



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:58 AM UTC

PDB ID : 9BRU / pdb_00009bru
EMDB ID : EMD-44844
Title : Intact V-ATPase State 1 in synaptophysin knock-out isolated synaptic vesicles
Authors : Wang, C.; Jiang, W.; Yang, K.; Wang, X.; Guo, Q.; Brunger, A.T.
Deposited on : 2024-05-11
Resolution : 4.40 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:

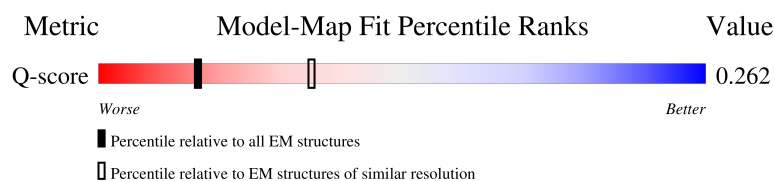
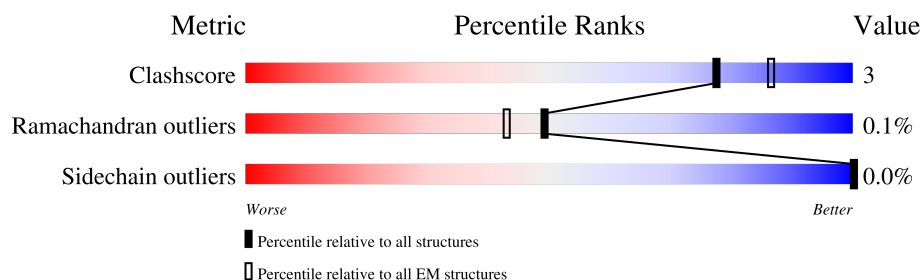
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	7	247	
2	8	226	
2	9	226	
2	Q	226	

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Mol	Chain	Length	Quality of chain
3	R	118	
3	T	118	
3	V	118	
4	6	382	
5	U	483	
6	a	838	
7	e	81	
8	f	98	
9	b	205	
10	g	155	
10	h	155	
10	i	155	
10	j	155	
10	k	155	
10	l	155	
10	m	155	
10	n	155	
10	o	155	
11	X	119	
12	d	351	
13	c	463	
14	p	350	
15	0	617	
15	1	617	
15	2	617	

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Mol	Chain	Length	Quality of chain
16	3	511	88% 10%
16	4	511	86% 6% 8%
16	5	511	87% 5% 8%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 65548 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 V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	208	Total	C	N	O	S	0	0
			1676	1064	303	304	5		

- Molecule 2 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
2	9	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
2	Q	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		

- Molecule 3 is a protein called V-type proton ATPase subunit G 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	114	Total	C	N	O	S	0	0
			925	552	192	176	5		
3	T	114	Total	C	N	O	S	0	0
			925	552	192	176	5		
3	V	114	Total	C	N	O	S	0	0
			925	552	192	176	5		

- Molecule 4 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	361	Total	C	N	O	S	0	0
			2931	1877	495	550	9		

- Molecule 5 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	426	Total	C	N	O	S	0	0
			3501	2224	604	648	25		

- Molecule 6 is a protein called V-type proton ATPase 116 kDa subunit a 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	752	Total	C	N	O	S	0	0
			6117	3991	1027	1058	41		

- Molecule 7 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	77	Total	C	N	O	S	0	0
			623	431	97	92	3		

- Molecule 8 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	85	Total	C	N	O	S	0	0
			658	434	102	115	7		

- Molecule 9 is a protein called V-type proton ATPase 21 kDa proteolipid subunit c".

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	200	Total	C	N	O	S	0	0
			1484	983	234	256	11		

- Molecule 10 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	g	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
10	h	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
10	i	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
10	j	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
10	k	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
10	l	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
10	n	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
10	o	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		

- Molecule 11 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	110	Total	C	N	O	S	0	0
			875	553	157	163	2		

- Molecule 12 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	351	Total	C	N	O	S	0	0
			2842	1834	461	532	15		

- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	203	Total	C	N	O	S	0	0
			1642	1079	259	295	9		

- Molecule 14 is a protein called Renin receptor cytoplasmic fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	49	Total	C	N	O	S	0	0
			407	277	57	71	2		

- Molecule 15 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	600	Total	C	N	O	S	0	0
			4656	2953	787	889	27		
15	0	602	Total	C	N	O	S	0	0
			4671	2961	789	894	27		
15	2	600	Total	C	N	O	S	0	0
			4656	2953	787	889	27		

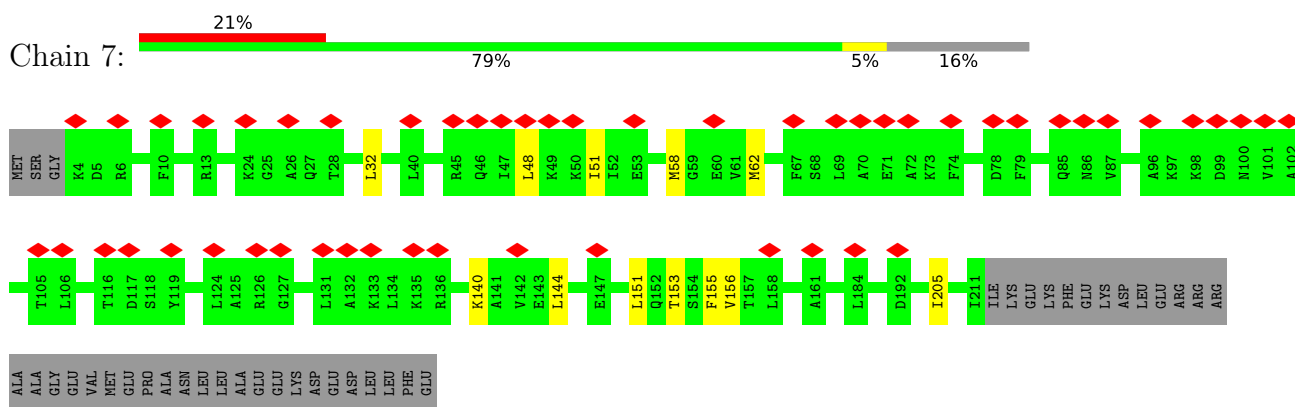
- Molecule 16 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	461	Total	C	N	O	S	0	0
			3610	2290	615	685	20		
16	4	468	Total	C	N	O	S	0	0
			3667	2326	623	698	20		
16	5	468	Total	C	N	O	S	0	0
			3667	2326	623	698	20		

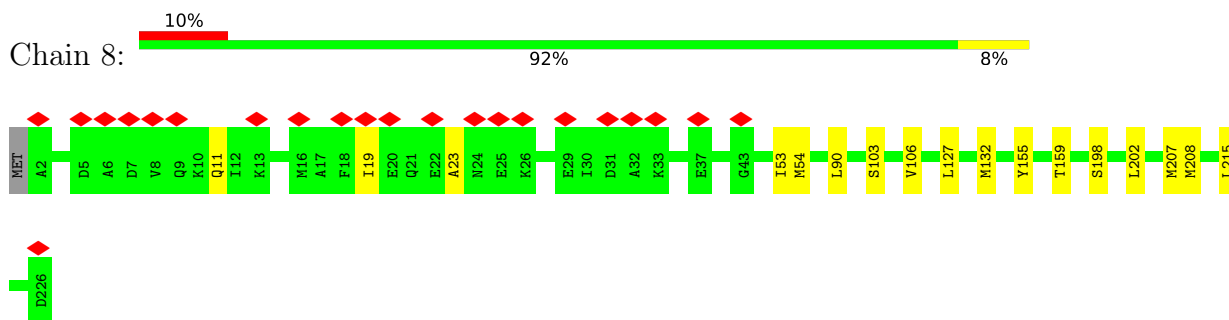
3 Residue-property plots

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.

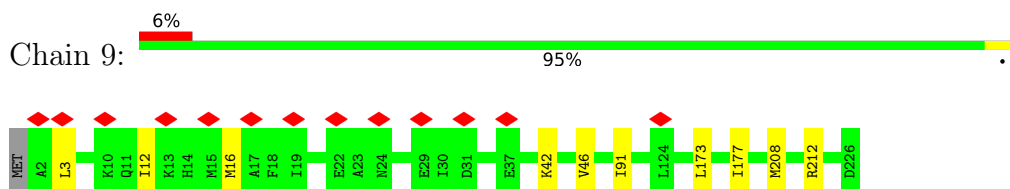
- Molecule 1: V-type proton ATPase subunit D



- Molecule 2: V-type proton ATPase subunit E 1

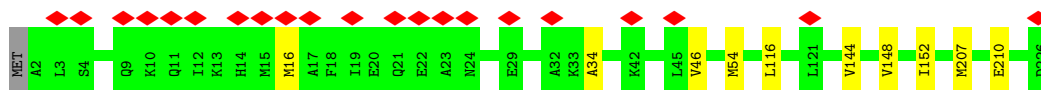


- Molecule 2: V-type proton ATPase subunit E 1

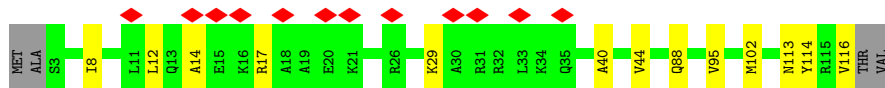
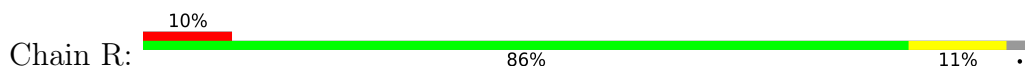


- Molecule 2: V-type proton ATPase subunit E 1

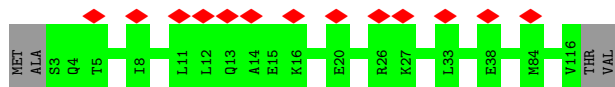




- Molecule 3: V-type proton ATPase subunit G 2



- Molecule 3: V-type proton ATPase subunit G 2



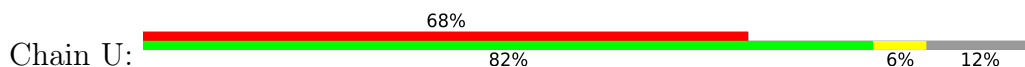
- Molecule 3: V-type proton ATPase subunit G 2

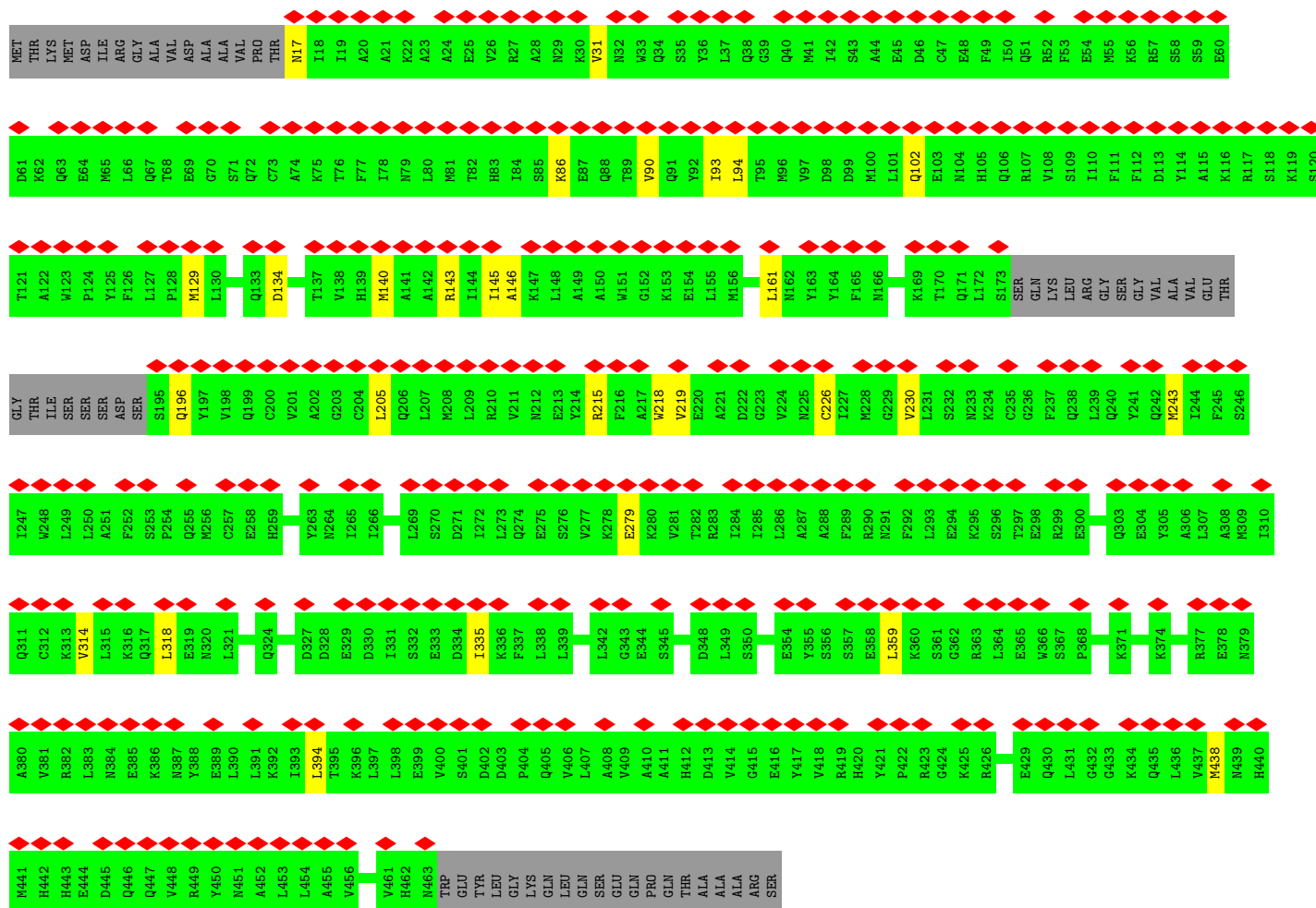


- Molecule 4: V-type proton ATPase subunit C 1

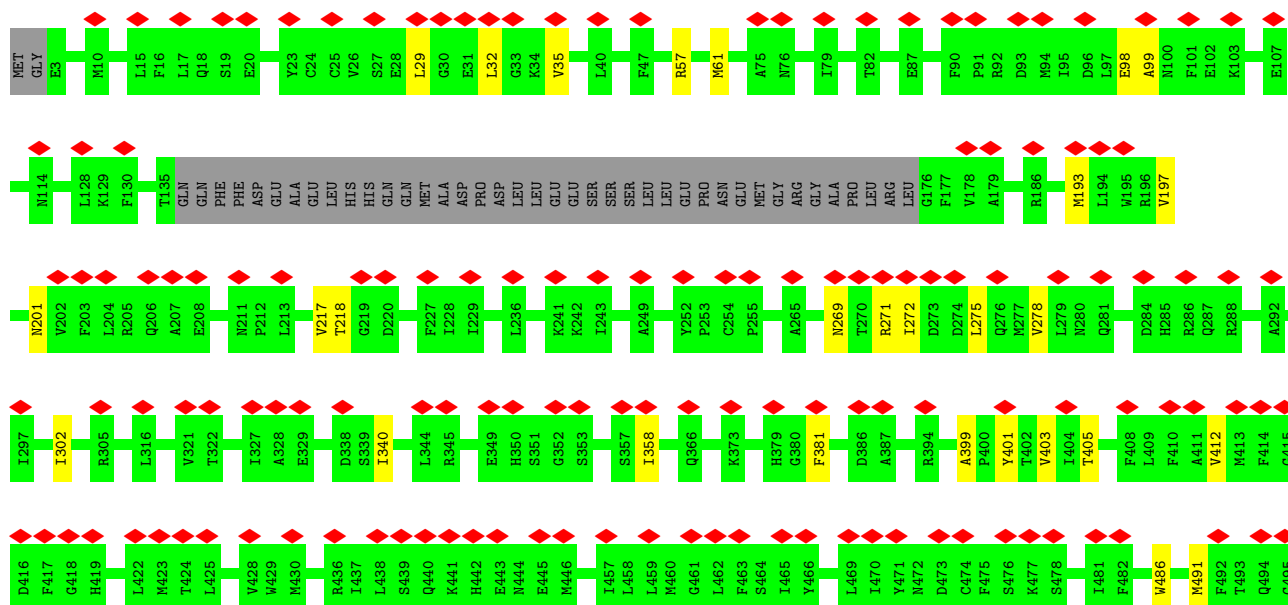
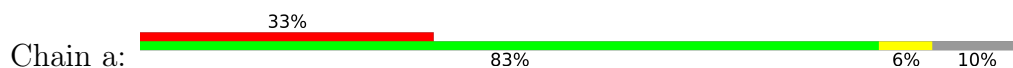


