Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 09:41 am GMT

PDB ID	:	5FN2
EMDB ID	:	EMD-3237
Title	:	Cryo-EM structure of gamma secretase in complex with a drug DAPT
Authors	:	Bai, X.C.; Rajendra, E.; Yang, G.H.; Shi, Y.G.; Scheres, S.H.W.
Deposited on	:	2015-11-10
Resolution	:	4.20 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:

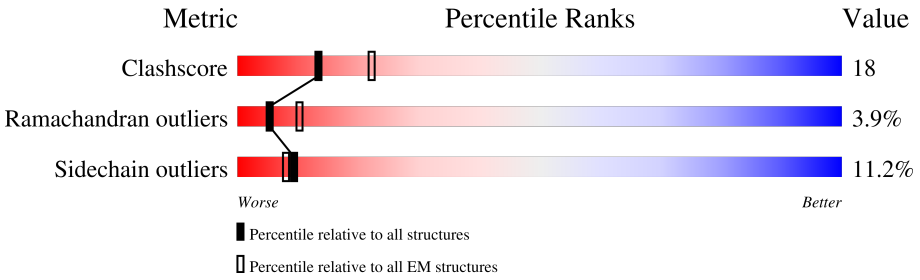
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	709	64% 25% 6%
2	B	467	29% 28% 6% 36%
3	C	265	63% 23% 6% 8%
4	D	101	8% 77% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10276 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
			Total	C	N	O	S		
1	A	665	5222	3312	888	1001	21	0	0

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	301	2339	1590	354	381	14	0	0

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
			Total	C	N	O	S		
3	C	243	1868	1252	299	313	4	0	0

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

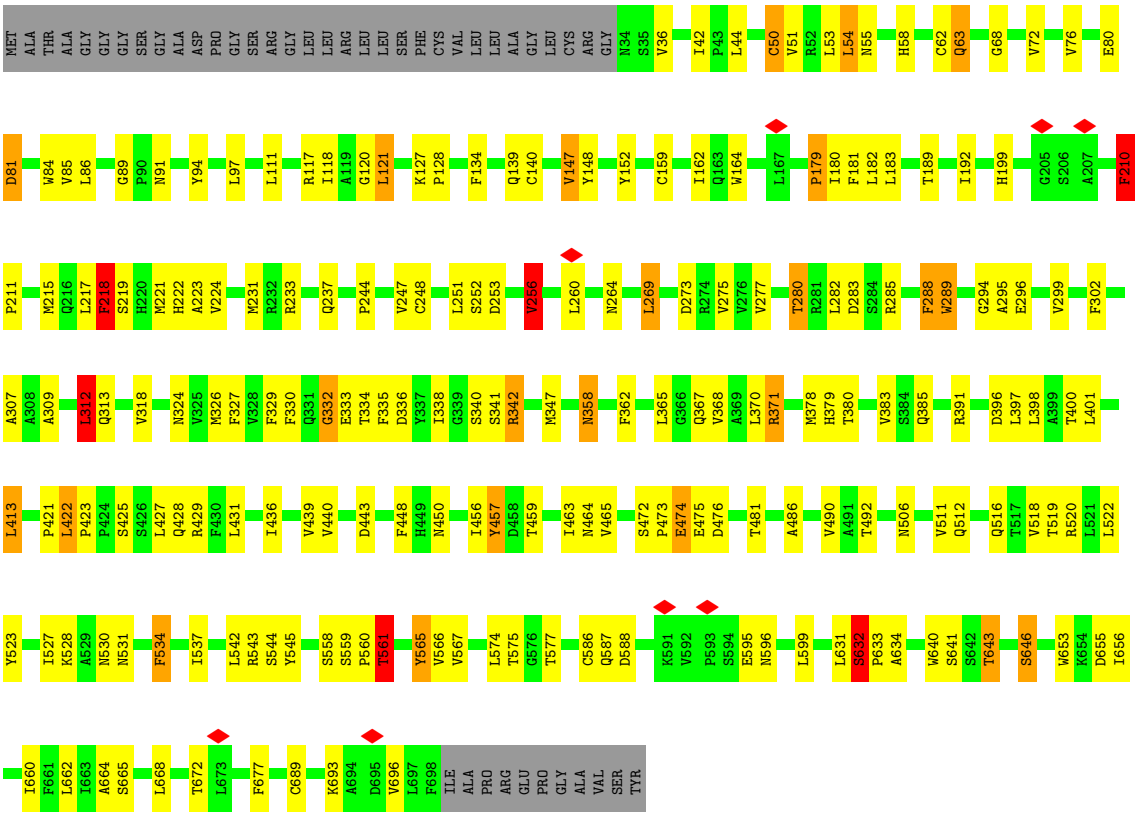
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	100	847	579	133	134	1	0	0

3 Residue-property plots (i)

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.

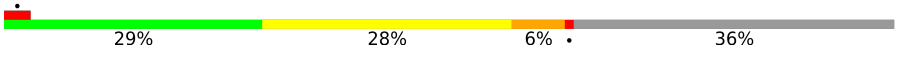
• Molecule 1: Nicastrin

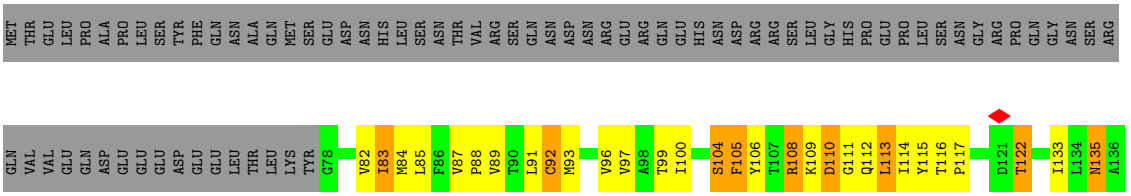
Chain A:

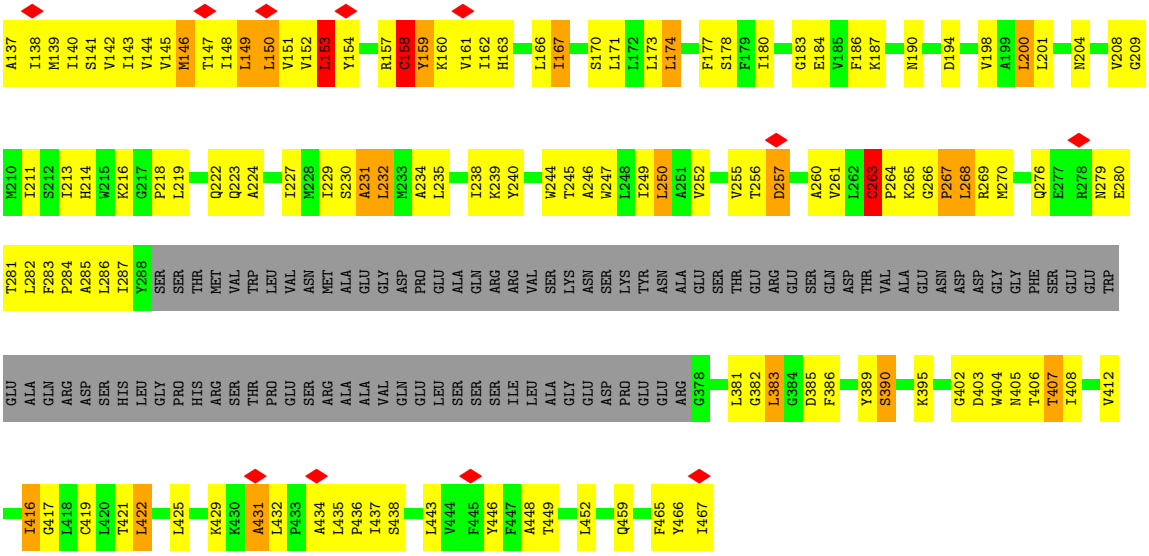


• Molecule 2: Presenilin-1

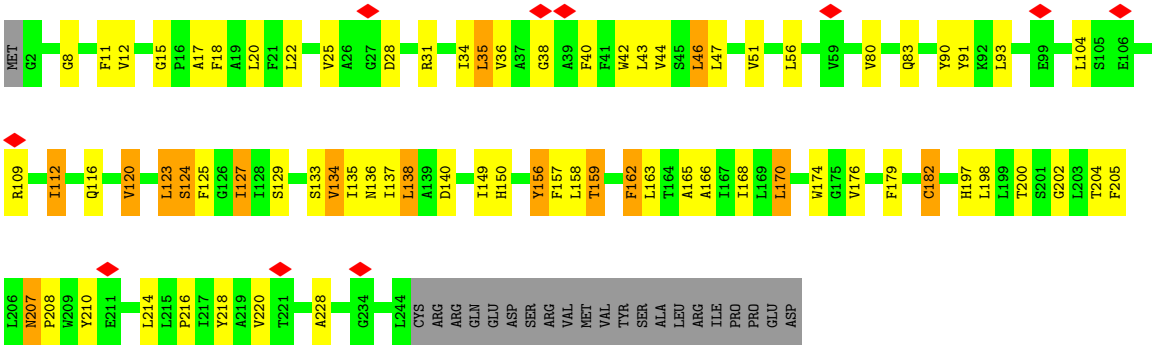
Chain B:



