Full wwPDB EM Validation Report ⓘ

Jul 27, 2024 – 02:47 PM EDT

PDB ID	:	9BRS
EMDB ID	:	EMD-44842
Title	:	Intact V-ATPase State 2 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:

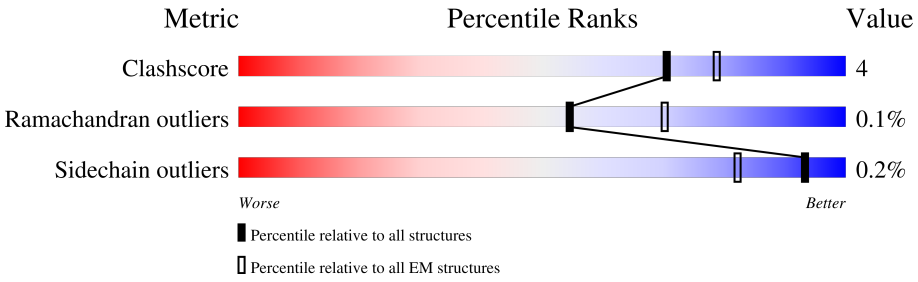
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	8	226	5% 91% 8%
1	9	226	· 92% 7%
1	Q	226	7% 92% 7%
2	R	118	6% 91% 6% ·
2	T	118	5% 87% 9% ·
2	V	118	· 90% 7% ·
3	6	382	16% 91% · 5%
4	U	483	51% 82% 6% 12%

