Full wwPDB EM Validation Report ⓘ

Sep 9, 2024 – 08:48 AM EDT

PDB ID	:	8VUR
EMDB ID	:	EMD-43537
Title	:	Human GluN1-2A with IgG 003-102 WT conformation
Authors	:	Michalski, K.; Furukawa, H.
Deposited on	:	2024-01-29
Resolution	:	3.84 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:

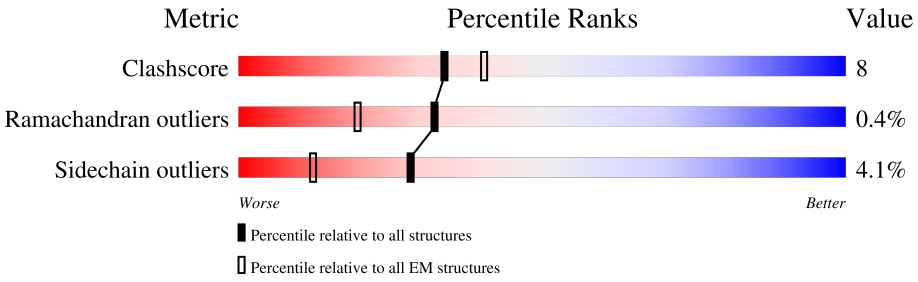
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 3.84 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	815	6% 77% 19%
2	B	808	8% 79% 17%
2	D	808	7% 77% 18%
3	C	815	7% 78% 18%
4	H	234	88% 12%
5	L	218	91% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24978 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	787	Total	C	N	O	S	0	0
			5778	3679	1012	1059	28		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	781	Total	C	N	O	S	0	0
			5547	3569	949	1002	27		
2	D	780	Total	C	N	O	S	0	0
			5412	3508	925	955	24		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	578I	CYS	ASN	conflict	UNP Q12879
B	578L	ASP	LYS	conflict	UNP Q12879
B	578N	ARG	LYS	conflict	UNP Q12879
B	578O	GLU	ALA	conflict	UNP Q12879
B	578Q	GLY	HIS	conflict	UNP Q12879
D	578I	CYS	ASN	conflict	UNP Q12879
D	578L	ASP	LYS	conflict	UNP Q12879
D	578N	ARG	LYS	conflict	UNP Q12879
D	578O	GLU	ALA	conflict	UNP Q12879
D	578Q	GLY	HIS	conflict	UNP Q12879

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	787	Total	C	N	O	S	0	0
			5496	3504	973	996	23		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	54	ALA	GLY	conflict	UNP Q05586
C	358	ARG	ASN	conflict	UNP Q05586

- Molecule 4 is a protein called 003-102 Heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	234	Total	C	N	O	S	0	0
			1456	912	269	271	4		

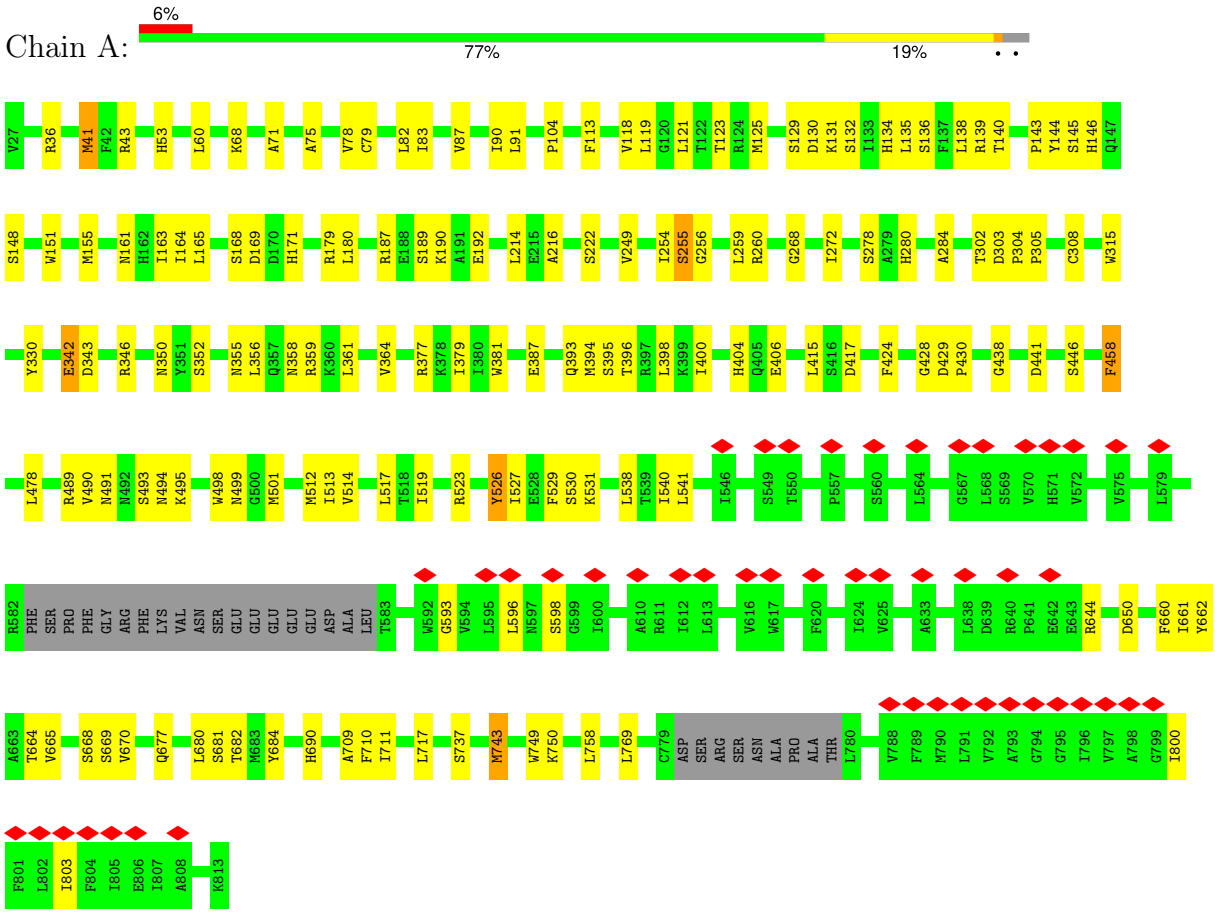
- Molecule 5 is a protein called 003-102 Light.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	218	Total	C	N	O	S	0	0
			1289	802	226	256	5		

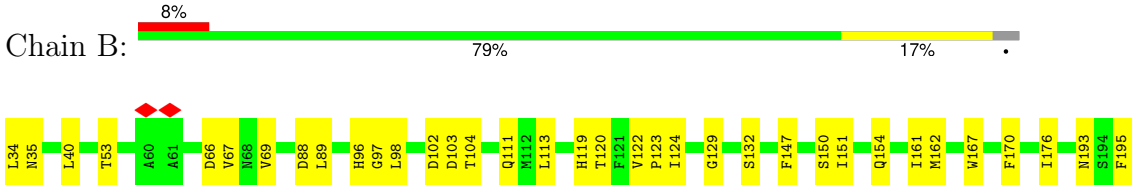
3 Residue-property plots (i)

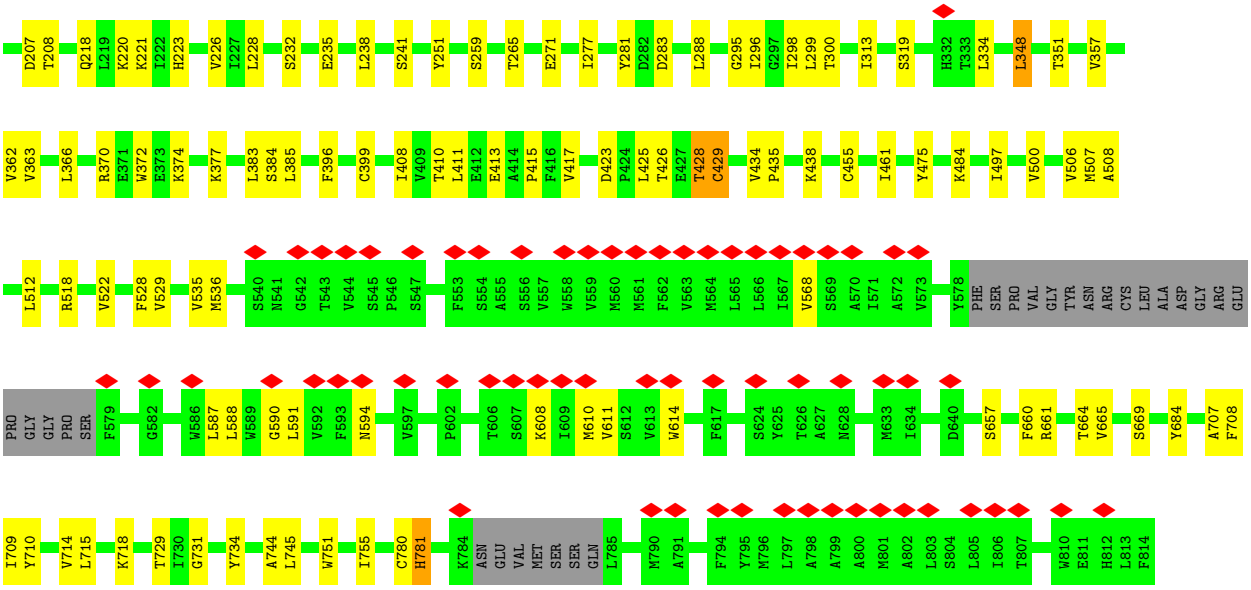
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Glutamate receptor ionotropic, NMDA 1



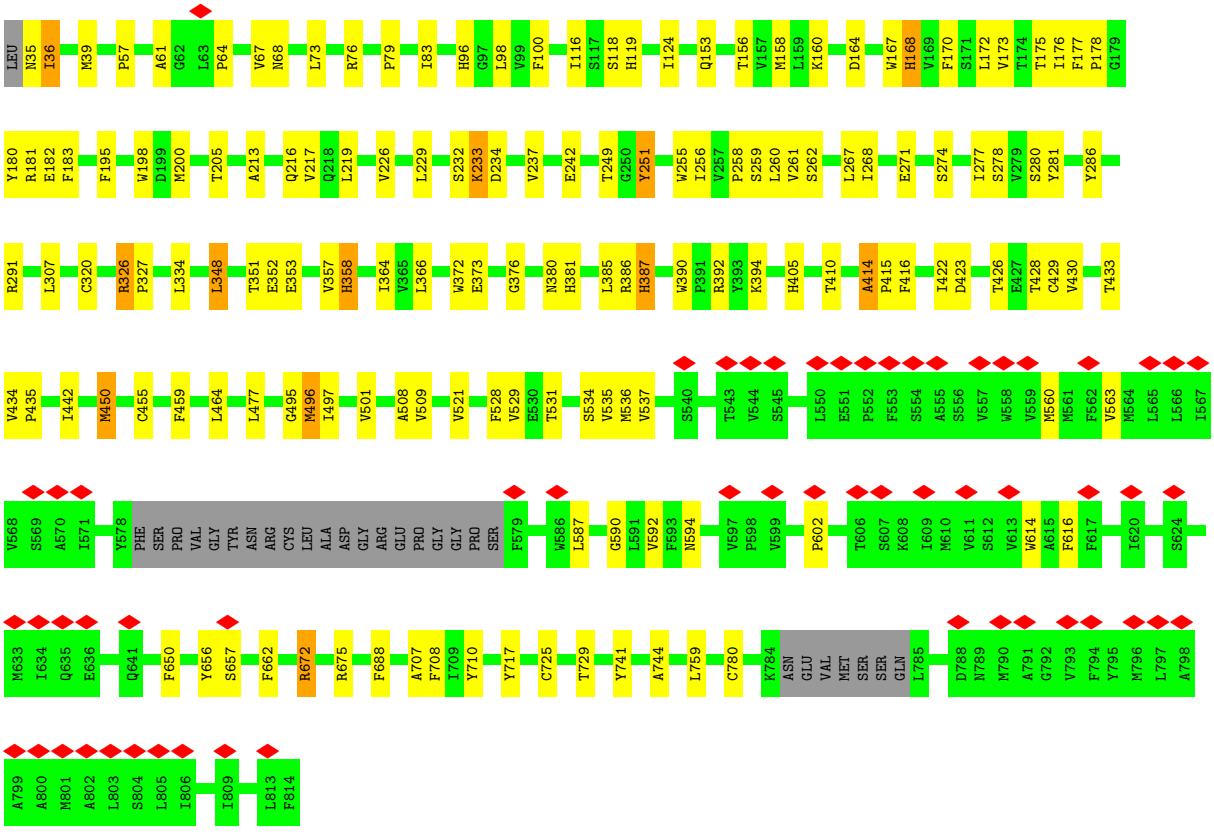
• Molecule 2: Glutamate receptor ionotropic, NMDA 2A