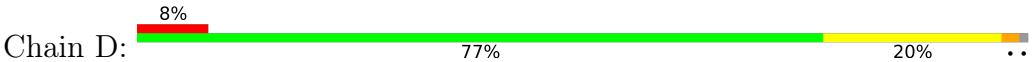


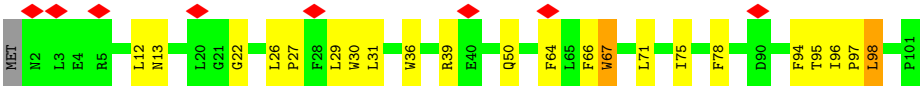


• Molecule 3: Gamma-secretase subunit APH-1A



• Molecule 4: Gamma-secretase subunit PEN-2





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51366	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 ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	252.0, 252.0, 252.0	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.47	0/5345	0.79	4/7284 (0.1%)
2	B	0.54	0/2399	0.90	1/3279 (0.0%)
3	C	0.54	0/1920	0.89	0/2619
4	D	0.52	0/880	0.76	0/1201
All	All	0.51	0/10544	0.83	5/14383 (0.0%)

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	2
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	PHE	CB-CG-CD1	7.91	126.33	120.80
1	A	218	PHE	CB-CG-CD2	-6.38	116.34	120.80
1	A	312	LEU	CA-CB-CG	5.51	127.98	115.30
2	B	263	CYS	C-N-CD	5.37	139.67	128.40
1	A	218	PHE	N-CA-CB	5.26	120.07	110.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	LEU	Peptide
1	A	256	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	288	PHE	Peptide
1	A	335	PHE	Peptide
1	A	91	ASN	Peptide
2	B	263	CYS	Peptide
2	B	402	GLY	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	113	0
2	B	2339	0	2453	214	0
3	C	1868	0	1907	55	0
4	D	847	0	836	16	0
All	All	10276	0	10316	372	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 18.