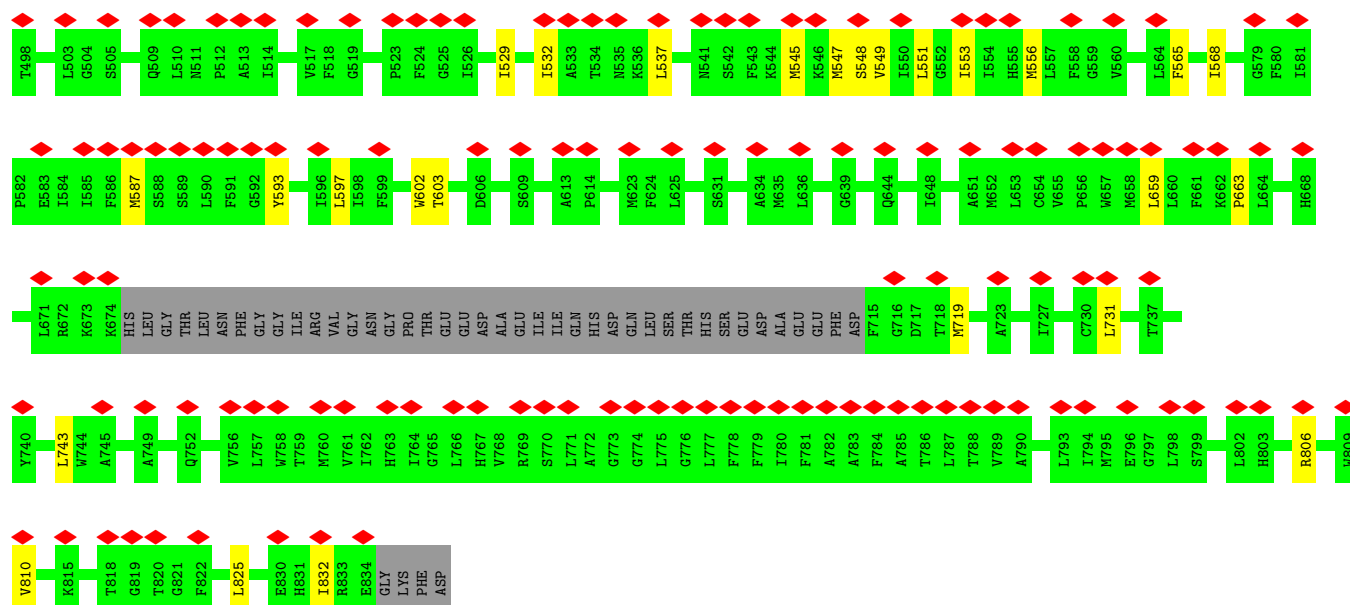
- Molecule 5: V-type proton ATPase subunit H



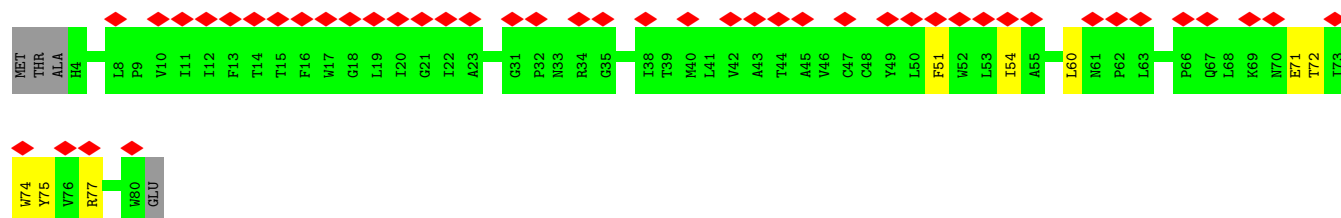
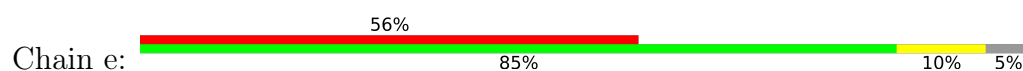


• Molecule 6: V-type proton ATPase 116 kDa subunit a 1

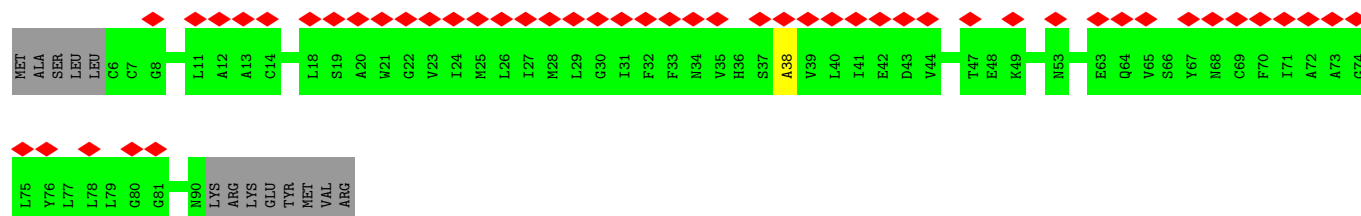
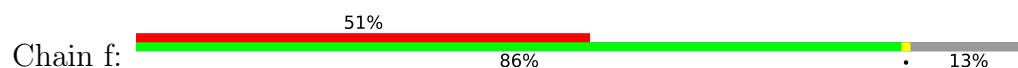




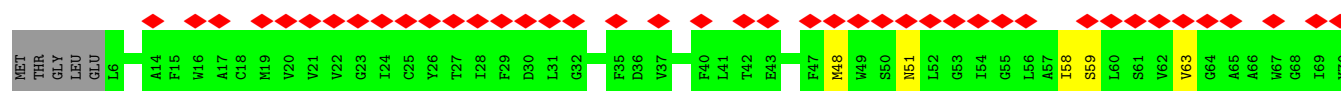
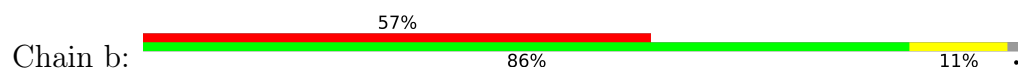
• Molecule 7: V-type proton ATPase subunit e 2

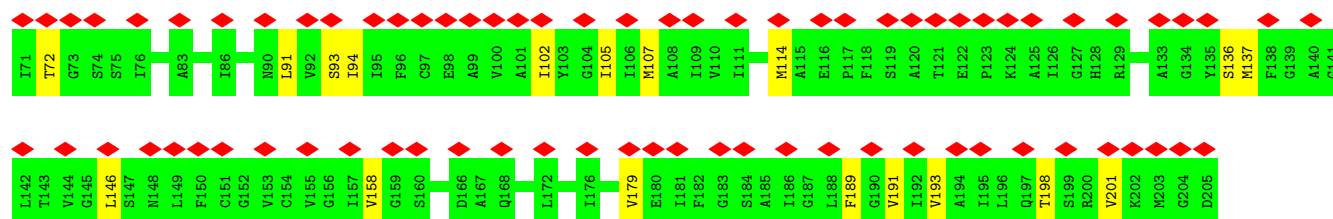


• Molecule 8: Ribonuclease kappa

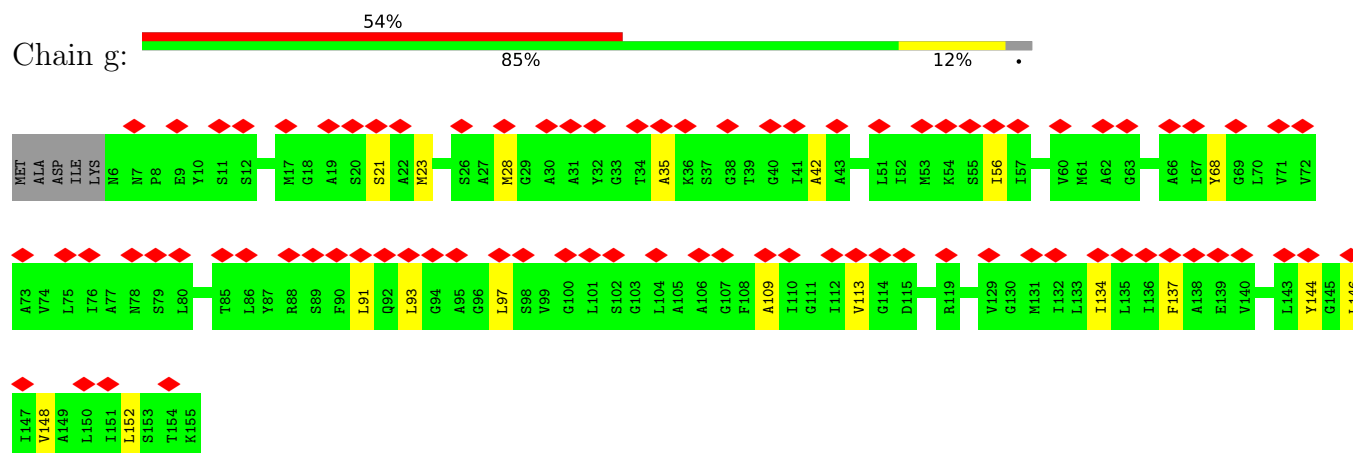


• Molecule 9: V-type proton ATPase 21 kDa proteolipid subunit c''

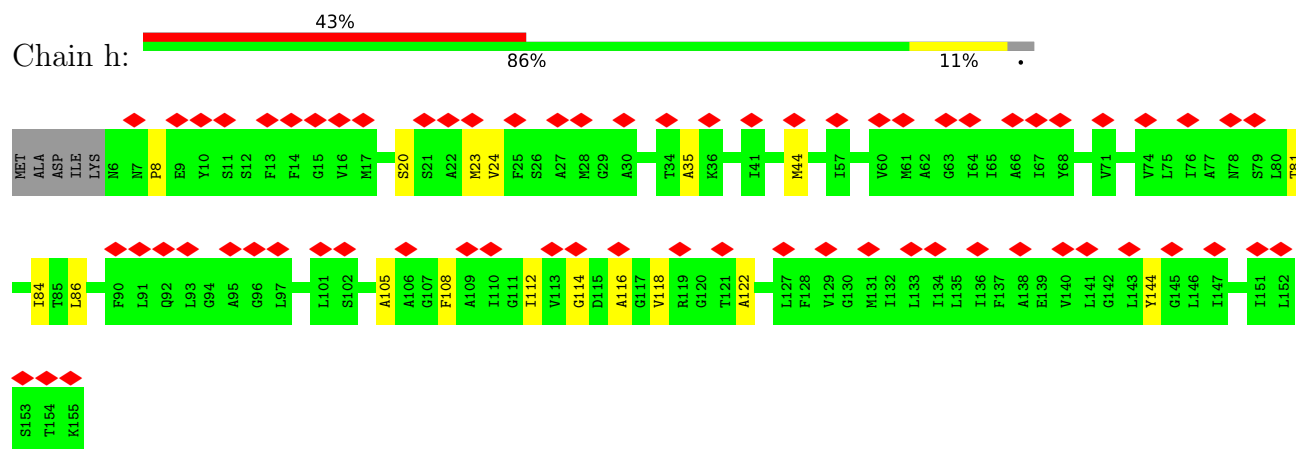




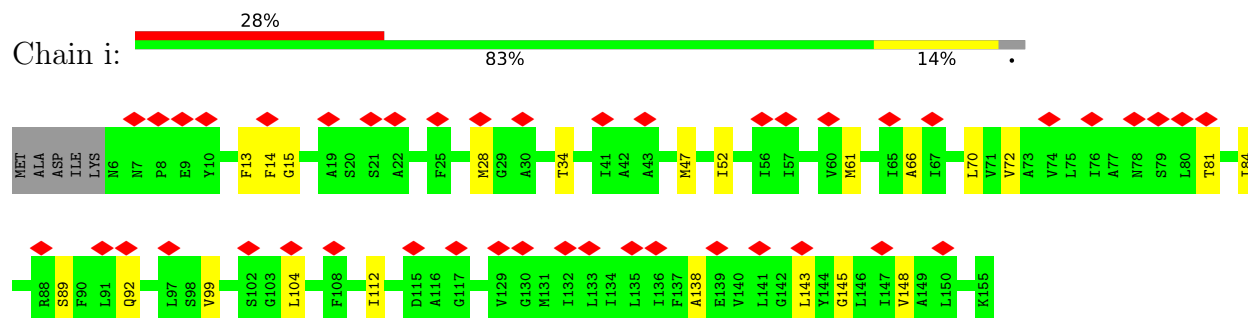
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c



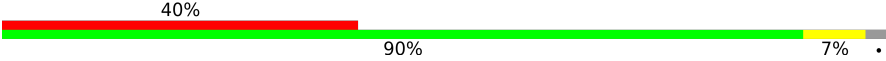
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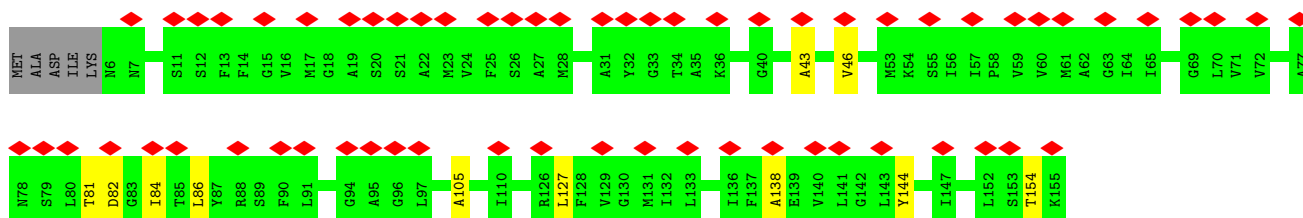


- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c



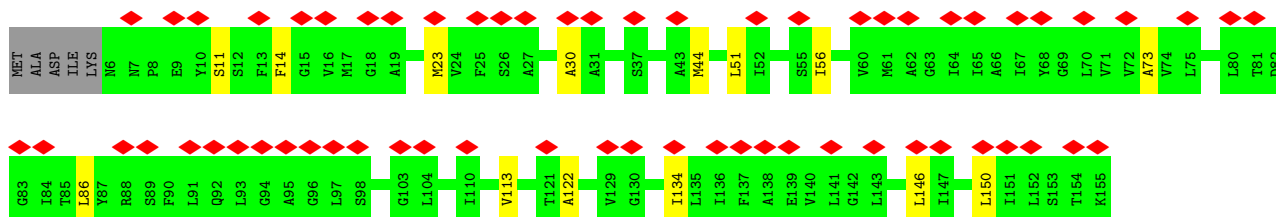
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c

Chain j: 



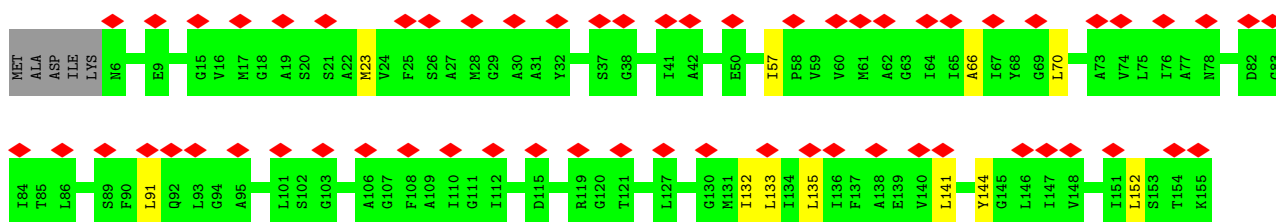
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c

Chain k: 