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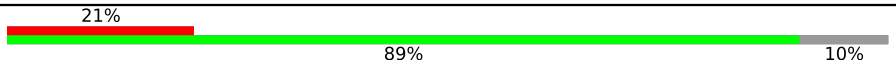
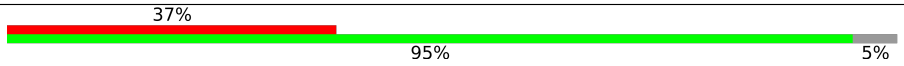
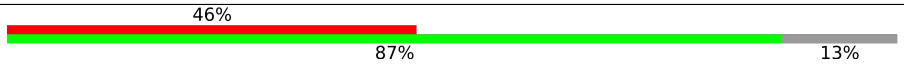
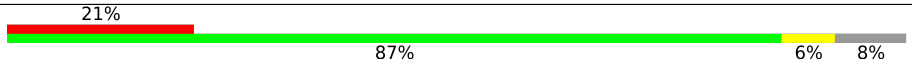
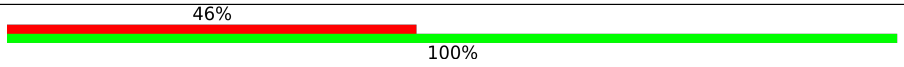
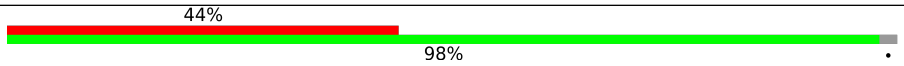
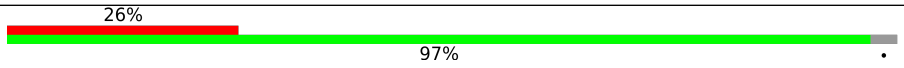
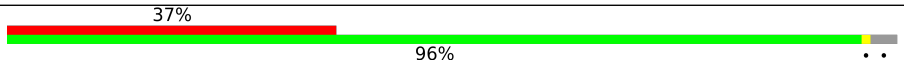
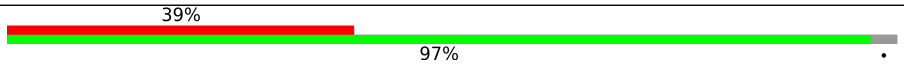
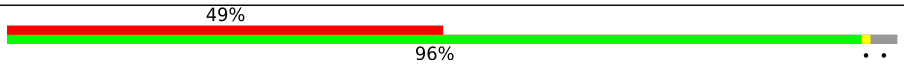
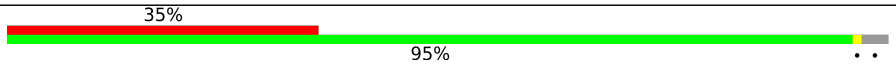
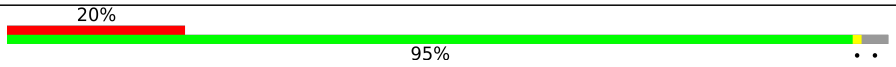
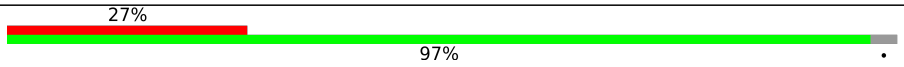
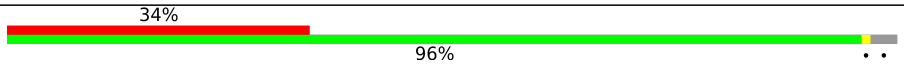
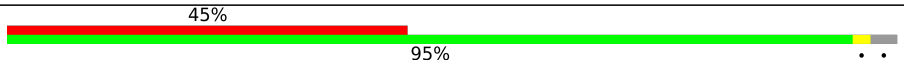
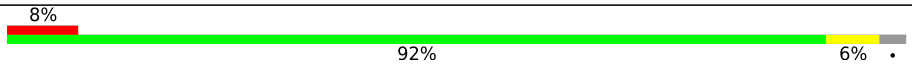
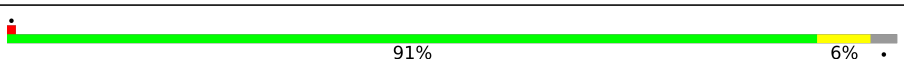
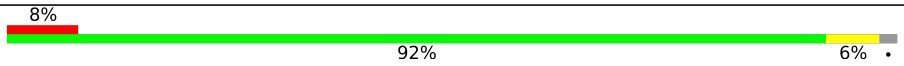
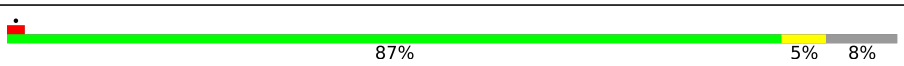
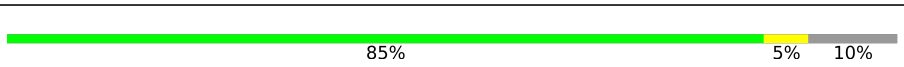
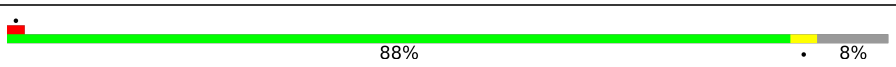
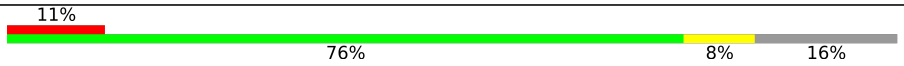
Mol	Chain	Length	Quality of chain
5	a	838	
6	e	81	
7	f	98	
8	X	119	
9	d	351	
10	c	463	
11	p	350	
12	b	205	
13	g	155	
13	h	155	
13	i	155	
13	j	155	
13	k	155	
13	l	155	
13	m	155	
13	n	155	
13	o	155	
14	0	617	
14	1	617	
14	2	617	
15	3	511	
15	4	511	
15	5	511	
16	7	247	

2 Entry composition (i)

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 E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
1	9	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
1	Q	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		

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

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

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	361	Total	C	N	O	S	0	0
			2931	1877	495	550	9		

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

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

- Molecule 5 is a protein called V-type proton ATPase 116 kDa subunit a 1.

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

- Molecule 6 is a protein called V-type proton ATPase subunit e 2.

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

- Molecule 7 is a protein called Ribonuclease kappa.

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

- Molecule 8 is a protein called V-type proton ATPase subunit F.

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

- Molecule 9 is a protein called V-type proton ATPase subunit d 1.

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

- Molecule 10 is a protein called V-type proton ATPase subunit S1.

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

- Molecule 11 is a protein called Renin receptor cytoplasmic fragment.

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

- Molecule 12 is a protein called V-type proton ATPase 21 kDa proteolipid subunit c".