All (372) 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:114:ILE:O	2:B:117:PRO:HD2	1.38	1.24
2:B:263:CYS:O	2:B:267:PRO:HD2	1.38	1.20
2:B:113:LEU:HD23	2:B:240:TYR:O	1.44	1.17
2:B:141:SER:O	2:B:145:VAL:HG23	1.47	1.13
2:B:144:VAL:O	2:B:147:THR:HG22	1.44	1.12
2:B:113:LEU:CD2	2:B:240:TYR:O	2.00	1.09
2:B:114:ILE:C	2:B:117:PRO:HD2	1.73	1.08
2:B:264:PRO:O	2:B:267:PRO:HB2	1.53	1.07
2:B:263:CYS:C	2:B:267:PRO:HD2	1.76	1.05
2:B:263:CYS:O	2:B:266:GLY:N	1.89	1.05
2:B:261:VAL:HG13	2:B:431:ALA:O	1.57	1.05
2:B:140:ILE:O	2:B:144:VAL:HG23	1.57	1.04
2:B:114:ILE:O	2:B:117:PRO:CD	2.06	1.04
2:B:117:PRO:HA	2:B:135:ASN:HB2	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:THR:O	2:B:284:PRO:HD3	1.56	1.01
2:B:116:THR:HG22	2:B:138:ILE:CG2	1.92	0.99
2:B:108:ARG:HE	2:B:108:ARG:HA	1.29	0.96
2:B:263:CYS:O	2:B:267:PRO:CD	2.15	0.94
2:B:261:VAL:HA	2:B:265:LYS:HZ2	1.35	0.90
2:B:261:VAL:HG22	2:B:265:LYS:HZ1	1.36	0.89
2:B:116:THR:HB	2:B:135:ASN:O	1.74	0.88
2:B:149:LEU:HD23	2:B:150:LEU:N	1.89	0.87
2:B:260:ALA:O	2:B:264:PRO:HD2	1.77	0.85
2:B:265:LYS:HA	2:B:268:LEU:HB3	1.58	0.83
2:B:163:HIS:ND1	2:B:280:GLU:OE1	2.11	0.83
2:B:261:VAL:HG22	2:B:265:LYS:NZ	1.95	0.82
2:B:117:PRO:HA	2:B:135:ASN:CB	2.10	0.82
2:B:260:ALA:HA	2:B:264:PRO:HD2	1.62	0.82
3:C:179:PHE:HA	3:C:182:CYS:SG	2.20	0.81
2:B:116:THR:HG22	2:B:138:ILE:HB	1.62	0.81
2:B:261:VAL:HA	2:B:265:LYS:NZ	1.96	0.80
2:B:116:THR:HG22	2:B:138:ILE:CB	2.11	0.79
2:B:114:ILE:O	2:B:117:PRO:CG	2.30	0.79
2:B:264:PRO:O	2:B:267:PRO:CB	2.30	0.79
2:B:261:VAL:HG22	2:B:265:LYS:CE	2.14	0.78
2:B:281:THR:O	2:B:284:PRO:CD	2.32	0.78
2:B:147:THR:O	2:B:151:VAL:HG23	1.84	0.77
2:B:213:ILE:O	2:B:281:THR:CG2	2.33	0.77
2:B:144:VAL:O	2:B:147:THR:CG2	2.32	0.75
1:A:260:LEU:HD11	1:A:318:VAL:HG13	1.69	0.74
3:C:17:ALA:HB1	3:C:127:ILE:HD11	1.70	0.73
2:B:108:ARG:HG3	2:B:109:LYS:N	2.03	0.73
2:B:148:ILE:O	2:B:152:VAL:HG23	1.87	0.73
2:B:263:CYS:O	2:B:266:GLY:CA	2.35	0.73
2:B:110:ASP:C	2:B:113:LEU:HG	2.08	0.73
2:B:116:THR:HG22	2:B:138:ILE:HG22	1.70	0.72
2:B:466:TYR:HB2	3:C:204:THR:HG21	1.72	0.72
1:A:260:LEU:HD13	1:A:312:LEU:HD11	1.70	0.72
2:B:261:VAL:HA	2:B:265:LYS:CE	2.19	0.72
2:B:110:ASP:O	2:B:113:LEU:HG	1.90	0.72
2:B:213:ILE:O	2:B:281:THR:HG21	1.90	0.72
1:A:42:ILE:HD12	3:C:149:ILE:HG12	1.72	0.71
2:B:108:ARG:HG3	2:B:109:LYS:H	1.54	0.71
2:B:261:VAL:N	2:B:265:LYS:HE3	2.06	0.71
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD11	1:A:223:ALA:HB1	1.73	0.71
3:C:40:PHE:O	3:C:44:VAL:HG23	1.91	0.71
2:B:261:VAL:CA	2:B:265:LYS:HE3	2.21	0.70
2:B:116:THR:CG2	2:B:138:ILE:HB	2.21	0.70
2:B:112:GLN:O	2:B:113:LEU:HB2	1.93	0.69
2:B:113:LEU:HD22	2:B:240:TYR:O	1.91	0.69
2:B:108:ARG:HE	2:B:108:ARG:CA	2.04	0.69
2:B:104:SER:O	2:B:106:TYR:N	2.25	0.68
2:B:146:MET:HE2	2:B:149:LEU:HD22	1.75	0.68
2:B:257:ASP:O	2:B:261:VAL:HG23	1.94	0.67
2:B:150:LEU:C	2:B:150:LEU:HD13	2.14	0.67
2:B:117:PRO:CA	2:B:135:ASN:HB2	2.23	0.67
2:B:260:ALA:CA	2:B:264:PRO:HD2	2.25	0.67
2:B:82:VAL:HG22	2:B:422:LEU:HG	1.76	0.67
2:B:116:THR:CG2	2:B:138:ILE:HG22	2.25	0.67
2:B:149:LEU:HD23	2:B:149:LEU:C	2.15	0.67
2:B:116:THR:CB	2:B:135:ASN:O	2.42	0.66
1:A:282:LEU:HD11	1:A:567:VAL:HG21	1.77	0.66
2:B:108:ARG:HA	2:B:108:ARG:NE	2.08	0.66
1:A:55:ASN:N	1:A:58:HIS:O	2.29	0.66
1:A:653:TRP:CD1	1:A:656:ILE:HG23	2.31	0.66
2:B:466:TYR:CZ	3:C:163:LEU:HD23	2.31	0.66
2:B:279:ASN:HB2	2:B:280:GLU:HA	1.78	0.66
2:B:282:LEU:HD23	2:B:282:LEU:O	1.96	0.66
2:B:281:THR:C	2:B:284:PRO:HD3	2.17	0.65
2:B:261:VAL:HA	2:B:265:LYS:HE3	1.79	0.65
2:B:282:LEU:HD23	2:B:282:LEU:C	2.18	0.64
2:B:113:LEU:HD23	2:B:240:TYR:C	2.15	0.64
2:B:114:ILE:O	2:B:117:PRO:HG2	1.98	0.63
1:A:371:ARG:HH22	1:A:486:ALA:HB1	1.64	0.63
2:B:116:THR:CG2	2:B:138:ILE:CG2	2.74	0.63
1:A:397:LEU:HD21	1:A:439:VAL:HG23	1.82	0.62
1:A:36:VAL:HG21	3:C:137:ILE:HG22	1.80	0.62
2:B:186:PHE:HB3	4:D:95:THR:HG21	1.81	0.62
4:D:31:LEU:HD13	4:D:64:PHE:CE2	2.35	0.62
2:B:110:ASP:OD1	2:B:110:ASP:N	2.33	0.62
2:B:404:TRP:O	2:B:407:THR:HG22	2.00	0.61
1:A:183:LEU:HD12	1:A:189:THR:HG22	1.82	0.61
1:A:307:ALA:HB2	1:A:518:VAL:HG22	1.82	0.60
2:B:111:GLY:HA2	2:B:112:GLN:C	2.22	0.60
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:THR:HA	2:B:434:ALA:HB3	1.84	0.59
4:D:26:LEU:O	4:D:29:LEU:N	2.36	0.59
3:C:35:LEU:O	3:C:124:SER:HB2	2.03	0.58
2:B:465:PHE:HB3	3:C:205:PHE:HA	1.84	0.58
3:C:116:GLN:O	3:C:120:VAL:HG13	2.03	0.58
1:A:164:TRP:CH2	1:A:423:PRO:HA	2.38	0.58
3:C:159:THR:HG21	3:C:210:TYR:CD1	2.37	0.58
1:A:672:THR:HG23	3:C:158:LEU:HD13	1.84	0.58
1:A:280:THR:HG21	1:A:302:PHE:HA	1.85	0.58
2:B:116:THR:O	2:B:135:ASN:HB2	2.04	0.58
3:C:17:ALA:HB1	3:C:127:ILE:CD1	2.34	0.58
1:A:42:ILE:HD12	3:C:149:ILE:CG1	2.33	0.57
3:C:34:ILE:O	3:C:90:TYR:OH	2.19	0.57
2:B:88:PRO:CB	2:B:286:LEU:HD21	2.35	0.57
2:B:173:LEU:HD21	2:B:232:LEU:HD11	1.86	0.57
1:A:233:ARG:HD3	4:D:96:ILE:HG21	1.86	0.57
2:B:84:MET:O	2:B:88:PRO:CD	2.53	0.57
1:A:51:VAL:HG21	1:A:289:TRP:CD1	2.39	0.57
2:B:260:ALA:C	2:B:264:PRO:HD2	2.24	0.57
2:B:92:CYS:SG	2:B:390:SER:OG	2.46	0.57
2:B:141:SER:O	2:B:145:VAL:CG2	2.39	0.57
2:B:260:ALA:HA	2:B:264:PRO:CD	2.34	0.57
2:B:114:ILE:CB	2:B:117:PRO:CD	2.83	0.56
3:C:174:TRP:CH2	3:C:197:HIS:HA	2.40	0.56
1:A:63:GLN:NE2	1:A:221:MET:O	2.36	0.56
2:B:135:ASN:HD21	2:B:245:THR:CG2	2.18	0.56
2:B:100:ILE:HD11	2:B:238:ILE:HD13	1.87	0.56
2:B:173:LEU:HD21	2:B:232:LEU:CD1	2.36	0.56
2:B:114:ILE:CB	2:B:117:PRO:HD3	2.36	0.56
2:B:265:LYS:O	2:B:266:GLY:C	2.44	0.55
1:A:516:GLN:O	1:A:519:THR:HG22	2.07	0.55
2:B:186:PHE:O	2:B:190:ASN:N	2.40	0.55
2:B:151:VAL:O	2:B:154:TYR:N	2.38	0.55
2:B:116:THR:CG2	2:B:138:ILE:CB	2.83	0.54
4:D:22:GLY:HA3	4:D:30:TRP:NE1	2.22	0.54
2:B:114:ILE:C	2:B:117:PRO:CD	2.63	0.54
2:B:158:CYS:HB3	2:B:159:TYR:HA	1.89	0.54
2:B:261:VAL:CG1	2:B:431:ALA:O	2.43	0.54
1:A:162:ILE:HD11	1:A:164:TRP:CD2	2.42	0.54
1:A:309:ALA:HA	1:A:327:PHE:CZ	2.43	0.54
2:B:106:TYR:HA	2:B:239:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:ILE:HG13	3:C:83:GLN:HE22	1.72	0.54
2:B:200:LEU:HD13	4:D:71:LEU:HD13	1.90	0.54
2:B:218:PRO:HB3	4:D:36:TRP:CD1	2.42	0.54
1:A:632:SER:HB2	1:A:646:SER:OG	2.09	0.53
2:B:113:LEU:HA	2:B:240:TYR:HB3	1.91	0.53
2:B:425:LEU:O	2:B:429:LYS:N	2.42	0.53
1:A:260:LEU:HD13	1:A:312:LEU:CD1	2.38	0.53
1:A:152:TYR:CZ	1:A:383:VAL:HG11	2.44	0.53
2:B:110:ASP:HB3	2:B:113:LEU:HD11	1.90	0.53
1:A:365:LEU:N	1:A:365:LEU:HD12	2.24	0.52
2:B:465:PHE:CB	3:C:205:PHE:HA	2.39	0.52
3:C:8:GLY:O	3:C:12:VAL:HG23	2.09	0.52
1:A:401:LEU:HD11	1:A:439:VAL:HG21	1.91	0.52
2:B:223:GLN:O	2:B:227:ILE:HG23	2.09	0.52
2:B:261:VAL:CA	2:B:265:LYS:CE	2.85	0.52
2:B:261:VAL:CA	2:B:265:LYS:HZ2	2.17	0.52
1:A:256:VAL:HG21	1:A:567:VAL:HG12	1.91	0.52
2:B:214:HIS:HA	2:B:281:THR:HG21	1.92	0.52
2:B:187:LYS:HE3	4:D:95:THR:HG23	1.92	0.52
2:B:261:VAL:CG2	2:B:265:LYS:CE	2.85	0.52
2:B:268:LEU:HD13	2:B:269:ARG:N	2.24	0.52
3:C:42:TRP:CH2	3:C:46:LEU:HD12	2.45	0.52
3:C:42:TRP:CZ2	3:C:129:SER:HA	2.45	0.52
2:B:264:PRO:HA	2:B:267:PRO:HG2	1.92	0.52
3:C:11:PHE:O	3:C:15:GLY:HA3	2.10	0.52
2:B:150:LEU:HD22	2:B:150:LEU:O	2.10	0.51
2:B:157:ARG:HG2	2:B:158:CYS:C	2.30	0.51
1:A:147:VAL:HG22	1:A:428:GLN:HB2	1.92	0.51
1:A:423:PRO:HG2	1:A:440:VAL:HG11	1.93	0.51
2:B:116:THR:HG21	2:B:139:MET:N	2.26	0.51
3:C:176:VAL:HG11	3:C:228:ALA:HB1	1.91	0.51
2:B:204:ASN:O	2:B:208:VAL:HG13	2.10	0.51
1:A:277:VAL:HG11	1:A:362:PHE:CE2	2.46	0.51
2:B:151:VAL:O	2:B:154:TYR:HB2	2.11	0.51
1:A:282:LEU:HD12	1:A:302:PHE:CG	2.46	0.50
2:B:231:ALA:O	2:B:234:ALA:N	2.45	0.50
1:A:218:PHE:N	1:A:218:PHE:CD1	2.80	0.50
1:A:528:LYS:O	1:A:531:ASN:ND2	2.44	0.50
1:A:218:PHE:N	1:A:218:PHE:HD1	2.09	0.50
1:A:219:SER:HA	1:A:656:ILE:HG22	1.93	0.50
1:A:312:LEU:C	1:A:312:LEU:HD12	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:ALA:O	2:B:452:LEU:N	2.41	0.50
1:A:474:GLU:O	1:A:476:ASP:N	2.45	0.50
2:B:105:PHE:CZ	2:B:239:LYS:HE3	2.46	0.50
3:C:134:VAL:HG22	3:C:138:LEU:HD13	1.92	0.50
2:B:261:VAL:CG2	2:B:265:LYS:NZ	2.73	0.50
1:A:42:ILE:HD11	3:C:150:HIS:NE2	2.26	0.50
1:A:379:HIS:HB2	1:A:440:VAL:HB	1.94	0.50
2:B:163:HIS:O	2:B:167:ILE:HG23	2.12	0.49
2:B:284:PRO:CD	2:B:285:ALA:HA	2.42	0.49
1:A:523:TYR:CE1	1:A:527:ILE:HG21	2.46	0.49
3:C:200:THR:O	3:C:204:THR:HG23	2.12	0.49
2:B:265:LYS:CA	2:B:268:LEU:HB3	2.36	0.49