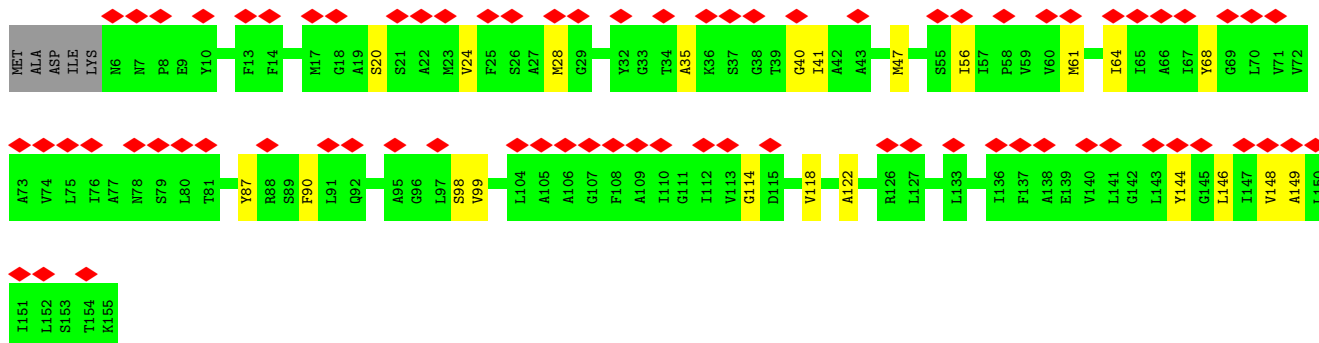
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c

Chain l: 



- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c

Chain m: 



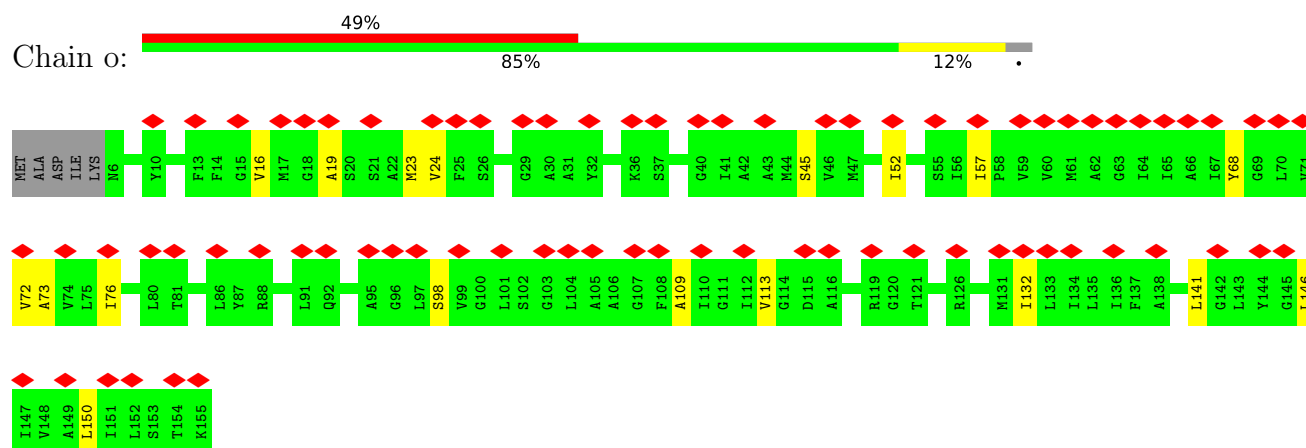
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c

Chain n: 

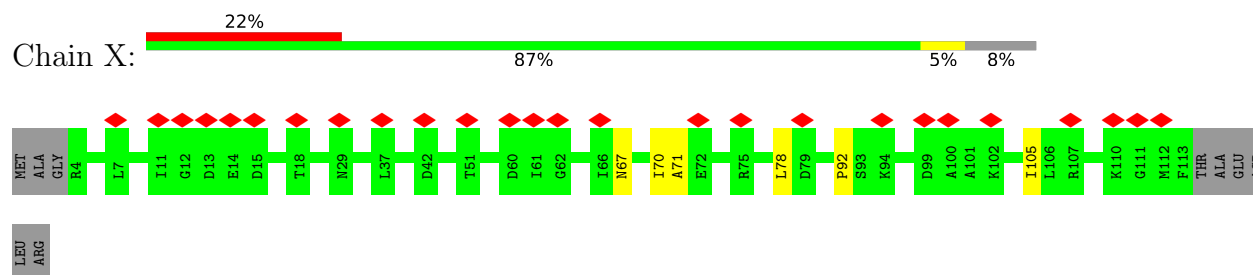




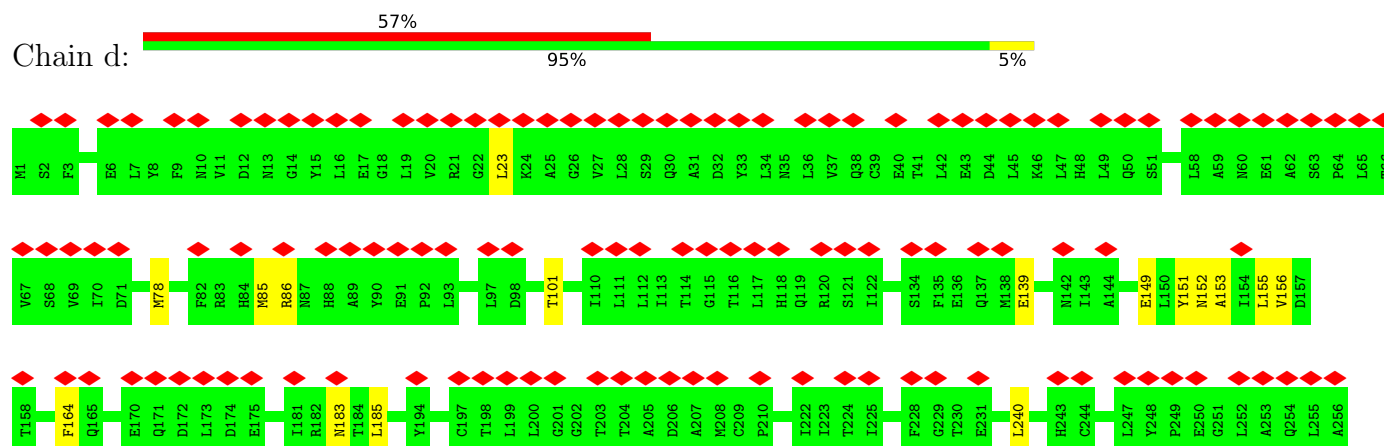
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit c



- Molecule 11: V-type proton ATPase subunit F

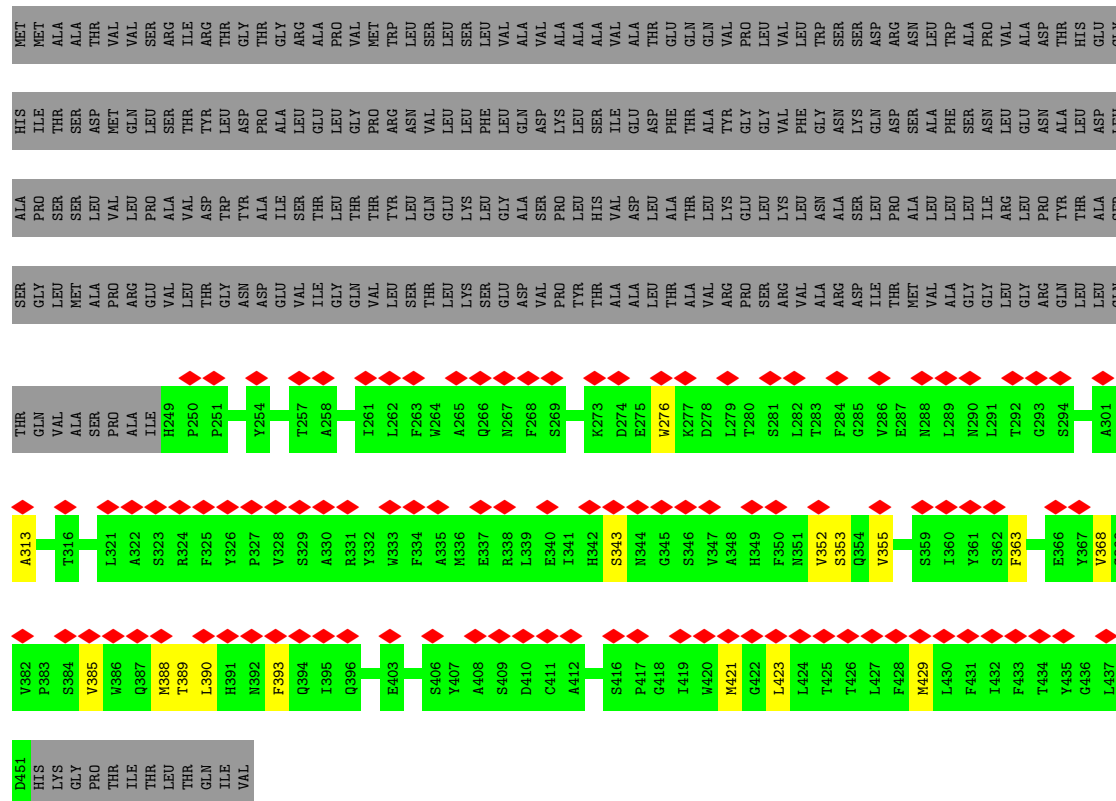
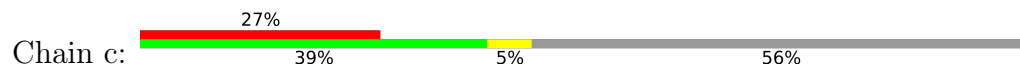


- Molecule 12: V-type proton ATPase subunit d 1

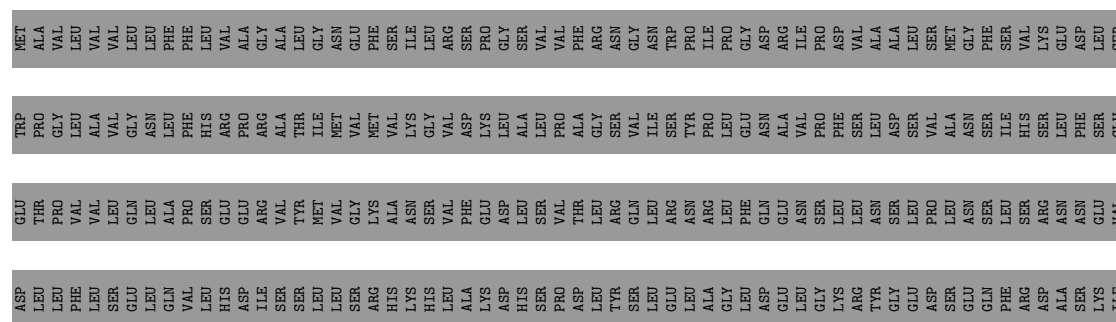


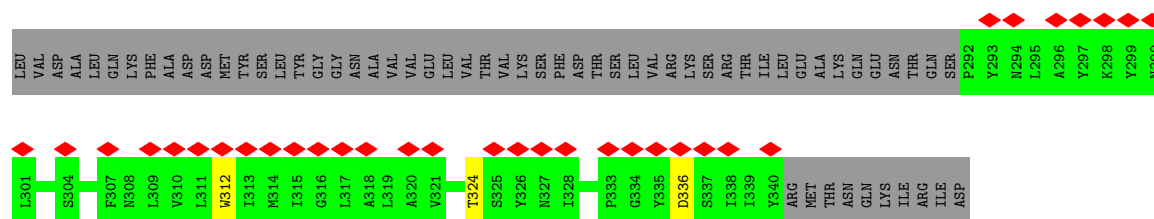


• Molecule 13: V-type proton ATPase subunit S1

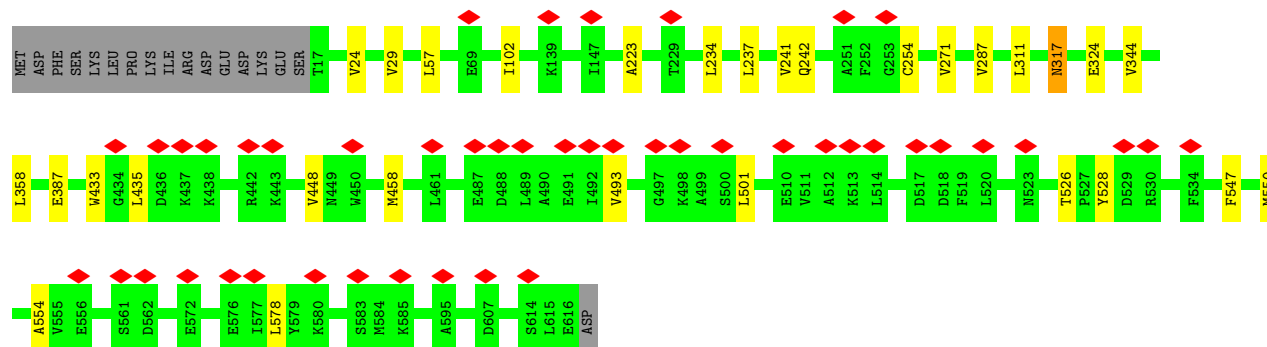
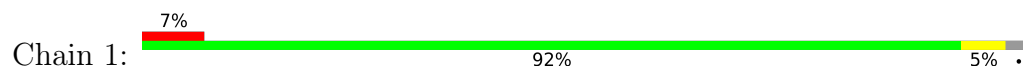


• Molecule 14: Renin receptor cytoplasmic fragment

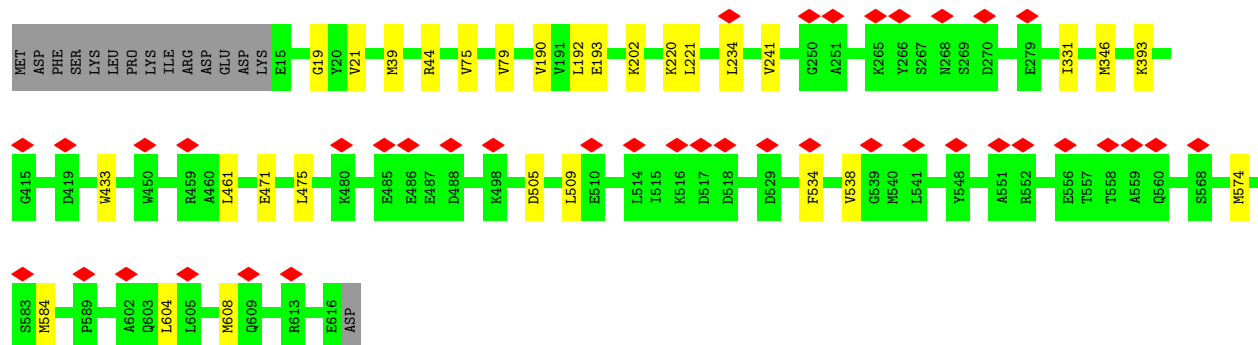




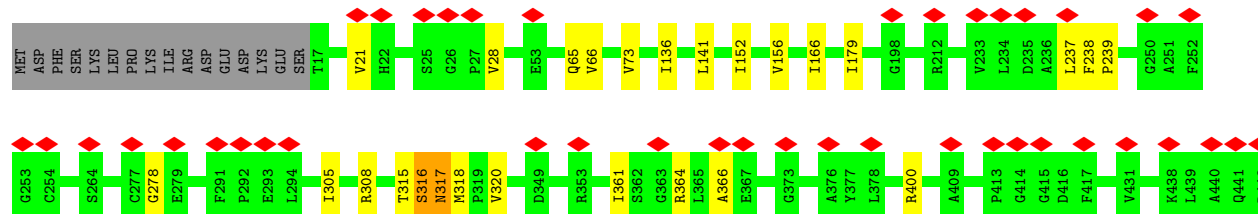
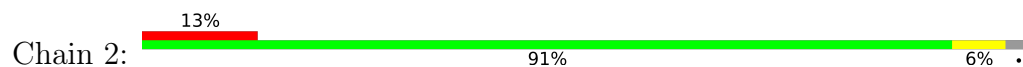
• Molecule 15: V-type proton ATPase catalytic subunit A

