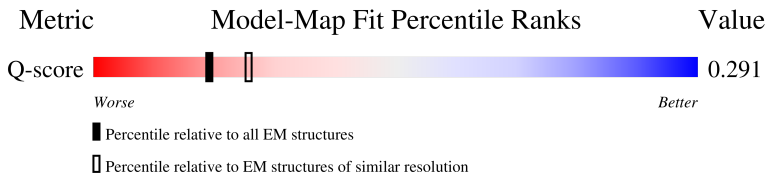
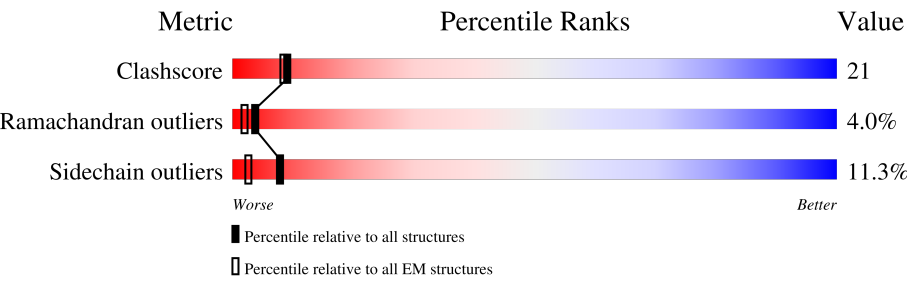
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.10 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	6458 (3.60 - 4.60)

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	12% 68% 21% 5% 6%
2	B	467	12% 27% 24% 8% 39%
3	C	265	12% 61% 26% 8%
4	D	101	8% 79% 19%

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Mol	Chain	Length	Quality of chain
5	G	24	63% 38% 33% 21% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10291 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	286	Total	C	N	O	S	0	0
			2234	1523	335	363	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	256	THR	TYR	conflict	UNP P49768

- 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		

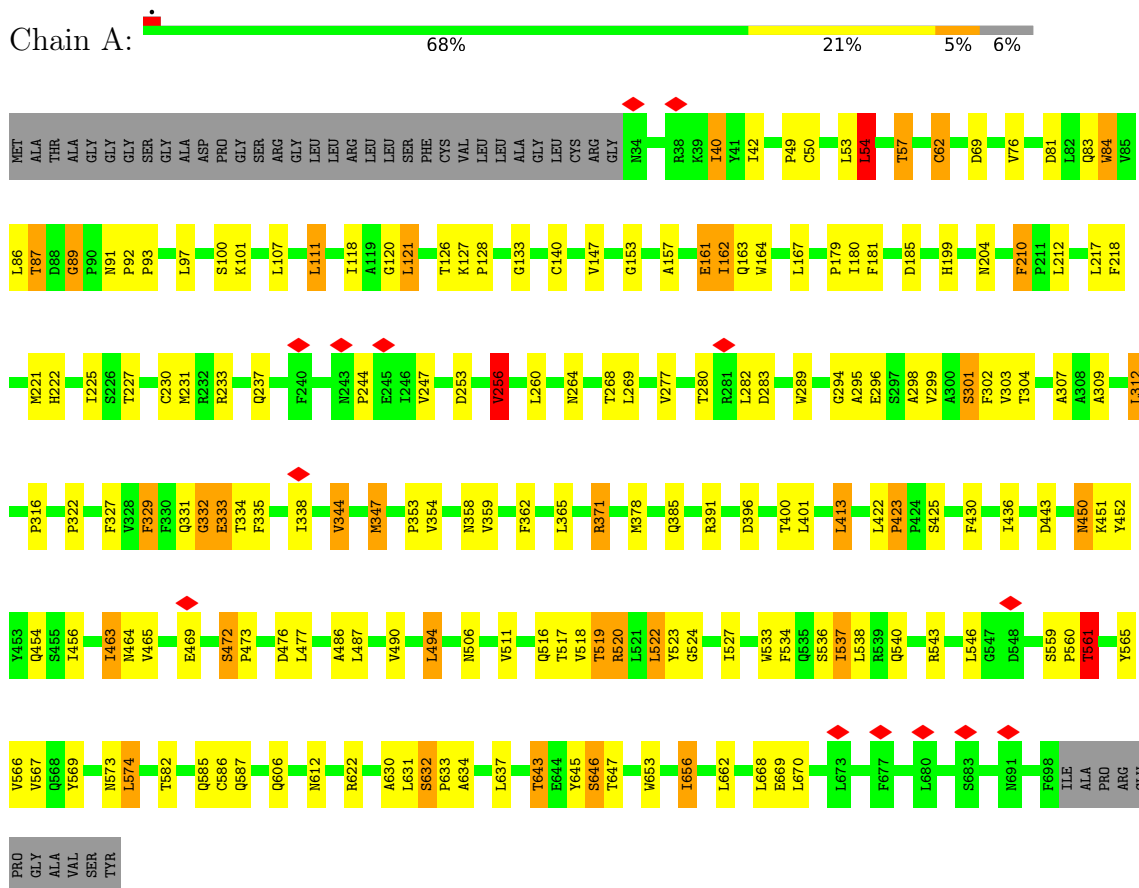
- Molecule 5 is a protein called POLY ALA CHAIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	24	Total	C	N	O	0	0
			120	72	24	24		

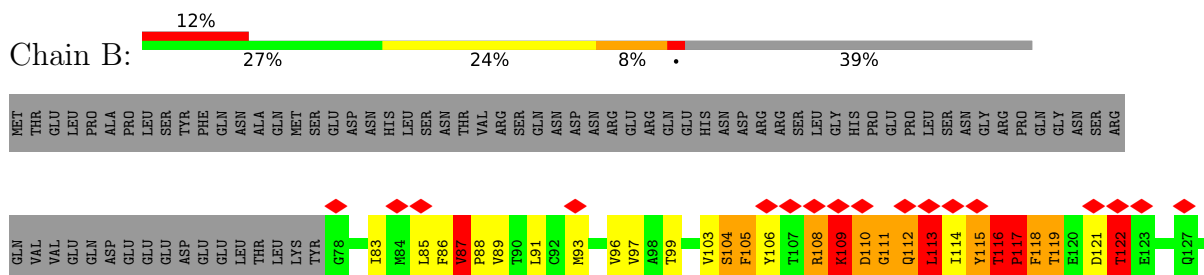
3 Residue-property plots

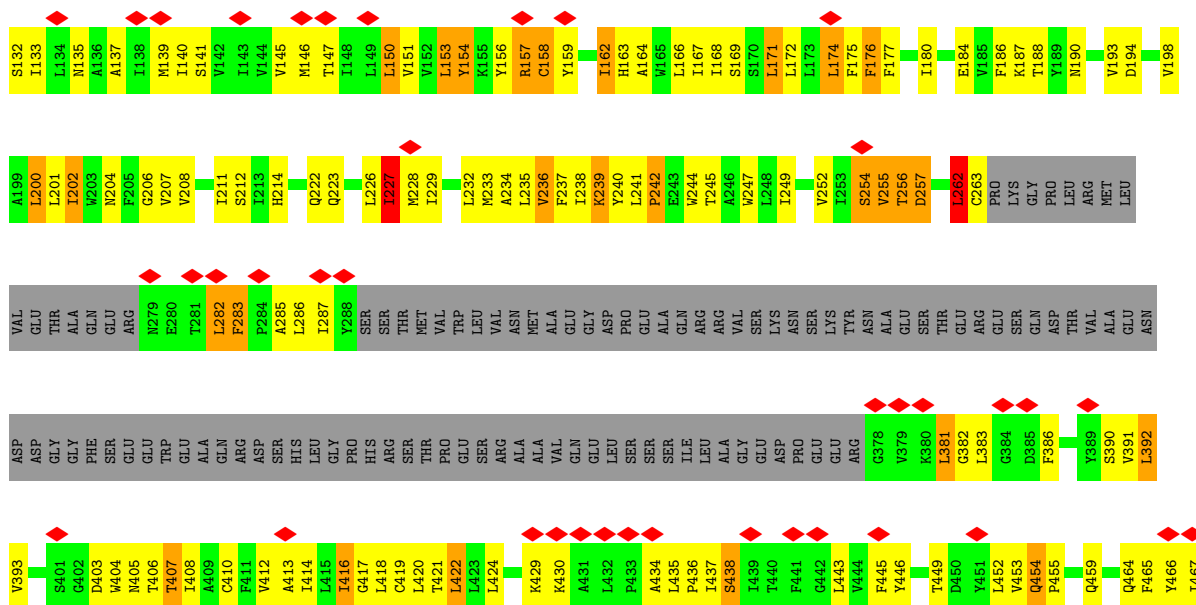
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

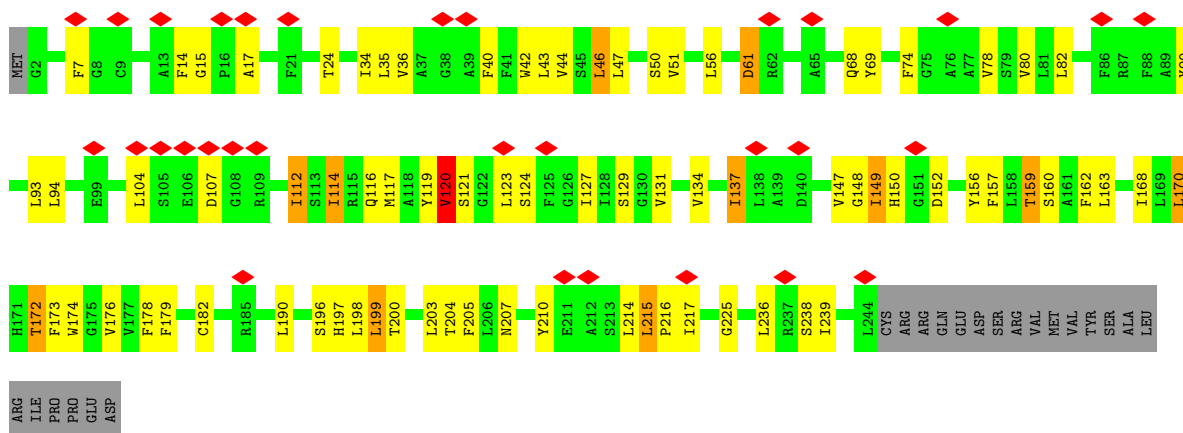


• Molecule 2: Presenilin-1

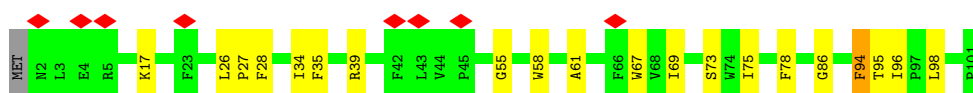
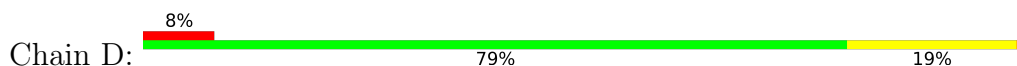