1:A:260:LEU:HD11	1:A:318:VAL:CG1	2.41	0.49
1:A:181:PHE:CD1	1:A:217:LEU:HD21	2.48	0.49
2:B:110:ASP:HB3	2:B:113:LEU:HD21	1.93	0.49
2:B:108:ARG:CG	2:B:109:LYS:N	2.76	0.49
2:B:143:ILE:O	2:B:146:MET:HB3	2.12	0.49
2:B:147:THR:HG23	2:B:148:ILE:N	2.28	0.49
2:B:435:LEU:N	2:B:436:PRO:HD2	2.27	0.49
3:C:25:VAL:HG13	3:C:31:ARG:HB3	1.95	0.49
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.95	0.49
1:A:492:THR:HG23	1:A:512:GLN:HA	1.95	0.48
2:B:260:ALA:O	2:B:264:PRO:CD	2.54	0.48
1:A:72:VAL:HG13	1:A:94:TYR:CD1	2.48	0.48
1:A:120:GLY:HA2	1:A:179:PRO:O	2.14	0.48
4:D:31:LEU:HD13	4:D:64:PHE:CZ	2.49	0.48
1:A:256:VAL:HG21	1:A:567:VAL:CG1	2.44	0.48
1:A:275:VAL:HG12	1:A:324:ASN:HB3	1.95	0.48
1:A:120:GLY:C	1:A:121:LEU:HD23	2.34	0.48
2:B:87:VAL:N	2:B:88:PRO:CD	2.76	0.48
2:B:194:ASP:HB3	4:D:78:PHE:CE1	2.49	0.48
2:B:183:GLY:O	2:B:187:LYS:HG2	2.13	0.48
1:A:486:ALA:O	1:A:490:VAL:HG23	2.13	0.48
2:B:198:VAL:HG21	4:D:94:PHE:CD2	2.49	0.48
2:B:261:VAL:CG2	2:B:265:LYS:HZ1	2.18	0.48
1:A:542:LEU:O	1:A:545:TYR:N	2.43	0.47
2:B:246:ALA:HA	2:B:249:ILE:HG22	1.96	0.47
2:B:250:LEU:HD11	2:B:443:LEU:HD21	1.95	0.47
2:B:416:ILE:HG12	3:C:40:PHE:CG	2.49	0.47
1:A:380:THR:HG21	1:A:398:LEU:HD11	1.95	0.47
1:A:181:PHE:CE1	1:A:217:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HB2	1:A:247:VAL:HG23	1.95	0.47
1:A:164:TRP:HB3	1:A:448:PHE:CE2	2.50	0.47
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.95	0.47
1:A:338:ILE:HG22	1:A:646:SER:OG	2.15	0.47
2:B:263:CYS:O	2:B:266:GLY:HA3	2.13	0.47
2:B:149:LEU:HD23	2:B:150:LEU:CA	2.45	0.47
2:B:265:LYS:O	2:B:268:LEU:N	2.48	0.47
2:B:284:PRO:N	2:B:285:ALA:HA	2.30	0.47
2:B:466:TYR:CE1	3:C:163:LEU:HD23	2.49	0.47
3:C:12:VAL:O	3:C:165:ALA:HB2	2.15	0.47
1:A:147:VAL:HG23	1:A:148:TYR:CD2	2.50	0.47
2:B:108:ARG:CA	2:B:108:ARG:NE	2.73	0.47
2:B:108:ARG:CG	2:B:109:LYS:H	2.25	0.47
2:B:144:VAL:C	2:B:147:THR:HG22	2.27	0.47
3:C:20:LEU:HB3	3:C:123:LEU:HD11	1.97	0.47
1:A:307:ALA:CB	1:A:518:VAL:HG22	2.44	0.46
1:A:368:VAL:HG11	1:A:490:VAL:HG11	1.97	0.46
2:B:116:THR:HG22	2:B:138:ILE:HG21	1.91	0.46
2:B:239:LYS:HG2	2:B:240:TYR:CE1	2.50	0.46
2:B:143:ILE:O	2:B:146:MET:CB	2.63	0.46
1:A:237:GLN:HB3	1:A:244:PRO:HB2	1.97	0.46
1:A:342:ARG:NE	1:A:632:SER:O	2.43	0.46
2:B:232:LEU:HA	2:B:235:LEU:HD12	1.97	0.46
2:B:383:LEU:O	2:B:386:PHE:HB3	2.15	0.46
2:B:209:GLY:O	2:B:213:ILE:HG12	2.15	0.46
2:B:261:VAL:CA	2:B:265:LYS:NZ	2.73	0.46
2:B:406:THR:HA	2:B:449:THR:HG21	1.97	0.45
3:C:216:PRO:O	3:C:220:VAL:HG23	2.16	0.45
4:D:22:GLY:HA3	4:D:30:TRP:CE2	2.52	0.45
2:B:84:MET:O	2:B:88:PRO:HD3	2.16	0.45
1:A:148:TYR:CZ	1:A:421:PRO:O	2.70	0.45
1:A:50:CYS:SG	1:A:62:CYS:N	2.90	0.45
1:A:299:VAL:HA	1:A:302:PHE:CE2	2.52	0.45
2:B:110:ASP:HB3	2:B:113:LEU:CG	2.47	0.45
2:B:385:ASP:HB2	2:B:435:LEU:HD13	1.99	0.45
2:B:157:ARG:HA	2:B:158:CYS:CB	2.45	0.45
2:B:200:LEU:CD1	4:D:71:LEU:HD13	2.46	0.45
2:B:386:PHE:HA	2:B:389:TYR:CD2	2.52	0.45
1:A:662:LEU:HD13	3:C:149:ILE:HA	1.99	0.45
2:B:412:VAL:HG11	3:C:43:LEU:CD1	2.46	0.45
1:A:396:ASP:O	1:A:400:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:PRO:HG2	2:B:265:LYS:H	1.82	0.44
1:A:534:PHE:CZ	1:A:566:VAL:HG11	2.53	0.44
1:A:215:MET:HA	1:A:660:ILE:HA	1.99	0.44
1:A:397:LEU:CD2	1:A:439:VAL:HG23	2.46	0.44
1:A:693:LYS:HD2	1:A:696:VAL:HG21	1.99	0.44
2:B:110:ASP:CB	2:B:113:LEU:HD11	2.48	0.44
2:B:177:PHE:HA	2:B:180:ILE:HD12	2.00	0.44
1:A:313:GLN:HG2	1:A:575:THR:O	2.17	0.44
1:A:282:LEU:HD12	1:A:302:PHE:CD2	2.53	0.44
2:B:108:ARG:O	2:B:109:LYS:HB2	2.17	0.44
3:C:170:LEU:HG	3:C:174:TRP:CZ2	2.53	0.44
1:A:44:LEU:CD1	1:A:192:ILE:HD11	2.48	0.44
1:A:295:ALA:HA	1:A:299:VAL:HB	2.00	0.44
1:A:457:TYR:C	1:A:459:THR:HG23	2.38	0.44
2:B:416:ILE:HD12	3:C:36:VAL:HG12	2.00	0.44
3:C:202:GLY:HA2	3:C:205:PHE:CD2	2.53	0.44
1:A:147:VAL:HG11	1:A:431:LEU:HB3	2.00	0.44
2:B:154:TYR:CD2	2:B:268:LEU:HD23	2.52	0.44
2:B:170:SER:HB3	2:B:282:LEU:HD11	2.00	0.44
1:A:309:ALA:HB2	1:A:327:PHE:CD2	2.52	0.44
2:B:116:THR:C	2:B:135:ASN:HB2	2.37	0.44
2:B:434:ALA:O	2:B:437:ILE:HG22	2.18	0.44
1:A:560:PRO:HG2	1:A:565:TYR:CZ	2.53	0.44
1:A:596:ASN:HD22	1:A:599:LEU:HD13	1.83	0.44
1:A:199:HIS:NE2	1:A:662:LEU:HD21	2.33	0.43
1:A:330:PHE:CD2	1:A:340:SER:HA	2.53	0.43
1:A:341:SER:HA	1:A:429:ARG:HD2	1.99	0.43
2:B:85:LEU:HD13	2:B:422:LEU:CD2	2.48	0.43
3:C:156:TYR:CD1	3:C:157:PHE:N	2.86	0.43
2:B:84:MET:O	2:B:88:PRO:HD2	2.18	0.43
2:B:417:GLY:HA3	2:B:438:SER:HA	1.99	0.43
3:C:134:VAL:O	3:C:135:ILE:C	2.56	0.43
2:B:137:ALA:HA	2:B:140:ILE:HD12	1.99	0.43
3:C:20:LEU:HB2	3:C:123:LEU:HD21	2.01	0.43
2:B:434:ALA:HB1	2:B:437:ILE:HG22	1.99	0.43
2:B:109:LYS:O	2:B:239:LYS:NZ	2.52	0.43
2:B:135:ASN:ND2	2:B:245:THR:OG1	2.51	0.43
2:B:174:LEU:O	2:B:178:SER:HB3	2.19	0.43
2:B:89:VAL:HG22	2:B:386:PHE:CD2	2.54	0.43
2:B:282:LEU:C	2:B:282:LEU:CD2	2.85	0.43
1:A:85:VAL:HG11	1:A:118:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASP:OD2	1:A:332:GLY:N	2.50	0.42
2:B:163:HIS:CG	2:B:280:GLU:OE1	2.70	0.42
2:B:186:PHE:CB	4:D:95:THR:HG21	2.49	0.42
1:A:456:ILE:HD12	1:A:456:ILE:N	2.34	0.42
2:B:247:TRP:CZ2	2:B:395:LYS:HB3	2.54	0.42
1:A:560:PRO:O	1:A:561:THR:HG22	2.19	0.42
2:B:405:ASN:OD1	3:C:136:ASN:ND2	2.52	0.42
3:C:162:PHE:HB3	3:C:214:LEU:HD11	2.00	0.42
2:B:381:LEU:HD22	2:B:382:GLY:N	2.35	0.42
2:B:412:VAL:HG11	3:C:43:LEU:HD12	2.01	0.42
3:C:162:PHE:CB	3:C:214:LEU:HD21	2.49	0.42
1:A:632:SER:HB2	1:A:646:SER:HG	1.84	0.42
2:B:260:ALA:O	2:B:265:LYS:HG2	2.20	0.42
1:A:86:LEU:O	1:A:117:ARG:NE	2.52	0.42
1:A:199:HIS:CE1	1:A:662:LEU:HD21	2.54	0.42
2:B:99:THR:CG2	2:B:235:LEU:HD21	2.50	0.42
1:A:86:LEU:HA	1:A:117:ARG:HD3	2.01	0.42
1:A:252:SER:CB	1:A:631:LEU:HA	2.50	0.42
2:B:153:LEU:HD23	2:B:162:ILE:HB	2.01	0.42
1:A:378:MET:CE	1:A:413:LEU:HD22	2.50	0.42
2:B:261:VAL:HG13	2:B:265:LYS:NZ	2.35	0.42
2:B:417:GLY:HA3	2:B:438:SER:CB	2.49	0.42
2:B:93:MET:O	2:B:97:VAL:HG23	2.19	0.42
2:B:142:VAL:O	2:B:146:MET:HB2	2.20	0.42
3:C:91:TYR:CE2	3:C:182:CYS:HB2	2.54	0.42
1:A:182:LEU:HB2	1:A:288:PHE:CG	2.55	0.41
2:B:114:ILE:CB	2:B:117:PRO:HD2	2.50	0.41
2:B:208:VAL:O	2:B:211:ILE:HG13	2.20	0.41
2:B:285:ALA:HB1	2:B:383:LEU:HG	2.02	0.41
3:C:38:GLY:O	3:C:125:PHE:CE1	2.73	0.41
3:C:47:LEU:O	3:C:51:VAL:HG23	2.20	0.41
3:C:162:PHE:HB3	3:C:214:LEU:HD21	2.02	0.41
1:A:269:LEU:HD23	1:A:358:ASN:ND2	2.34	0.41
1:A:542:LEU:O	1:A:544:SER:N	2.54	0.41
1:A:256:VAL:HG22	1:A:329:PHE:HB2	2.01	0.41
1:A:332:GLY:O	1:A:334:THR:N	2.53	0.41
1:A:385:GLN:O	1:A:391:ARG:HB2	2.20	0.41
2:B:224:ALA:O	2:B:227:ILE:HG12	2.21	0.41
1:A:76:VAL:HG13	1:A:81:ASP:HB2	2.02	0.41
2:B:87:VAL:HB	2:B:88:PRO:HD3	2.03	0.41
2:B:252:VAL:O	2:B:256:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:ASN:N	3:C:208:PRO:CD	2.83	0.41
4:D:27:PRO:HG3	4:D:67:TRP:CG	2.55	0.41
1:A:664:ALA:HB1	1:A:668:LEU:HD22	2.02	0.41
1:A:62:CYS:SG	1:A:180:ILE:HD12	2.60	0.41
1:A:210:PHE:CD1	1:A:665:SER:HA	2.56	0.41
2:B:166:LEU:HB3	2:B:282:LEU:HD13	2.03	0.41
1:A:127:LYS:N	1:A:128:PRO:HD2	2.36	0.41
2:B:421:THR:HG23	2:B:434:ALA:HB3	2.01	0.41
1:A:273:ASP:O	1:A:358:ASN:ND2	2.53	0.41
2:B:167:ILE:HG22	2:B:214:HIS:NE2	2.36	0.41
3:C:18:PHE:CZ	3:C:22:LEU:HD11	2.56	0.41
1:A:421:PRO:O	1:A:422:LEU:CB	2.69	0.41
2:B:83:ILE:O	2:B:87:VAL:HG23	2.20	0.41
3:C:80:VAL:HG13	3:C:197:HIS:ND1	2.36	0.41
4:D:97:PRO:O	4:D:98:LEU:C	2.59	0.41
2:B:432:LEU:HD22	2:B:435:LEU:HD11	2.03	0.41
2:B:285:ALA:CB	2:B:383:LEU:HB2	2.51	0.40
3:C:166:ALA:O	3:C:170:LEU:HB2	2.21	0.40
1:A:632:SER:OG	1:A:634:ALA:N	2.54	0.40
2:B:150:LEU:C	2:B:150:LEU:CD1	2.85	0.40
2:B:239:LYS:HG3	2:B:240:TYR:CD1	2.56	0.40
1:A:164:TRP:CH2	1:A:423:PRO:CA	3.04	0.40
2:B:159:TYR:O	2:B:161:VAL:N	2.54	0.40
3:C:80:VAL:HG11	3:C:198:LEU:HD12	2.03	0.40
1:A:210:PHE:N	1:A:211:PRO:CD	2.84	0.40
1:A:280:THR:HG21	1:A:302:PHE:CA	2.50	0.40
2:B:96:VAL:HG21	2:B:390:SER:HB3	2.03	0.40
2:B:114:ILE:CA	2:B:117:PRO:HD2	2.46	0.40
1:A:164:TRP:CZ2	1:A:423:PRO:HA	2.56	0.40
1:A:362:PHE:CD1	1:A:427:LEU:HD13	2.56	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%)	528 (80%)	102 (15%)	33 (5%)	2 23
2	B	297/467 (64%)	262 (88%)	20 (7%)	15 (5%)	2 22
3	C	241/265 (91%)	217 (90%)	22 (9%)	2 (1%)	19 60
4	D	98/101 (97%)	86 (88%)	11 (11%)	1 (1%)	15 54
All	All	1299/1542 (84%)	1093 (84%)	155 (12%)	51 (4%)	5 27