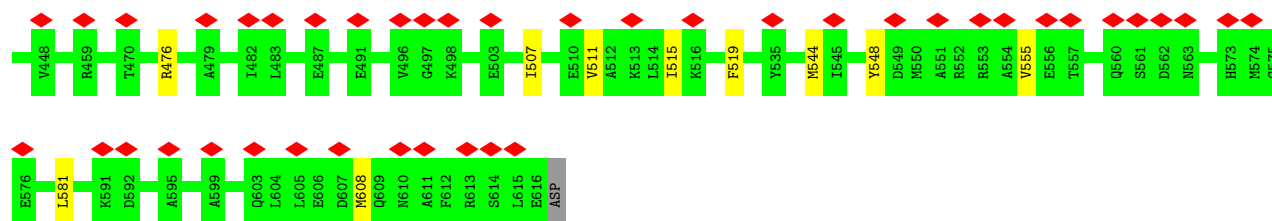


• Molecule 15: V-type proton ATPase catalytic subunit A



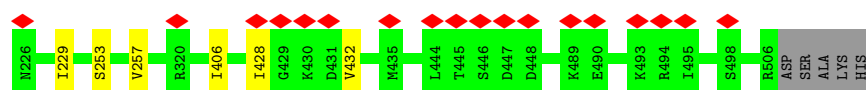
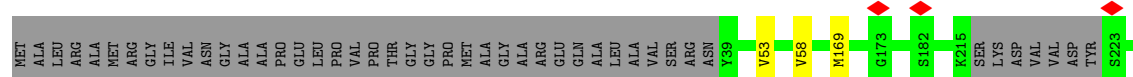
• Molecule 15: V-type proton ATPase catalytic subunit A





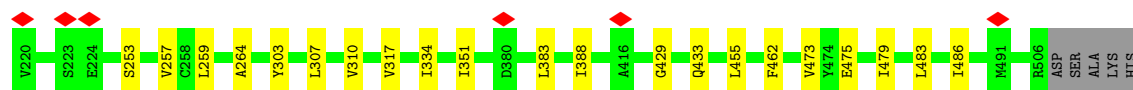
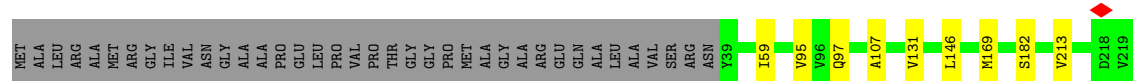
- Molecule 16: V-type proton ATPase subunit B, brain isoform

Chain 3: 88% 10%



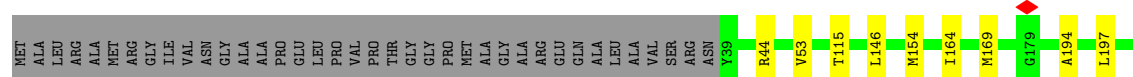
- Molecule 16: V-type proton ATPase subunit B, brain isoform

Chain 4: 86% 6% 8%



- Molecule 16: V-type proton ATPase subunit B, brain isoform

Chain 5: 87% 5% 8%



HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	495.6672, 495.6672, 495.6672	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1064, 1.1064, 1.1064	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	7	0.21	0/1694	0.43	0/2267
2	8	0.22	0/1840	0.44	0/2462
2	9	0.20	0/1840	0.43	0/2462
2	Q	0.21	0/1840	0.48	0/2462
3	R	0.25	0/930	0.41	0/1237
3	T	0.20	0/930	0.42	0/1237
3	V	0.20	0/930	0.39	0/1237
4	6	0.19	0/2985	0.43	1/4032 (0.0%)
5	U	0.18	0/3568	0.43	0/4806
6	a	0.21	0/6274	0.45	0/8486
7	e	0.25	0/648	0.46	0/891
8	f	0.22	0/674	0.43	0/915
9	b	0.21	0/1518	0.46	0/2061
10	g	0.23	0/1084	0.46	0/1466
10	h	0.21	0/1084	0.41	0/1466
10	i	0.32	0/1084	0.58	0/1466
10	j	0.19	0/1084	0.44	0/1466
10	k	0.21	0/1084	0.49	0/1466
10	l	0.22	0/1084	0.47	0/1466
10	m	0.25	0/1084	0.52	0/1466
10	n	0.23	0/1084	0.51	0/1466
10	o	0.24	0/1084	0.53	0/1466
11	X	0.16	0/889	0.37	0/1199
12	d	0.19	0/2908	0.40	0/3937
13	c	0.25	0/1697	0.54	1/2311 (0.0%)
14	p	0.16	0/420	0.33	0/576
15	0	0.18	0/4767	0.41	0/6453
15	1	0.17	0/4752	0.40	0/6433
15	2	0.19	0/4752	0.44	0/6433
16	3	0.18	0/3681	0.42	0/4987
16	4	0.19	0/3740	0.43	0/5069
16	5	0.18	0/3740	0.40	0/5069
All	All	0.20	0/66773	0.44	2/90216 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	c	373	LYS	N-CA-C	-5.72	98.61	110.80
4	6	291	PHE	N-CA-CB	5.03	118.08	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7	1676	0	1781	9	0
2	8	1823	0	1895	17	0
2	9	1823	0	1895	7	0
2	Q	1823	0	1895	9	0
3	R	925	0	935	12	0
3	T	925	0	935	0	0
3	V	925	0	935	5	0
4	6	2931	0	2969	10	0
5	U	3501	0	3481	19	0
6	a	6117	0	6154	42	0
7	e	623	0	641	11	0
8	f	658	0	652	1	0
9	b	1484	0	1528	19	0
10	g	1069	0	1136	23	0
10	h	1069	0	1136	14	0
10	i	1069	0	1136	19	0
10	j	1069	0	1136	10	0
10	k	1069	0	1136	11	0
10	l	1069	0	1136	9	0
10	m	1069	0	1136	25	0
10	n	1069	0	1136	13	0
10	o	1069	0	1136	14	0
11	X	875	0	883	4	0
12	d	2842	0	2782	11	0
13	c	1642	0	1568	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	p	407	0	403	3	0
15	0	4671	0	4654	19	0
15	1	4656	0	4643	24	0
15	2	4656	0	4643	40	0
16	3	3610	0	3613	6	0
16	4	3667	0	3667	22	0
16	5	3667	0	3667	21	0
All	All	65548	0	66443	381	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 3.