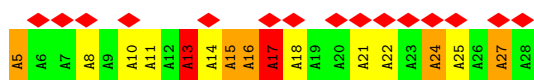
• Molecule 3: Gamma-secretase subunit APH-1A



• 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	63873	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	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	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	0.68	0/5345	1.12	15/7284 (0.2%)
2	B	0.84	2/2291 (0.1%)	1.42	14/3130 (0.4%)
3	C	0.79	0/1920	1.39	3/2619 (0.1%)
4	D	0.71	0/880	1.17	0/1201
5	G	0.47	0/119	0.96	1/165 (0.6%)
All	All	0.74	2/10555 (0.0%)	1.24	33/14399 (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	5
2	B	0	15
5	G	0	8
All	All	0	28

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	122	THR	CA-C	5.94	1.60	1.52
2	B	262	LEU	CA-C	5.03	1.59	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASN	CA-C-N	10.13	130.82	120.38
1	A	91	ASN	C-N-CA	10.13	130.82	120.38
1	A	92	PRO	N-CA-C	8.87	121.52	110.70
2	B	256	THR	CB-CA-C	-8.30	97.85	110.88
2	B	117	PRO	CA-N-CD	-7.38	101.66	112.00
1	A	162	ILE	N-CA-C	7.34	118.12	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLY	CA-C-N	7.09	126.62	119.24
1	A	153	GLY	C-N-CA	7.09	126.62	119.24
1	A	573	ASN	N-CA-CB	6.72	119.76	110.01
2	B	116	THR	CA-C-N	-6.59	111.61	119.84
2	B	116	THR	C-N-CA	-6.59	111.61	119.84
2	B	255	VAL	N-CA-CB	6.26	117.88	110.55
3	C	69	TYR	CA-CB-CG	6.21	125.07	113.90
3	C	199	LEU	CA-C-O	-6.12	114.06	120.55
2	B	87	VAL	O-C-N	6.05	124.29	120.42
2	B	454	GLN	O-C-N	5.83	126.09	120.55
2	B	157	ARG	N-CA-C	5.78	118.64	109.96
3	C	120	VAL	N-CA-CB	5.77	118.39	110.54
1	A	256	VAL	N-CA-C	-5.75	103.79	110.05
1	A	199	HIS	N-CA-C	5.69	120.75	113.18
2	B	227	ILE	N-CA-CB	5.62	118.19	110.54
1	A	669	GLU	CB-CA-C	-5.52	102.21	110.88
2	B	176	PHE	N-CA-C	-5.38	104.46	111.02
2	B	214	HIS	N-CA-C	5.26	119.17	112.12
2	B	262	LEU	CA-C-N	5.24	131.13	121.70
2	B	262	LEU	C-N-CA	5.24	131.13	121.70
5	G	17	ALA	CB-CA-C	-5.23	110.52	116.54
1	A	519	THR	N-CA-CB	5.13	117.45	110.01
1	A	423	PRO	N-CA-C	5.12	116.95	110.70
2	B	256	THR	N-CA-CB	5.11	117.42	110.01
1	A	574	LEU	N-CA-C	5.04	116.46	110.97
1	A	54	LEU	N-CA-C	5.03	116.84	109.24
1	A	40	ILE	N-CA-C	5.01	119.76	109.34

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	VAL	Peptide
1	A	335	PHE	Peptide
1	A	57	THR	Peptide
1	A	62	CYS	Peptide
1	A	622	ARG	Peptide
2	B	108	ARG	Peptide
2	B	109	LYS	Peptide
2	B	110	ASP	Peptide
2	B	111	GLY	Peptide
2	B	112	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	113	LEU	Peptide
2	B	115	TYR	Peptide
2	B	116	THR	Peptide
2	B	117	PRO	Peptide
2	B	118	PHE	Peptide
2	B	156	TYR	Peptide
2	B	157	ARG	Peptide
2	B	242	PRO	Peptide
2	B	283	PHE	Peptide
2	B	86	PHE	Peptide
5	G	13	ALA	Peptide
5	G	14	ALA	Peptide
5	G	15	ALA	Peptide
5	G	16	ALA	Peptide
5	G	17	ALA	Peptide
5	G	24	ALA	Peptide
5	G	27	ALA	Peptide
5	G	5	ALA	Peptide

5.2 Too-close contacts [i](#)

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	95	0
2	B	2234	0	2344	268	0
3	C	1868	0	1907	57	0
4	D	847	0	836	11	0
5	G	120	0	119	58	0
All	All	10291	0	10326	425	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 21.