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	TRP
1	A	333	GLU
1	A	422	LEU
1	A	472	SER
1	A	475	GLU
1	A	511	VAL
1	A	558	SER
1	A	646	SER
2	B	122	THR
2	B	160	LYS
2	B	263	CYS
3	C	156	TYR
1	A	159	CYS
1	A	248	CYS
1	A	336	ASP
1	A	358	ASN
1	A	436	ILE
1	A	543	ARG
2	B	104	SER
2	B	105	PHE
2	B	216	LYS
1	A	63	GLN
1	A	89	GLY
1	A	179	PRO
1	A	253	ASP
1	A	294	GLY
1	A	530	ASN
1	A	559	SER
1	A	561	THR
1	A	632	SER

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Mol	Chain	Res	Type
2	B	158	CYS
2	B	276	GLN
1	A	371	ARG
1	A	633	PRO
1	A	640	TRP
1	A	643	THR
2	B	159	TYR
2	B	446	TYR
4	D	98	LEU
1	A	210	PHE
1	A	332	GLY
1	A	473	PRO
1	A	595	GLU
1	A	655	ASP
2	B	153	LEU
2	B	231	ALA
2	B	431	ALA
2	B	113	LEU
2	B	403	ASP
1	A	68	GLY
3	C	112	ILE

5.3.2 Protein sidechains (i)

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%)	529 (91%)	54 (9%)	9 31
2	B	250/408 (61%)	208 (83%)	42 (17%)	2 14
3	C	192/214 (90%)	170 (88%)	22 (12%)	5 24
4	D	87/89 (98%)	80 (92%)	7 (8%)	12 38
All	All	1112/1323 (84%)	987 (89%)	125 (11%)	9 25

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

Mol	Chain	Res	Type
1	A	50	CYS
1	A	53	LEU
1	A	54	LEU
1	A	80	GLU
1	A	81	ASP
1	A	84	TRP
1	A	97	LEU
1	A	111	LEU
1	A	121	LEU
1	A	134	PHE
1	A	139	GLN
1	A	140	CYS
1	A	147	VAL
1	A	210	PHE
1	A	218	PHE
1	A	224	VAL
1	A	231	MET
1	A	256	VAL
1	A	264	ASN
1	A	269	LEU
1	A	280	THR
1	A	285	ARG
1	A	296	GLU
1	A	312	LEU
1	A	326	MET
1	A	342	ARG
1	A	347	MET
1	A	367	GLN
1	A	370	LEU
1	A	413	LEU
1	A	425	SER
1	A	443	ASP
1	A	450	ASN
1	A	457	TYR
1	A	464	ASN
1	A	474	GLU
1	A	481	THR
1	A	506	ASN
1	A	520	ARG
1	A	522	LEU
1	A	534	PHE
1	A	537	ILE
1	A	561	THR

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Mol	Chain	Res	Type
1	A	565	TYR
1	A	574	LEU
1	A	577	THR
1	A	586	CYS
1	A	587	GLN
1	A	588	ASP
1	A	632	SER
1	A	641	SER
1	A	643	THR
1	A	677	PHE
1	A	689	CYS
2	B	83	ILE
2	B	91	LEU
2	B	92	CYS
2	B	108	ARG
2	B	110	ASP
2	B	115	TYR
2	B	122	THR
2	B	133	ILE
2	B	135	ASN
2	B	146	MET
2	B	149	LEU
2	B	150	LEU
2	B	153	LEU
2	B	158	CYS
2	B	167	ILE
2	B	171	LEU
2	B	174	LEU
2	B	184	GLU
2	B	200	LEU
2	B	201	LEU
2	B	219	LEU
2	B	222	GLN
2	B	229	ILE
2	B	230	SER
2	B	232	LEU
2	B	244	TRP
2	B	250	LEU
2	B	255	VAL
2	B	257	ASP
2	B	267	PRO
2	B	268	LEU