All (381) 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)
10:m:47:MET:CE	10:m:122:ALA:HB1	1.81	1.10
10:o:23:MET:HE2	10:o:73:ALA:HB3	1.41	0.99
15:0:220:LYS:HG2	16:5:242:ARG:NH1	1.80	0.97
10:m:28:MET:HE2	10:n:105:ALA:HB2	1.51	0.92
10:h:35:ALA:HB1	10:i:112:ILE:HG21	1.51	0.90
15:0:220:LYS:HG2	16:5:242:ARG:HH12	1.36	0.88
10:m:47:MET:HE2	10:m:122:ALA:HB1	1.55	0.85
5:U:438:MET:HE1	6:a:278:VAL:HG21	1.58	0.85
10:m:35:ALA:HB1	10:n:112:ILE:HG21	1.59	0.83
15:2:239:PRO:HD2	15:2:476:ARG:HH22	1.41	0.82
15:2:581:LEU:HD21	15:2:608:MET:HE1	1.63	0.79
10:m:24:VAL:HG13	10:n:101:LEU:HD11	1.67	0.77
10:g:28:MET:HE2	10:h:105:ALA:HB2	1.65	0.76
10:m:47:MET:SD	10:m:122:ALA:CB	2.76	0.74
15:2:239:PRO:CD	15:2:476:ARG:NH2	2.51	0.73
6:a:381:PHE:CD2	6:a:403:VAL:HG22	2.24	0.73
2:Q:148:VAL:O	2:Q:152:ILE:HD12	1.90	0.72
15:2:237:LEU:O	15:2:476:ARG:NH2	2.22	0.71
15:2:239:PRO:CD	15:2:476:ARG:HH22	2.04	0.70
9:b:94:ILE:HG21	10:g:137:PHE:CD2	2.27	0.70
15:2:239:PRO:HD2	15:2:476:ARG:NH2	2.06	0.69
2:9:173:LEU:HD23	2:9:177:ILE:HG21	1.75	0.69
5:U:205:LEU:HD11	5:U:218:TRP:CZ3	2.28	0.68
2:8:207:MET:HE1	3:R:102:MET:HE3	1.74	0.68
16:4:429:GLY:C	16:4:455:LEU:HD11	2.19	0.68
10:k:30:ALA:HB1	10:l:141:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:n:68:TYR:CD2	10:n:146:LEU:HD22	2.29	0.67
10:g:97:LEU:HD13	13:c:429:MET:HE2	1.76	0.67
10:m:24:VAL:HG13	10:n:101:LEU:CD1	2.24	0.67
15:2:315:THR:O	15:2:316:SER:C	2.37	0.67
9:b:136:SER:HA	10:o:16:VAL:HG21	1.77	0.67
9:b:105:ILE:HB	10:g:144:TYR:HE2	1.60	0.67
2:8:19:ILE:HD11	3:R:14:ALA:HB2	1.76	0.67
10:m:47:MET:SD	10:m:122:ALA:HB1	2.35	0.66
2:9:212:ARG:HB2	16:5:146:LEU:HD11	1.78	0.66
15:1:317:ASN:ND2	15:1:317:ASN:O	2.29	0.66
10:m:28:MET:CE	10:n:105:ALA:HB2	2.26	0.65
9:b:107:MET:HE3	9:b:191:VAL:HG13	1.78	0.65
10:m:47:MET:HE1	10:m:122:ALA:HB1	1.77	0.65
15:0:190:VAL:HG21	15:0:202:LYS:HD3	1.79	0.65
10:g:113:VAL:HG21	10:g:134:ILE:HG21	1.79	0.65
10:o:68:TYR:CG	10:o:146:LEU:HD22	2.32	0.65
16:4:213:VAL:HG23	16:4:473:VAL:HG21	1.79	0.64
10:n:66:ALA:CB	10:o:141:LEU:HD22	2.27	0.64
15:2:28:VAL:HG13	15:2:66:VAL:O	1.97	0.64
9:b:158:VAL:HG21	9:b:179:VAL:HG11	1.79	0.64
10:g:68:TYR:CD1	10:g:146:LEU:HD22	2.34	0.62
15:1:287:VAL:HG11	15:1:311:LEU:HD21	1.81	0.62
15:2:239:PRO:HD3	15:2:476:ARG:NH2	2.13	0.62
6:a:545:MET:O	6:a:549:VAL:HG23	1.99	0.61
6:a:401:TYR:CZ	6:a:405:THR:HG21	2.36	0.61
16:4:303:TYR:OH	16:4:334:ILE:HD11	2.00	0.60
6:a:532:ILE:CD1	7:e:72:THR:HG21	2.31	0.60
10:g:35:ALA:HB1	10:h:112:ILE:HG21	1.82	0.60
16:5:238:MET:SD	16:5:242:ARG:HD3	2.42	0.60
2:Q:34:ALA:HB1	3:V:32:ARG:HD2	1.84	0.59
6:a:271:ARG:O	6:a:275:LEU:HD23	2.02	0.59
15:0:241:VAL:HG12	15:0:461:LEU:HD21	1.84	0.59
10:k:56:ILE:HD11	10:l:133:LEU:HD22	1.85	0.59
6:a:825:LEU:HD12	6:a:825:LEU:O	2.02	0.59
10:h:35:ALA:CB	10:i:112:ILE:HG21	2.31	0.59
15:2:239:PRO:CD	15:2:476:ARG:NH1	2.66	0.59
10:m:47:MET:CE	10:m:122:ALA:CB	2.70	0.58
15:1:526:THR:HG21	15:1:528:TYR:CZ	2.38	0.58
6:a:602:TRP:CH2	7:e:54:ILE:HG23	2.38	0.58
12:d:86:ARG:HH12	12:d:101:THR:HG21	1.68	0.58
15:2:239:PRO:HD3	15:2:476:ARG:CZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:379:VAL:HG23	16:5:391:PRO:O	2.03	0.58
9:b:58:ILE:HD11	10:g:148:VAL:HG11	1.86	0.58
16:4:351:ILE:O	16:4:351:ILE:HG23	2.04	0.57
6:a:532:ILE:HD11	7:e:72:THR:HG21	1.86	0.57
15:2:507:ILE:HD11	15:2:555:VAL:HG21	1.87	0.56
15:0:584:MET:HE2	15:0:604:LEU:HD12	1.86	0.56
10:k:44:MET:SD	10:k:122:ALA:HB2	2.45	0.56
2:Q:207:MET:HE3	2:Q:210:GLU:OE1	2.05	0.56
15:2:239:PRO:CD	15:2:476:ARG:CZ	2.84	0.56
10:m:41:ILE:HD13	10:m:56:ILE:HD13	1.88	0.56
15:2:238:PHE:HA	15:2:476:ARG:NH2	2.21	0.56
16:5:194:ALA:H	16:5:197:LEU:HD12	1.71	0.56
12:d:164:PHE:CE1	12:d:185:LEU:HD22	2.41	0.56
5:U:438:MET:HE1	6:a:278:VAL:CG2	2.34	0.56
9:b:146:LEU:HD13	10:o:24:VAL:HG11	1.88	0.55
4:6:72:VAL:HG22	4:6:136:LEU:CD2	2.37	0.55
5:U:17:ASN:N	5:U:196:GLN:HE21	2.05	0.55
15:1:57:LEU:CD1	16:4:107:ALA:HB2	2.36	0.55
6:a:603:THR:HG22	7:e:60:LEU:HD23	1.89	0.55
15:0:234:LEU:HD13	15:0:433:TRP:CE3	2.42	0.55
15:0:574:MET:HE1	15:0:608:MET:SD	2.47	0.55
15:0:234:LEU:HD22	15:0:433:TRP:CG	2.42	0.55
13:c:390:LEU:HD22	13:c:393:PHE:CD1	2.42	0.54
4:6:93:ALA:HB1	4:6:291:PHE:CZ	2.43	0.54
10:n:114:GLY:O	10:n:118:VAL:HG23	2.08	0.54
15:2:316:SER:O	15:2:317:ASN:C	2.50	0.54
15:1:493:VAL:HG12	15:1:501:LEU:HD21	1.89	0.54
10:m:20:SER:O	10:m:24:VAL:HG23	2.08	0.54
10:m:61:MET:O	10:m:64:ILE:HG22	2.08	0.53
1:7:205:ILE:CD1	16:4:317:VAL:HG22	2.37	0.53
2:8:208:MET:HE2	16:4:146:LEU:CD1	2.38	0.53
11:X:71:ALA:HB1	11:X:78:LEU:HD22	1.90	0.53
16:5:154:MET:HE3	16:5:154:MET:O	2.09	0.53
10:i:72:VAL:HG11	10:i:99:VAL:HG11	1.91	0.53
15:2:519:PHE:HB2	15:2:544:MET:HE1	1.90	0.53
5:U:226:CYS:O	5:U:230:VAL:HG23	2.09	0.53
10:g:113:VAL:HG21	10:g:134:ILE:CG2	2.39	0.53
5:U:145:ILE:HD11	5:U:161:LEU:HD22	1.91	0.53
10:o:23:MET:HE2	10:o:73:ALA:CB	2.26	0.53
15:1:102:ILE:HG22	15:1:102:ILE:O	2.09	0.53
15:1:234:LEU:HD22	15:1:433:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:86:LYS:O	5:U:90:VAL:HG12	2.10	0.52
15:2:239:PRO:CD	15:2:476:ARG:HH12	2.22	0.52
12:d:183:ASN:HB3	12:d:240:LEU:HD22	1.92	0.52
10:g:21:SER:HB2	10:g:97:LEU:HD23	1.90	0.52
3:R:8:ILE:O	3:R:12:LEU:HD23	2.10	0.52
10:h:108:PHE:O	10:h:112:ILE:HG22	2.09	0.52
16:5:197:LEU:HD13	16:5:379:VAL:HG13	1.92	0.52
10:k:14:PHE:CE2	10:k:86:LEU:HD11	2.45	0.52
12:d:139:GLU:OE1	12:d:153:ALA:HB1	2.10	0.51
15:1:317:ASN:ND2	15:1:317:ASN:C	2.68	0.51
10:g:97:LEU:HD22	13:c:429:MET:HE1	1.92	0.51
16:5:44:ARG:NH2	16:5:115:THR:HG22	2.25	0.51
1:7:62:MET:HE1	11:X:92:PRO:O	2.10	0.51
10:k:14:PHE:CD2	10:k:86:LEU:HD11	2.46	0.51
10:o:68:TYR:HB3	10:o:146:LEU:HD13	1.93	0.51
15:2:511:VAL:HG21	15:2:548:TYR:HB2	1.93	0.51
10:k:113:VAL:HG21	10:k:134:ILE:HG21	1.91	0.51
15:2:28:VAL:HG11	15:2:65:GLN:OE1	2.11	0.51
9:b:137:MET:HE1	9:b:198:THR:HG22	1.93	0.51
10:i:28:MET:CE	10:j:105:ALA:HB2	2.40	0.51
10:m:40:GLY:C	10:m:118:VAL:HG11	2.35	0.51
15:2:581:LEU:HD21	15:2:608:MET:CE	2.36	0.51
9:b:102:ILE:HA	9:b:105:ILE:HG22	1.91	0.51
10:o:19:ALA:HB2	10:o:76:ILE:HG21	1.93	0.51
10:g:109:ALA:O	10:g:113:VAL:HG12	2.11	0.50
15:0:534:PHE:O	15:0:538:VAL:HG23	2.11	0.50
15:2:239:PRO:HD2	15:2:476:ARG:HH12	1.75	0.50
10:g:93:LEU:CD1	10:g:97:LEU:HD11	2.41	0.50
10:m:47:MET:SD	10:m:122:ALA:HB2	2.51	0.50
16:5:238:MET:HE1	16:5:239:GLU:OE2	2.10	0.50
2:Q:16:MET:HE2	3:V:11:LEU:HD23	1.94	0.50
3:R:40:ALA:O	3:R:44:VAL:HG23	2.12	0.50
2:8:23:ALA:HB1	3:R:17:ARG:HG2	1.92	0.50
6:a:399:ALA:O	6:a:403:VAL:HG23	2.12	0.50
2:8:90:LEU:HD23	3:R:88:GLN:OE1	2.11	0.50
10:l:132:ILE:HD13	10:l:135:LEU:HD12	1.94	0.49
13:c:313:ALA:HB1	13:c:343:SER:OG	2.12	0.49
16:5:241:ALA:HB1	16:5:261:LEU:HD22	1.92	0.49
2:8:155:TYR:O	2:8:159:THR:HG22	2.12	0.49
6:a:401:TYR:CE2	6:a:405:THR:HG21	2.46	0.49
12:d:78:MET:HE1	12:d:319:VAL:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:152:ASN:O	12:d:156:VAL:HG23	2.11	0.49
5:U:94:LEU:HD11	5:U:140:MET:HE3	1.94	0.49
15:0:221:LEU:HD11	15:0:393:LYS:CD	2.43	0.49
6:a:32:LEU:HD21	6:a:340:ILE:CD1	2.43	0.49
10:l:91:LEU:HD21	10:l:152:LEU:HB3	1.95	0.49
16:3:169:MET:CE	16:3:406:ILE:HG22	2.41	0.49
2:8:127:LEU:HD23	2:8:132:MET:HG2	1.95	0.49
4:6:5:TRP:CD1	4:6:371:TYR:HH	2.31	0.49
6:a:547:MET:HE1	7:e:51:PHE:HA	1.95	0.49
13:c:368:VAL:O	13:c:368:VAL:HG13	2.13	0.49
13:c:423:LEU:HD11	14:p:312:TRP:CZ2	2.48	0.49
15:1:223:ALA:HB1	15:1:241:VAL:HG21	1.95	0.49
15:0:471:GLU:OE1	15:0:475:LEU:HD11	2.13	0.49
2:8:207:MET:CE	3:R:102:MET:HE3	2.43	0.49
10:i:66:ALA:O	10:i:70:LEU:HD23	2.12	0.49
10:j:81:THR:HG22	10:j:82:ASP:H	1.78	0.49
15:0:505:ASP:O	15:0:509:LEU:HD23	2.13	0.49
4:6:68:VAL:O	4:6:72:VAL:HG23	2.12	0.48
15:2:156:VAL:HG23	15:2:166:ILE:HD11	1.94	0.48
2:9:42:LYS:O	2:9:46:VAL:HG23	2.13	0.48
10:o:109:ALA:O	10:o:113:VAL:HG22	2.13	0.48
15:0:331:ILE:HD13	15:0:346:MET:HE1	1.95	0.48
16:4:59:ILE:HD12	16:4:95:VAL:HG22	1.96	0.48
2:9:91:ILE:HG21	2:9:208:MET:HE1	1.95	0.48
16:4:462:PHE:HB2	16:4:483:LEU:HD11	1.95	0.48
16:5:169:MET:HE1	16:5:213:VAL:HG11	1.95	0.48
6:a:486:TRP:CH2	6:a:529:ILE:HG21	2.49	0.48
6:a:659:LEU:O	6:a:719:MET:HE1	2.14	0.48
15:1:287:VAL:CG1	15:1:311:LEU:HD21	2.44	0.48
2:8:155:TYR:CZ	2:8:159:THR:HG21	2.49	0.48
10:i:104:LEU:HD22	14:p:324:THR:HG21	1.96	0.48
10:m:68:TYR:CE1	10:m:146:LEU:HD22	2.48	0.48
10:o:57:ILE:HD13	10:o:132:ILE:HD12	1.96	0.48
12:d:164:PHE:CD1	12:d:185:LEU:HD22	2.49	0.48
6:a:548:SER:OG	6:a:743:LEU:HD22	2.14	0.48
9:b:51:ASN:OD1	10:g:91:LEU:HD13	2.14	0.48
10:i:15:GLY:HA2	10:i:92:GLN:HB3	1.96	0.48
4:6:72:VAL:HG22	4:6:136:LEU:HD21	1.96	0.48
10:m:47:MET:HE2	10:m:122:ALA:CB	2.37	0.48
2:Q:54:MET:HE3	2:Q:54:MET:HA	1.94	0.47
4:6:208:VAL:HG12	4:6:229:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:412:VAL:CG1	6:a:743:LEU:HD11	2.45	0.47
10:i:66:ALA:HB1	10:j:144:TYR:CE2	2.49	0.47
2:8:198:SER:O	2:8:202:LEU:HD23	2.14	0.47
6:a:565:PHE:HA	6:a:568:ILE:HG22	1.94	0.47
9:b:189:PHE:O	9:b:193:VAL:HG23	2.14	0.47
10:l:70:LEU:HD11	10:m:144:TYR:HB3	1.96	0.47
16:5:197:LEU:HD13	16:5:379:VAL:CG1	2.45	0.47
4:6:207:MET:H	4:6:207:MET:HE2	1.78	0.47
10:g:35:ALA:CB	10:h:112:ILE:HG21	2.44	0.47
9:b:137:MET:HE2	9:b:201:VAL:HG21	1.96	0.47
10:k:11:SER:HA	10:k:86:LEU:HD13	1.96	0.47
1:7:32:LEU:HG	16:5:438:VAL:HG22	1.97	0.47
9:b:58:ILE:CD1	10:g:148:VAL:HG11	2.44	0.47
10:h:81:THR:HG23	10:h:84:ILE:HD13	1.97	0.47
10:i:28:MET:HB2	10:i:104:LEU:HD21	1.97	0.47
16:4:131:VAL:HG22	16:4:259:LEU:HD12	1.97	0.47
6:a:217:VAL:HG23	6:a:218:THR:HG23	1.97	0.47
10:h:44:MET:HG2	10:h:122:ALA:HB2	1.97	0.47
2:8:103:SER:O	2:8:106:VAL:HG12	2.15	0.47
6:a:491:MET:HE3	7:e:77:ARG:HG2	1.96	0.47
12:d:151:TYR:CZ	12:d:155:LEU:HD11	2.50	0.47
10:i:145:GLY:O	10:i:148:VAL:HG12	2.14	0.47
11:X:67:ASN:OD1	11:X:70:ILE:HD12	2.15	0.47
3:R:113:ASN:O	3:R:114:TYR:C	2.55	0.46
5:U:230:VAL:HG12	5:U:243:MET:HE1	1.97	0.46
6:a:731:LEU:CD1	10:i:143:LEU:HD22	2.45	0.46
10:n:53:MET:HE2	10:n:53:MET:N	2.30	0.46
2:8:11:GLN:HG2	6:a:358:ILE:HD12	1.97	0.46
6:a:412:VAL:HG13	6:a:743:LEU:HD11	1.95	0.46
10:g:93:LEU:HD11	10:g:97:LEU:HD11	1.98	0.46
16:3:53:VAL:HG12	16:3:58:VAL:HG22	1.97	0.46
5:U:318:LEU:HD12	5:U:335:ILE:HG23	1.97	0.46
6:a:537:LEU:HD13	10:j:154:THR:HG21	1.97	0.46
7:e:75:TYR:CE1	8:f:38:ALA:HB1	2.51	0.46
5:U:143:ARG:HH11	5:U:146:ALA:HB3	1.81	0.46
10:i:81:THR:HG23	10:i:84:ILE:CD1	2.46	0.46
4:6:207:MET:HE2	4:6:207:MET:N	2.30	0.46
15:0:19:GLY:O	15:0:79:VAL:HB	2.16	0.46
3:V:96:LEU:O	3:V:100:LEU:HD23	2.15	0.46
15:0:192:LEU:HD23	15:0:193:GLU:N	2.31	0.46
5:U:314:VAL:HG12	5:U:318:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:61:MET:HG2	6:a:98:GLU:HG2	1.98	0.46
6:a:603:THR:CG2	7:e:60:LEU:HD23	2.45	0.46
10:i:14:PHE:HB2	10:i:89:SER:HB3	1.96	0.46
10:k:23:MET:HE3	10:k:73:ALA:CB	2.46	0.46
15:1:57:LEU:HD12	16:4:107:ALA:HB2	1.98	0.46
10:g:91:LEU:HD21	10:g:152:LEU:HD12	1.98	0.45
10:o:45:SER:HA	10:o:52:ILE:HD12	1.98	0.45
6:a:269:ASN:HA	6:a:272:ILE:HD12	1.99	0.45
10:m:114:GLY:O	10:m:118:VAL:HG23	2.17	0.45
15:1:237:LEU:O	15:1:458:MET:HE1	2.17	0.45
15:1:526:THR:HG21	15:1:528:TYR:CE1	2.51	0.45
2:9:12:ILE:HG22	2:9:16:MET:SD	2.57	0.45
6:a:29:LEU:HD22	6:a:35:VAL:HG21	1.98	0.45
6:a:302:ILE:HD13	6:a:832:ILE:O	2.17	0.45
15:2:366:ALA:CB	16:5:317:VAL:HG21	2.46	0.45
9:b:72:THR:HG21	9:b:93:SER:HB2	1.99	0.45
10:i:52:ILE:HD11	10:j:127:LEU:CD2	2.47	0.45
10:k:146:LEU:HD11	10:k:150:LEU:HD21	1.99	0.45
15:2:239:PRO:HD2	15:2:476:ARG:NH1	2.31	0.45
15:2:152:ILE:HD11	15:2:400:ARG:NH1	2.32	0.45
15:2:515:ILE:HG12	15:2:544:MET:HE2	1.99	0.45
16:3:428:ILE:O	16:3:432:VAL:HG23	2.16	0.45
6:a:593:TYR:O	6:a:597:LEU:HD13	2.17	0.44
10:g:42:ALA:HB2	10:h:116:ALA:HB1	1.98	0.44
15:0:21:VAL:O	15:0:75:VAL:HG23	2.17	0.44
5:U:145:ILE:CD1	5:U:161:LEU:HD22	2.47	0.44
10:o:72:VAL:HG22	10:o:150:LEU:HD21	1.99	0.44
12:d:149:GLU:O	12:d:153:ALA:HB2	2.17	0.44
13:c:355:VAL:HG13	13:c:363:PHE:CD2	2.52	0.44
15:1:324:GLU:OE1	15:1:358:LEU:HD21	2.17	0.44
16:4:97:GLN:OE1	16:4:310:VAL:HG23	2.17	0.44
2:9:3:LEU:HD11	6:a:201:ASN:HD21	1.82	0.44
2:Q:148:VAL:HG13	2:Q:152:ILE:HD11	1.99	0.44
10:m:24:VAL:CG1	10:n:101:LEU:HD11	2.40	0.44
15:2:364:ARG:O	15:2:364:ARG:HG3	2.17	0.44
10:i:47:MET:HE1	14:p:336:ASP:OD2	2.17	0.44
13:c:276:TRP:CZ3	13:c:389:THR:HG22	2.52	0.44
10:i:70:LEU:HD21	10:j:144:TYR:CG	2.52	0.44
10:l:23:MET:SD	10:m:148:VAL:HG11	2.57	0.44
15:0:44:ARG:O	15:0:79:VAL:HA	2.16	0.44
2:8:215:LEU:HD21	3:R:95:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:h:23:MET:SD	10:i:148:VAL:HG11	2.58	0.44
15:1:271:VAL:HB	15:1:344:VAL:HG12	2.00	0.44
10:h:8:PRO:HD2	10:h:86:LEU:HD11	2.00	0.43
12:d:335:CYS:SG	12:d:344:ILE:HD12	2.58	0.43
15:0:584:MET:CE	15:0:604:LEU:HD12	2.48	0.43
1:7:51:ILE:HG22	1:7:151:LEU:HD21	1.99	0.43
2:8:53:ILE:HD11	3:R:44:VAL:CG1	2.48	0.43
10:g:97:LEU:HB3	13:c:429:MET:HE1	2.00	0.43
9:b:48:MET:HE1	13:c:421:MET:HB3	2.01	0.43
1:7:58:MET:N	1:7:58:MET:HE2	2.34	0.43
2:8:19:ILE:CD1	3:R:14:ALA:HB2	2.47	0.43
15:2:511:VAL:O	15:2:515:ILE:HG13	2.19	0.43
16:4:307:LEU:HA	16:4:310:VAL:HG12	2.01	0.43
15:2:21:VAL:HG11	15:2:73:VAL:HG21	1.99	0.43
16:5:194:ALA:N	16:5:197:LEU:HD12	2.33	0.43
6:a:193:MET:O	6:a:197:VAL:HG22	2.19	0.43
10:g:23:MET:HE1	10:h:144:TYR:HB3	2.00	0.43
10:l:23:MET:HE2	10:m:98:SER:HB3	1.99	0.43
9:b:114:MET:HE2	9:b:201:VAL:HG12	2.00	0.43
10:n:120:GLY:C	10:n:127:LEU:HD22	2.44	0.43
4:6:132:ILE:O	4:6:136:LEU:HD13	2.19	0.43
15:1:254:CYS:SG	15:1:435:LEU:HD23	2.58	0.43
16:4:383:LEU:HD22	16:4:388:ILE:HD12	2.01	0.43
10:j:84:ILE:HG22	10:j:86:LEU:H	1.84	0.43
10:m:87:TYR:HA	10:m:90:PHE:CE1	2.53	0.43
13:c:373:LYS:HD3	13:c:374:LYS:H	1.84	0.43
15:1:234:LEU:HD21	15:1:448:VAL:HG11	2.01	0.43
15:2:278:GLY:HA2	15:2:316:SER:H	1.84	0.43
6:a:549:VAL:HG12	6:a:553:ILE:HD12	2.00	0.42
16:4:169:MET:HE1	16:4:182:SER:HB3	2.01	0.42
1:7:48:LEU:HD13	1:7:155:PHE:CZ	2.54	0.42
1:7:153:THR:O	1:7:156:VAL:HG12	2.19	0.42
2:Q:46:VAL:HG11	3:V:40:ALA:HB1	2.00	0.42
5:U:215:ARG:O	5:U:219:VAL:HG22	2.17	0.42
15:2:237:LEU:O	15:2:476:ARG:CZ	2.67	0.42
10:g:56:ILE:HG22	10:g:56:ILE:O	2.17	0.42
15:1:24:VAL:HG12	15:1:29:VAL:HG23	2.01	0.42
15:2:305:ILE:HG22	15:2:305:ILE:O	2.19	0.42
5:U:359:LEU:HD22	5:U:394:LEU:HD21	2.00	0.42
15:2:239:PRO:HD2	15:2:476:ARG:CZ	2.50	0.42
10:i:61:MET:HE1	10:i:138:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:376:ASN:O	13:c:377:LEU:HB3	2.19	0.42
5:U:129:MET:HE1	5:U:140:MET:HE1	2.01	0.42
10:g:97:LEU:HD22	13:c:429:MET:CE	2.49	0.42
6:a:57:ARG:HH22	6:a:99:ALA:HB2	1.84	0.42
15:1:387:GLU:OE1	16:4:264:ALA:HB3	2.19	0.42
16:3:169:MET:HE2	16:3:406:ILE:HG22	2.02	0.42
15:2:308:ARG:O	15:2:308:ARG:HG2	2.19	0.42
2:Q:34:ALA:HB1	3:V:32:ARG:CD	2.49	0.42
6:a:491:MET:HE2	7:e:74:TRP:HA	2.02	0.42
7:e:71:GLU:OE2	7:e:72:THR:HG23	2.20	0.42
16:5:164:ILE:HD11	16:5:342:GLU:HB3	2.01	0.42
16:5:212:LEU:HD11	16:5:227:PHE:CD1	2.55	0.42
13:c:385:VAL:HG23	13:c:385:VAL:O	2.20	0.42
16:3:229:ILE:HB	16:3:257:VAL:HG22	2.02	0.42
10:l:66:ALA:O	10:l:70:LEU:HD13	2.18	0.41
15:1:550:MET:HE3	15:1:554:ALA:HB2	2.02	0.41
15:2:136:ILE:HG23	15:2:136:ILE:O	2.19	0.41
16:3:253:SER:O	16:3:257:VAL:HG23	2.20	0.41
16:4:475:GLU:OE2	16:4:479:ILE:HD11	2.20	0.41
2:9:212:ARG:HG3	16:5:146:LEU:HD21	2.01	0.41
10:m:99:VAL:HB	10:m:149:ALA:HB2	2.02	0.41
16:4:303:TYR:CZ	16:4:334:ILE:HD11	2.55	0.41
6:a:412:VAL:HG23	7:e:51:PHE:HE1	1.85	0.41
15:1:317:ASN:C	15:1:317:ASN:HD22	2.19	0.41
15:2:28:VAL:HG11	15:2:65:GLN:CD	2.46	0.41
15:2:141:LEU:HD22	15:2:179:ILE:HD11	2.01	0.41
16:4:253:SER:O	16:4:257:VAL:HG23	2.20	0.41
10:h:20:SER:O	10:h:24:VAL:HG23	2.21	0.41
15:0:39:MET:HE2	16:5:53:VAL:HG13	2.01	0.41
15:2:320:VAL:HG12	15:2:361:ILE:HG23	2.02	0.41
1:7:140:LYS:O	1:7:144:LEU:HD23	2.21	0.41
10:n:23:MET:SD	10:o:98:SER:HB2	2.60	0.41
12:d:23:LEU:HD11	12:d:85:MET:HE3	2.01	0.41
13:c:380:THR:HG22	13:c:381:ASN:N	2.35	0.41
3:R:29:LYS:HE2	3:R:29:LYS:HA	2.03	0.41
10:k:23:MET:HE1	10:l:144:TYR:OH	2.21	0.41
13:c:352:VAL:HG12	13:c:353:SER:N	2.35	0.41
15:1:234:LEU:HD11	15:1:448:VAL:HG21	2.03	0.41
15:2:317:ASN:O	15:2:318:MET:C	2.63	0.41
10:h:114:GLY:O	10:h:118:VAL:HG23	2.20	0.41
13:c:370:SER:CB	13:c:377:LEU:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:59:SER:O	9:b:63:VAL:HG23	2.21	0.41
10:j:81:THR:HG22	10:j:82:ASP:N	2.35	0.41
2:8:208:MET:HE2	16:4:146:LEU:HD11	2.03	0.41
5:U:31:VAL:HG11	5:U:93:ILE:HD13	2.02	0.41
5:U:102:GLN:HA	5:U:143:ARG:HE	1.86	0.41
9:b:91:LEU:HD22	9:b:94:ILE:HD12	2.03	0.41
2:8:54:MET:HE3	2:8:54:MET:HA	2.02	0.41
10:k:51:LEU:HD12	10:k:51:LEU:O	2.21	0.41
15:2:21:VAL:HG11	15:2:73:VAL:CG2	2.50	0.41
6:a:806:ARG:O	6:a:810:VAL:HG23	2.21	0.40
16:4:433:GLN:HE21	16:4:433:GLN:HB3	1.64	0.40
15:1:241:VAL:HG22	15:1:242:GLN:N	2.37	0.40
15:1:547:PHE:CZ	15:1:578:LEU:HD21	2.56	0.40
16:4:483:LEU:O	16:4:486:ILE:HG22	2.21	0.40
10:j:43:ALA:O	10:j:46:VAL:HG22	2.21	0.40
10:o:68:TYR:CD1	10:o:146:LEU:HD22	2.56	0.40
4:6:50:VAL:HG12	4:6:50:VAL:O	2.21	0.40
6:a:547:MET:HE3	6:a:551:LEU:HG	2.03	0.40
6:a:663:PRO:HG3	6:a:719:MET:SD	2.62	0.40
9:b:48:MET:HE1	13:c:421:MET:CB	2.51	0.40
10:i:34:THR:HG21	10:j:138:ALA:HB2	2.04	0.40
1:7:155:PHE:HD2	11:X:105:ILE:HD11	1.86	0.40
2:Q:116:LEU:HD21	2:Q:144:VAL:HA	2.03	0.40
5:U:31:VAL:HG11	5:U:93:ILE:HA	2.03	0.40
6:a:556:MET:HG2	6:a:587:MET:HE1	2.04	0.40
10:n:84:ILE:HD12	10:n:89:SER:OG	2.22	0.40
16:5:286:ALA:CB	16:5:348:ILE:HD11	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	206/247 (83%)	197 (96%)	9 (4%)	0	100	100
2	8	223/226 (99%)	219 (98%)	4 (2%)	0	100	100
2	9	223/226 (99%)	220 (99%)	3 (1%)	0	100	100
2	Q	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
3	R	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
3	T	112/118 (95%)	112 (100%)	0	0	100	100
3	V	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
4	6	357/382 (94%)	339 (95%)	18 (5%)	0	100	100
5	U	422/483 (87%)	394 (93%)	26 (6%)	2 (0%)	24	62
6	a	746/838 (89%)	697 (93%)	49 (7%)	0	100	100
7	e	75/81 (93%)	71 (95%)	4 (5%)	0	100	100
8	f	83/98 (85%)	79 (95%)	4 (5%)	0	100	100
9	b	198/205 (97%)	192 (97%)	6 (3%)	0	100	100
10	g	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	h	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
10	i	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
10	j	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
10	k	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
10	l	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	18	55
10	m	148/155 (96%)	136 (92%)	12 (8%)	0	100	100
10	n	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	o	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
11	X	108/119 (91%)	103 (95%)	5 (5%)	0	100	100
12	d	349/351 (99%)	330 (95%)	19 (5%)	0	100	100
13	c	201/463 (43%)	166 (83%)	33 (16%)	2 (1%)	12	47
14	p	47/350 (13%)	43 (92%)	4 (8%)	0	100	100
15	0	600/617 (97%)	563 (94%)	37 (6%)	0	100	100
15	1	598/617 (97%)	564 (94%)	34 (6%)	0	100	100
15	2	598/617 (97%)	552 (92%)	44 (7%)	2 (0%)	36	71
16	3	457/511 (89%)	429 (94%)	28 (6%)	0	100	100
16	4	466/511 (91%)	442 (95%)	24 (5%)	0	100	100
16	5	466/511 (91%)	451 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8314/9428 (88%)	7877 (95%)	430 (5%)	7 (0%)	49 83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	U	134	ASP
13	c	388	MET
15	2	316	SER
15	2	317	ASN
10	l	57	ILE
13	c	373	LYS
5	U	279	GLU