All (425) 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)
5:G:15:ALA:C	5:G:17:ALA:HB3	1.31	1.47
2:B:146:MET:HE1	5:G:25:ALA:N	1.50	1.27
2:B:112:GLN:CD	5:G:15:ALA:HB2	1.61	1.25
5:G:15:ALA:O	5:G:17:ALA:CB	1.89	1.19
2:B:146:MET:CE	5:G:25:ALA:H	1.56	1.18
5:G:15:ALA:O	5:G:17:ALA:HB3	0.98	1.16
5:G:15:ALA:C	5:G:17:ALA:CB	2.17	1.16
2:B:139:MET:CE	5:G:22:ALA:HB1	1.81	1.10
2:B:108:ARG:HG3	2:B:109:LYS:HB3	1.20	1.09
2:B:233:MET:HE3	2:B:237:PHE:HZ	1.21	1.06
2:B:109:LYS:HG3	2:B:110:ASP:HB2	1.39	1.03
2:B:108:ARG:O	2:B:239:LYS:NZ	1.90	1.03
2:B:146:MET:CE	5:G:25:ALA:HB3	1.91	1.00
2:B:117:PRO:CD	2:B:135:ASN:HB2	1.90	1.00
2:B:117:PRO:HD3	2:B:135:ASN:HB2	1.47	0.97
5:G:11:ALA:O	5:G:16:ALA:HB2	1.64	0.97
2:B:108:ARG:CG	2:B:109:LYS:HB3	1.97	0.93
5:G:17:ALA:HB3	5:G:18:ALA:HB2	1.47	0.93
2:B:139:MET:HE1	5:G:22:ALA:HB1	1.47	0.93
2:B:118:PHE:HB2	2:B:135:ASN:HB3	1.49	0.93
2:B:116:THR:HB	2:B:118:PHE:CE2	2.05	0.92
2:B:242:PRO:HD2	2:B:245:THR:HB	1.52	0.92
5:G:17:ALA:HB3	5:G:18:ALA:CB	1.96	0.92
2:B:233:MET:HG2	2:B:237:PHE:HE2	1.34	0.91
2:B:108:ARG:HG3	2:B:109:LYS:CB	2.01	0.90
2:B:146:MET:HE1	5:G:25:ALA:H	0.76	0.90
2:B:169:SER:OG	5:G:24:ALA:HB1	1.72	0.89
2:B:132:SER:HA	2:B:135:ASN:ND2	1.88	0.89
2:B:109:LYS:HB2	2:B:110:ASP:CG	1.99	0.88
2:B:117:PRO:CG	2:B:135:ASN:HB2	2.04	0.87
2:B:113:LEU:HD23	2:B:113:LEU:H	1.39	0.87
2:B:106:TYR:HA	2:B:239:LYS:HD2	1.58	0.86
2:B:112:GLN:OE1	5:G:15:ALA:HB2	1.75	0.85
2:B:139:MET:HE1	5:G:22:ALA:CB	2.05	0.85
2:B:112:GLN:CG	5:G:15:ALA:HB2	2.06	0.85
2:B:113:LEU:HD12	2:B:116:THR:HA	1.60	0.83
2:B:108:ARG:O	2:B:109:LYS:HG2	1.78	0.83
2:B:85:LEU:HD22	2:B:418:LEU:HD21	1.59	0.83
2:B:233:MET:HG2	2:B:237:PHE:CE2	2.13	0.83
2:B:392:LEU:HD22	2:B:414:ILE:HD11	1.60	0.82
2:B:106:TYR:HA	2:B:239:LYS:CD	2.10	0.81
2:B:169:SER:OG	5:G:24:ALA:CB	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:PRO:HA	2:B:118:PHE:HB2	1.63	0.80
2:B:233:MET:HE3	2:B:237:PHE:CZ	2.11	0.80
2:B:117:PRO:HA	2:B:135:ASN:CB	2.12	0.79
2:B:116:THR:HG22	2:B:118:PHE:N	1.97	0.79
2:B:146:MET:CE	5:G:25:ALA:CB	2.59	0.79
2:B:113:LEU:HA	2:B:114:ILE:O	1.82	0.79
2:B:232:LEU:O	2:B:236:VAL:HG23	1.83	0.78
2:B:114:ILE:CB	2:B:115:TYR:HA	2.14	0.77
2:B:146:MET:HE3	5:G:25:ALA:HB3	1.66	0.77
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.66	0.77
2:B:177:PHE:CE2	5:G:21:ALA:HB2	2.21	0.76
2:B:105:PHE:C	2:B:239:LYS:HE2	2.11	0.75
2:B:113:LEU:HB3	2:B:116:THR:O	1.86	0.75
2:B:112:GLN:CG	5:G:15:ALA:CB	2.64	0.75
2:B:146:MET:HE1	5:G:25:ALA:CA	2.17	0.74
2:B:146:MET:HE1	5:G:25:ALA:CB	2.17	0.74
2:B:132:SER:HA	2:B:135:ASN:HD21	1.53	0.74
2:B:163:HIS:O	2:B:167:ILE:N	2.19	0.73
2:B:112:GLN:CD	5:G:15:ALA:CB	2.54	0.73
2:B:113:LEU:CD1	2:B:116:THR:HG23	2.19	0.73
2:B:108:ARG:NE	2:B:109:LYS:HB3	2.03	0.73
2:B:117:PRO:HA	2:B:135:ASN:HB2	1.70	0.73
2:B:105:PHE:CG	2:B:239:LYS:HE2	2.23	0.72
2:B:174:LEU:HG	2:B:229:ILE:HD11	1.70	0.72
2:B:113:LEU:H	2:B:113:LEU:CD2	2.01	0.72
2:B:113:LEU:HD12	2:B:116:THR:HG23	1.71	0.72
2:B:117:PRO:CA	2:B:135:ASN:HB2	2.19	0.72
2:B:113:LEU:CD1	2:B:116:THR:HA	2.19	0.71
1:A:256:VAL:HG21	1:A:567:VAL:HG12	1.72	0.71
2:B:237:PHE:HA	2:B:241:LEU:HD13	1.73	0.70
2:B:237:PHE:CA	2:B:241:LEU:HD13	2.21	0.70
2:B:240:TYR:HE2	5:G:15:ALA:HB1	1.55	0.70
2:B:116:THR:HG22	2:B:118:PHE:H	1.56	0.70
2:B:105:PHE:CZ	2:B:239:LYS:HE3	2.27	0.70
2:B:242:PRO:HD2	2:B:245:THR:CB	2.21	0.70
2:B:118:PHE:CB	2:B:135:ASN:HB3	2.21	0.69
2:B:139:MET:HE3	5:G:22:ALA:HB1	1.75	0.69
2:B:105:PHE:CE2	2:B:239:LYS:HD3	2.28	0.69
2:B:139:MET:CE	5:G:22:ALA:CB	2.62	0.69
2:B:112:GLN:HB2	2:B:113:LEU:C	2.18	0.69
2:B:237:PHE:O	2:B:241:LEU:HD13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ARG:HG3	2:B:109:LYS:HD3	1.76	0.68
2:B:113:LEU:HD23	2:B:113:LEU:N	2.07	0.68
2:B:146:MET:CE	5:G:25:ALA:N	2.33	0.68
2:B:283:PHE:HZ	5:G:27:ALA:O	1.77	0.68
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.76	0.68
2:B:285:ALA:HB2	2:B:383:LEU:HB2	1.76	0.67
2:B:177:PHE:HE2	5:G:21:ALA:HB2	1.58	0.67
2:B:116:THR:HB	2:B:118:PHE:CD2	2.29	0.67
1:A:162:ILE:HD11	1:A:164:TRP:CD2	2.29	0.67
1:A:299:VAL:HA	1:A:302:PHE:CE2	2.29	0.67
2:B:112:GLN:HB2	2:B:114:ILE:N	2.10	0.67
1:A:378:MET:HE3	1:A:413:LEU:HD22	1.76	0.67
2:B:177:PHE:HE2	5:G:21:ALA:CB	2.08	0.66
2:B:238:ILE:HD11	2:B:391:VAL:O	1.96	0.66
2:B:233:MET:CE	2:B:237:PHE:HZ	2.04	0.66
2:B:137:ALA:HA	2:B:140:ILE:HD12	1.79	0.65
2:B:105:PHE:CE1	2:B:239:LYS:HE3	2.32	0.65
2:B:177:PHE:CE2	5:G:21:ALA:CB	2.80	0.65
2:B:150:LEU:O	2:B:153:LEU:HG	1.96	0.65
2:B:233:MET:O	2:B:236:VAL:HB	1.97	0.64
2:B:153:LEU:HD13	2:B:162:ILE:HG13	1.80	0.63
1:A:260:LEU:HD22	1:A:312:LEU:HD13	1.81	0.63
2:B:117:PRO:HD3	2:B:135:ASN:CB	2.27	0.62
2:B:207:VAL:HB	4:D:26:LEU:HD21	1.82	0.62
3:C:170:LEU:HG	3:C:174:TRP:CZ2	2.35	0.61
5:G:5:ALA:O	5:G:8:ALA:N	2.34	0.61
2:B:150:LEU:HD22	2:B:153:LEU:HD21	1.82	0.61
2:B:240:TYR:HE2	5:G:15:ALA:CB	2.14	0.61
2:B:108:ARG:C	2:B:109:LYS:HG2	2.25	0.61
2:B:435:LEU:N	2:B:436:PRO:HD2	2.16	0.60
2:B:163:HIS:O	2:B:167:ILE:HG23	2.01	0.60
3:C:40:PHE:O	3:C:44:VAL:HG23	2.02	0.60
2:B:113:LEU:HA	2:B:114:ILE:C	2.26	0.60
2:B:121:ASP:O	2:B:122:THR:OG1	2.17	0.59
2:B:175:PHE:CE1	2:B:206:GLY:HA3	2.37	0.59
2:B:116:THR:CG2	2:B:118:PHE:CD2	2.85	0.59
1:A:120:GLY:C	1:A:121:LEU:HD23	2.27	0.59
5:G:16:ALA:C	5:G:18:ALA:HB3	2.28	0.59
2:B:240:TYR:CE2	5:G:15:ALA:HB1	2.35	0.59
2:B:153:LEU:HD22	2:B:162:ILE:HG23	1.84	0.59
3:C:116:GLN:O	3:C:120:VAL:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:16:ALA:N	5:G:17:ALA:CB	2.64	0.59
1:A:280:THR:HG21	1:A:302:PHE:HA	1.84	0.58
2:B:105:PHE:CD2	2:B:239:LYS:CE	2.86	0.58
2:B:105:PHE:CD2	2:B:239:LYS:HE2	2.38	0.58
2:B:283:PHE:CZ	5:G:27:ALA:O	2.57	0.58
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.85	0.58
2:B:198:VAL:HG21	4:D:94:PHE:CE2	2.38	0.58
1:A:40:ILE:CG1	3:C:147:VAL:HG22	2.33	0.58
2:B:108:ARG:CD	2:B:109:LYS:HB3	2.33	0.58
2:B:117:PRO:N	2:B:118:PHE:HD2	2.03	0.57
3:C:35:LEU:O	3:C:124:SER:HB2	2.04	0.57
2:B:252:VAL:O	2:B:256:THR:HG23	2.04	0.57
5:G:5:ALA:O	5:G:8:ALA:HB3	2.04	0.57
2:B:233:MET:CG	2:B:237:PHE:CE2	2.85	0.57
2:B:237:PHE:HB3	2:B:241:LEU:HD22	1.86	0.57
1:A:516:GLN:O	1:A:519:THR:HG22	2.04	0.56
2:B:237:PHE:O	2:B:241:LEU:HB2	2.04	0.56
2:B:85:LEU:HD13	2:B:422:LEU:HD23	1.88	0.56
2:B:146:MET:CE	5:G:25:ALA:CA	2.81	0.56
2:B:151:VAL:O	2:B:154:TYR:HD1	1.89	0.56
1:A:371:ARG:NH2	1:A:486:ALA:HB1	2.20	0.55
2:B:112:GLN:OE1	2:B:240:TYR:CE2	2.59	0.55
2:B:116:THR:CB	2:B:118:PHE:CE2	2.85	0.55
2:B:111:GLY:CA	2:B:240:TYR:CD2	2.89	0.55
5:G:11:ALA:C	5:G:16:ALA:HB2	2.30	0.55
1:A:662:LEU:HD22	3:C:148:GLY:HA3	1.88	0.55
2:B:252:VAL:O	2:B:255:VAL:HG22	2.07	0.55
2:B:223:GLN:O	2:B:227:ILE:HG23	2.07	0.55
2:B:105:PHE:CE2	2:B:239:LYS:CD	2.89	0.55
2:B:105:PHE:CD2	2:B:239:LYS:HD3	2.41	0.55
2:B:118:PHE:O	2:B:119:THR:OG1	2.24	0.55
2:B:112:GLN:HG2	5:G:15:ALA:CB	2.37	0.55
2:B:240:TYR:OH	5:G:15:ALA:HA	2.07	0.55
2:B:237:PHE:C	2:B:241:LEU:HD13	2.32	0.55
1:A:303:VAL:HG11	1:A:522:LEU:HD13	1.88	0.55
1:A:534:PHE:CE2	1:A:566:VAL:HG11	2.42	0.55
2:B:445:PHE:O	2:B:449:THR:OG1	2.24	0.55
1:A:164:TRP:CH2	1:A:423:PRO:HA	2.42	0.54
2:B:93:MET:O	2:B:97:VAL:HG23	2.06	0.54
1:A:53:LEU:O	1:A:54:LEU:HD23	2.07	0.54
3:C:42:TRP:CH2	3:C:46:LEU:HD12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:10:ALA:O	5:G:13:ALA:HB3	2.07	0.54
2:B:115:TYR:O	2:B:116:THR:OG1	2.26	0.54
1:A:40:ILE:HG12	3:C:147:VAL:HG22	1.90	0.54
1:A:233:ARG:HD3	4:D:96:ILE:HG21	1.89	0.54
2:B:117:PRO:HG3	2:B:135:ASN:HB2	1.85	0.54
2:B:158:CYS:HB2	2:B:162:ILE:HG12	1.89	0.54
2:B:109:LYS:CG	2:B:110:ASP:HB2	2.25	0.53
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.90	0.53
2:B:117:PRO:CD	2:B:118:PHE:HD2	2.20	0.53
2:B:141:SER:O	2:B:145:VAL:HG23	2.08	0.53
2:B:108:ARG:CZ	2:B:109:LYS:HA	2.37	0.53
3:C:134:VAL:O	3:C:137:ILE:HG13	2.08	0.53
1:A:309:ALA:HA	1:A:327:PHE:CZ	2.43	0.53
2:B:112:GLN:N	2:B:113:LEU:HA	2.24	0.53
2:B:113:LEU:CD1	2:B:116:THR:CG2	2.86	0.53
3:C:200:THR:O	3:C:204:THR:HG23	2.08	0.53
2:B:162:ILE:N	2:B:162:ILE:HD13	2.23	0.53
2:B:105:PHE:CE2	2:B:239:LYS:CE	2.91	0.52
2:B:234:ALA:HA	2:B:391:VAL:HG22	1.91	0.52
2:B:236:VAL:O	2:B:239:LYS:HB3	2.09	0.52
1:A:49:PRO:HB3	1:A:181:PHE:CZ	2.45	0.52
1:A:62:CYS:SG	1:A:180:ILE:HD12	2.49	0.52
3:C:24:THR:HG21	3:C:119:TYR:CE1	2.44	0.52
1:A:222:HIS:HB2	1:A:247:VAL:HG23	1.91	0.52
2:B:233:MET:CE	2:B:237:PHE:CZ	2.86	0.52
1:A:299:VAL:O	1:A:303:VAL:HG23	2.09	0.52
1:A:540:GLN:HA	1:A:606:GLN:HE21	1.74	0.52
2:B:166:LEU:HD11	2:B:282:LEU:HB2	1.92	0.52
2:B:256:THR:OG1	2:B:257:ASP:N	2.42	0.52
2:B:99:THR:CG2	2:B:235:LEU:HD21	2.40	0.52
2:B:464:GLN:O	3:C:207:ASN:ND2	2.42	0.52
1:A:303:VAL:HG21	1:A:522:LEU:CD1	2.41	0.51
1:A:347:MET:SD	1:A:354:VAL:O	2.68	0.51
1:A:538:LEU:HD11	1:A:546:LEU:HD11	1.92	0.51
2:B:392:LEU:HD23	2:B:393:VAL:N	2.24	0.51
2:B:108:ARG:HG3	2:B:109:LYS:CG	2.40	0.51
1:A:295:ALA:HA	1:A:299:VAL:HB	1.93	0.51
1:A:653:TRP:CD1	1:A:656:ILE:HG23	2.46	0.51
2:B:283:PHE:HB2	2:B:285:ALA:HB2	1.92	0.51
2:B:117:PRO:HD3	2:B:118:PHE:HD2	1.74	0.51
3:C:236:LEU:HA	3:C:239:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:GLY:HA2	2:B:240:TYR:CD2	2.45	0.51
2:B:108:ARG:NE	2:B:109:LYS:CB	2.73	0.51
2:B:117:PRO:CG	2:B:135:ASN:CB	2.86	0.51
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.45	0.51
1:A:101:LYS:HG3	1:A:126:THR:HG21	1.93	0.51
1:A:463:ILE:CG2	1:A:465:VAL:HG23	2.41	0.51
2:B:186:PHE:HB3	4:D:95:THR:HG21	1.93	0.51
2:B:283:PHE:HB2	2:B:383:LEU:HB2	1.93	0.50