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Mol	Chain	Res	Type
2	B	270	MET
2	B	283	PHE
2	B	287	ILE
2	B	383	LEU
2	B	390	SER
2	B	407	THR
2	B	408	ILE
2	B	416	ILE
2	B	419	CYS
2	B	422	LEU
2	B	459	GLN
3	C	28	ASP
3	C	35	LEU
3	C	46	LEU
3	C	56	LEU
3	C	93	LEU
3	C	104	LEU
3	C	109	ARG
3	C	112	ILE
3	C	120	VAL
3	C	123	LEU
3	C	124	SER
3	C	127	ILE
3	C	133	SER
3	C	134	VAL
3	C	138	LEU
3	C	140	ASP
3	C	159	THR
3	C	162	PHE
3	C	170	LEU
3	C	182	CYS
3	C	207	ASN
3	C	218	TYR
4	D	12	LEU
4	D	13	ASN
4	D	39	ARG
4	D	50	GLN
4	D	66	PHE
4	D	67	TRP
4	D	75	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	91	ASN
1	A	142	ASN
1	A	237	GLN
1	A	462	ASN
1	A	596	ASN
2	B	135	ASN
3	C	136	ASN
3	C	207	ASN

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 monosaccharides 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.

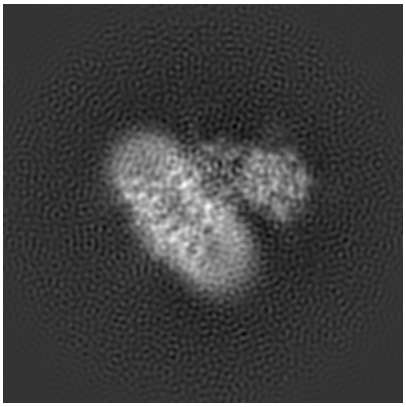
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3237. These allow visual inspection of the internal detail of the map and identification of artifacts.

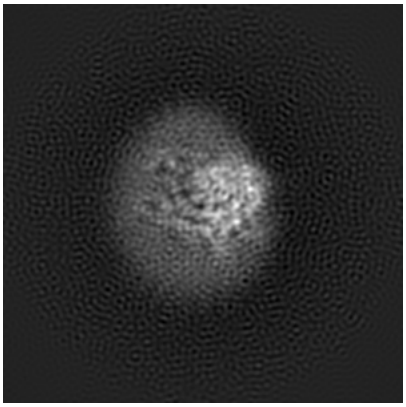
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

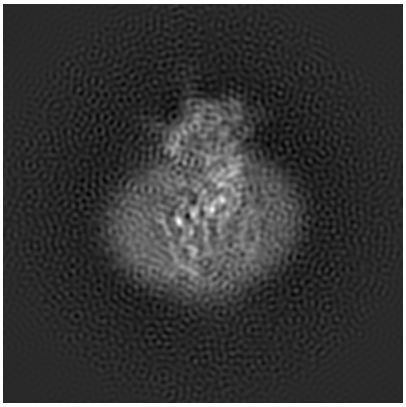
6.1.1 Primary map



X



Y

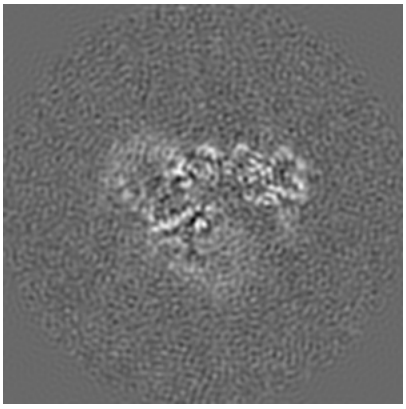


Z

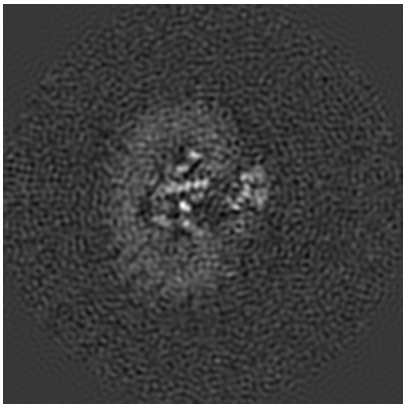
The images above show the map projected in three orthogonal directions.

6.2 Central slices

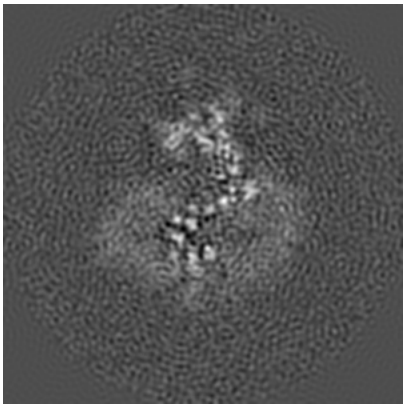
6.2.1 Primary map



X Index: 90



Y Index: 90

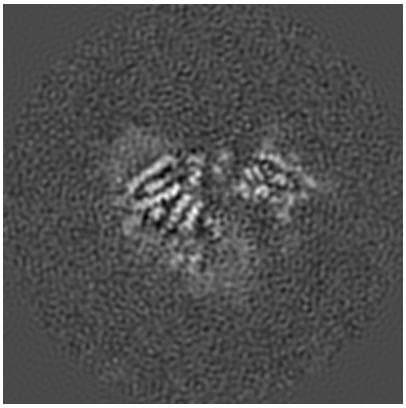


Z Index: 90

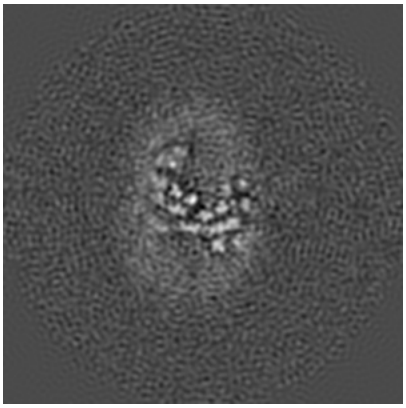
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

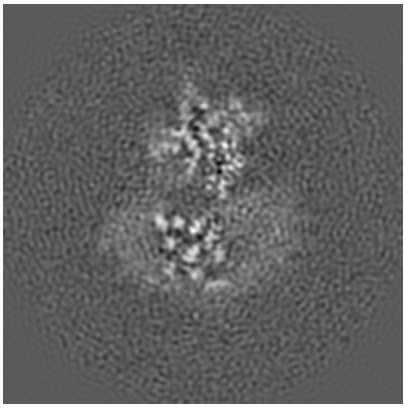
6.3.1 Primary map



X Index: 85



Y Index: 81



Z Index: 97

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

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.

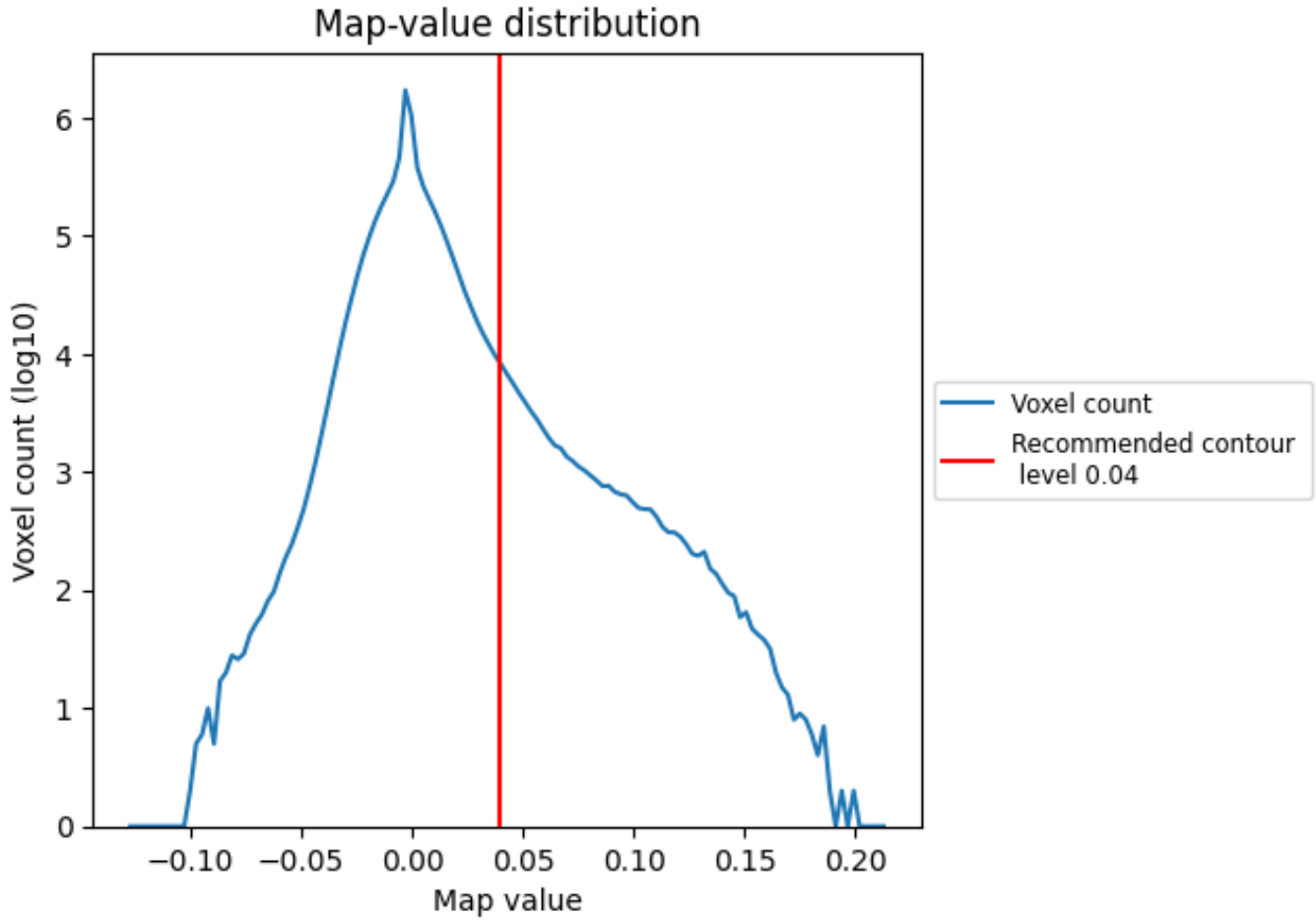
6.5 Mask visualisation (i)