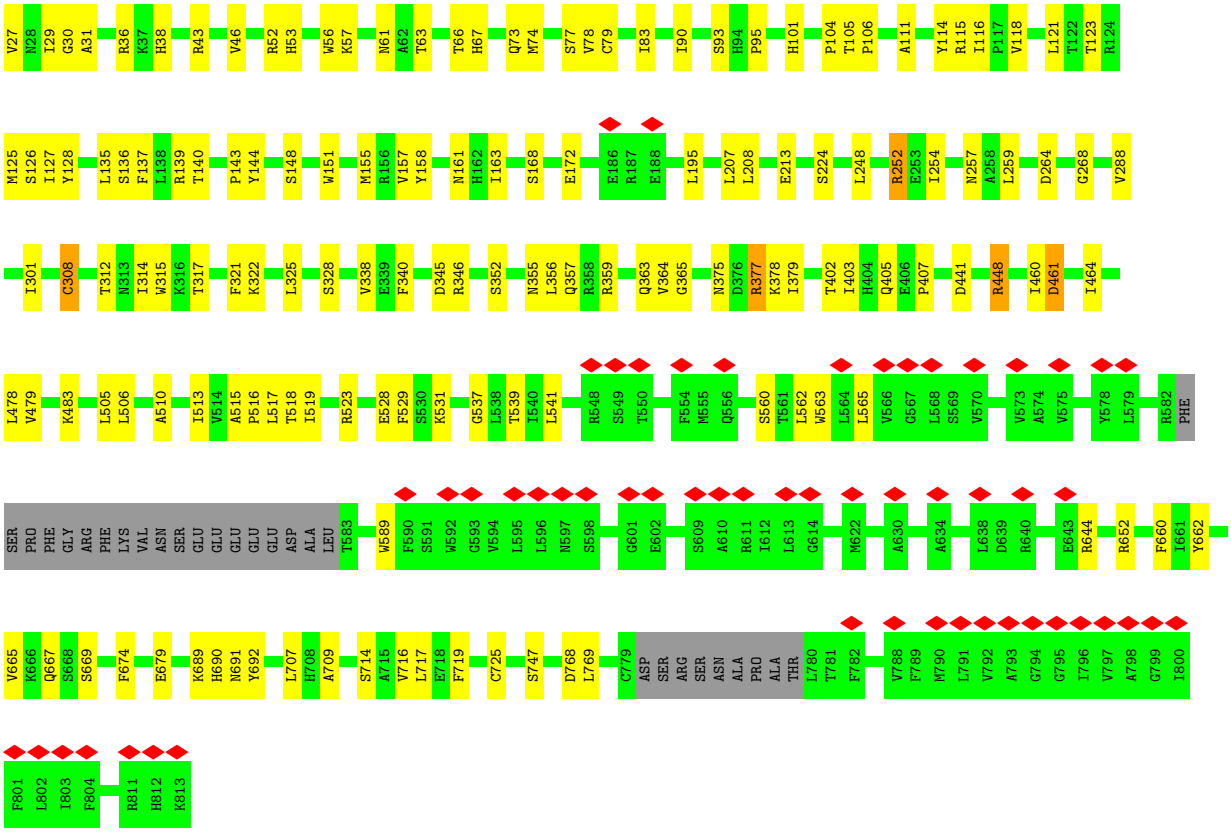
• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain D:



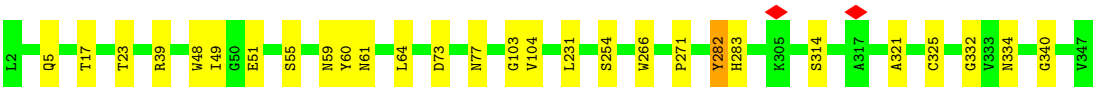
• Molecule 3: Glutamate receptor ionotropic, NMDA 1

Chain C:



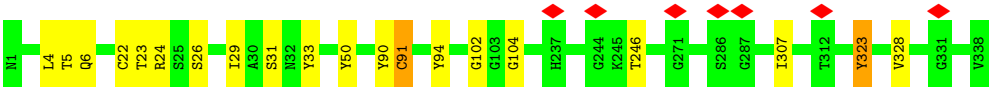
• Molecule 4: 003-102 Heavy

Chain H:



• Molecule 5: 003-102 Light

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133432	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.743	Depositor
Minimum map value	-0.426	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0509	Depositor
Map size (Å)	342.4, 342.4, 342.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.856, 0.856, 0.856	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	0.26	0/5903	0.50	0/8045
2	B	0.26	0/5673	0.48	1/7762 (0.0%)
2	D	0.25	0/5538	0.48	1/7600 (0.0%)
3	C	0.25	0/5618	0.47	0/7701
4	H	0.24	0/1495	0.49	0/2071
5	L	0.27	0/1315	0.49	0/1821
All	All	0.26	0/25542	0.48	2/35000 (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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	89	LEU	CA-CB-CG	6.62	130.53	115.30
2	D	348	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	428	THR	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	5778	0	5401	98	0
2	B	5547	0	5008	85	0
2	D	5412	0	4730	88	0
3	C	5496	0	4885	87	0
4	H	1456	0	1037	18	0
5	L	1289	0	871	12	0
All	All	24978	0	21932	374	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 8.