1:A:167:LEU:HD23	1:A:451:LYS:HA	1.92	0.50
1:A:524:GLY:HA3	1:A:534:PHE:CZ	2.46	0.50
2:B:146:MET:CE	5:G:22:ALA:O	2.60	0.50
1:A:260:LEU:HD13	1:A:312:LEU:CD1	2.42	0.50
2:B:108:ARG:HG3	2:B:109:LYS:CD	2.40	0.50
2:B:238:ILE:HD11	2:B:391:VAL:HA	1.93	0.50
2:B:381:LEU:HD22	2:B:382:GLY:N	2.26	0.50
1:A:301:SER:O	1:A:304:THR:OG1	2.23	0.50
2:B:117:PRO:HG3	2:B:135:ASN:CB	2.42	0.50
1:A:630:ALA:O	1:A:632:SER:N	2.45	0.50
2:B:208:VAL:O	2:B:211:ILE:HG13	2.11	0.50
2:B:112:GLN:HB2	2:B:113:LEU:CA	2.42	0.49
1:A:533:TRP:O	1:A:536:SER:OG	2.27	0.49
2:B:106:TYR:HA	2:B:239:LYS:HD3	1.89	0.49
2:B:237:PHE:HB3	2:B:241:LEU:CD2	2.42	0.49
2:B:104:SER:O	2:B:106:TYR:N	2.46	0.49
2:B:453:VAL:HA	3:C:50:SER:CB	2.42	0.49
3:C:42:TRP:CZ2	3:C:129:SER:HA	2.47	0.49
2:B:111:GLY:HA3	2:B:240:TYR:CD2	2.47	0.49
3:C:90:TYR:CZ	3:C:94:LEU:HD21	2.47	0.49
3:C:112:ILE:HD13	3:C:112:ILE:N	2.26	0.49
1:A:42:ILE:HD12	3:C:149:ILE:HG12	1.93	0.49
2:B:117:PRO:HA	2:B:135:ASN:HB3	1.92	0.49
2:B:105:PHE:CG	2:B:239:LYS:CE	2.94	0.49
1:A:230:CYS:HA	1:A:233:ARG:HG2	1.95	0.49
3:C:47:LEU:O	3:C:51:VAL:HG23	2.13	0.49
3:C:121:SER:O	3:C:124:SER:OG	2.31	0.49
2:B:186:PHE:O	2:B:190:ASN:N	2.46	0.48
1:A:268:THR:HG23	1:A:353:PRO:O	2.13	0.48
1:A:283:ASP:OD1	1:A:334:THR:HG22	2.13	0.48
1:A:338:ILE:HG22	1:A:646:SER:OG	2.14	0.48
2:B:404:TRP:O	2:B:407:THR:HG22	2.13	0.48
3:C:74:PHE:O	3:C:78:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:15:ALA:HB1	5:G:18:ALA:CB	2.44	0.48
1:A:294:GLY:O	1:A:298:ALA:N	2.47	0.48
2:B:113:LEU:HD13	2:B:116:THR:C	2.39	0.48
3:C:137:ILE:C	3:C:137:ILE:HD12	2.39	0.48
3:C:168:ILE:O	3:C:172:THR:OG1	2.32	0.48
2:B:113:LEU:HD12	2:B:116:THR:CA	2.40	0.47
2:B:113:LEU:CD1	2:B:116:THR:CA	2.92	0.47
2:B:208:VAL:HG13	4:D:26:LEU:HD23	1.96	0.47
2:B:247:TRP:CZ2	2:B:446:TYR:CE2	3.02	0.47
5:G:15:ALA:O	5:G:17:ALA:CA	2.60	0.47
1:A:126:THR:HG22	1:A:128:PRO:HG2	1.97	0.47
1:A:227:THR:HG21	1:A:647:THR:HB	1.97	0.47
2:B:117:PRO:C	2:B:119:THR:H	2.23	0.47
1:A:385:GLN:O	1:A:391:ARG:HB2	2.14	0.47
2:B:116:THR:CB	2:B:118:PHE:CD2	2.96	0.47
2:B:118:PHE:HB2	2:B:135:ASN:CB	2.32	0.47
2:B:238:ILE:CG1	2:B:391:VAL:HG13	2.45	0.47
2:B:117:PRO:HD3	2:B:118:PHE:CD2	2.48	0.47
2:B:416:ILE:CD1	3:C:36:VAL:HG12	2.45	0.47
1:A:396:ASP:O	1:A:400:THR:HG23	2.15	0.47
2:B:113:LEU:HD13	2:B:118:PHE:H	1.80	0.47
2:B:140:ILE:HG12	2:B:252:VAL:HG11	1.97	0.47
2:B:153:LEU:CD2	2:B:162:ILE:HG23	2.44	0.47
3:C:114:ILE:HA	3:C:117:MET:HE3	1.96	0.46
2:B:392:LEU:HD21	2:B:410:CYS:HB3	1.96	0.46
2:B:392:LEU:HD22	2:B:414:ILE:CD1	2.36	0.46
3:C:90:TYR:CE2	3:C:94:LEU:HD21	2.49	0.46
1:A:83:GLN:O	1:A:87:THR:N	2.37	0.46
1:A:162:ILE:HD11	1:A:164:TRP:CG	2.51	0.46
2:B:186:PHE:CE1	2:B:193:VAL:HG21	2.51	0.46
1:A:365:LEU:N	1:A:365:LEU:HD12	2.30	0.46
2:B:177:PHE:CZ	5:G:21:ALA:HB2	2.50	0.46
1:A:127:LYS:N	1:A:128:PRO:HD2	2.31	0.46
1:A:133:GLY:CA	1:A:167:LEU:HD21	2.45	0.46
1:A:450:ASN:O	1:A:452:TYR:N	2.45	0.46
1:A:632:SER:OG	1:A:634:ALA:N	2.48	0.46
2:B:109:LYS:HB2	2:B:110:ASP:OD1	2.15	0.46
2:B:117:PRO:C	2:B:119:THR:N	2.73	0.46
2:B:175:PHE:HD1	2:B:202:ILE:HG23	1.81	0.46
1:A:277:VAL:HG11	1:A:362:PHE:CD2	2.51	0.46
1:A:53:LEU:C	1:A:54:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:VAL:HA	3:C:50:SER:HB2	1.96	0.46
2:B:466:TYR:HB2	3:C:204:THR:HG21	1.98	0.46
2:B:108:ARG:CG	2:B:109:LYS:HD3	2.45	0.46
2:B:117:PRO:O	2:B:119:THR:N	2.48	0.46
2:B:118:PHE:CG	2:B:135:ASN:HB3	2.51	0.46
2:B:174:LEU:HD22	2:B:206:GLY:HA2	1.97	0.46
2:B:383:LEU:O	2:B:386:PHE:HB3	2.16	0.46
2:B:113:LEU:HD13	2:B:116:THR:O	2.15	0.45
1:A:365:LEU:HD11	1:A:494:LEU:HD11	1.97	0.45
2:B:108:ARG:HA	2:B:108:ARG:HD2	1.66	0.45
2:B:413:ALA:HB2	2:B:445:PHE:CD2	2.51	0.45
3:C:200:THR:HA	3:C:203:LEU:HD12	1.97	0.45
2:B:236:VAL:O	2:B:239:LYS:N	2.49	0.45
1:A:329:PHE:N	1:A:329:PHE:CD1	2.85	0.45
2:B:105:PHE:CE2	2:B:239:LYS:HE3	2.52	0.45
2:B:240:TYR:CE2	5:G:15:ALA:CB	2.98	0.45
2:B:421:THR:HG23	2:B:434:ALA:HB3	1.98	0.45
2:B:118:PHE:CD2	2:B:135:ASN:CB	2.99	0.45
2:B:449:THR:HA	2:B:453:VAL:HB	1.99	0.45
3:C:163:LEU:HD11	3:C:217:ILE:HD13	1.99	0.45
2:B:454:GLN:N	2:B:455:PRO:CD	2.79	0.45
1:A:212:LEU:O	1:A:662:LEU:HA	2.16	0.45
2:B:112:GLN:CG	5:G:15:ALA:HB3	2.45	0.45
2:B:118:PHE:C	2:B:119:THR:HG23	2.41	0.45
1:A:181:PHE:CD1	1:A:217:LEU:HD21	2.52	0.45
1:A:560:PRO:HG2	1:A:565:TYR:CZ	2.51	0.45
3:C:80:VAL:HG11	3:C:198:LEU:HD12	2.00	0.44
2:B:85:LEU:CD1	2:B:422:LEU:HD23	2.48	0.44
2:B:172:LEU:O	2:B:176:PHE:N	2.48	0.44
1:A:237:GLN:O	1:A:244:PRO:HB3	2.17	0.44
3:C:163:LEU:HD11	3:C:204:THR:HG22	2.00	0.44
1:A:76:VAL:HG13	1:A:81:ASP:HB2	1.98	0.44
1:A:523:TYR:CE1	1:A:527:ILE:HG21	2.53	0.44
2:B:194:ASP:HB3	4:D:78:PHE:CE1	2.52	0.44
3:C:215:LEU:N	3:C:216:PRO:HD2	2.32	0.44
1:A:282:LEU:HD12	1:A:302:PHE:CD2	2.52	0.44
2:B:117:PRO:CB	2:B:135:ASN:HB2	2.48	0.44
3:C:159:THR:HG21	3:C:210:TYR:CE1	2.52	0.44
2:B:175:PHE:O	2:B:176:PHE:C	2.61	0.44
3:C:196:SER:O	3:C:200:THR:HG23	2.18	0.44
4:D:27:PRO:HG3	4:D:67:TRP:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PHE:CE1	1:A:212:LEU:HD12	2.52	0.44
2:B:103:VAL:HG13	2:B:188:THR:OG1	2.18	0.44
2:B:113:LEU:CA	2:B:114:ILE:C	2.90	0.44
2:B:116:THR:HG22	2:B:118:PHE:CD2	2.53	0.44
2:B:392:LEU:HD12	2:B:443:LEU:HD23	2.00	0.44
1:A:476:ASP:OD1	1:A:476:ASP:N	2.50	0.44
2:B:87:VAL:N	2:B:88:PRO:CD	2.81	0.44
2:B:114:ILE:CB	2:B:115:TYR:CA	2.93	0.44
2:B:164:ALA:HA	2:B:167:ILE:HG13	2.00	0.44
1:A:282:LEU:HD12	1:A:302:PHE:CG	2.53	0.43
2:B:233:MET:HE1	5:G:25:ALA:HA	2.00	0.43
3:C:14:PHE:O	3:C:15:GLY:C	2.61	0.43
2:B:238:ILE:HG12	2:B:391:VAL:HG13	2.01	0.43
2:B:435:LEU:N	2:B:436:PRO:CD	2.80	0.43
1:A:303:VAL:HG21	1:A:522:LEU:HD12	1.99	0.43
2:B:117:PRO:HA	2:B:118:PHE:CB	2.39	0.43
2:B:187:LYS:HE3	4:D:95:THR:HG23	1.99	0.43
1:A:546:LEU:HD21	1:A:566:VAL:HG22	2.00	0.43
1:A:560:PRO:O	1:A:561:THR:HG22	2.18	0.43
1:A:298:ALA:O	1:A:299:VAL:C	2.61	0.43
2:B:381:LEU:HD11	2:B:386:PHE:HD2	1.82	0.43
3:C:34:ILE:O	3:C:90:TYR:OH	2.31	0.43
4:D:34:ILE:HD11	4:D:61:ALA:HA	2.01	0.43
1:A:256:VAL:HG21	1:A:567:VAL:CG1	2.43	0.43
1:A:456:ILE:HD12	1:A:456:ILE:N	2.33	0.43
2:B:118:PHE:CD2	2:B:135:ASN:HB3	2.54	0.43
3:C:199:LEU:O	3:C:203:LEU:HG	2.19	0.43
2:B:200:LEU:HD23	2:B:200:LEU:C	2.44	0.43
2:B:412:VAL:HG11	3:C:43:LEU:HD12	2.01	0.43
1:A:662:LEU:CD1	3:C:149:ILE:HD12	2.48	0.42
2:B:112:GLN:HB2	2:B:114:ILE:O	2.19	0.42
2:B:234:ALA:O	2:B:238:ILE:HG13	2.19	0.42
2:B:416:ILE:HD12	3:C:36:VAL:HG12	2.01	0.42
2:B:241:LEU:HD12	2:B:241:LEU:N	2.34	0.42
2:B:465:PHE:HB3	3:C:205:PHE:HA	2.01	0.42
1:A:179:PRO:HG2	1:A:217:LEU:HD22	2.01	0.42
2:B:417:GLY:HA3	2:B:438:SER:HA	2.00	0.42
2:B:381:LEU:HD22	2:B:382:GLY:H	1.83	0.42
2:B:405:ASN:O	2:B:408:ILE:HG22	2.20	0.42
3:C:35:LEU:HA	3:C:124:SER:HB3	2.02	0.42
3:C:162:PHE:HB3	3:C:214:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:HA2	1:A:179:PRO:O	2.19	0.42
1:A:477:LEU:HB3	1:A:520:ARG:HD2	2.02	0.42
2:B:147:THR:HG22	5:G:27:ALA:CB	2.49	0.42
2:B:424:LEU:C	2:B:424:LEU:HD13	2.44	0.42
3:C:90:TYR:CE2	3:C:94:LEU:HD11	2.54	0.42
3:C:94:LEU:HD12	3:C:179:PHE:HE2	1.85	0.42
3:C:170:LEU:HG	3:C:174:TRP:CH2	2.55	0.42
3:C:173:PHE:CG	3:C:225:GLY:HA2	2.54	0.42
3:C:178:PHE:CE1	3:C:182:CYS:SG	3.13	0.42
1:A:537:ILE:HG21	1:A:569:TYR:O	2.20	0.42
5:G:15:ALA:HB1	5:G:18:ALA:HB1	2.01	0.42
2:B:113:LEU:HB2	2:B:114:ILE:HA	2.01	0.42
2:B:167:ILE:O	2:B:171:LEU:N	2.32	0.42
2:B:113:LEU:HD12	2:B:116:THR:CG2	2.43	0.41
2:B:416:ILE:HG12	3:C:40:PHE:CG	2.55	0.41
3:C:112:ILE:HG13	3:C:117:MET:CG	2.50	0.41
2:B:113:LEU:HB2	2:B:116:THR:HA	2.02	0.41
3:C:148:GLY:O	3:C:150:HIS:N	2.53	0.41
1:A:307:ALA:HB2	1:A:518:VAL:HG22	2.01	0.41
2:B:228:MET:O	2:B:232:LEU:HD13	2.19	0.41
2:B:452:LEU:O	2:B:455:PRO:HD2	2.20	0.41
2:B:392:LEU:HD23	2:B:392:LEU:C	2.45	0.41
4:D:55:GLY:O	4:D:58:TRP:HB3	2.19	0.41
1:A:164:TRP:CZ2	1:A:423:PRO:HA	2.55	0.41
2:B:262:LEU:HB2	2:B:263:CYS:HA	2.02	0.41
2:B:105:PHE:O	2:B:239:LYS:HE2	2.18	0.41
2:B:146:MET:HE1	5:G:22:ALA:O	2.20	0.41
2:B:406:THR:HA	2:B:449:THR:HG21	2.03	0.41
3:C:172:THR:O	3:C:176:VAL:HG23	2.20	0.41
1:A:111:LEU:CD2	1:A:118:ILE:HG21	2.51	0.41
1:A:260:LEU:CD2	1:A:312:LEU:HD13	2.49	0.41
2:B:167:ILE:O	2:B:171:LEU:HB3	2.21	0.41
1:A:283:ASP:OD2	1:A:332:GLY:N	2.51	0.41
1:A:164:TRP:CH2	1:A:423:PRO:CA	3.04	0.40
1:A:344:VAL:HG21	1:A:430:PHE:HA	2.03	0.40
1:A:582:THR:HG22	1:A:585:GLN:OE1	2.21	0.40
2:B:204:ASN:O	2:B:208:VAL:HG22	2.20	0.40
1:A:486:ALA:O	1:A:490:VAL:HG23	2.21	0.40
1:A:540:GLN:HA	1:A:606:GLN:NE2	2.35	0.40
2:B:381:LEU:HD11	2:B:386:PHE:CD2	2.56	0.40
1:A:40:ILE:HD11	3:C:157:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:C	1:A:338:ILE:HD12	2.46	0.40
2:B:89:VAL:HG22	2:B:386:PHE:CD2	2.56	0.40
2:B:241:LEU:N	2:B:241:LEU:CD1	2.85	0.40
2:B:416:ILE:HG21	3:C:40:PHE:CE1	2.56	0.40
5:G:17:ALA:CB	5:G:18:ALA:CB	2.78	0.40
1:A:84:TRP:O	1:A:89:GLY:N	2.54	0.40
1:A:221:MET:HE1	1:A:653:TRP:CD2	2.57	0.40
1:A:633:PRO:HG2	1:A:645:TYR:HB3	2.04	0.40
2:B:117:PRO:HG3	2:B:135:ASN:CG	2.47	0.40
2:B:204:ASN:HB3	4:D:28:PHE:HB2	2.04	0.40
2:B:233:MET:HA	2:B:236:VAL:CG2	2.51	0.40
2:B:254:SER:HA	2:B:436:PRO:HB3	2.03	0.40
2:B:434:ALA:O	2:B:437:ILE:HG22	2.21	0.40
5:G:16:ALA:CA	5:G:18:ALA:HB3	2.51	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%)	534 (80%)	99 (15%)	30 (4%)	2	19
2	B	280/467 (60%)	248 (89%)	16 (6%)	16 (6%)	1	16
3	C	241/265 (91%)	221 (92%)	16 (7%)	4 (2%)	7	36
4	D	98/101 (97%)	89 (91%)	8 (8%)	1 (1%)	12	46
5	G	22/24 (92%)	20 (91%)	1 (4%)	1 (4%)	2	19
All	All	1304/1566 (83%)	1112 (85%)	140 (11%)	52 (4%)	4	21