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

- Molecule 13 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

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

- Molecule 14 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	600	Total	C	N	O	S	0	0
			4656	2953	787	889	27		
14	2	602	Total	C	N	O	S	0	0
			4671	2961	789	894	27		
14	0	600	Total	C	N	O	S	0	0
			4656	2953	787	889	27		

- Molecule 15 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	461	Total	C	N	O	S	0	0
			3610	2290	615	685	20		
15	5	468	Total	C	N	O	S	0	0
			3667	2326	623	698	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	468	Total	C	N	O	S	0	0
			3667	2326	623	698	20		

- Molecule 16 is a protein called V-type proton ATPase subunit D.

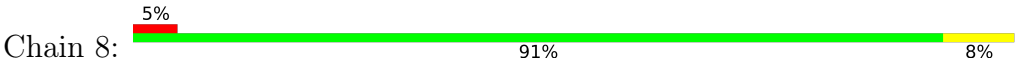
Mol	Chain	Residues	Atoms					AltConf	Trace
16	7	208	Total	C	N	O	S	0	0
			1676	1064	303	304	5		

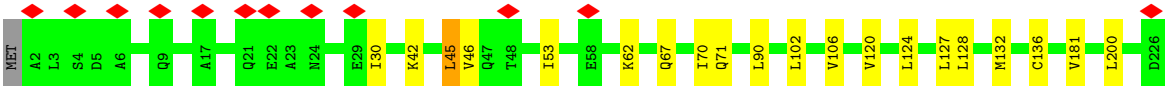
3 Residue-property plots (i)

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: V-type proton ATPase subunit E 1

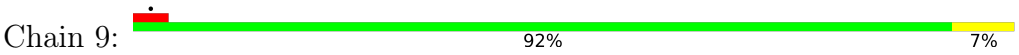
Chain 8:

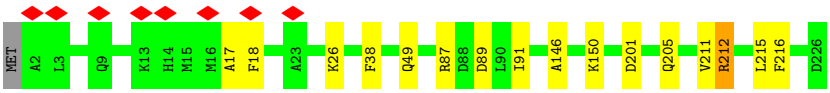




• Molecule 1: V-type proton ATPase subunit E 1

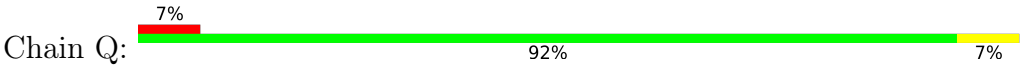
Chain 9:

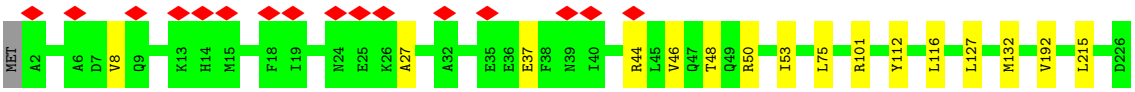




• Molecule 1: V-type proton ATPase subunit E 1

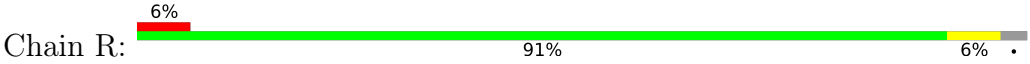
Chain Q:

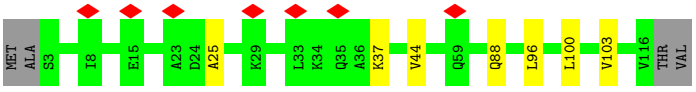




• Molecule 2: V-type proton ATPase subunit G 2

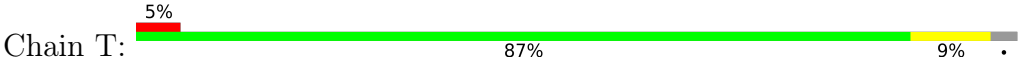
Chain R:

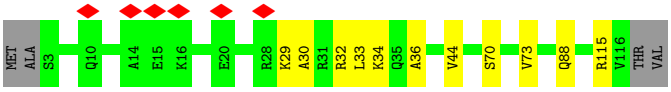




• Molecule 2: V-type proton ATPase subunit G 2

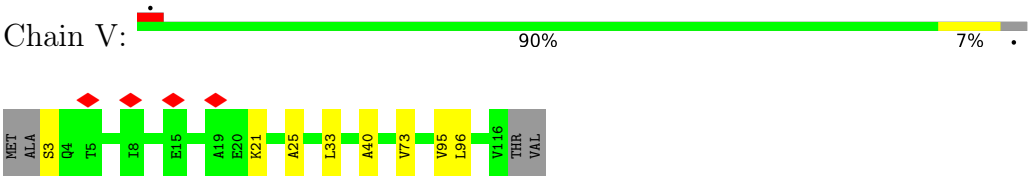
Chain T:





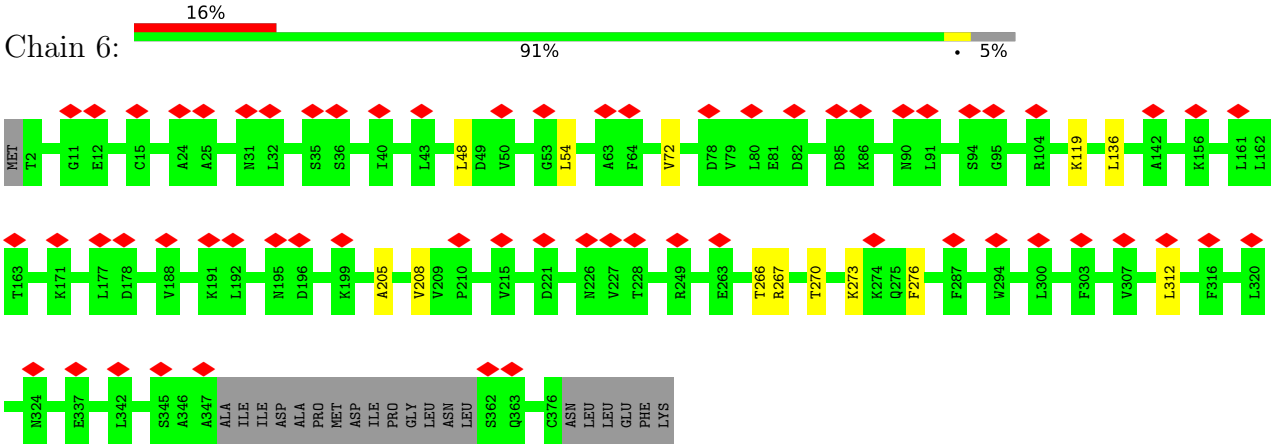
• Molecule 2: V-type proton ATPase subunit G 2

Chain V:



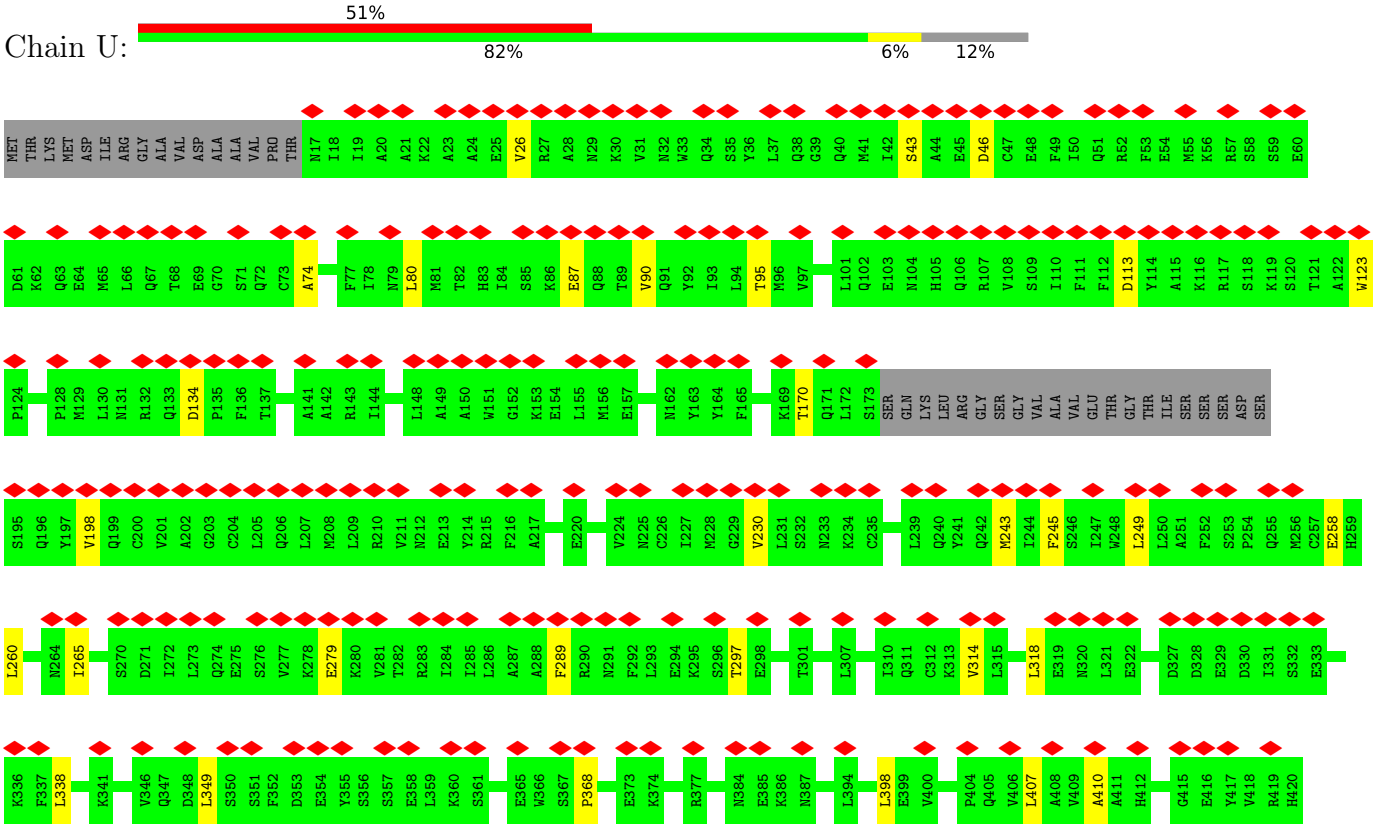
• Molecule 3: V-type proton ATPase subunit C 1