All (374) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:MET:HB3	1:A:513:ILE:HD11	1.67	0.76
1:A:512:MET:HG2	1:A:514:VAL:HG23	1.71	0.72
2:B:271:GLU:N	2:B:271:GLU:OE2	2.24	0.70
3:C:148:SER:HA	3:C:151:TRP:HD1	1.57	0.70
2:B:34:LEU:HD23	2:B:96:HIS:HD2	1.57	0.69
2:D:258:PRO:O	2:D:260:LEU:N	2.26	0.69
1:A:381:TRP:NE1	1:A:387:GLU:O	2.25	0.69
3:C:93:SER:HB2	3:C:121:LEU:HD12	1.74	0.69
1:A:441:ASP:HB2	1:A:446:SER:HB3	1.75	0.69
1:A:359:ARG:NH1	4:H:103:GLY:O	2.26	0.68
2:D:39:MET:HG3	2:D:98:LEU:HD11	1.73	0.68
2:D:251:TYR:O	2:D:392:ARG:NH1	2.25	0.68
3:C:155:MET:HG3	3:C:163:ILE:HD11	1.76	0.68
5:L:24:ARG:HD3	5:L:29:ILE:HD11	1.76	0.68
2:B:425:LEU:HG	2:B:426:THR:HG22	1.77	0.67
3:C:27:VAL:N	3:C:57:LYS:O	2.26	0.67
1:A:119:LEU:HD12	1:A:138:LEU:HB2	1.77	0.67
1:A:130:ASP:O	1:A:132:SER:N	2.26	0.67
1:A:364:VAL:HG21	1:A:379:ILE:HG23	1.76	0.66
2:B:40:LEU:HD11	2:B:288:LEU:HD21	1.78	0.66
2:B:590:GLY:O	2:B:594:ASN:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:GLN:NE2	2:D:242:GLU:OE2	2.28	0.65
3:C:195:LEU:HB3	3:C:207:LEU:HD11	1.79	0.65
2:D:508:ALA:HB3	2:D:744:ALA:HB3	1.78	0.65
1:A:155:MET:HE2	1:A:163:ILE:HG21	1.79	0.65
1:A:255:SER:OG	1:A:256:GLY:N	2.29	0.65
1:A:800:ILE:HA	1:A:803:ILE:HD12	1.80	0.64
2:D:326:ARG:HG2	2:D:327:PRO:HD2	1.79	0.64
2:B:34:LEU:N	2:B:66:ASP:O	2.31	0.64
2:D:536:MET:HA	2:D:729:THR:HA	1.81	0.63
2:B:232:SER:HB3	2:B:235:GLU:HG3	1.81	0.63
3:C:301:ILE:HA	3:C:317:THR:HG21	1.81	0.62
2:B:34:LEU:HB2	2:B:67:VAL:HG12	1.81	0.62
3:C:312:THR:HG21	2:D:76:ARG:HB3	1.82	0.62
3:C:505:LEU:HD22	3:C:513:ILE:HG21	1.80	0.62
1:A:41:MET:SD	1:A:278:SER:OG	2.51	0.62
2:D:392:ARG:HH21	2:D:405:HIS:HB2	1.65	0.62
3:C:36:ARG:O	3:C:36:ARG:NH1	2.33	0.61
4:H:73:ASP:O	4:H:77:ASN:N	2.33	0.61
3:C:505:LEU:HA	3:C:510:ALA:HA	1.83	0.61
1:A:91:LEU:HD23	1:A:119:LEU:HB3	1.82	0.61
1:A:523:ARG:HH12	1:A:669:SER:HB2	1.64	0.60
1:A:358:ASN:ND2	4:H:51:GLU:OE1	2.33	0.60
3:C:363:GLN:NE2	3:C:365:GLY:O	2.34	0.60
4:H:39:ARG:HD3	4:H:49:ILE:HD11	1.83	0.60
3:C:135:LEU:O	3:C:322:LYS:NZ	2.35	0.60
3:C:137:PHE:HE2	3:C:139:ARG:HD3	1.66	0.60
2:B:408:ILE:HD12	2:B:408:ILE:H	1.67	0.60
3:C:83:ILE:HG21	3:C:308:CYS:HB3	1.84	0.60
3:C:144:TYR:OH	3:C:252:ARG:NH2	2.35	0.60
3:C:537:GLY:H	3:C:714:SER:HB2	1.67	0.60
1:A:125:MET:O	1:A:139:ARG:NH2	2.36	0.59
1:A:355:ASN:OD1	1:A:356:LEU:N	2.36	0.59
2:B:423:ASP:OD1	2:B:423:ASP:N	2.35	0.58
2:B:660:PHE:O	2:B:684:TYR:OH	2.14	0.58
2:B:415:PRO:HG2	2:B:714:VAL:HG22	1.84	0.58
2:D:450:MET:SD	2:D:450:MET:N	2.71	0.58
5:L:246:THR:HA	5:L:307:ILE:O	2.03	0.58
3:C:359:ARG:NH2	4:H:332:GLY:O	2.33	0.58
3:C:127:ILE:HG23	3:C:128:TYR:HD1	1.69	0.58
3:C:325:LEU:O	3:C:328:SER:OG	2.18	0.58
4:H:231:LEU:HA	4:H:254:SER:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:314:SER:O	4:H:314:SER:OG	2.22	0.57
1:A:677:GLN:NE2	1:A:684:TYR:OH	2.37	0.57
5:L:24:ARG:NE	5:L:26:SER:O	2.30	0.57
1:A:90:ILE:HB	1:A:118:VAL:HG12	1.86	0.56
1:A:664:THR:HB	1:A:711:ILE:HG13	1.86	0.56
3:C:483:LYS:NZ	3:C:667:GLN:O	2.39	0.56
3:C:461:ASP:HB3	3:C:769:LEU:HD11	1.87	0.56
1:A:143:PRO:O	1:A:145:SER:N	2.39	0.56
2:B:123:PRO:HG3	2:B:334:LEU:HD11	1.86	0.56
5:L:90:TYR:CE1	5:L:104:GLY:HA2	2.41	0.56
2:D:280:SER:OG	2:D:281:TYR:N	2.39	0.56
3:C:375:ASN:OD1	3:C:377:ARG:NH2	2.40	0.55
2:D:35:ASN:N	2:D:68:ASN:OD1	2.40	0.55
3:C:407:PRO:HG3	3:C:716:VAL:HA	1.88	0.55
1:A:489:ARG:NH2	1:A:494:ASN:OD1	2.39	0.55
3:C:31:ALA:HA	3:C:90:ILE:HG13	1.88	0.55
2:B:97:GLY:HA2	2:B:123:PRO:O	2.05	0.55
2:D:464:LEU:HD22	2:D:509:VAL:HG11	1.87	0.55
2:B:413:GLU:H	2:B:417:VAL:HG23	1.72	0.55
1:A:664:THR:HG23	1:A:665:VAL:H	1.71	0.54
3:C:254:ILE:HD13	3:C:268:GLY:HA3	1.90	0.54
3:C:364:VAL:HG11	3:C:379:ILE:HD11	1.90	0.54
1:A:541:LEU:HB3	1:A:710:PHE:HB3	1.90	0.54
1:A:596:LEU:HD22	2:D:616:PHE:HB2	1.90	0.54
3:C:151:TRP:HZ3	3:C:248:LEU:HD22	1.72	0.54
2:B:162:MET:HE1	2:B:228:LEU:HD12	1.90	0.54
2:D:416:PHE:O	2:D:459:PHE:N	2.39	0.54
4:H:334:ASN:H	5:L:323:TYR:HE2	1.55	0.54
1:A:129:SER:O	1:A:129:SER:OG	2.25	0.53
4:H:271:PRO:HD3	4:H:321:ALA:HA	1.90	0.53
2:B:265:THR:HB	2:B:372:TRP:CD1	2.44	0.53
2:D:233:LYS:H	2:D:261:VAL:HG22	1.73	0.53
3:C:136:SER:HA	3:C:322:LYS:NZ	2.23	0.53
2:D:426:THR:O	2:D:428:THR:N	2.39	0.53
2:B:428:THR:O	2:B:429:CYS:HB3	2.07	0.53
4:H:17:THR:O	4:H:17:THR:HG22	2.09	0.53
2:B:167:TRP:HB3	2:B:226:VAL:HG21	1.91	0.53
2:D:205:THR:HG22	2:D:205:THR:O	2.08	0.53
2:B:417:VAL:HG12	2:B:461:ILE:HG12	1.90	0.52
2:D:422:ILE:HD12	2:D:423:ASP:H	1.74	0.52
1:A:82:LEU:HD22	1:A:87:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:LEU:HG	2:B:385:LEU:HD13	1.90	0.52
2:D:79:PRO:O	2:D:83:ILE:HG12	2.08	0.52
2:D:380:ASN:O	2:D:381:HIS:ND1	2.42	0.52
3:C:560:SER:O	3:C:563:TRP:HB2	2.08	0.52
1:A:424:PHE:HB3	1:A:428:GLY:HA2	1.92	0.52
2:B:150:SER:OG	2:B:151:ILE:N	2.43	0.52
1:A:134:HIS:O	1:A:136:SER:N	2.42	0.52
1:A:259:LEU:O	1:A:359:ARG:NH2	2.39	0.52
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.08	0.52
2:B:120:THR:HG22	2:B:122:VAL:HG22	1.91	0.52
2:B:506:VAL:HG12	2:B:507:MET:HG2	1.92	0.52
3:C:114:TYR:HA	3:C:314:ILE:HG22	1.90	0.52
1:A:36:ARG:O	1:A:36:ARG:NH1	2.43	0.52
2:B:508:ALA:HB3	2:B:744:ALA:HB3	1.91	0.52
4:H:325:CYS:O	4:H:340:GLY:N	2.35	0.52
2:D:351:THR:OG1	2:D:352:GLU:OE2	2.26	0.51
2:B:608:LYS:HG2	3:C:589:TRP:HB3	1.90	0.51
3:C:30:GLY:HA2	3:C:63:THR:H	1.75	0.51
3:C:441:ASP:O	3:C:448:ARG:NH2	2.43	0.51
3:C:662:TYR:HA	3:C:709:ALA:HB3	1.92	0.51
2:D:36:ILE:H	2:D:96:HIS:HA	1.75	0.51
1:A:530:SER:OG	1:A:531:LYS:N	2.44	0.51
2:B:536:MET:HG3	2:B:729:THR:HA	1.93	0.51
3:C:478:LEU:HD23	3:C:479:VAL:N	2.26	0.51
1:A:664:THR:HG23	1:A:665:VAL:N	2.26	0.51
2:B:207:ASP:OD1	2:B:208:THR:N	2.44	0.51
2:B:296:ILE:O	2:B:300:THR:HG22	2.10	0.51
3:C:104:PRO:HG3	3:C:123:THR:HG21	1.93	0.51
2:D:158:MET:SD	2:D:258:PRO:HB3	2.51	0.50
2:B:34:LEU:HD23	2:B:96:HIS:CD2	2.43	0.50
2:D:274:SER:HA	2:D:366:LEU:HB3	1.93	0.50
3:C:105:THR:HG23	3:C:106:PRO:HD3	1.93	0.50
3:C:151:TRP:CZ3	3:C:248:LEU:HB3	2.46	0.50
2:D:233:LYS:HA	2:D:261:VAL:HG13	1.93	0.50
2:D:587:LEU:HD22	2:D:602:PRO:HD3	1.93	0.50
5:L:4:LEU:HD12	5:L:22:CYS:SG	2.51	0.50
1:A:151:TRP:HH2	1:A:222:SER:HB2	1.76	0.50
1:A:668:SER:OG	1:A:669:SER:N	2.44	0.50
3:C:74:MET:O	3:C:78:VAL:HG12	2.11	0.50
3:C:101:HIS:O	3:C:101:HIS:ND1	2.44	0.50
1:A:168:SER:OG	1:A:169:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:LEU:HD23	2:B:614:TRP:HD1	1.77	0.50
2:D:83:ILE:HD13	2:D:116:ILE:HD11	1.93	0.50
3:C:541:LEU:HD22	3:C:717:LEU:HD22	1.93	0.49
2:D:118:SER:OG	2:D:119:HIS:N	2.44	0.49
2:B:497:ILE:HD12	2:B:522:VAL:HG11	1.93	0.49
1:A:121:LEU:HD22	1:A:280:HIS:HB3	1.93	0.49
1:A:415:LEU:HG	1:A:417:ASP:H	1.77	0.49
1:A:526:TYR:O	1:A:526:TYR:HD1	1.95	0.49
3:C:691:ASN:OD1	3:C:692:TYR:N	2.45	0.49
4:H:266:TRP:NE1	4:H:325:CYS:SG	2.85	0.49
2:B:96:HIS:O	2:B:98:LEU:N	2.45	0.49
2:B:500:VAL:HG21	2:B:508:ALA:HB2	1.93	0.49
1:A:541:LEU:HD22	1:A:717:LEU:HD22	1.94	0.49
2:B:176:ILE:HG12	2:B:207:ASP:HA	1.93	0.49
3:C:52:ARG:O	3:C:53:HIS:ND1	2.46	0.49
3:C:264:ASP:N	3:C:264:ASP:OD1	2.42	0.49
5:L:91:CYS:O	5:L:102:GLY:N	2.46	0.49
1:A:393:GLN:HG3	1:A:394:MET:H	1.78	0.49
1:A:490:VAL:HG23	1:A:493:SER:HB2	1.95	0.48
1:A:249:VAL:O	1:A:268:GLY:HA2	2.13	0.48
2:B:102:ASP:OD1	2:B:103:ASP:N	2.46	0.48
3:C:135:LEU:HD23	3:C:135:LEU:H	1.77	0.48
3:C:126:SER:N	3:C:172:GLU:OE2	2.38	0.48
1:A:104:PRO:HG3	1:A:123:THR:HG21	1.95	0.48
1:A:681:SER:HA	1:A:684:TYR:CD2	2.48	0.48
1:A:540:ILE:HD12	1:A:711:ILE:HG23	1.95	0.48
2:B:150:SER:O	2:B:154:GLN:NE2	2.46	0.48
2:D:61:ALA:HB3	2:D:64:PRO:HG3	1.95	0.48
2:D:173:VAL:O	2:D:229:LEU:HA	2.14	0.48
2:D:249:THR:HG22	2:D:255:TRP:HE1	1.78	0.48
3:C:519:ILE:HA	3:C:529:PHE:HE2	1.79	0.47
1:A:148:SER:HA	1:A:151:TRP:CE3	2.49	0.47
1:A:302:THR:HG22	1:A:303:ASP:H	1.79	0.47
2:D:35:ASN:N	2:D:35:ASN:OD1	2.46	0.47
1:A:254:ILE:HD13	1:A:268:GLY:HA3	1.95	0.47
1:A:272:ILE:HD13	1:A:350:ASN:HB3	1.96	0.47
3:C:66:THR:OG1	3:C:67:HIS:N	2.48	0.47
3:C:345:ASP:OD1	3:C:345:ASP:N	2.44	0.47
1:A:140:THR:O	1:A:346:ARG:NH1	2.47	0.47
2:B:661:ARG:O	2:B:707:ALA:HB3	2.15	0.47
3:C:519:ILE:HG12	3:C:529:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:434:VAL:O	2:D:455:CYS:HB2	2.15	0.47
2:D:495:GLY:O	2:D:497:ILE:N	2.48	0.47
3:C:127:ILE:HG23	3:C:128:TYR:CD1	2.48	0.47
3:C:148:SER:HA	3:C:151:TRP:CD1	2.45	0.47
5:L:5:THR:OG1	5:L:23:THR:OG1	2.33	0.47
4:H:5:GLN:O	4:H:23:THR:OG1	2.33	0.47
3:C:118:VAL:HG22	3:C:137:PHE:HA	1.97	0.47
3:C:157:VAL:HG23	3:C:157:VAL:O	2.15	0.47