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	333	GLU
1	A	473	PRO
1	A	643	THR
2	B	116	THR
2	B	117	PRO
2	B	122	THR
2	B	236	VAL
3	C	156	TYR
5	G	13	ALA
1	A	89	GLY
1	A	371	ARG
1	A	436	ILE
1	A	511	VAL
1	A	543	ARG
1	A	561	THR
1	A	632	SER
1	A	646	SER
2	B	286	LEU
2	B	287	ILE
3	C	61	ASP
3	C	149	ILE
1	A	358	ASN
1	A	464	ASN
1	A	472	SER
1	A	631	LEU
2	B	105	PHE
2	B	109	LYS
2	B	239	LYS
2	B	262	LEU
1	A	225	ILE
1	A	332	GLY
1	A	422	LEU
2	B	159	TYR
2	B	403	ASP
2	B	429	LYS
2	B	430	LYS
4	D	86	GLY
1	A	185	ASP
1	A	210	PHE
1	A	253	ASP
1	A	289	TRP
1	A	322	PRO

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Mol	Chain	Res	Type
1	A	612	ASN
2	B	104	SER
2	B	119	THR
3	C	107	ASP
1	A	161	GLU
1	A	359	VAL
1	A	93	PRO
1	A	316	PRO
1	A	559	SER

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%)	528 (91%)	55 (9%)	8	28
2	B	240/408 (59%)	201 (84%)	39 (16%)	2	13
3	C	192/214 (90%)	169 (88%)	23 (12%)	5	20
4	D	87/89 (98%)	79 (91%)	8 (9%)	8	29
All	All	1102/1323 (83%)	977 (89%)	125 (11%)	8	22

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	54	LEU
1	A	57	THR
1	A	69	ASP
1	A	84	TRP
1	A	86	LEU
1	A	87	THR
1	A	97	LEU
1	A	100	SER
1	A	107	LEU
1	A	111	LEU
1	A	121	LEU

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Mol	Chain	Res	Type
1	A	140	CYS
1	A	147	VAL
1	A	161	GLU
1	A	163	GLN
1	A	204	ASN
1	A	218	PHE
1	A	231	MET
1	A	256	VAL
1	A	264	ASN
1	A	269	LEU
1	A	296	GLU
1	A	301	SER
1	A	312	LEU
1	A	329	PHE
1	A	331	GLN
1	A	333	GLU
1	A	344	VAL
1	A	347	MET
1	A	401	LEU
1	A	413	LEU
1	A	425	SER
1	A	443	ASP
1	A	450	ASN
1	A	454	GLN
1	A	463	ILE
1	A	469	GLU
1	A	472	SER
1	A	487	LEU
1	A	494	LEU
1	A	506	ASN
1	A	517	THR
1	A	520	ARG
1	A	522	LEU
1	A	537	ILE
1	A	561	THR
1	A	574	LEU
1	A	586	CYS
1	A	587	GLN
1	A	637	LEU
1	A	643	THR
1	A	656	ILE
1	A	668	LEU