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

7 Map analysis

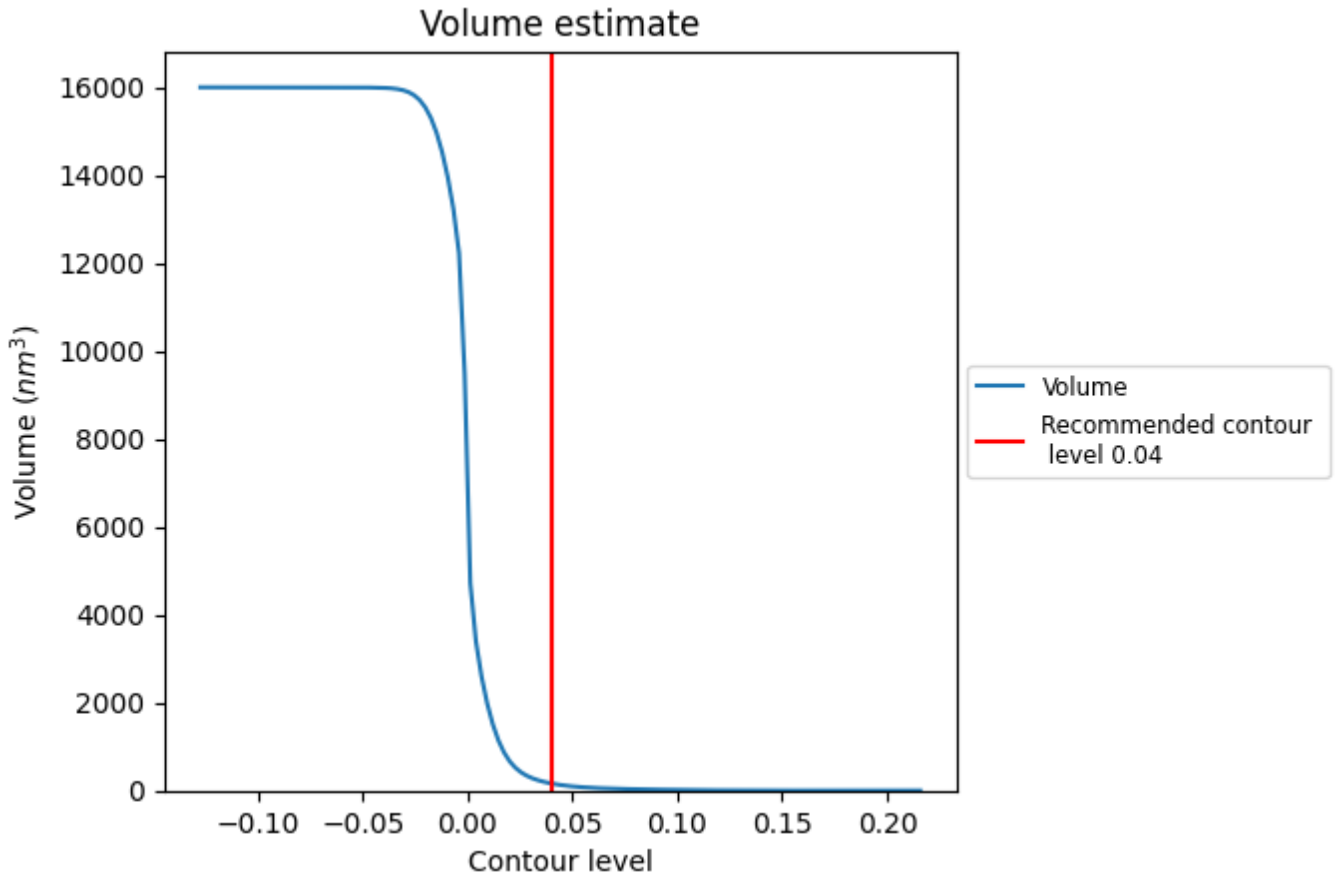
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

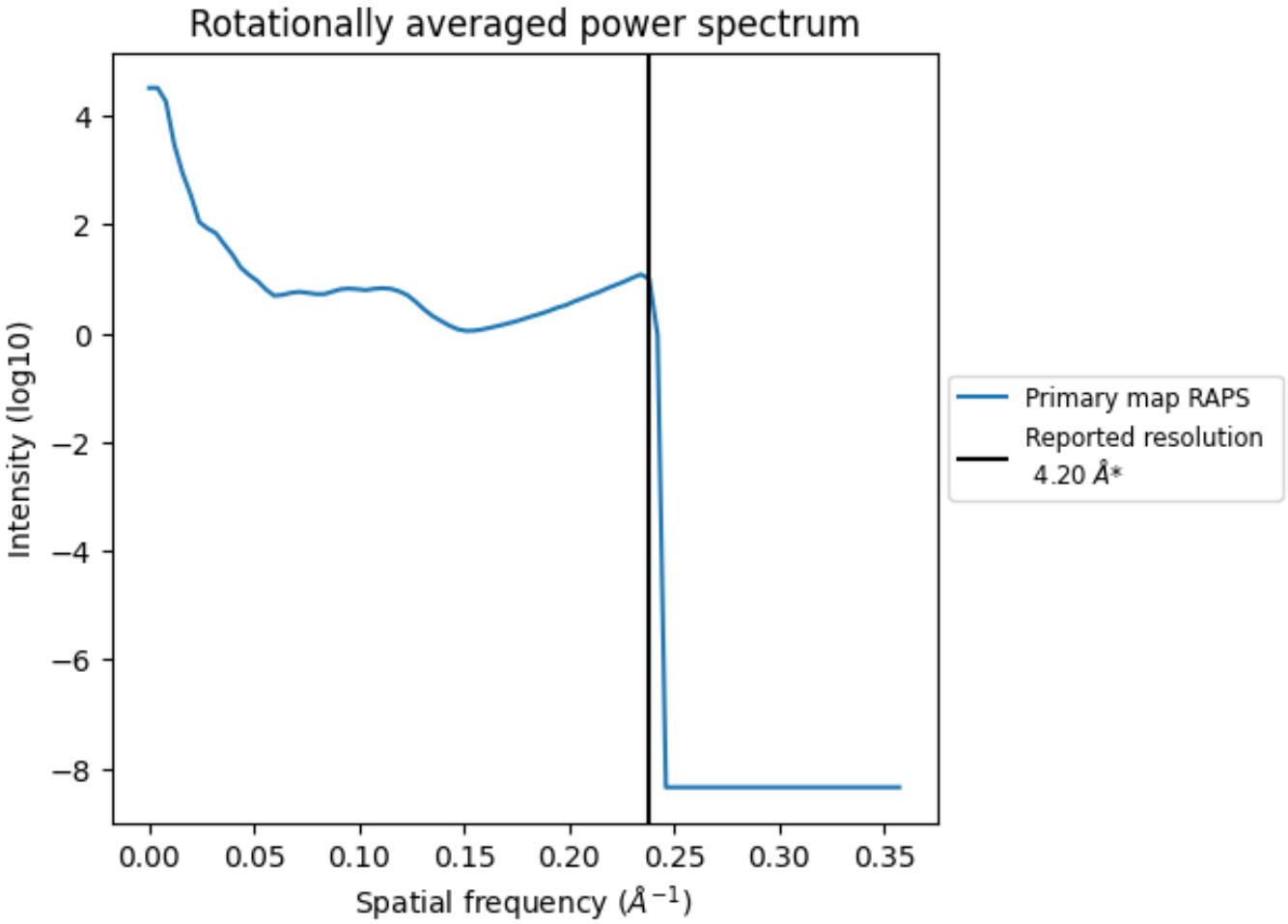
7.2 Volume estimate



The volume at the recommended contour level is 162 nm^3; this corresponds to an approximate mass of 146 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 (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