5:L:6:GLN:NE2	5:L:102:GLY:HA3	2.30	0.47
2:D:560:MET:HA	2:D:563:VAL:HG22	1.97	0.47
1:A:135:LEU:HD11	2:B:111:GLN:HE22	1.81	0.46
1:A:538:LEU:HD21	1:A:670:VAL:HG22	1.97	0.46
1:A:146:HIS:CE1	1:A:179:ARG:HH12	2.33	0.46
2:D:251:TYR:CE1	2:D:394:LYS:HA	2.50	0.46
2:D:429:CYS:HB3	2:D:433:THR:HG23	1.97	0.46
1:A:189:SER:OG	1:A:190:LYS:N	2.48	0.46
2:B:408:ILE:HD13	2:B:475:TYR:HB2	1.98	0.46
1:A:119:LEU:HD23	1:A:284:ALA:HB1	1.96	0.46
1:A:192:GLU:HG2	1:A:214:LEU:HD23	1.97	0.46
2:B:129:GLY:O	2:B:132:SER:HB3	2.15	0.46
2:B:710:TYR:HB3	2:B:715:LEU:HD21	1.97	0.46
2:D:268:ILE:HD11	2:D:372:TRP:HE1	1.81	0.46
2:B:434:VAL:HG11	2:B:475:TYR:HE2	1.80	0.46
1:A:662:TYR:HB3	1:A:709:ALA:HB3	1.98	0.46
2:D:172:LEU:HD11	2:D:183:PHE:HE1	1.80	0.46
3:C:338:VAL:HG22	3:C:346:ARG:HH21	1.81	0.46
1:A:71:ALA:HB1	2:B:119:HIS:CE1	2.50	0.45
2:B:745:LEU:HD11	2:B:755:ILE:HD12	1.97	0.45
2:D:170:PHE:CZ	2:D:200:MET:HB2	2.51	0.45
2:D:410:THR:HG22	2:D:477:LEU:HD21	1.99	0.45
2:B:610:MET:SD	2:B:611:VAL:N	2.89	0.45
1:A:79:CYS:HA	1:A:83:ILE:HB	1.99	0.45
2:B:102:ASP:OD1	2:B:104:THR:N	2.42	0.45
2:B:587:LEU:HD23	2:B:588:LEU:HD23	1.99	0.45
2:B:608:LYS:HA	2:B:608:LYS:HD2	1.72	0.45
3:C:407:PRO:HB3	3:C:719:PHE:CD2	2.51	0.45
2:D:73:LEU:HA	2:D:73:LEU:HD12	1.80	0.45
3:C:405:GLN:HG2	3:C:516:PRO:HG3	1.98	0.45
2:B:438:LYS:HE3	2:B:438:LYS:HB2	1.85	0.45
3:C:562:LEU:HD22	3:C:565:LEU:HD12	1.99	0.45
2:D:435:PRO:HA	2:D:455:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASP:OD1	1:A:650:ASP:N	2.49	0.45
2:B:161:ILE:HD11	2:B:363:VAL:HG21	1.99	0.45
2:B:435:PRO:HA	2:B:455:CYS:HA	1.98	0.45
3:C:518:THR:HG21	3:C:669:SER:HB2	1.99	0.45
2:D:415:PRO:HG3	2:D:717:TYR:CD1	2.52	0.45
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.81	0.44
2:D:352:GLU:HB2	2:D:353:GLU:H	1.67	0.44
1:A:495:LYS:HA	2:B:193:ASN:HB3	1.99	0.44
2:B:664:THR:OG1	2:B:665:VAL:N	2.50	0.44
2:D:153:GLN:O	2:D:156:THR:HG22	2.16	0.44
1:A:352:SER:O	1:A:352:SER:OG	2.33	0.44
2:B:366:LEU:HD11	2:B:370:ARG:HA	1.98	0.44
2:D:286:TYR:HE2	2:D:291:ARG:HG3	1.82	0.44
3:C:139:ARG:HH22	3:C:143:PRO:HB3	1.83	0.44
1:A:491:ASN:OD1	1:A:491:ASN:N	2.49	0.44
2:B:295:GLY:O	2:B:298:ILE:HG22	2.17	0.44
1:A:304:PRO:HA	1:A:305:PRO:HD3	1.87	0.44
1:A:260:ARG:HD2	5:L:31:SER:HA	2.00	0.44
1:A:342:GLU:HB3	1:A:343:ASP:H	1.68	0.44
2:D:592:VAL:HG23	2:D:614:TRP:HE1	1.83	0.44
3:C:402:THR:OG1	3:C:403:ILE:N	2.51	0.44
2:D:537:VAL:HG22	2:D:707:ALA:HA	1.99	0.44
2:D:725:CYS:HB2	2:D:780:CYS:HB2	1.67	0.44
1:A:458:PHE:HD1	1:A:769:LEU:HD22	1.82	0.43
1:A:593:GLY:O	1:A:598:SER:N	2.40	0.43
2:D:167:TRP:HB3	2:D:226:VAL:HG21	1.98	0.43
2:D:182:GLU:OE2	2:D:182:GLU:N	2.35	0.43
1:A:499:ASN:OD1	1:A:499:ASN:N	2.50	0.43
2:B:299:LEU:HD23	2:B:299:LEU:HA	1.86	0.43
3:C:692:TYR:CZ	3:C:707:LEU:HD11	2.52	0.43
2:D:180:TYR:OH	2:D:181:ARG:NH2	2.43	0.43
2:B:35:ASN:O	2:B:96:HIS:HB2	2.17	0.43
1:A:79:CYS:HB3	1:A:308:CYS:HB2	1.84	0.43
2:D:501:VAL:HG22	2:D:521:VAL:HG11	1.99	0.43
1:A:398:LEU:HD21	1:A:749:TRP:NE1	2.34	0.43
3:C:531:LYS:HD3	3:C:531:LYS:HA	1.76	0.43
1:A:356:LEU:HD13	1:A:361:LEU:HD22	2.00	0.43
3:C:679:GLU:CD	3:C:679:GLU:H	2.21	0.43
2:D:416:PHE:HA	2:D:459:PHE:HB3	1.99	0.43
2:B:512:LEU:HD12	2:B:512:LEU:HA	1.87	0.43
2:B:745:LEU:HD21	2:B:751:TRP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:THR:OG1	2:B:411:LEU:N	2.52	0.43
3:C:523:ARG:H	3:C:523:ARG:HG2	1.65	0.43
2:D:415:PRO:HG3	2:D:717:TYR:CG	2.53	0.43
2:B:518:ARG:NH1	2:B:669:SER:OG	2.52	0.43
2:D:160:LYS:HD2	2:D:160:LYS:HA	1.71	0.43
2:D:307:LEU:HD23	2:D:307:LEU:HA	1.91	0.43
2:D:672:ARG:HH11	2:D:675:ARG:HH12	1.67	0.43
2:B:238:LEU:HD23	2:B:238:LEU:HA	1.90	0.42
2:B:731:GLY:HA3	2:B:734:TYR:HB3	2.01	0.42
3:C:29:ILE:HG21	3:C:288:VAL:HG11	2.00	0.42
3:C:111:ALA:HB1	3:C:116:ILE:HG13	2.01	0.42
3:C:355:ASN:OD1	3:C:356:LEU:N	2.52	0.42
3:C:478:LEU:HD23	3:C:479:VAL:H	1.84	0.42
2:D:414:ALA:HB1	2:D:415:PRO:HD2	2.01	0.42
1:A:143:PRO:HD2	1:A:146:HIS:CD2	2.54	0.42
3:C:136:SER:HA	3:C:322:LYS:HZ3	1.84	0.42
2:D:364:ILE:HG22	2:D:373:GLU:O	2.18	0.42
2:D:376:GLY:HA2	2:D:385:LEU:HA	2.00	0.42
2:B:53:THR:HA	2:B:69:VAL:HG21	2.02	0.42
2:D:357:VAL:HG12	2:D:358:HIS:ND1	2.35	0.42
2:D:531:THR:HG21	2:D:741:TYR:CE1	2.54	0.42
2:D:168:HIS:HA	2:D:198:TRP:CD1	2.54	0.42
2:D:175:THR:OG1	2:D:176:ILE:N	2.51	0.42
2:D:219:LEU:HD12	2:D:219:LEU:HA	1.83	0.42
2:D:386:ARG:HE	2:D:387:HIS:CE1	2.38	0.42
2:D:590:GLY:O	2:D:594:ASN:N	2.51	0.42
1:A:517:LEU:HD12	1:A:517:LEU:HA	1.90	0.42
3:C:364:VAL:O	3:C:375:ASN:N	2.51	0.42
2:D:177:PHE:CG	2:D:178:PRO:HD2	2.54	0.42
2:D:278:SER:O	2:D:278:SER:OG	2.35	0.42
1:A:364:VAL:HG23	1:A:377:ARG:HB3	2.02	0.42
3:C:208:LEU:HD23	3:C:208:LEU:HA	1.87	0.42
2:D:57:PRO:HG2	2:D:67:VAL:HG21	2.02	0.42
2:D:759:LEU:HD23	2:D:759:LEU:HA	1.87	0.42
1:A:758:LEU:HD23	1:A:758:LEU:HA	1.93	0.42
2:B:241:SER:HB2	2:B:271:GLU:HG2	2.01	0.42
2:B:351:THR:HG23	2:B:357:VAL:HG22	2.01	0.42
3:C:506:LEU:HD23	3:C:506:LEU:HA	1.83	0.42
3:C:128:TYR:HD2	3:C:137:PHE:CZ	2.37	0.42
4:H:104:VAL:HB	5:L:33:TYR:HD2	1.85	0.42
1:A:523:ARG:O	1:A:527:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:O	3:C:77:SER:OG	2.27	0.42
3:C:140:THR:HG22	3:C:340:PHE:HZ	1.84	0.42
2:B:220:LYS:HE2	2:D:216:GLN:NE2	2.35	0.41
2:D:213:ALA:O	2:D:217:VAL:HG12	2.20	0.41
1:A:743:MET:CE	1:A:750:LYS:HA	2.49	0.41
2:B:113:LEU:HG	2:B:124:ILE:HG21	2.01	0.41
2:B:313:ILE:HD13	2:B:313:ILE:HA	1.88	0.41
2:B:384:SER:O	2:B:384:SER:OG	2.32	0.41
3:C:259:LEU:HD23	3:C:259:LEU:HA	1.87	0.41
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.90	0.41
1:A:438:GLY:HA3	1:A:478:LEU:HB2	2.01	0.41
2:B:170:PHE:HB3	2:B:226:VAL:HB	2.03	0.41
2:B:408:ILE:HG13	2:B:507:MET:HB2	2.01	0.41
2:D:177:PHE:CD1	2:D:178:PRO:HD2	2.55	0.41
1:A:489:ARG:HH21	2:B:195:PHE:HD2	1.69	0.41
2:B:218:GLN:HE21	2:B:218:GLN:HB2	1.72	0.41
3:C:213:GLU:OE1	3:C:213:GLU:HA	2.21	0.41
2:B:411:LEU:HD11	2:B:484:LYS:HG2	2.02	0.41
2:B:568:VAL:HG21	2:B:614:TRP:CZ3	2.56	0.41
3:C:115:ARG:HD3	3:C:115:ARG:HA	1.66	0.41
3:C:125:MET:H	3:C:139:ARG:HH12	1.68	0.41
1:A:161:ASN:OD1	1:A:187:ARG:NH1	2.54	0.41
2:B:528:PHE:HD1	2:B:529:VAL:HG23	1.85	0.41
2:B:780:CYS:SG	2:B:781:HIS:N	2.94	0.41
1:A:394:MET:O	1:A:396:THR:N	2.54	0.41
2:B:362:VAL:HG21	2:B:374:LYS:HD2	2.03	0.41
3:C:562:LEU:HA	3:C:565:LEU:HB2	2.02	0.41
2:D:98:LEU:HB3	2:D:124:ILE:HG23	2.03	0.41
2:D:672:ARG:NH1	2:D:675:ARG:HH12	2.18	0.41
2:B:348:LEU:H	2:B:348:LEU:HD23	1.86	0.41
2:B:718:LYS:HB2	2:B:718:LYS:HE2	1.73	0.41
3:C:67:HIS:CE1	3:C:95:PRO:HD3	2.55	0.41
2:D:232:SER:O	2:D:234:ASP:N	2.54	0.41
2:D:277:ILE:HD11	2:D:390:TRP:CZ2	2.56	0.41
4:H:48:TRP:CZ3	4:H:61:ASN:HB3	2.55	0.41
3:C:43:ARG:O	3:C:46:VAL:HG12	2.21	0.41
3:C:460:ILE:O	3:C:464:ILE:HG12	2.21	0.41
2:D:237:VAL:HG23	2:D:271:GLU:HB2	2.03	0.41
1:A:400:ILE:HG12	1:A:512:MET:HB3	2.02	0.40
1:A:164:ILE:HG23	1:A:216:ALA:HB3	2.03	0.40
1:A:395:SER:OG	1:A:396:THR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ILE:HG12	1:A:529:PHE:CD2	2.56	0.40
1:A:541:LEU:N	1:A:710:PHE:O	2.54	0.40
1:A:664:THR:CG2	1:A:665:VAL:H	2.34	0.40
3:C:515:ALA:O	3:C:517:LEU:N	2.52	0.40
3:C:539:THR:O	3:C:539:THR:OG1	2.33	0.40
2:D:534:SER:OG	2:D:535:VAL:N	2.55	0.40
2:D:650:PHE:HA	2:D:662:PHE:HZ	1.87	0.40
4:H:48:TRP:HZ2	4:H:51:GLU:HG3	1.87	0.40
4:H:282:TYR:HD1	4:H:283:HIS:N	2.19	0.40
5:L:323:TYR:HA	5:L:328:VAL:HA	2.03	0.40
1:A:75:ALA:O	1:A:78:VAL:HB	2.21	0.40
1:A:165:LEU:HD13	1:A:180:LEU:HD23	2.02	0.40
1:A:498:TRP:HE1	1:A:526:TYR:HH	1.68	0.40
1:A:644:ARG:HA	1:A:644:ARG:HD2	1.98	0.40
1:A:661:ILE:HD11	1:A:690:HIS:CG	2.56	0.40
1:A:677:GLN:HE22	1:A:680:LEU:HD21	1.85	0.40
2:B:161:ILE:HD13	2:B:277:ILE:HG21	2.03	0.40
2:D:98:LEU:HG	2:D:100:PHE:H	1.86	0.40
2:D:528:PHE:CD2	2:D:529:VAL:HG23	2.56	0.40
2:B:34:LEU:HB3	2:B:35:ASN:H	1.78	0.40
3:C:378:LYS:HE2	3:C:378:LYS:HB2	1.86	0.40
2:D:158:MET:HG2	2:D:256:ILE:HG22	2.03	0.40
2:D:268:ILE:HD11	2:D:372:TRP:NE1	2.37	0.40
4:H:73:ASP:O	4:H:77:ASN:CA	2.70	0.40
2:B:535:VAL:HG23	2:B:709:ILE:HG13	2.04	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	781/815 (96%)	685 (88%)	93 (12%)	3 (0%)	30 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	775/808 (96%)	682 (88%)	91 (12%)	2 (0%)	37 70
2	D	774/808 (96%)	662 (86%)	103 (13%)	9 (1%)	11 43
3	C	781/815 (96%)	698 (89%)	82 (10%)	1 (0%)	48 80
4	H	230/234 (98%)	201 (87%)	29 (13%)	0	100 100
5	L	214/218 (98%)	201 (94%)	13 (6%)	0	100 100
All	All	3555/3698 (96%)	3129 (88%)	411 (12%)	15 (0%)	32 65