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	7	179/212 (84%)	179 (100%)	0	100 100
2	8	197/198 (100%)	197 (100%)	0	100 100
2	9	197/198 (100%)	197 (100%)	0	100 100
2	Q	197/198 (100%)	197 (100%)	0	100 100
3	R	96/99 (97%)	95 (99%)	1 (1%)	68 76
3	T	96/99 (97%)	96 (100%)	0	100 100
3	V	96/99 (97%)	96 (100%)	0	100 100
4	6	326/344 (95%)	326 (100%)	0	100 100
5	U	384/429 (90%)	384 (100%)	0	100 100
6	a	669/741 (90%)	669 (100%)	0	100 100
7	e	65/68 (96%)	65 (100%)	0	100 100
8	f	71/83 (86%)	71 (100%)	0	100 100
9	b	154/158 (98%)	154 (100%)	0	100 100
10	g	109/113 (96%)	109 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	h	109/113 (96%)	109 (100%)	0	100	100
10	i	109/113 (96%)	108 (99%)	1 (1%)	70	76
10	j	109/113 (96%)	109 (100%)	0	100	100
10	k	109/113 (96%)	109 (100%)	0	100	100
10	l	109/113 (96%)	109 (100%)	0	100	100
10	m	109/113 (96%)	109 (100%)	0	100	100
10	n	109/113 (96%)	109 (100%)	0	100	100
10	o	109/113 (96%)	109 (100%)	0	100	100
11	X	94/100 (94%)	94 (100%)	0	100	100
12	d	306/306 (100%)	306 (100%)	0	100	100
13	c	180/395 (46%)	180 (100%)	0	100	100
14	p	44/309 (14%)	44 (100%)	0	100	100
15	0	509/524 (97%)	509 (100%)	0	100	100
15	1	507/524 (97%)	506 (100%)	1 (0%)	87	85
15	2	507/524 (97%)	507 (100%)	0	100	100
16	3	395/431 (92%)	395 (100%)	0	100	100
16	4	402/431 (93%)	402 (100%)	0	100	100
16	5	402/431 (93%)	402 (100%)	0	100	100
All	All	7054/7918 (89%)	7051 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	R	116	VAL
10	i	13	PHE
15	1	317	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	7	113	HIS
2	9	11	GLN
2	9	77	ASN
3	V	82	GLN
4	6	131	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	6	254	ASN
5	U	240	GLN
5	U	440	HIS
6	a	238	ASN
6	a	752	GLN
9	b	132	HIS
10	g	6	ASN
10	g	124	GLN
10	j	7	ASN
10	o	124	GLN
11	X	96	HIS
12	d	13	ASN
12	d	130	HIS
15	1	146	HIS
15	1	164	HIS
15	2	317	ASN
15	2	343	HIS
16	3	415	HIS
16	4	187	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 ⓘ

There are no chain breaks in this entry.

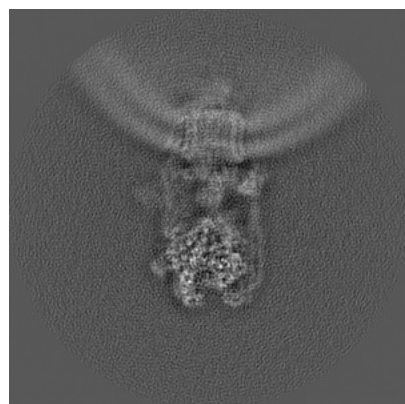
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44844. These allow visual inspection of the internal detail of the map and identification of artifacts.

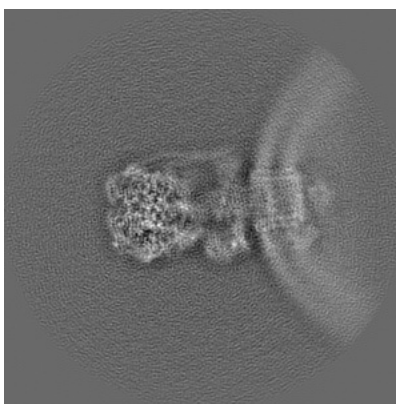
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

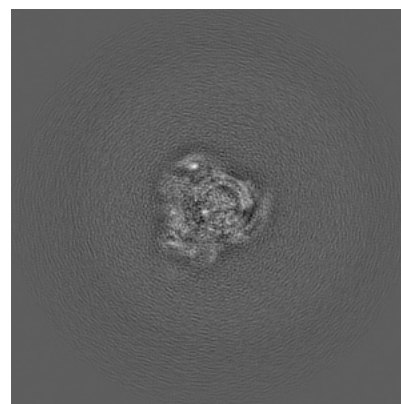
6.1.1 Primary map



X

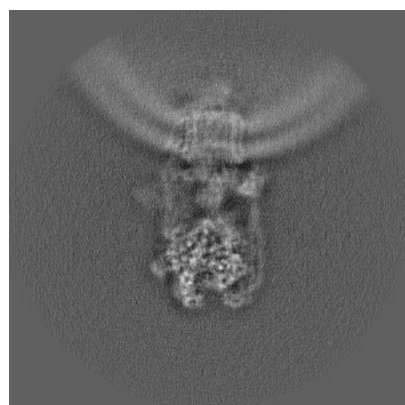


Y

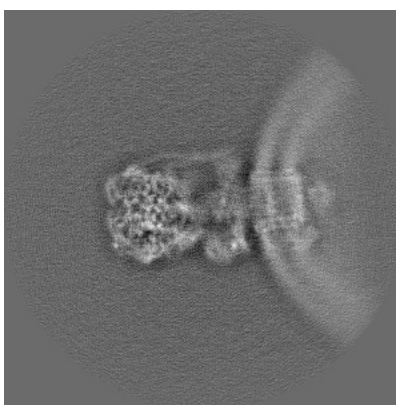


Z

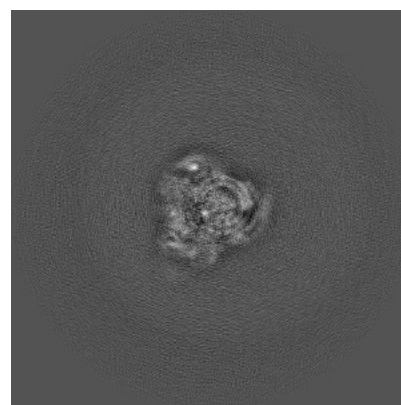
6.1.2 Raw map



X



Y

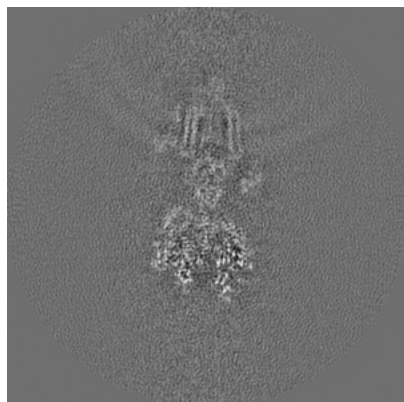


Z

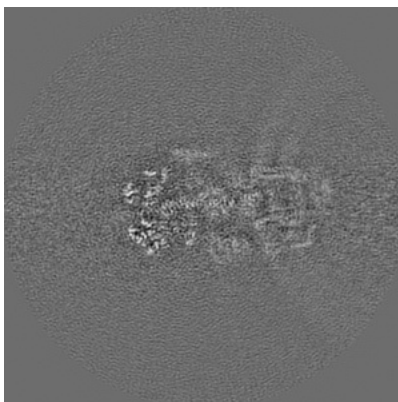
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