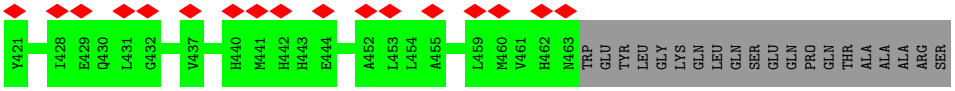
Chain 6:



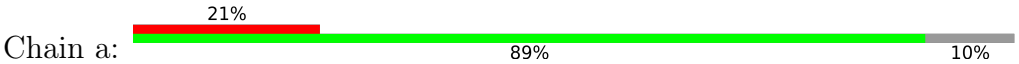
• Molecule 4: V-type proton ATPase subunit H

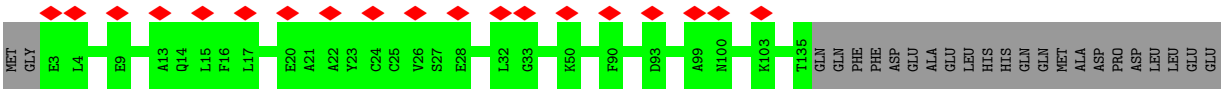
Chain U:

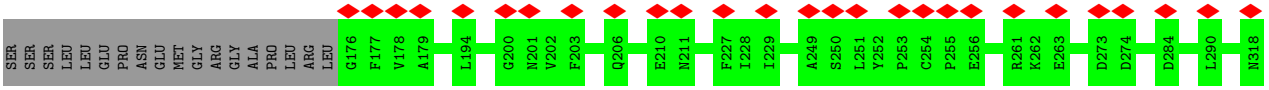


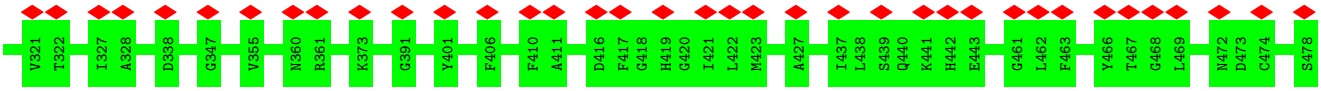


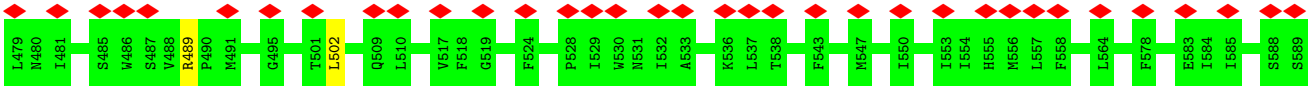
• Molecule 5: V-type proton ATPase 116 kDa subunit a 1