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TYR
2	D	259	SER
2	D	442	ILE
1	A	342	GLU
2	B	781	HIS
2	D	36	ILE
2	D	233	LYS
2	D	496	MET
2	D	657	SER
1	A	406	GLU
2	D	168	HIS
2	B	657	SER
2	D	430	VAL
2	D	414	ALA
3	C	665	VAL

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	555/703 (79%)	538 (97%)	17 (3%)	35 57
2	B	502/706 (71%)	487 (97%)	15 (3%)	36 58
2	D	446/706 (63%)	428 (96%)	18 (4%)	27 51

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	476/703 (68%)	448 (94%)	28 (6%)	16 42
4	H	87/202 (43%)	82 (94%)	5 (6%)	17 43
5	L	72/192 (38%)	68 (94%)	4 (6%)	17 44
All	All	2138/3212 (67%)	2051 (96%)	87 (4%)	28 51

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	43	ARG
1	A	53	HIS
1	A	68	LYS
1	A	113	PHE
1	A	131	LYS
1	A	171	HIS
1	A	255	SER
1	A	315	TRP
1	A	330	TYR
1	A	404	HIS
1	A	458	PHE
1	A	526	TYR
1	A	660	PHE
1	A	682	THR
1	A	737	SER
1	A	743	MET
2	B	88	ASP
2	B	147	PHE
2	B	221	LYS
2	B	223	HIS
2	B	251	TYR
2	B	259	SER
2	B	281	TYR
2	B	283	ASP
2	B	319	SER
2	B	348	LEU
2	B	377	LYS
2	B	396	PHE
2	B	399	CYS
2	B	429	CYS
2	B	708	PHE
3	C	38	HIS

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Mol	Chain	Res	Type
3	C	56	TRP
3	C	61	ASN
3	C	79	CYS
3	C	158	TYR
3	C	161	ASN
3	C	168	SER
3	C	224	SER
3	C	252	ARG
3	C	257	ASN
3	C	308	CYS
3	C	315	TRP
3	C	321	PHE
3	C	352	SER
3	C	357	GLN
3	C	377	ARG
3	C	448	ARG
3	C	461	ASP
3	C	528	GLU
3	C	644	ARG
3	C	652	ARG
3	C	660	PHE
3	C	674	PHE
3	C	689	LYS
3	C	690	HIS
3	C	725	CYS
3	C	747	SER
3	C	768	ASP
2	D	164	ASP
2	D	195	PHE
2	D	251	TYR
2	D	262	SER
2	D	267	LEU
2	D	320	CYS
2	D	326	ARG
2	D	334	LEU
2	D	348	LEU
2	D	358	HIS
2	D	387	HIS
2	D	450	MET
2	D	496	MET
2	D	656	TYR
2	D	672	ARG

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Mol	Chain	Res	Type
2	D	688	PHE
2	D	708	PHE
2	D	710	TYR
4	H	55	SER
4	H	59	ASN
4	H	60	TYR
4	H	64	LEU
4	H	282	TYR
5	L	50	TYR
5	L	91	CYS
5	L	94	TYR
5	L	323	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	677	GLN
2	B	96	HIS
2	B	111	GLN
2	D	68	ASN
5	L	6	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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	1
5	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	118:VAL	C	231:LEU	N	177.14
1	L	109:VAL	C	230:ASN	N	167.30

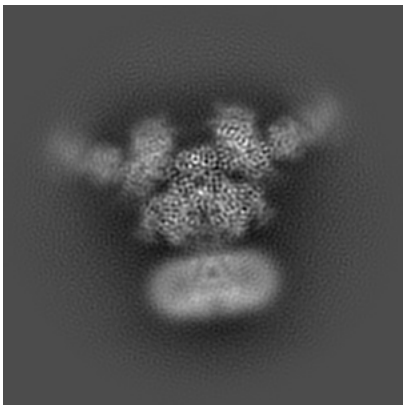
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43537. These allow visual inspection of the internal detail of the map and identification of artifacts.

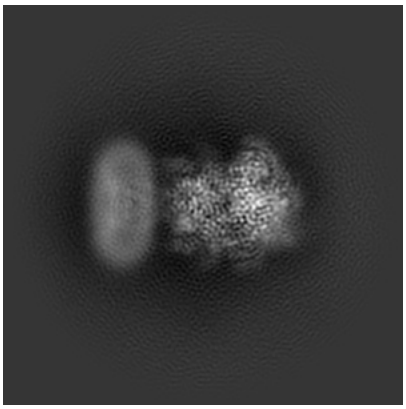
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

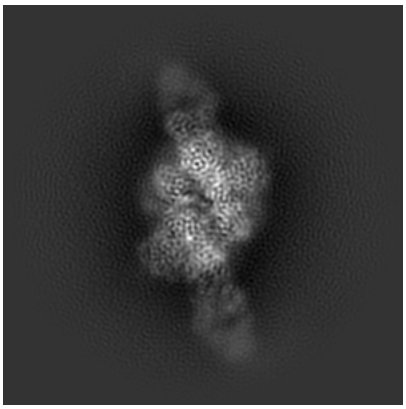
6.1.1 Primary map



X

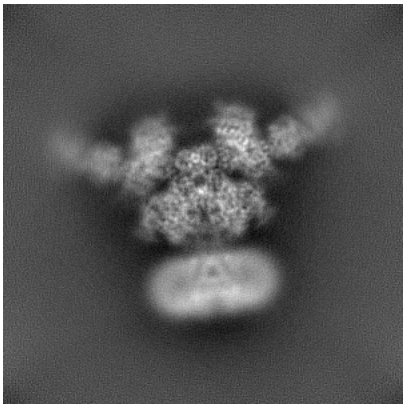


Y

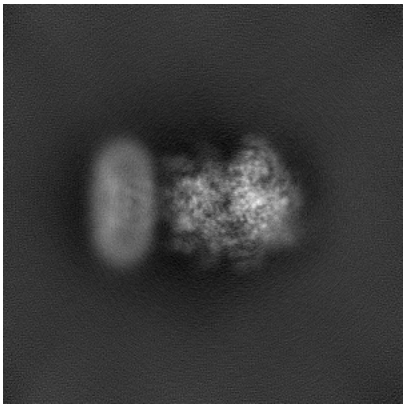


Z

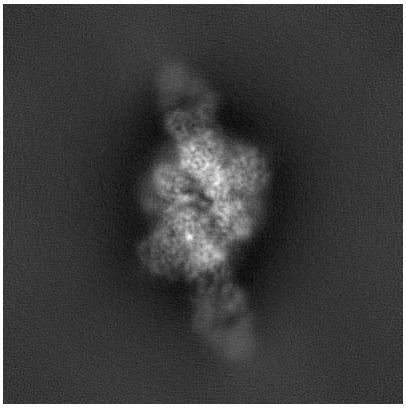
6.1.2 Raw map



X



Y

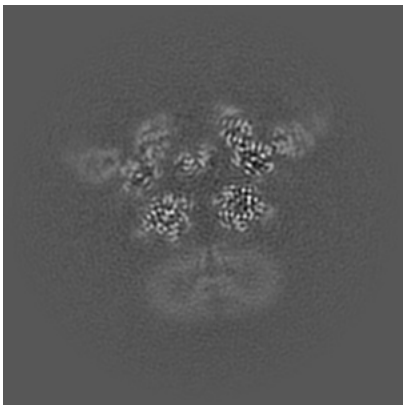


Z

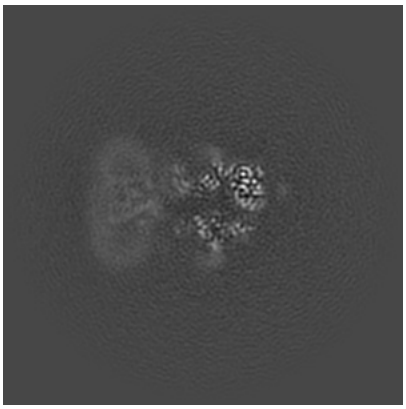
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