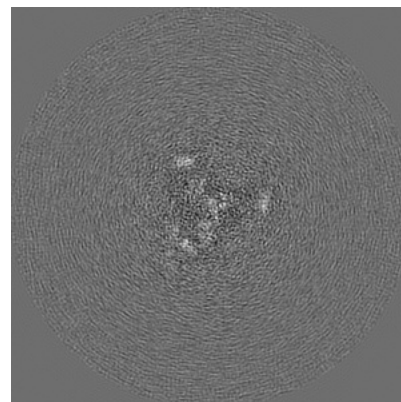
6.2.1 Primary map



X Index: 224

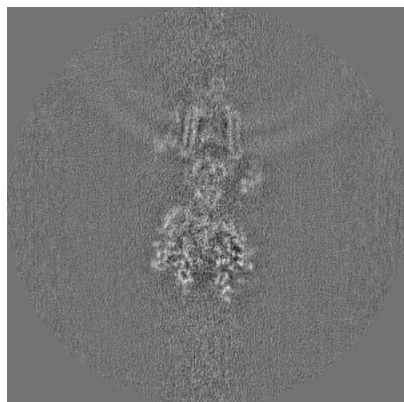


Y Index: 224



Z Index: 224

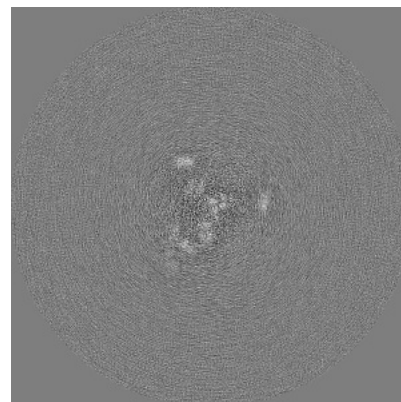
6.2.2 Raw map



X Index: 224



Y Index: 224



Z Index: 224

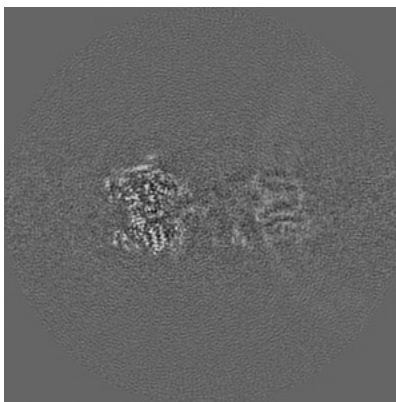
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

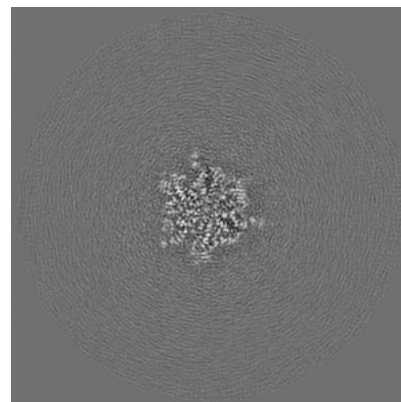
6.3.1 Primary map



X Index: 215

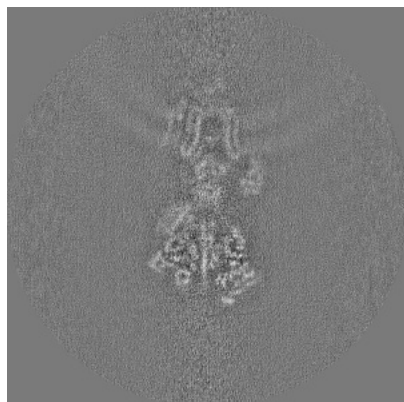


Y Index: 205

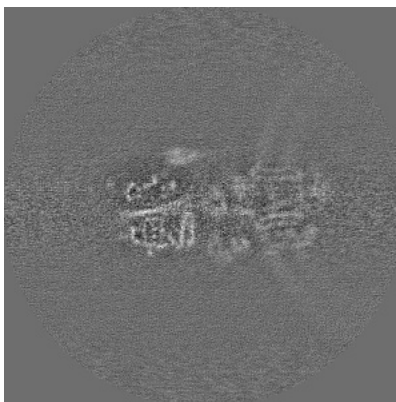


Z Index: 166

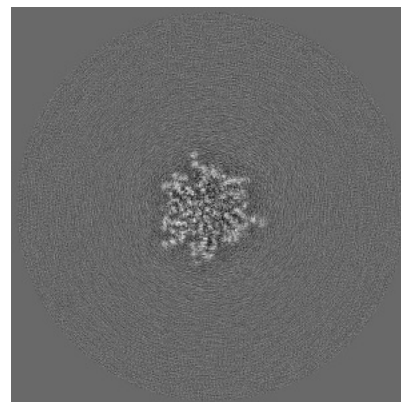
6.3.2 Raw map



X Index: 219



Y Index: 220

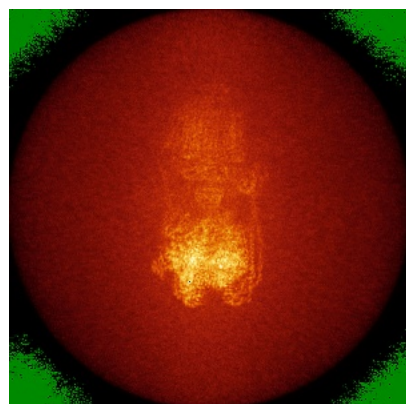


Z Index: 168

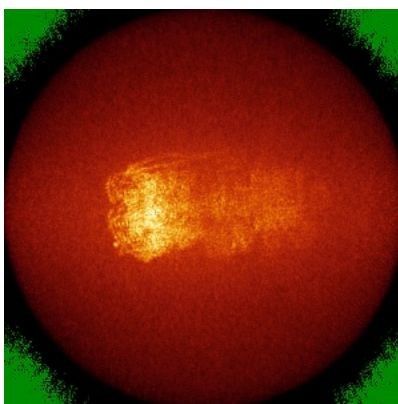
The images above show the largest variance slices of the map in three orthogonal directions.

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

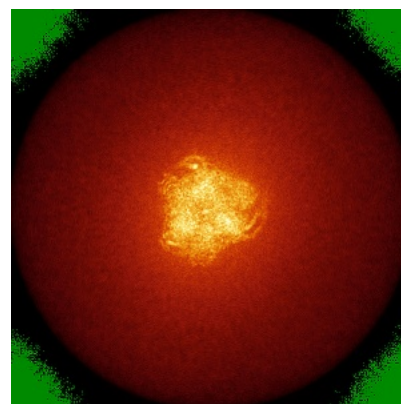
6.4.1 Primary map



X

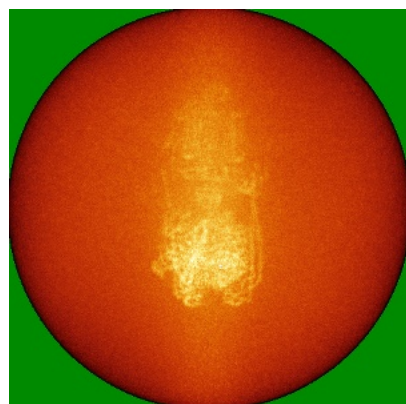


Y

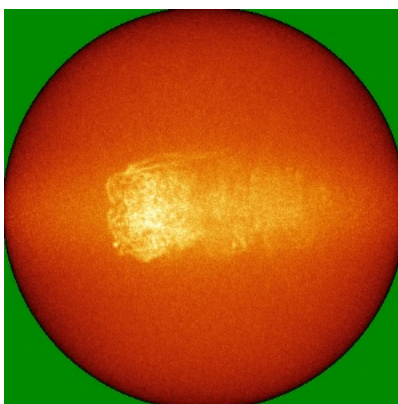


Z

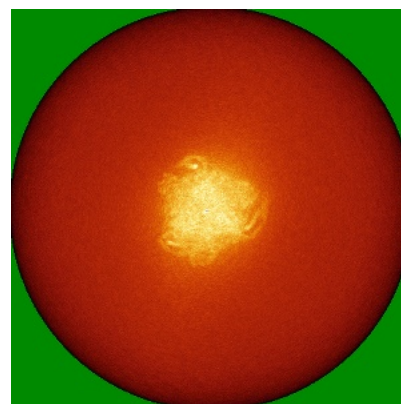
6.4.2 Raw map



X



Y

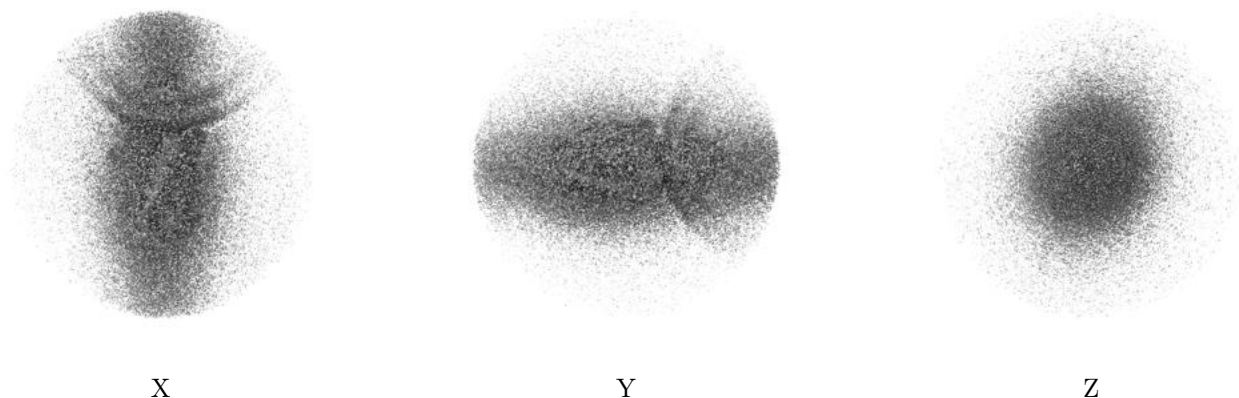


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

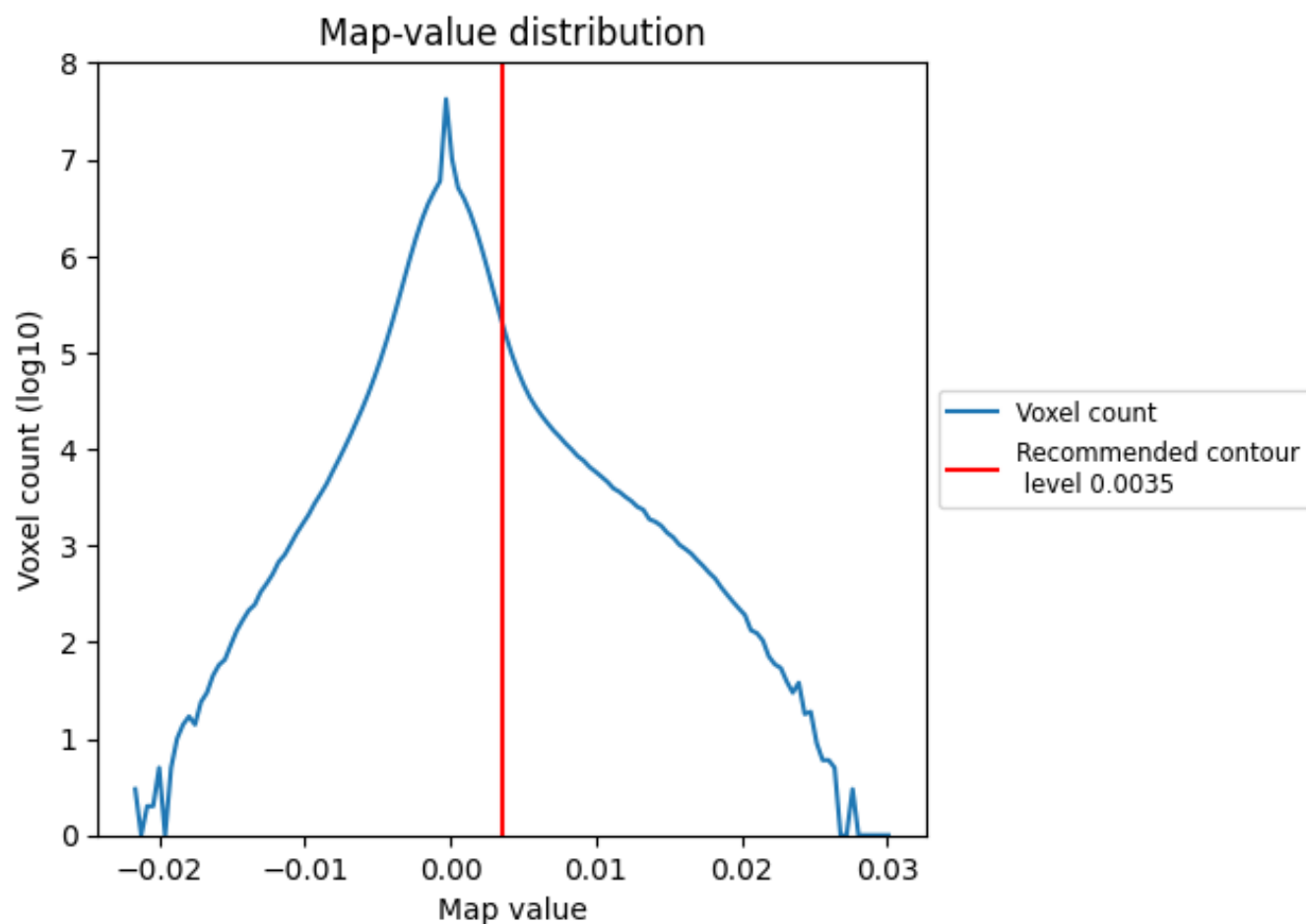
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

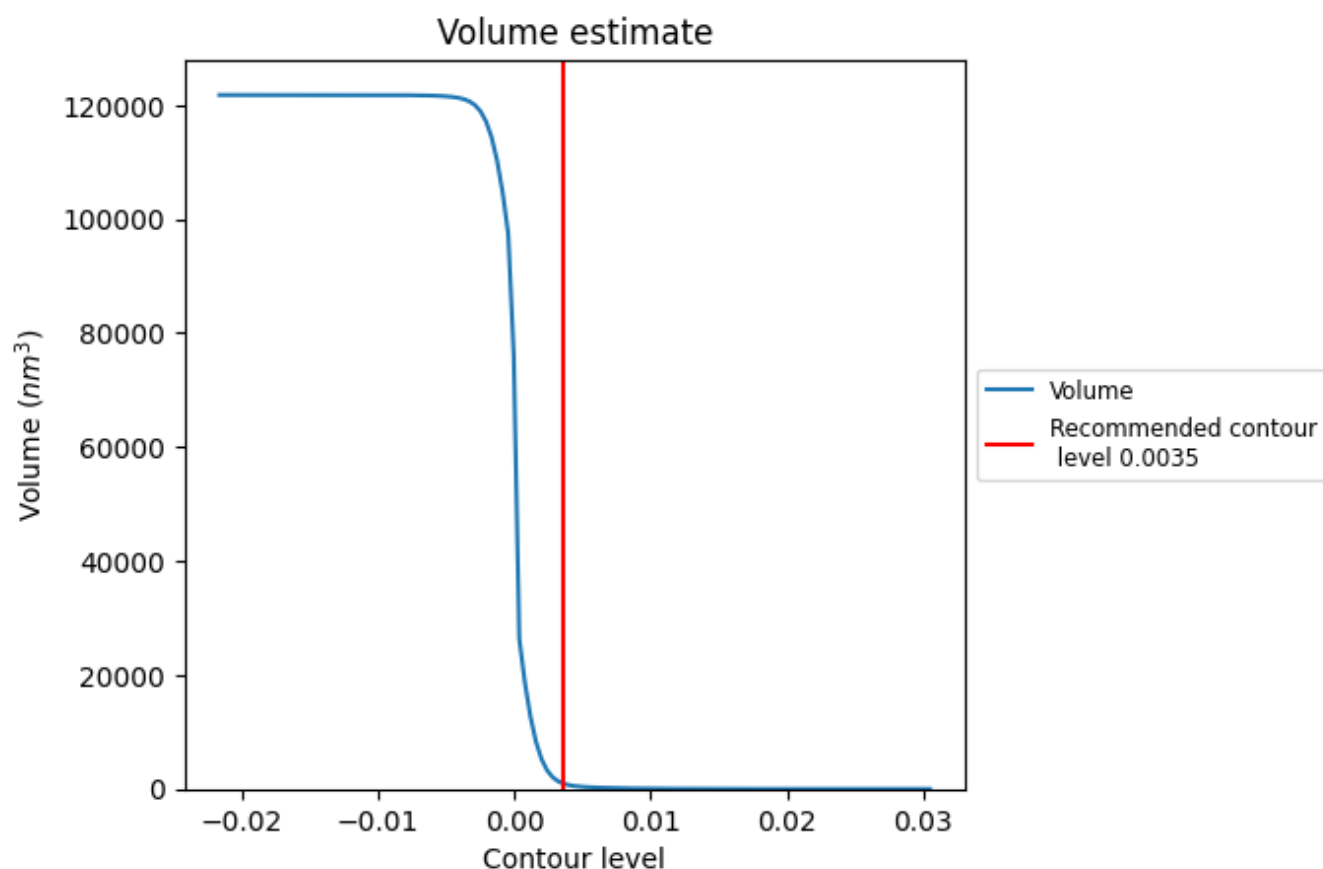
This section contains the results of statistical analysis of the map.