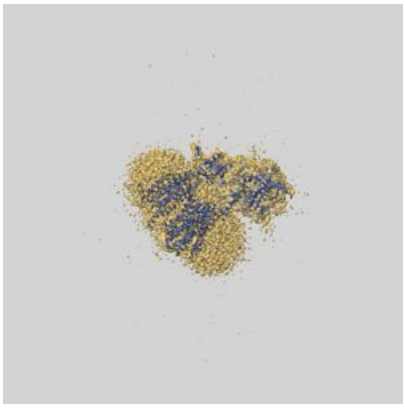
8 Fourier-Shell correlation (i)

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

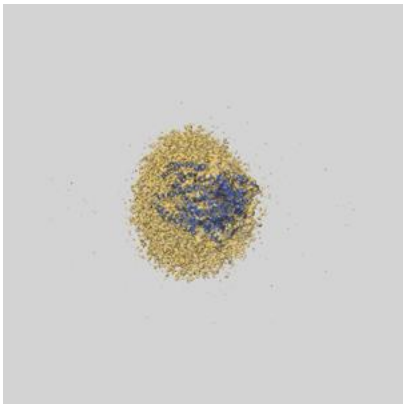
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3237 and PDB model 5FN2. Per-residue inclusion information can be found in section 3 on page 4.

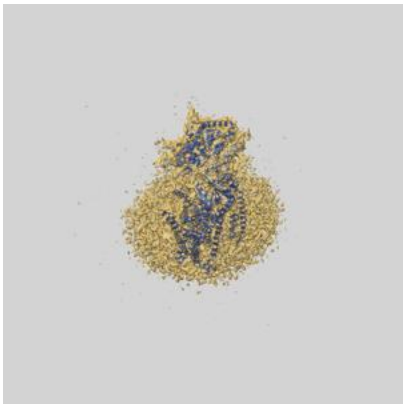
9.1 Map-model overlay



X



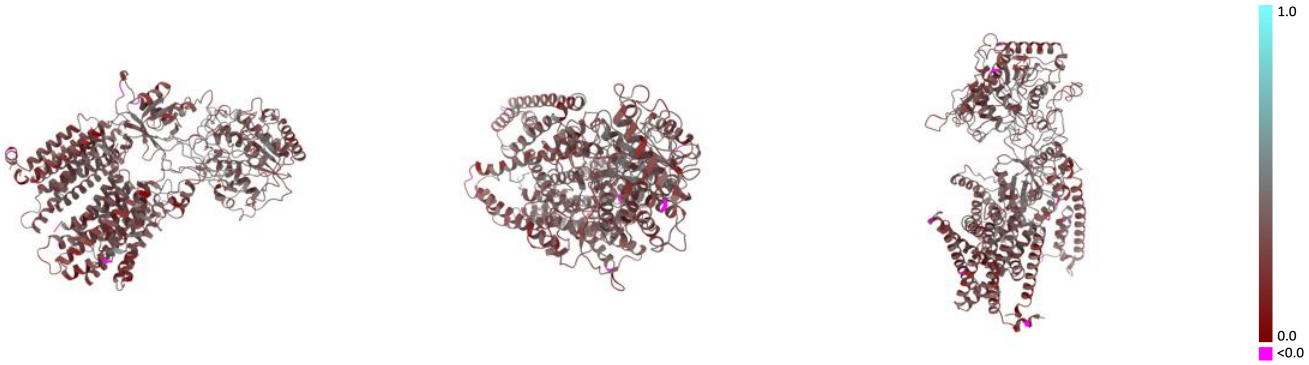
Y



Z

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

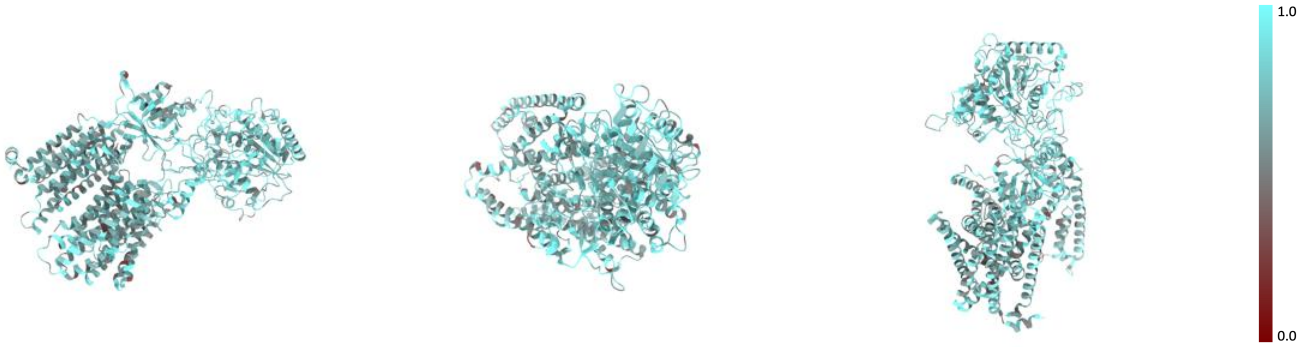
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

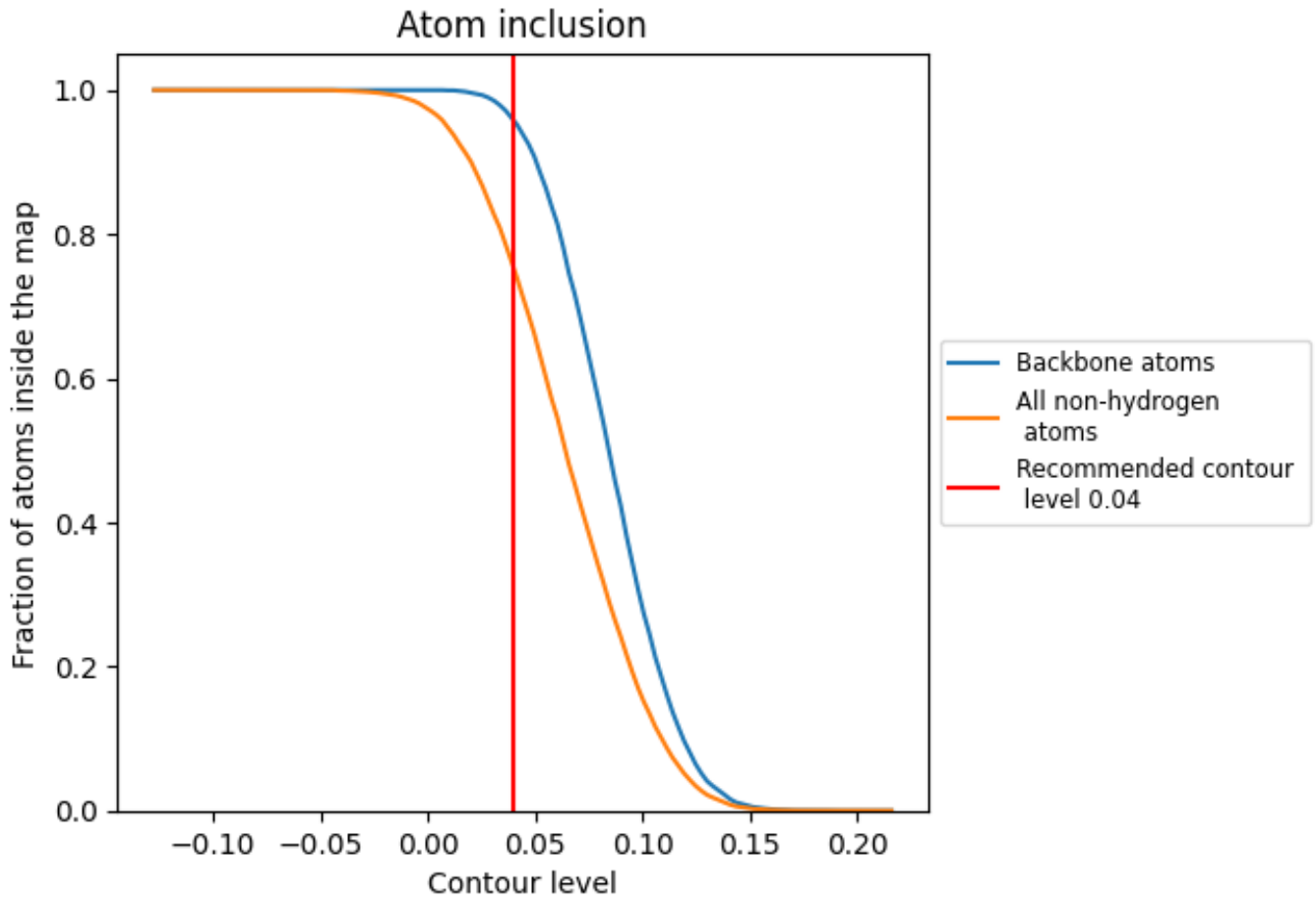
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 75% 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	0.7524	0.3230
A	0.7852	0.3450
B	0.7196	0.3080
C	0.7193	0.2960
D	0.7132	0.2910