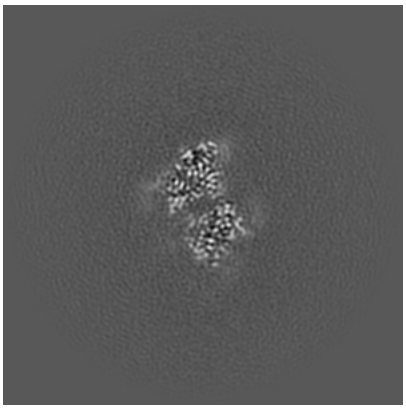
6.2.1 Primary map



X Index: 200

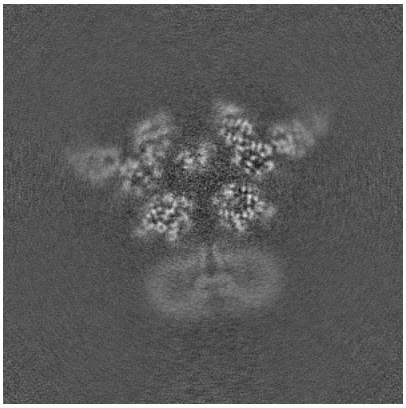


Y Index: 200

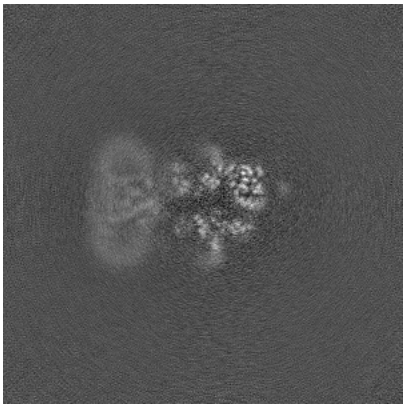


Z Index: 200

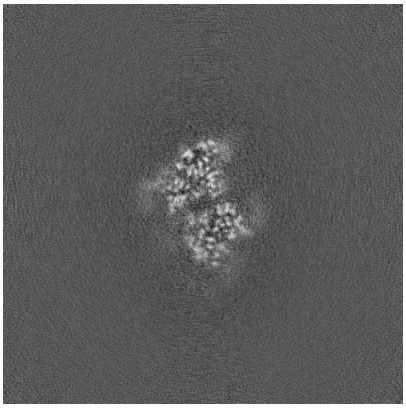
6.2.2 Raw map



X Index: 200



Y Index: 200

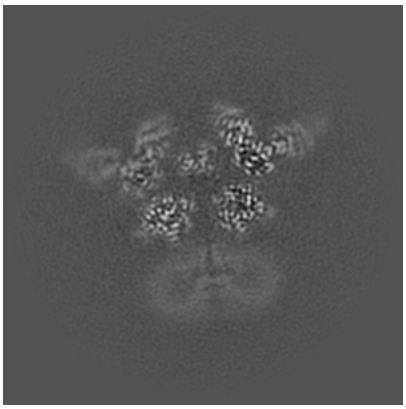


Z Index: 200

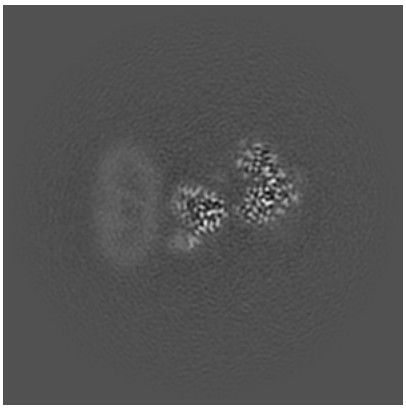
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

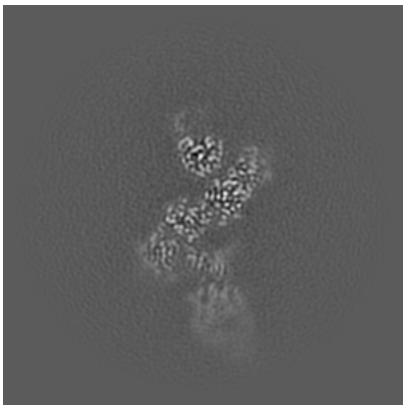
6.3.1 Primary map



X Index: 201

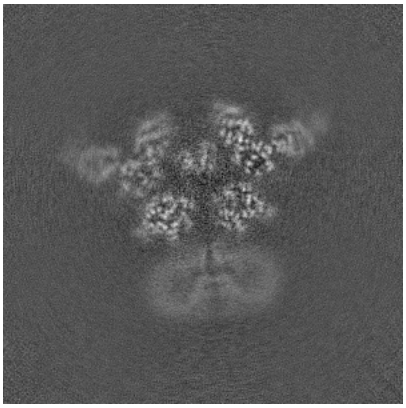


Y Index: 237

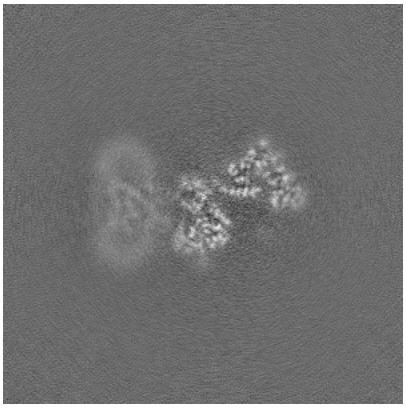


Z Index: 244

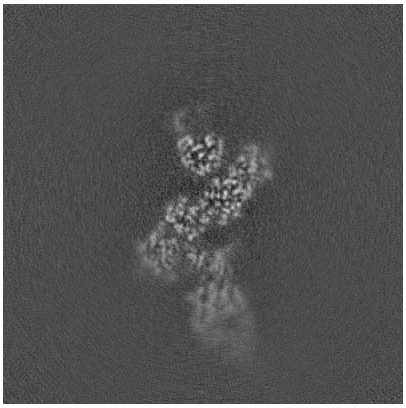
6.3.2 Raw map



X Index: 201



Y Index: 219

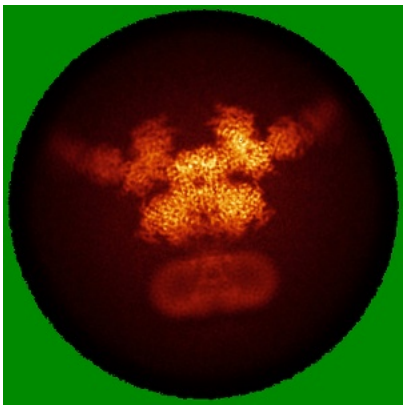


Z Index: 244

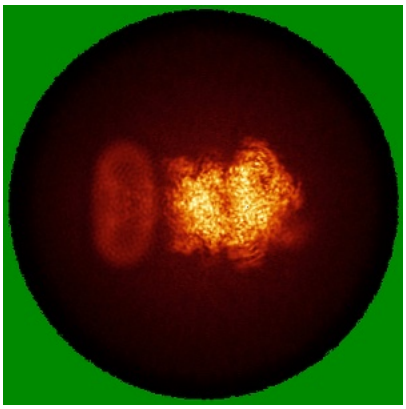
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

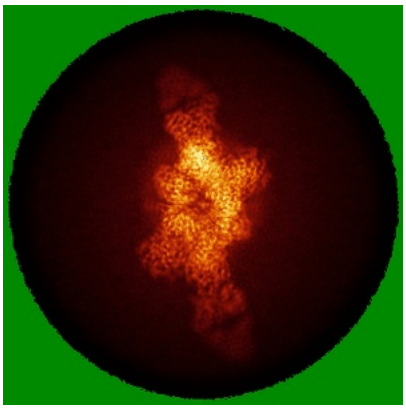
6.4.1 Primary map



X

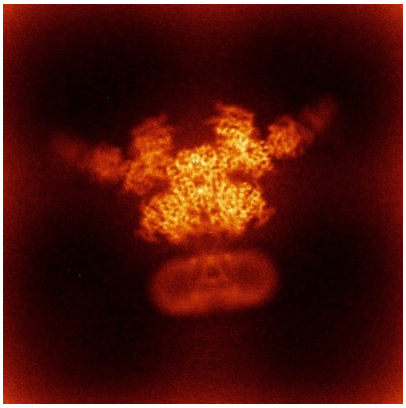


Y

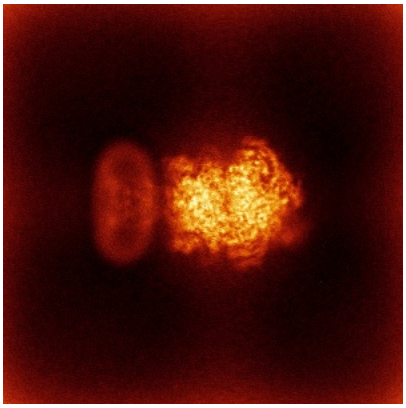


Z

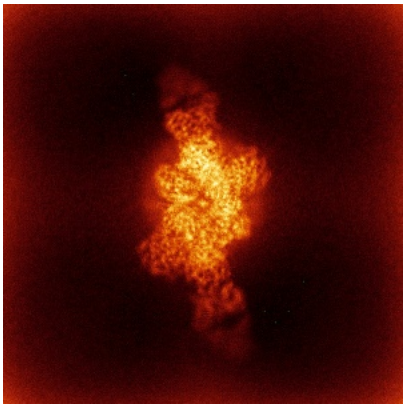
6.4.2 Raw map



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.

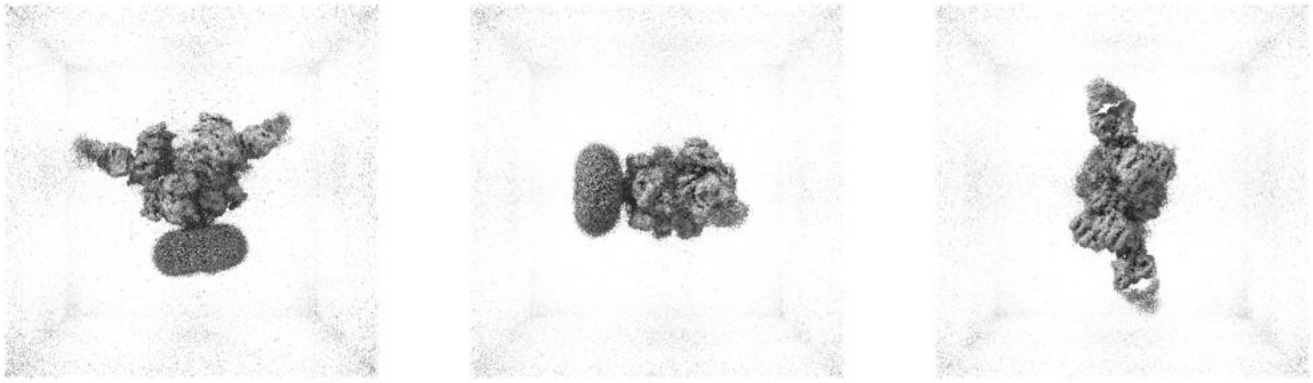
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0509. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