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.

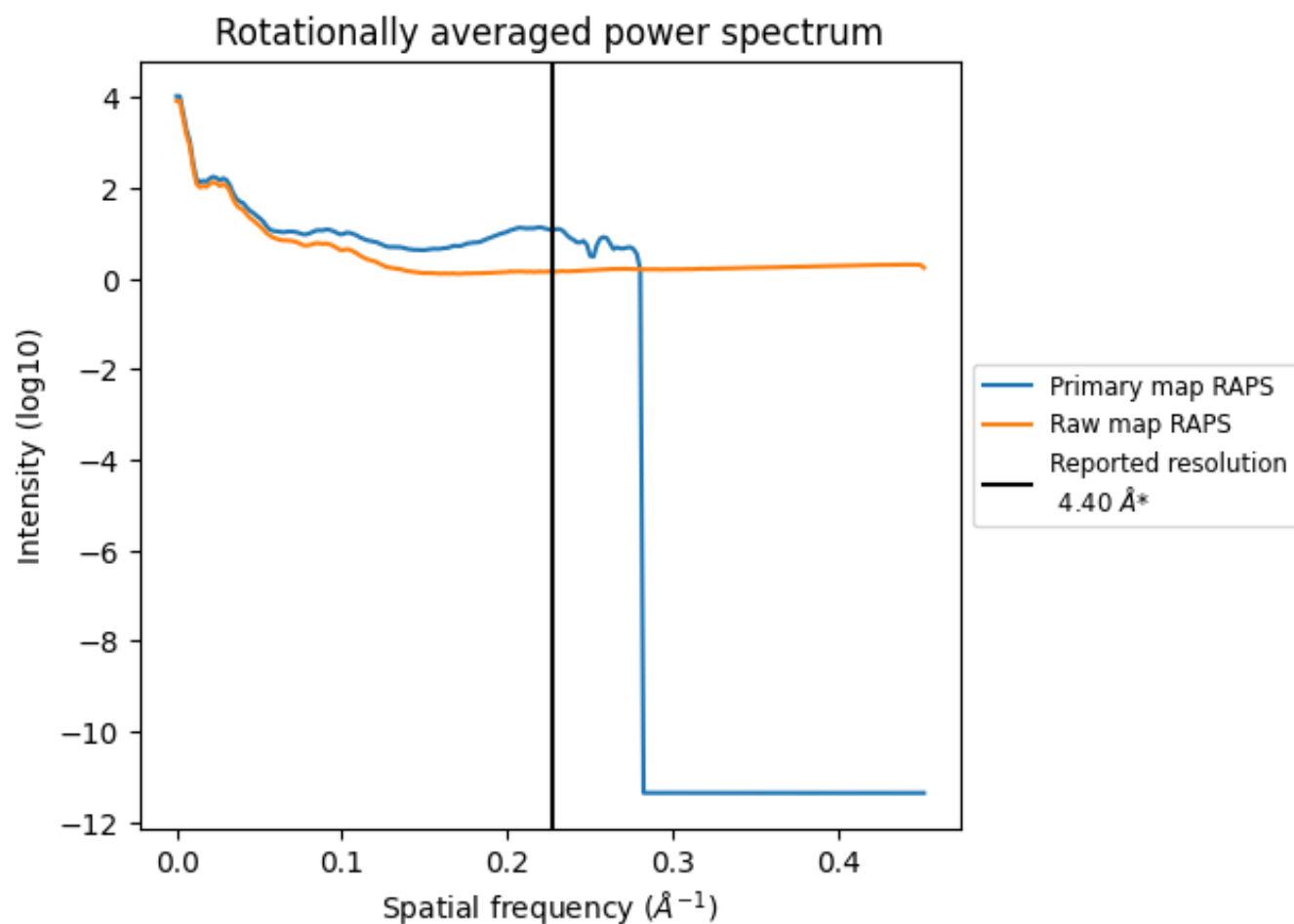
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1040 nm^3 ; this corresponds to an approximate mass of 940 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 ⓘ

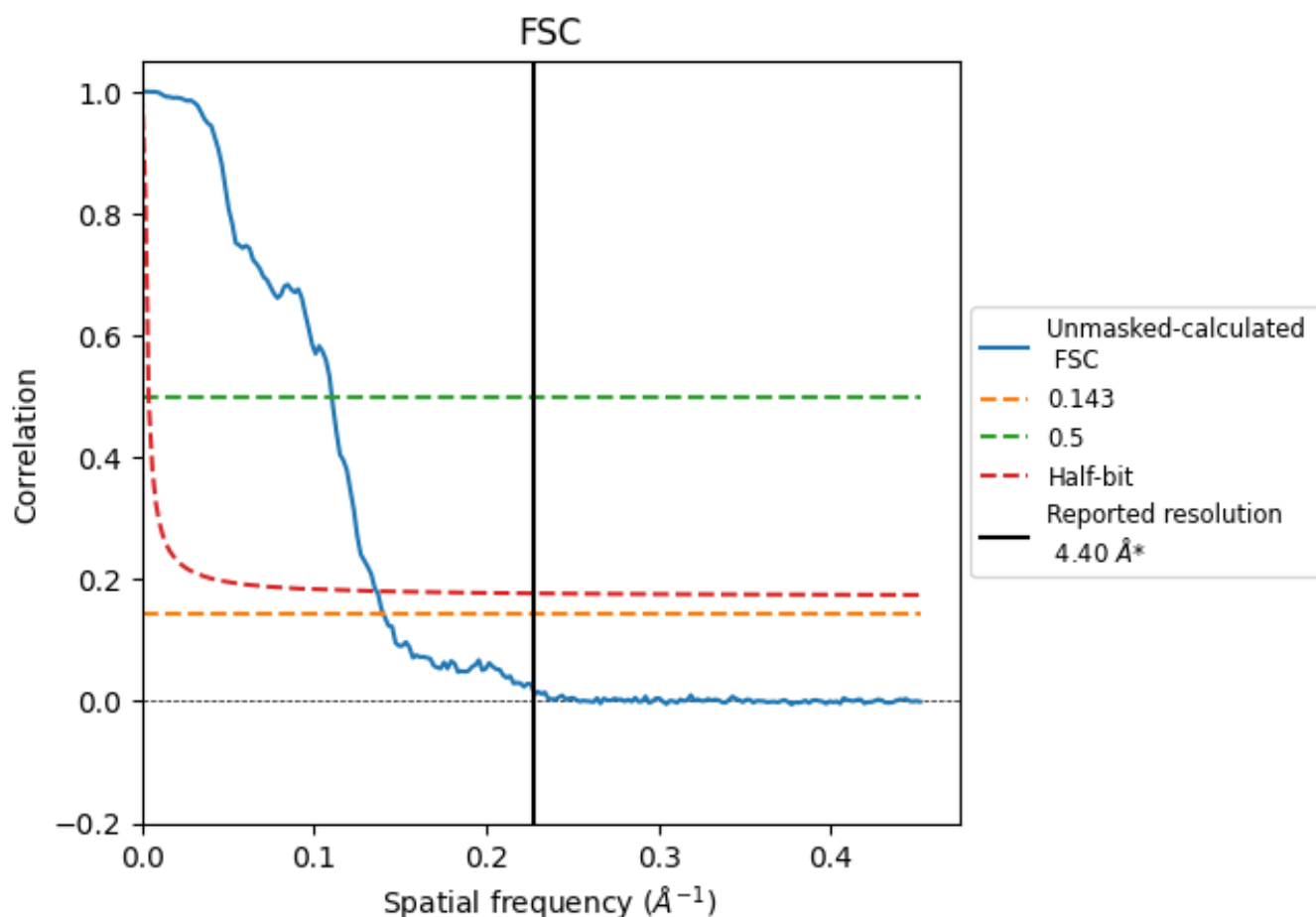


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.13	9.07	7.34

*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 7.13 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

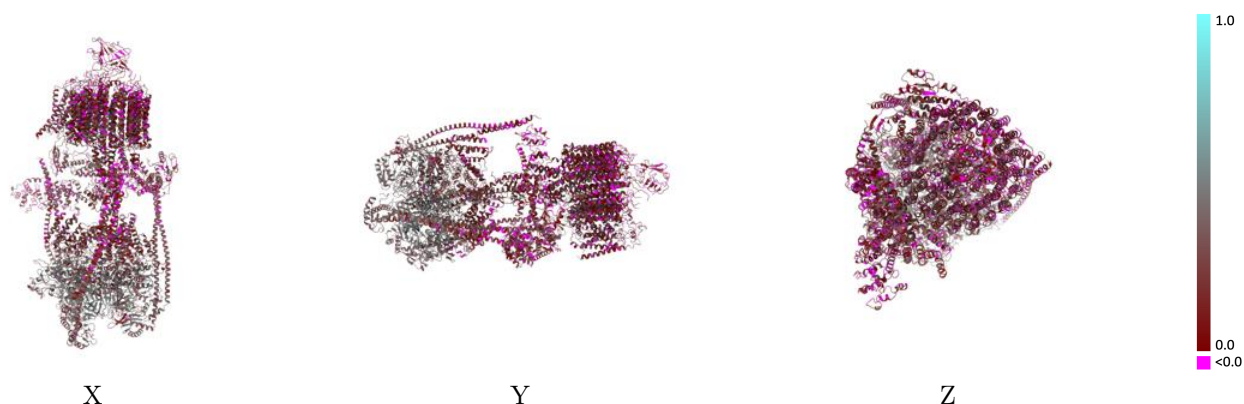
This section contains information regarding the fit between EMDB map EMD-44844 and PDB model 9BRU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



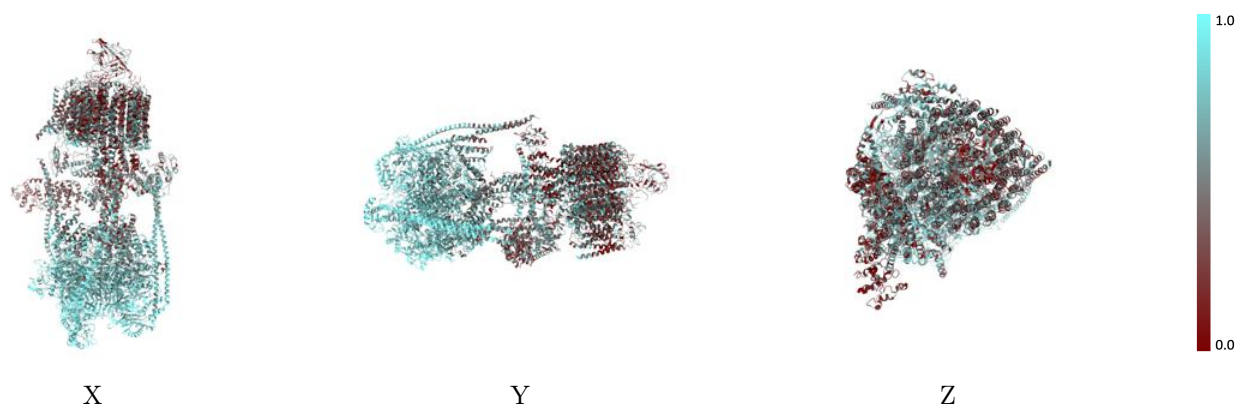
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



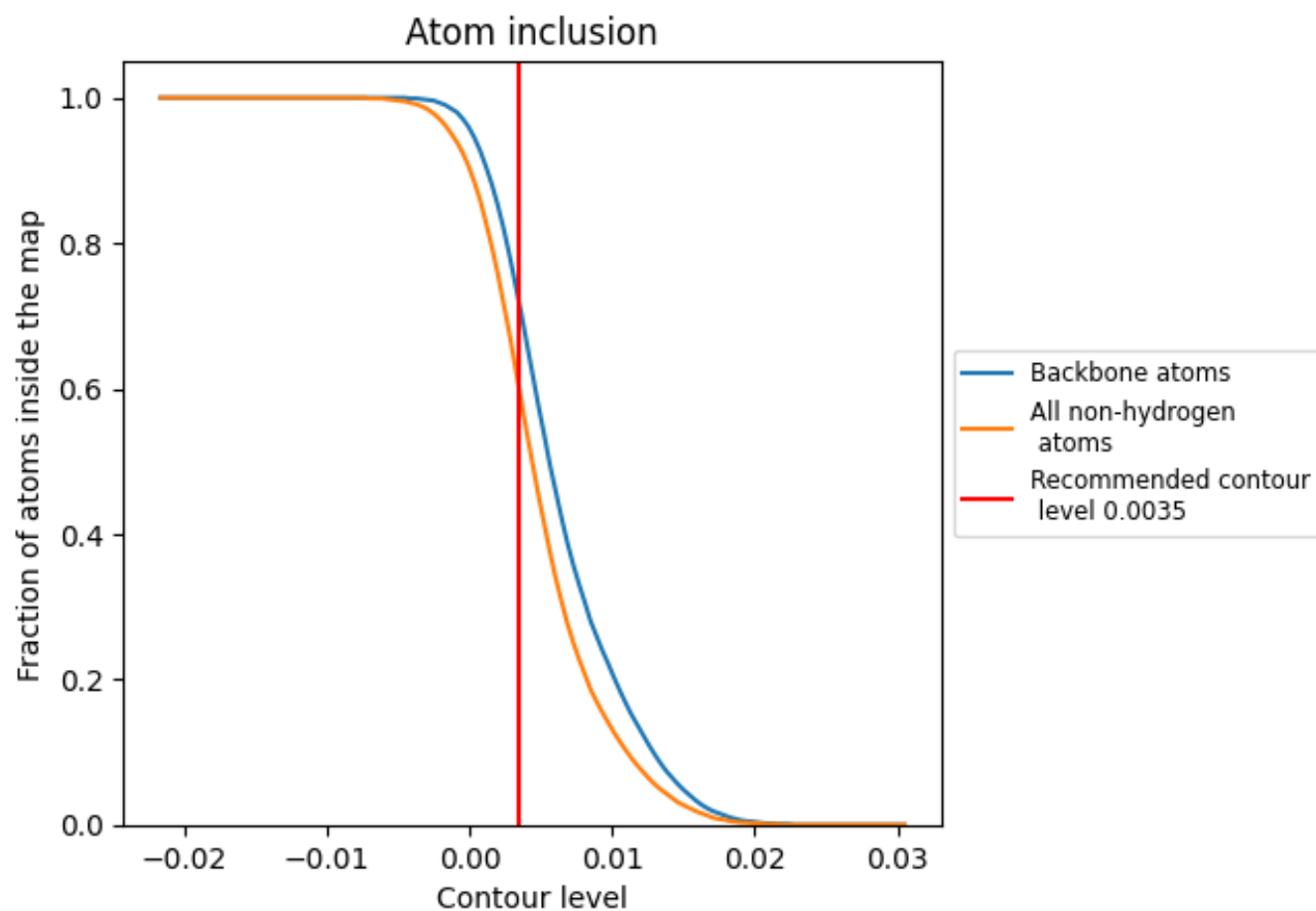
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 60% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5990	 0.2620
0	 0.7550	 0.3500
1	 0.7430	 0.3510
2	 0.6960	 0.2970
3	 0.7810	 0.3890
4	 0.7800	 0.3840
5	 0.7780	 0.3880
6	 0.5000	 0.1590
7	 0.5910	 0.2610
8	 0.7730	 0.3330
9	 0.7970	 0.3140
Q	 0.7560	 0.2960
R	 0.7270	 0.2370
T	 0.7700	 0.2550
U	 0.2680	 0.1390
V	 0.7270	 0.2120
X	 0.6140	 0.2340
a	 0.5040	 0.2070
b	 0.3850	 0.1660
c	 0.3270	 0.1450
d	 0.3670	 0.1760
e	 0.3780	 0.1540
f	 0.3620	 0.1860
g	 0.4100	 0.1740
h	 0.4610	 0.1830
i	 0.5360	 0.2170
j	 0.4850	 0.2140
k	 0.4590	 0.2050
l	 0.4780	 0.1730
m	 0.4470	 0.1810
n	 0.4390	 0.1430
o	 0.4370	 0.1890
p	 0.3440	 0.1630