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Mol	Chain	Res	Type
1	A	670	LEU
2	B	83	ILE
2	B	87	VAL
2	B	91	LEU
2	B	113	LEU
2	B	117	PRO
2	B	122	THR
2	B	133	ILE
2	B	150	LEU
2	B	153	LEU
2	B	154	TYR
2	B	158	CYS
2	B	162	ILE
2	B	168	ILE
2	B	171	LEU
2	B	174	LEU
2	B	180	ILE
2	B	184	GLU
2	B	200	LEU
2	B	201	LEU
2	B	202	ILE
2	B	212	SER
2	B	222	GLN
2	B	226	LEU
2	B	227	ILE
2	B	244	TRP
2	B	249	ILE
2	B	254	SER
2	B	257	ASP
2	B	282	LEU
2	B	381	LEU
2	B	392	LEU
2	B	407	THR
2	B	416	ILE
2	B	419	CYS
2	B	420	LEU
2	B	422	LEU
2	B	438	SER
2	B	459	GLN
2	B	467	ILE
3	C	7	PHE
3	C	46	LEU

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Mol	Chain	Res	Type
3	C	56	LEU
3	C	61	ASP
3	C	68	GLN
3	C	82	LEU
3	C	93	LEU
3	C	104	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	137	ILE
3	C	152	ASP
3	C	159	THR
3	C	160	SER
3	C	170	LEU
3	C	172	THR
3	C	190	LEU
3	C	215	LEU
3	C	238	SER
4	D	17	LYS
4	D	35	PHE
4	D	39	ARG
4	D	69	ILE
4	D	73	SER
4	D	75	ILE
4	D	94	PHE
4	D	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	197	GLN
1	A	305	GLN
1	A	313	GLN
1	A	331	GLN
1	A	358	ASN
1	A	367	GLN
1	A	379	HIS
1	A	450	ASN

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Mol	Chain	Res	Type
1	A	454	GLN
1	A	568	GLN
1	A	606	GLN
1	A	612	ASN
2	B	112	GLN
2	B	405	ASN
2	B	454	GLN
3	C	58	HIS
3	C	207	ASN
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.

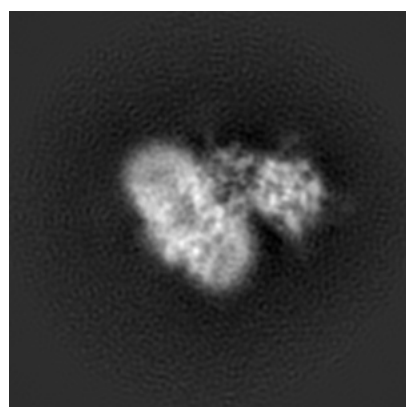
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3238. These allow visual inspection of the internal detail of the map and identification of artifacts.

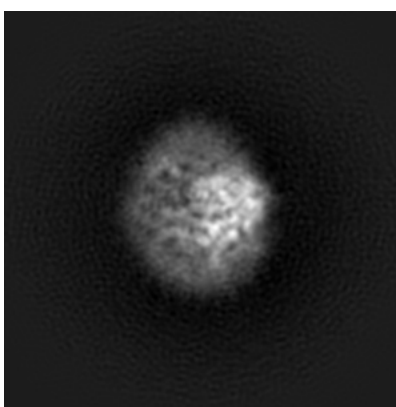
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

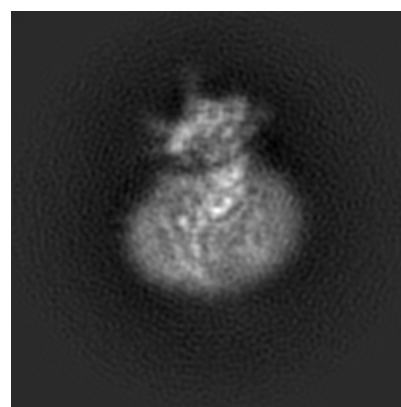
6.1.1 Primary map



X



Y

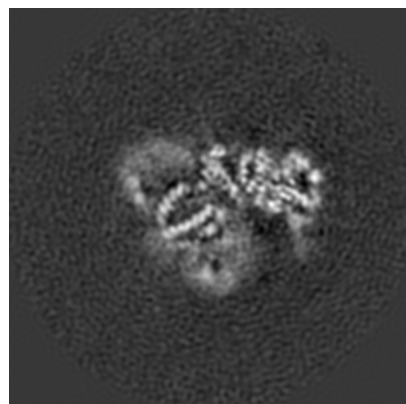


Z

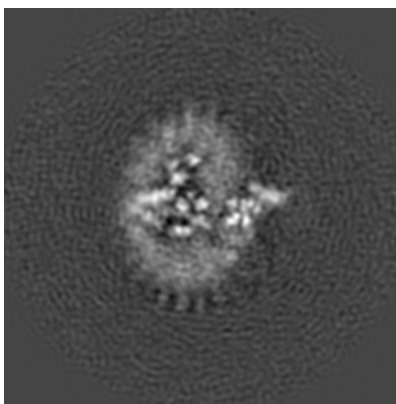
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

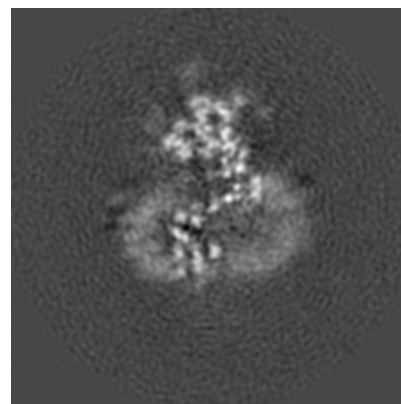
6.2.1 Primary map



X Index: 90



Y Index: 90

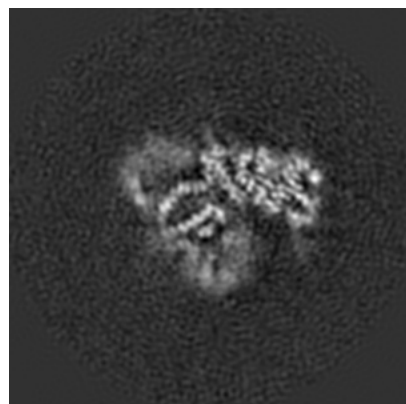


Z Index: 90

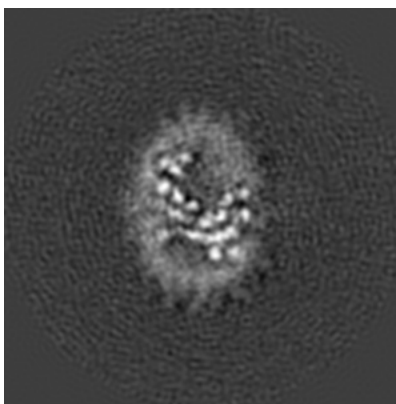
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

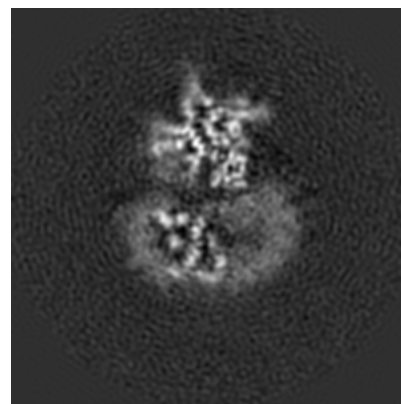
6.3.1 Primary map



X Index: 91



Y Index: 84

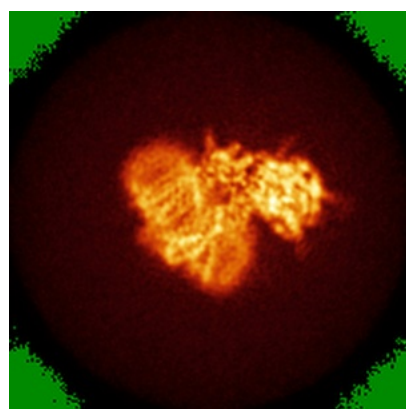


Z Index: 95

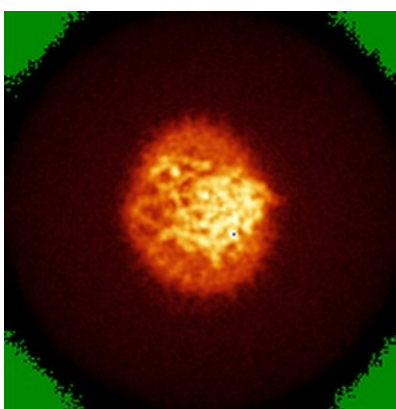
The images above show the largest variance slices of the map in three orthogonal directions.

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

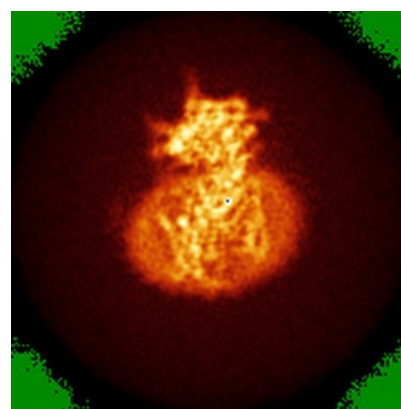
6.4.1 Primary map



X



Y

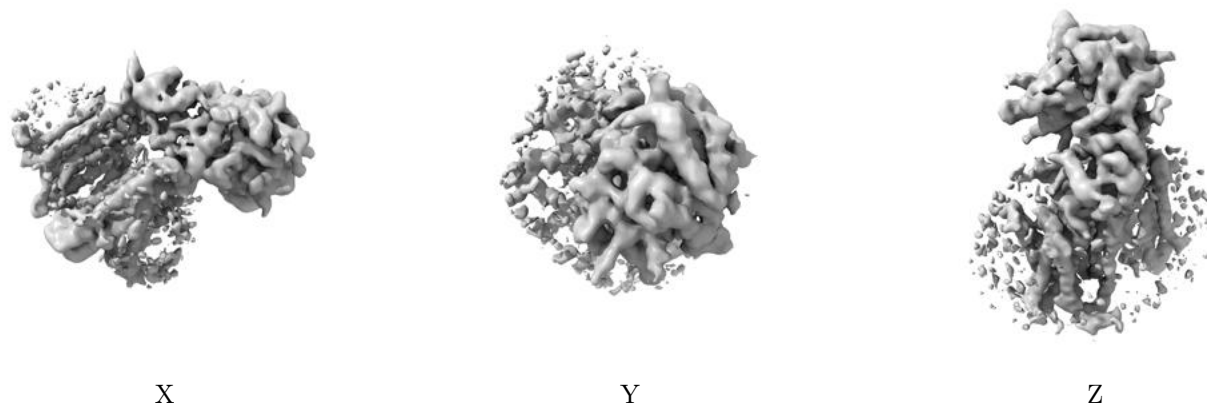


Z

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.