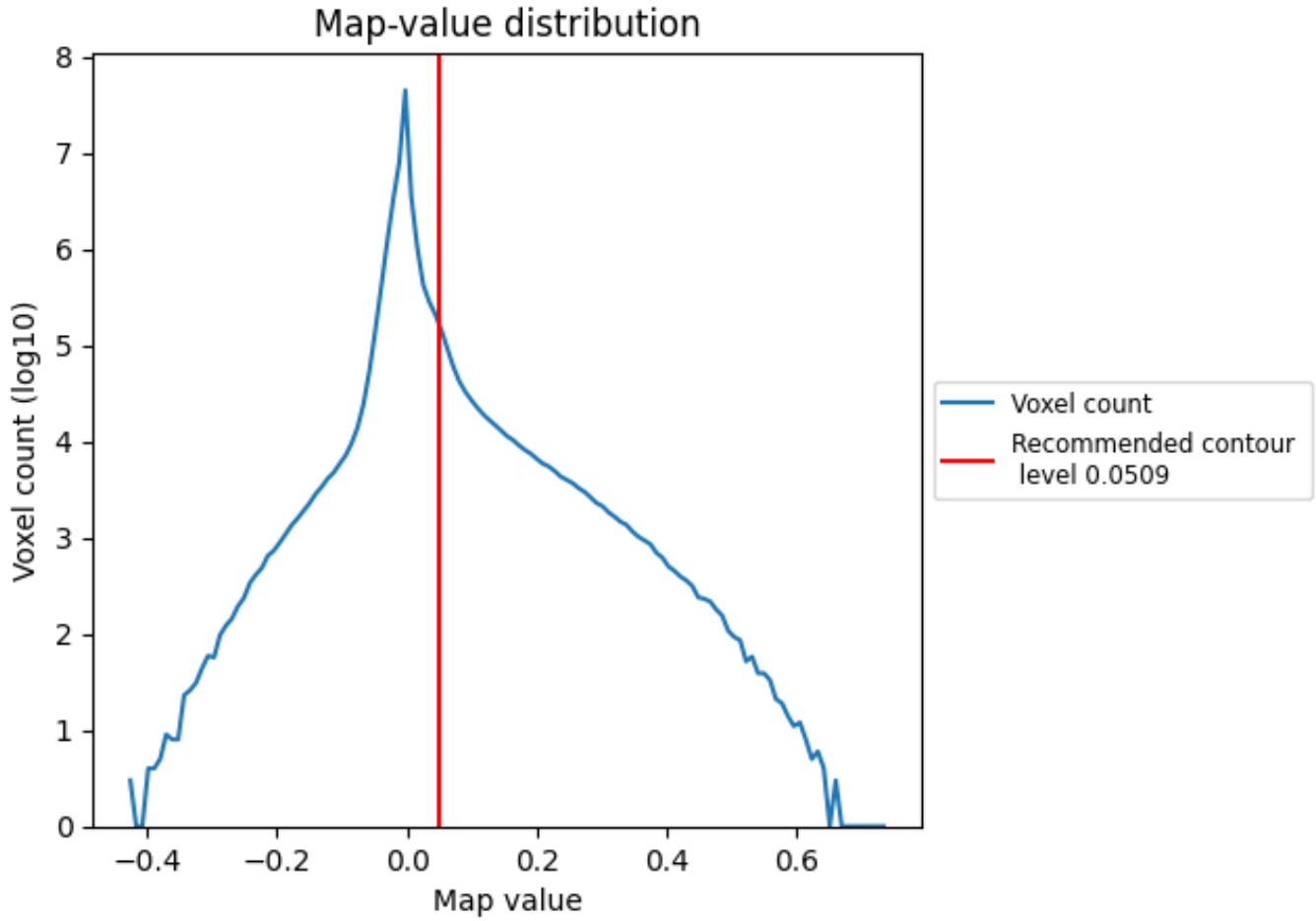
6.6 Mask visualisation (i)

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

7 Map analysis

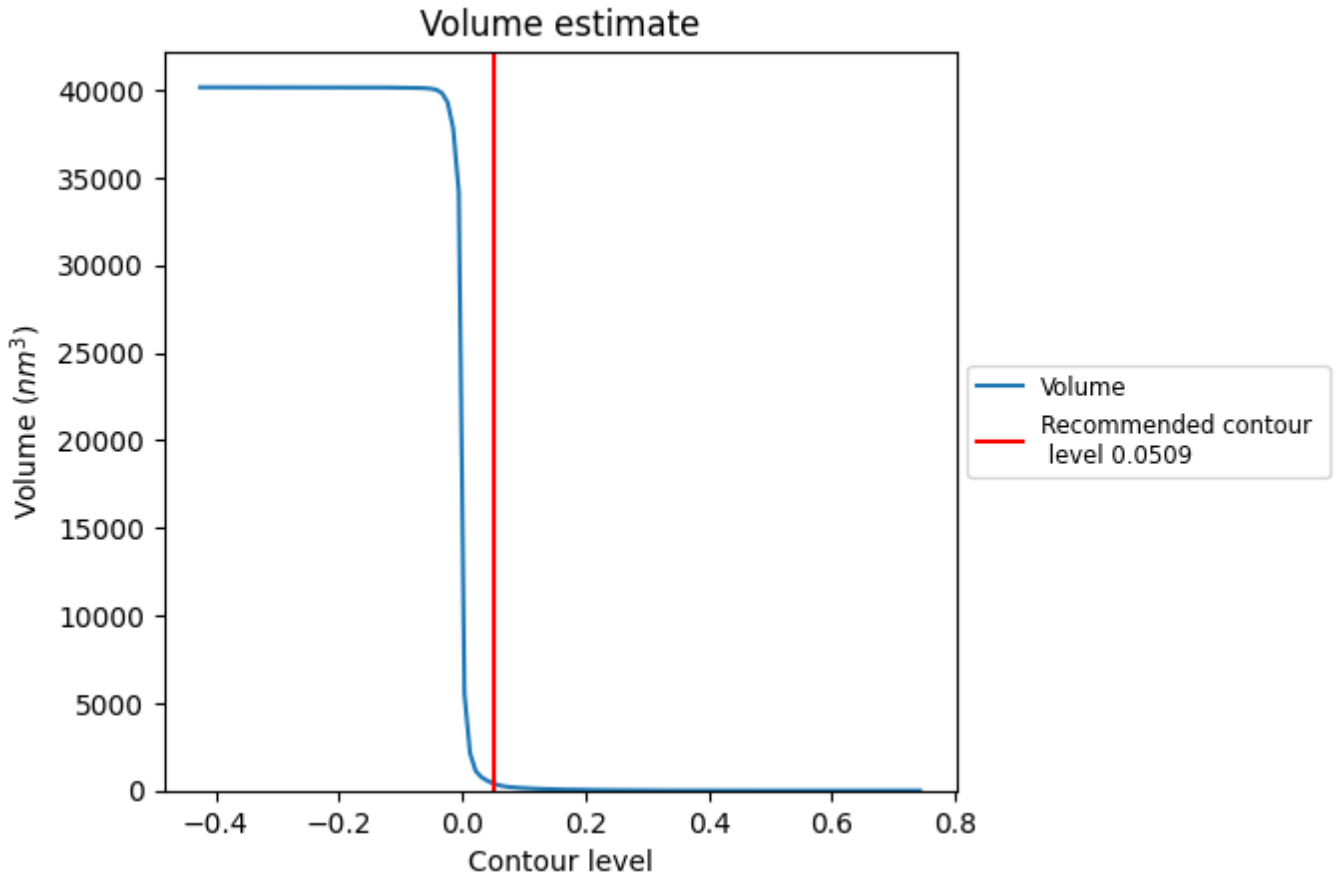
This section contains the results of statistical analysis of the map.

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.

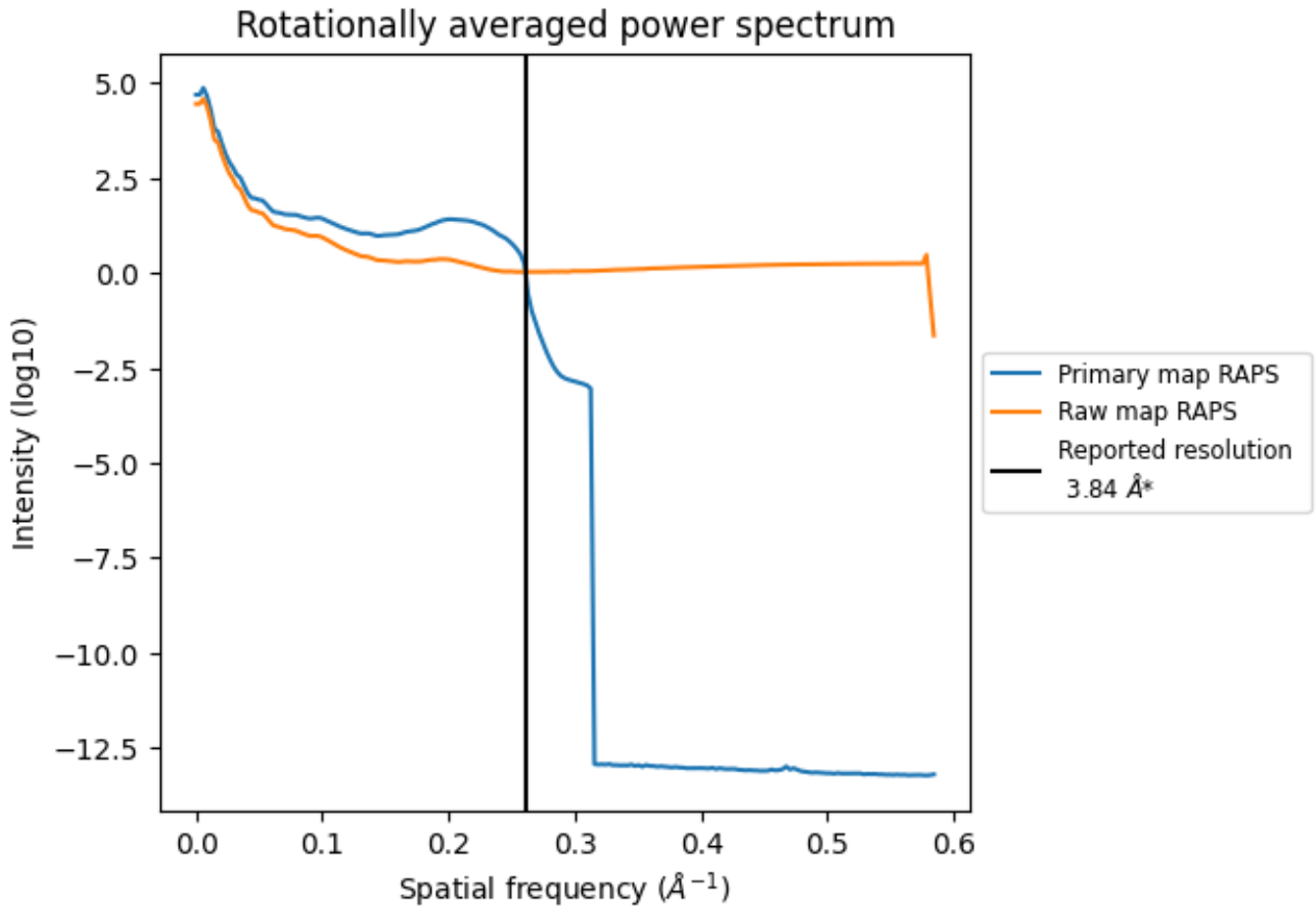
7.2 Volume estimate (i)



The volume at the recommended contour level is 404 nm^3; this corresponds to an approximate mass of 365 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)