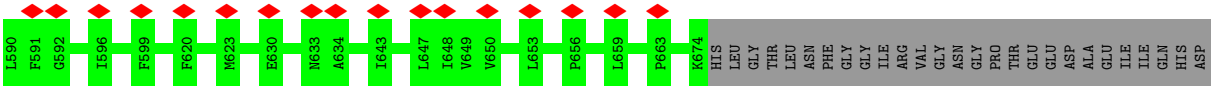


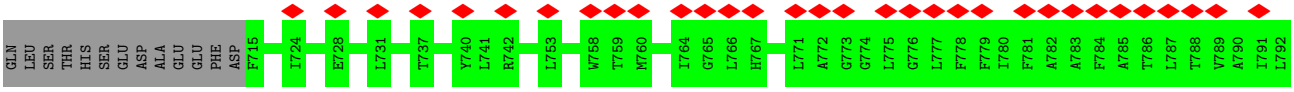


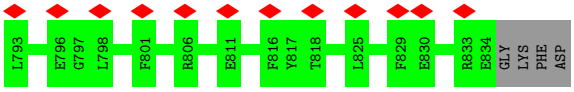




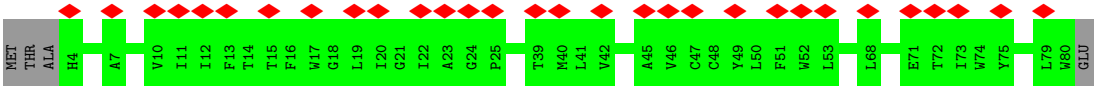




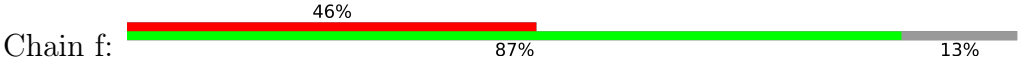


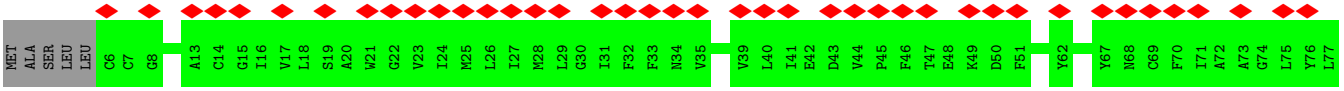


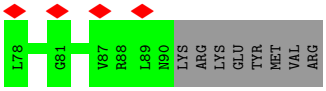
• Molecule 6: V-type proton ATPase subunit e 2



• Molecule 7: Ribonuclease kappa

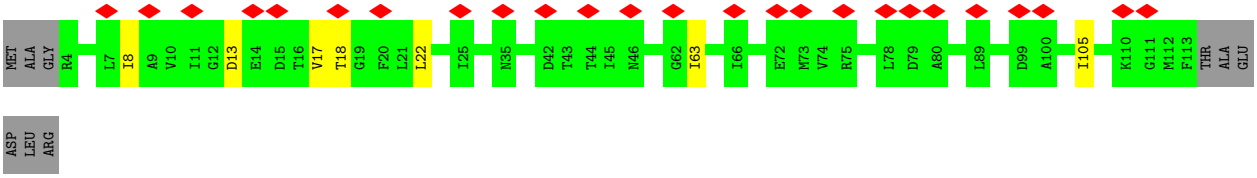






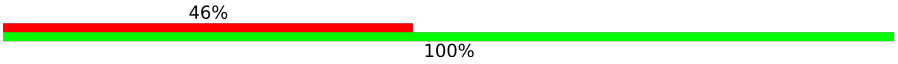
• Molecule 8: V-type proton ATPase subunit F