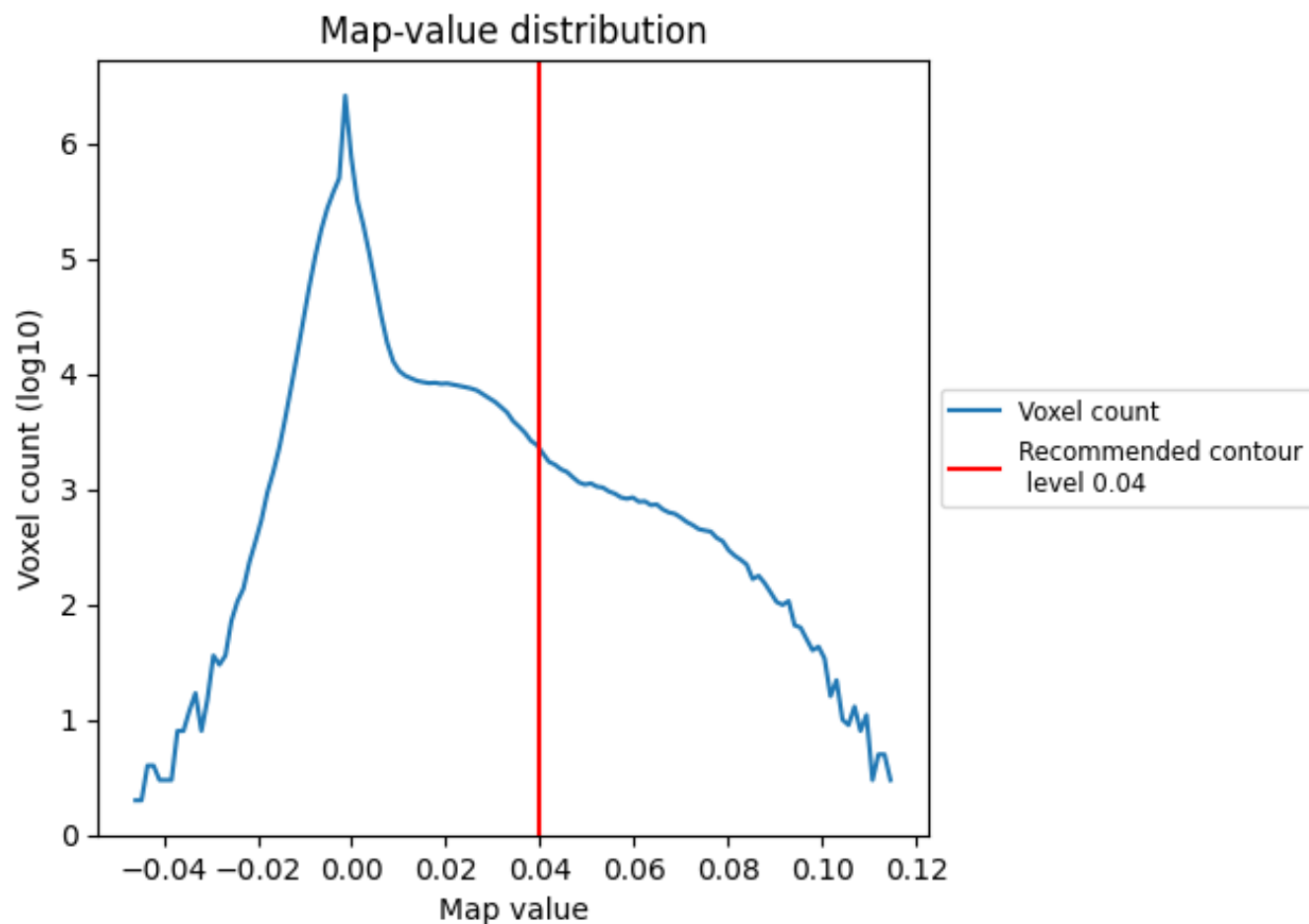
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

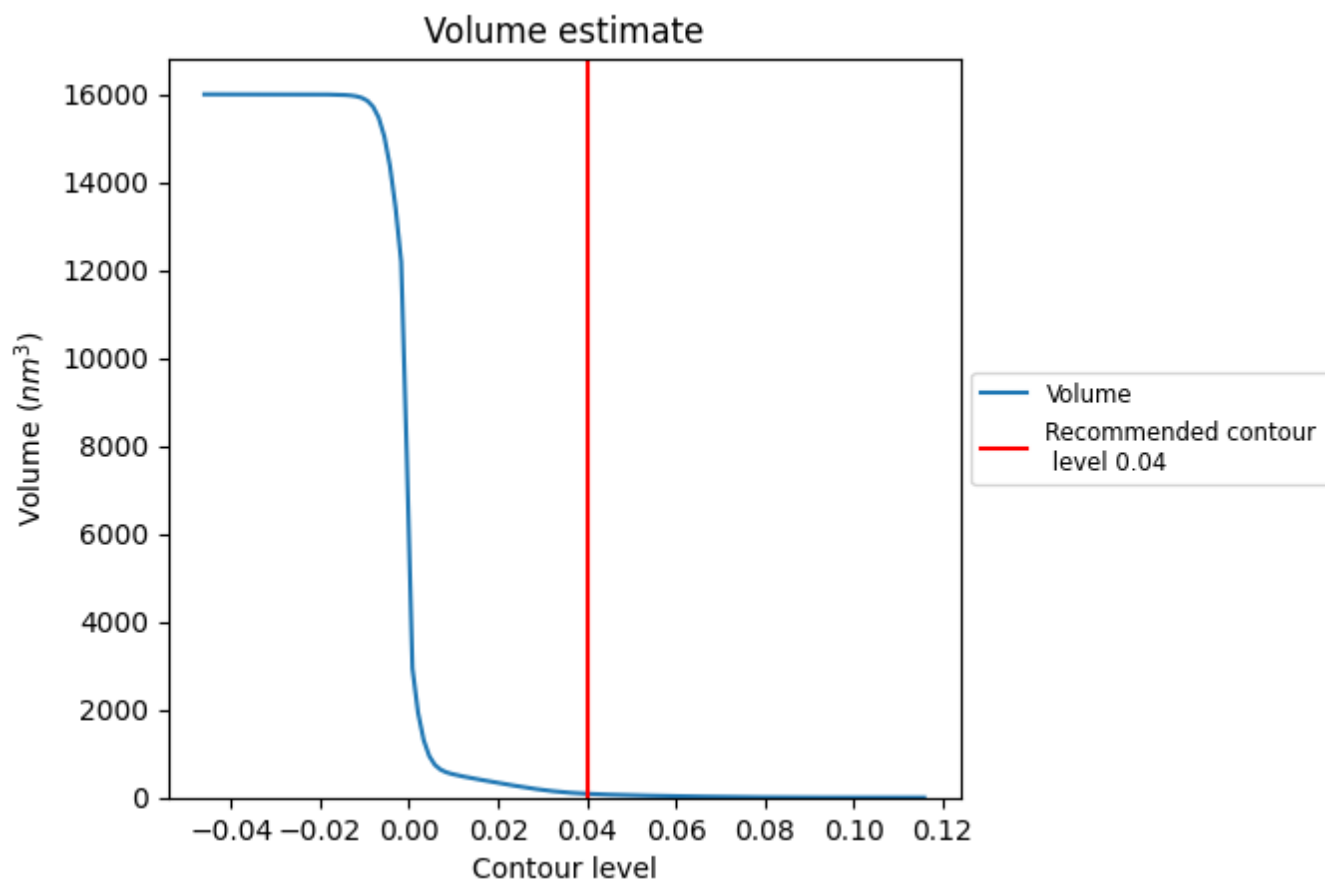
This section contains the results of statistical analysis of the map.

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.

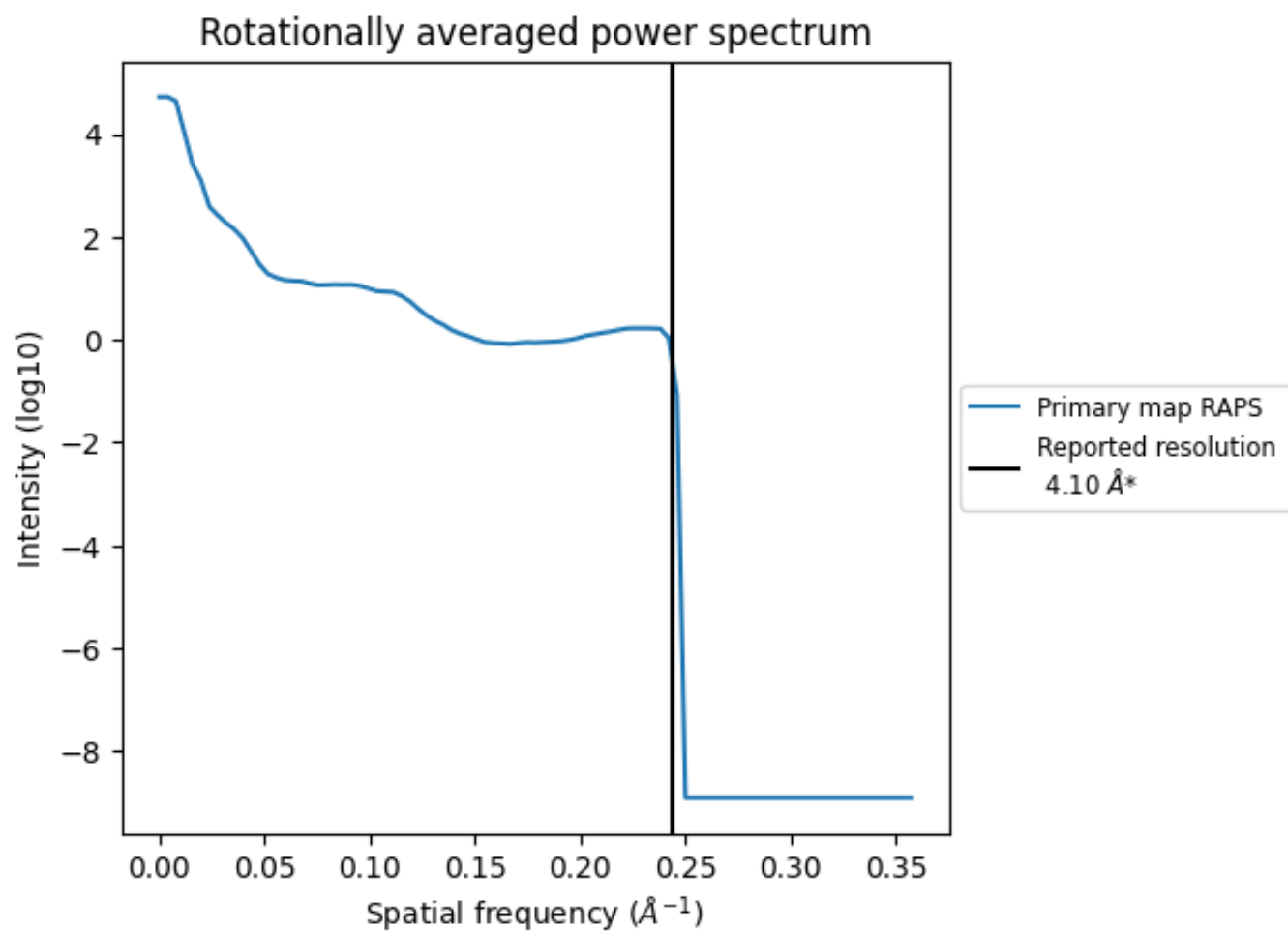
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 78 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 0.244 Å⁻¹