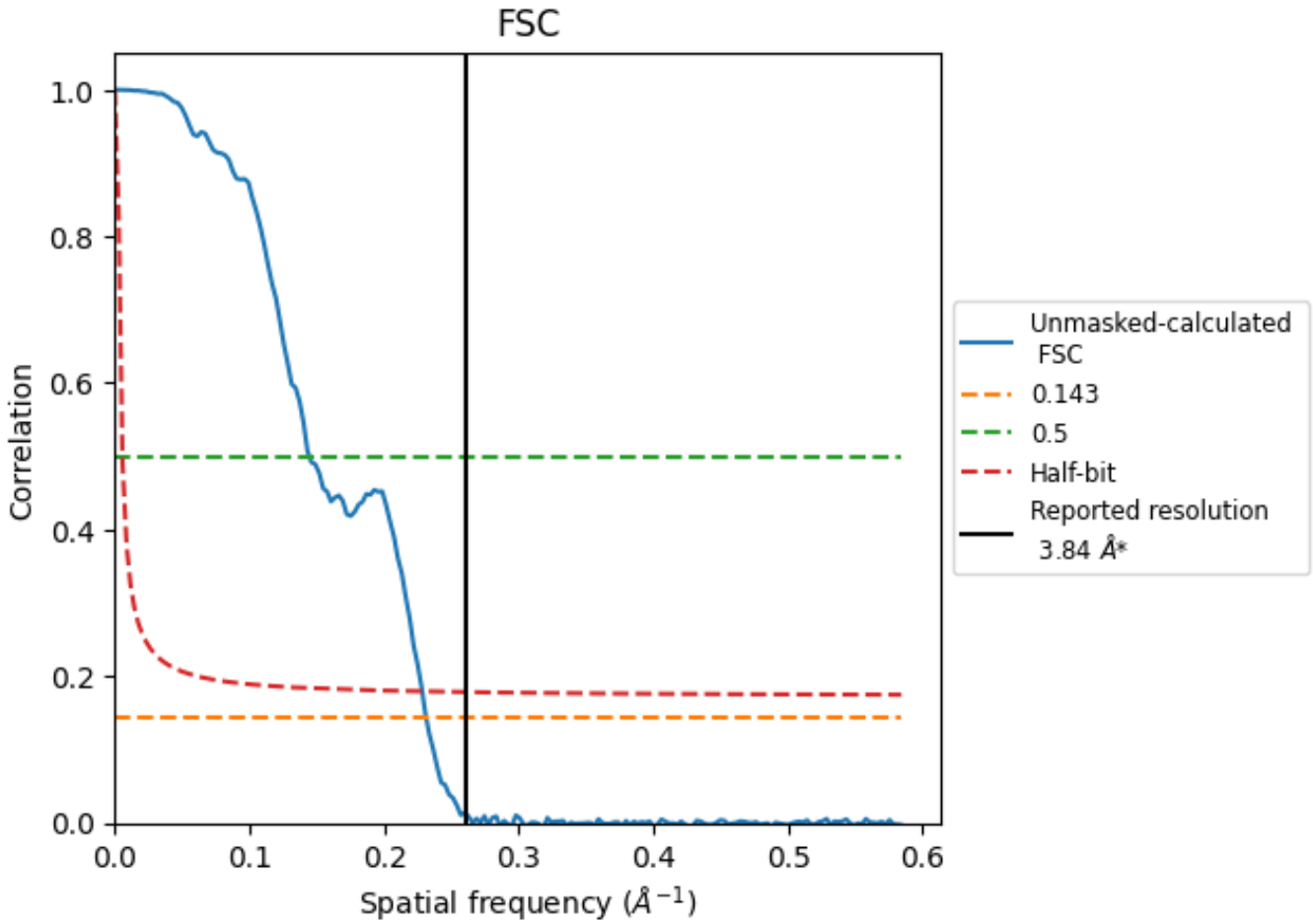


*Reported resolution corresponds to spatial frequency of 0.260 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

8.2 Resolution estimates (i)

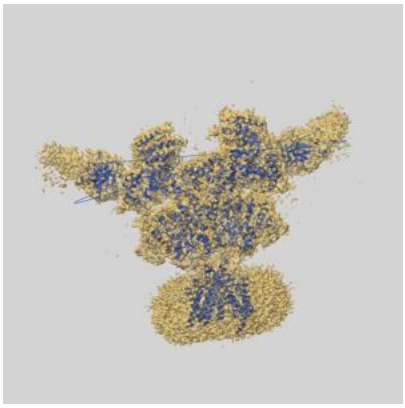
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	6.92	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.84 by more than 10 %

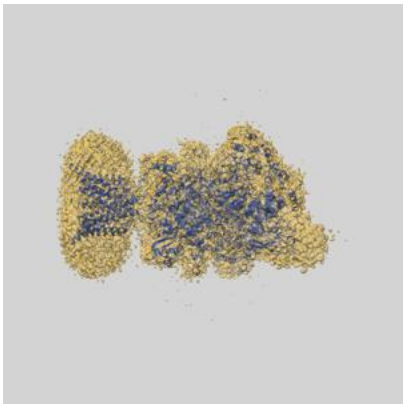
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43537 and PDB model 8VUR. Per-residue inclusion information can be found in section 3 on page 5.

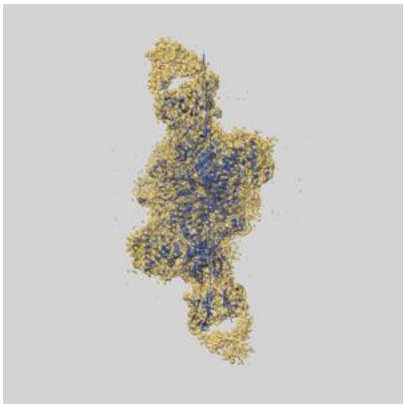
9.1 Map-model overlay



X



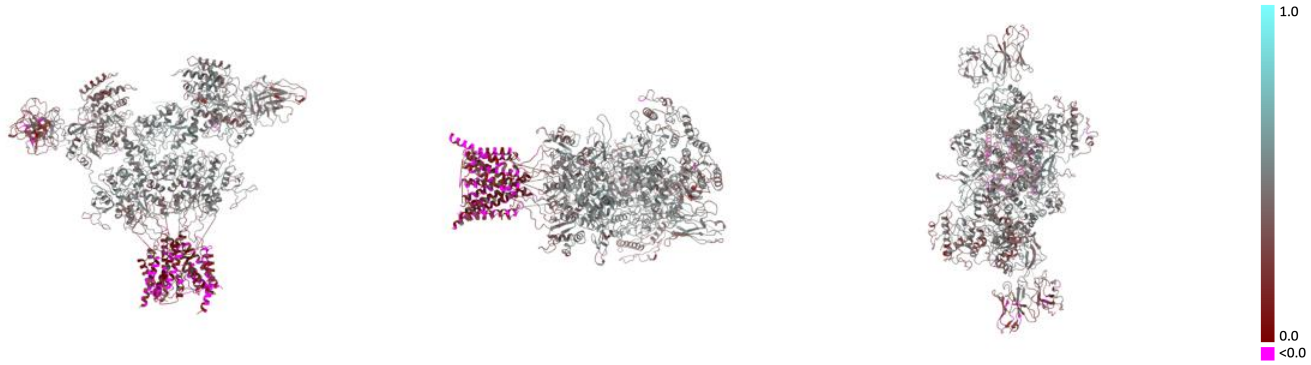
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0509 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

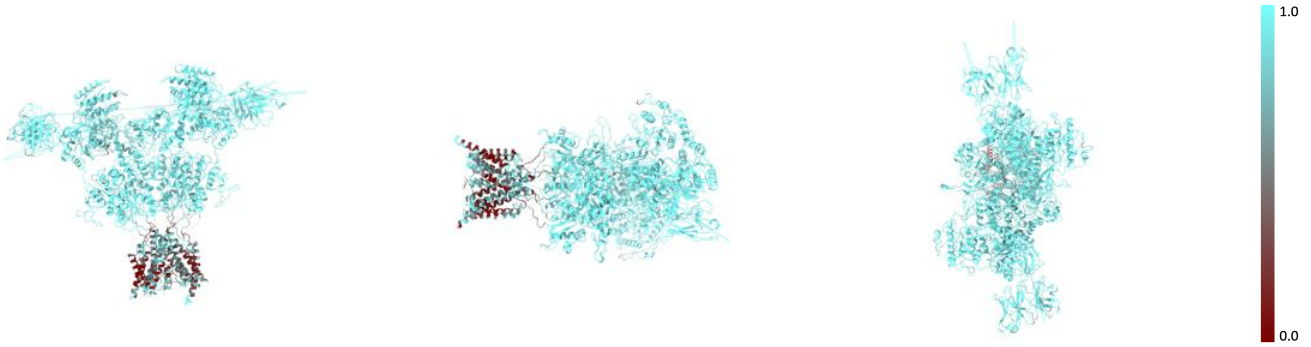
9.2 Q-score mapped to coordinate model



X Y Z

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

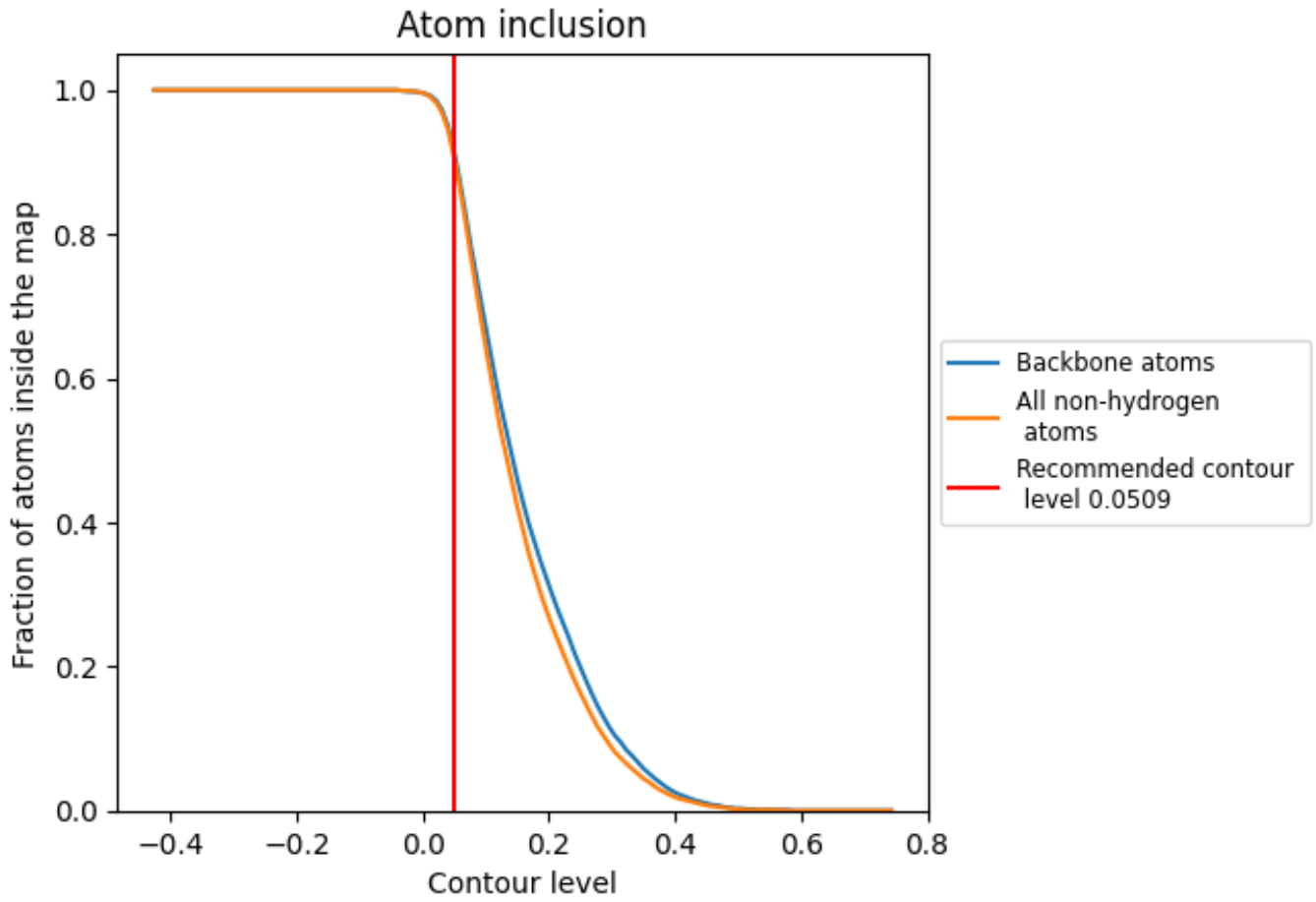
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0509).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.0509) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.4100
A	0.9120	0.4300
B	0.8940	0.4220
C	0.8890	0.3940
D	0.8930	0.4100
H	0.9530	0.3970
L	0.9330	0.3500