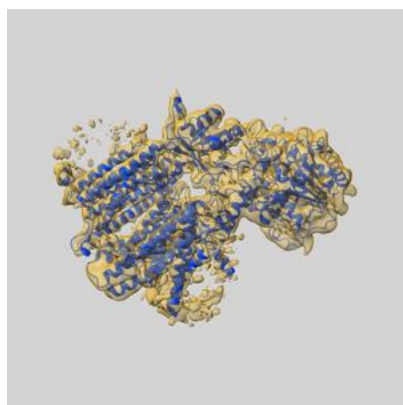
8 Fourier-Shell correlation ⓘ

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

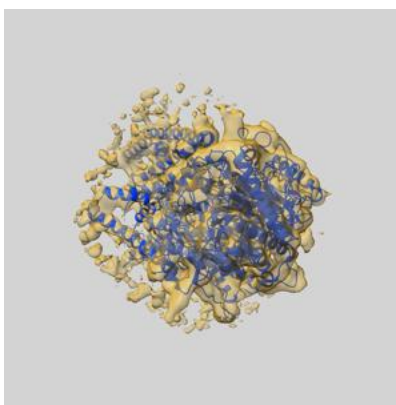
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3238 and PDB model 5FN3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

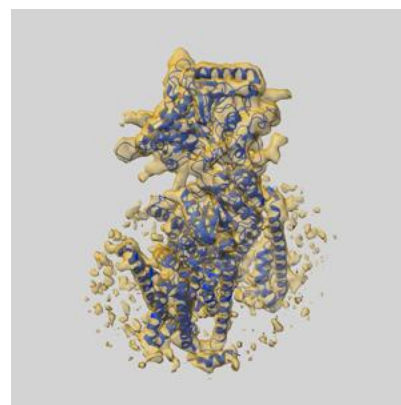
9.1 Map-model overlay [i](#)



X



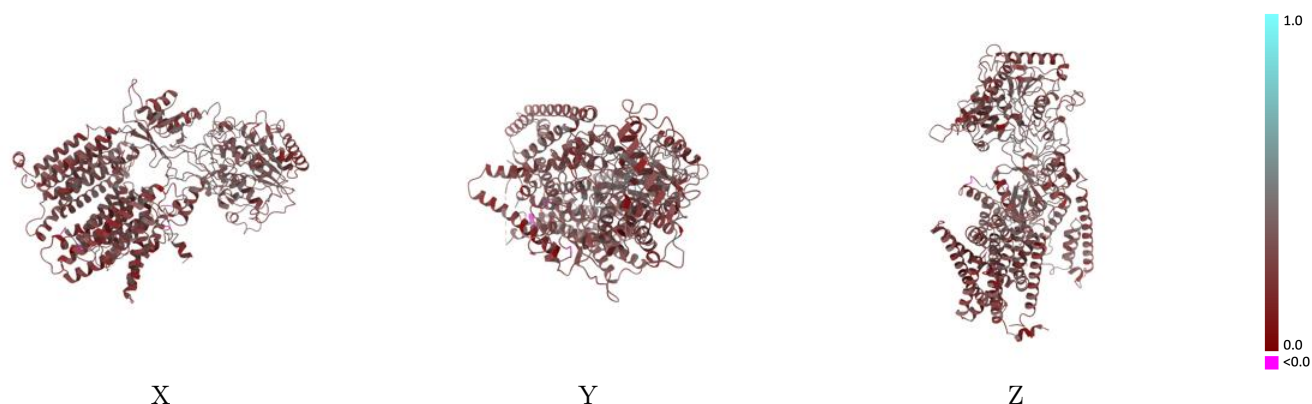
Y



Z

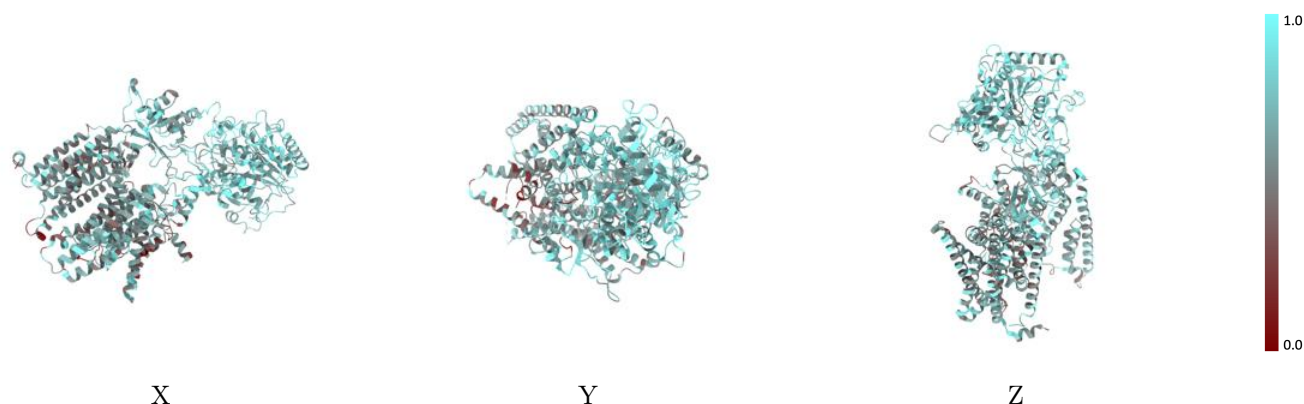
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



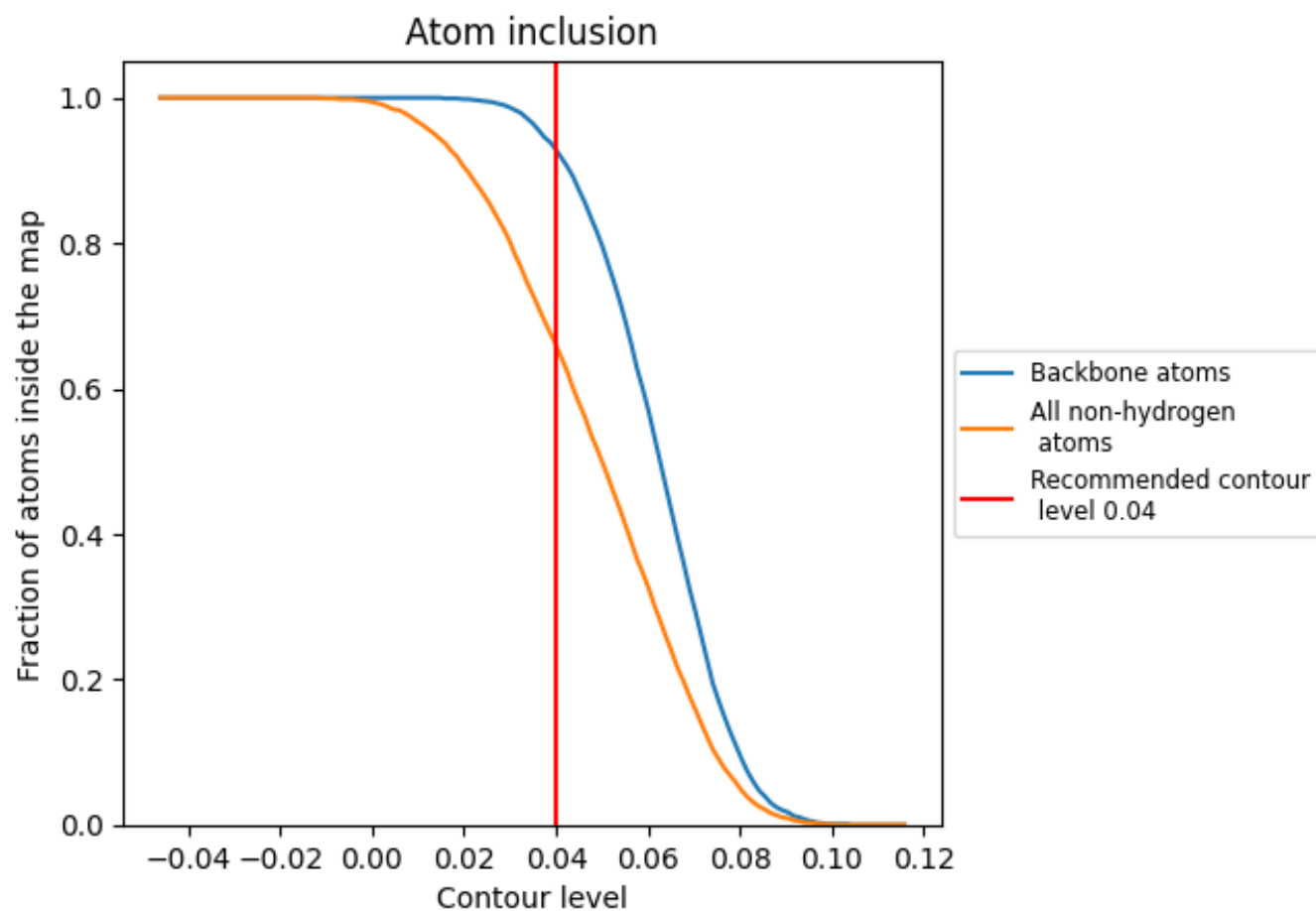
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 66% 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	0.6600	0.2910
A	0.7370	0.3200
B	0.5540	0.2630
C	0.5970	0.2580
D	0.6440	0.2560
G	0.3670	0.3380