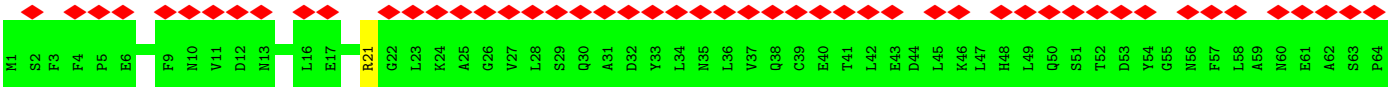
Chain X:

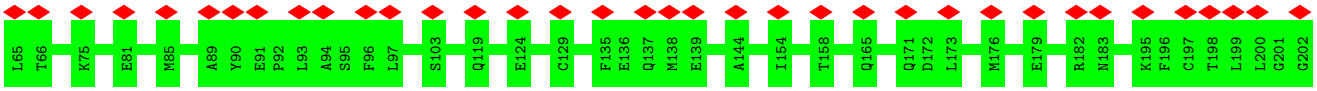


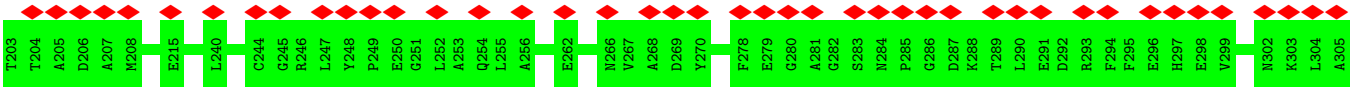
• Molecule 9: V-type proton ATPase subunit d 1

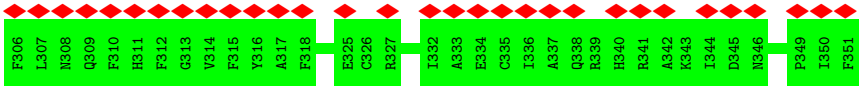
Chain d:





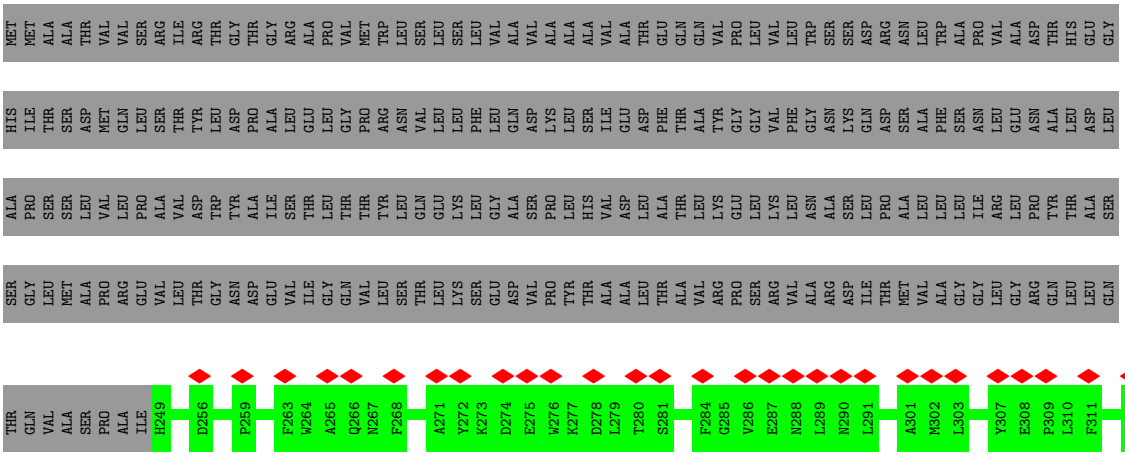


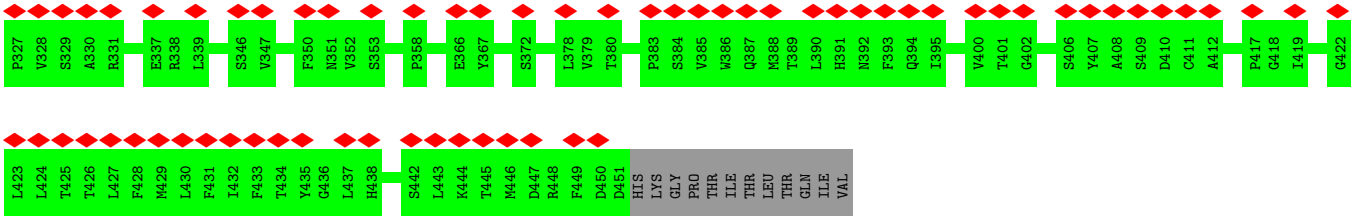




• Molecule 10: V-type proton ATPase subunit S1

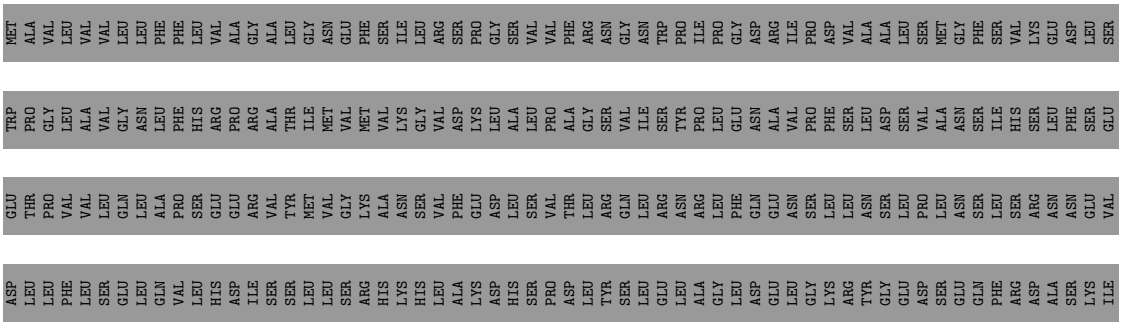
Chain c:

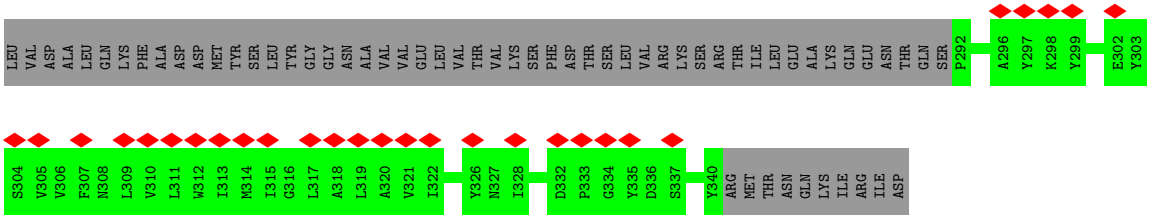




• Molecule 11: Renin receptor cytoplasmic fragment

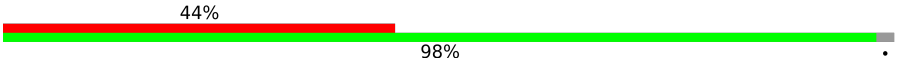
Chain p:

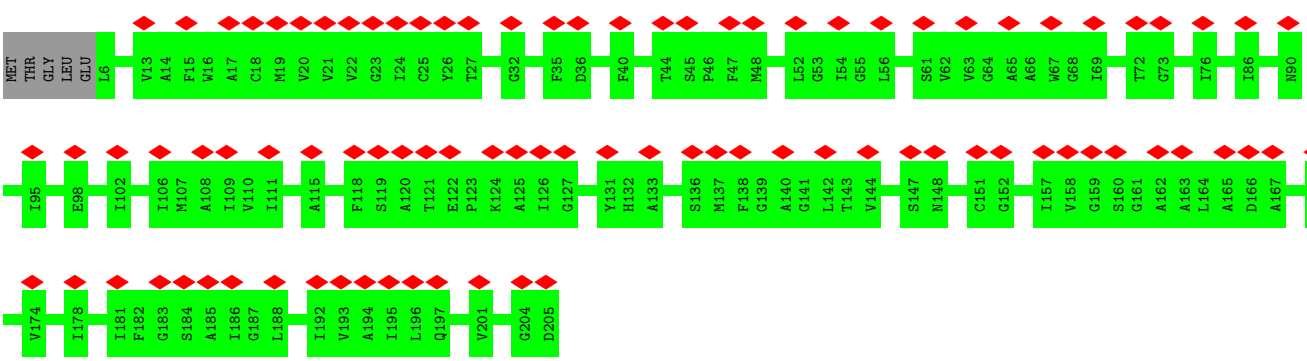




• Molecule 12: V-type proton ATPase 21 kDa proteolipid subunit c"

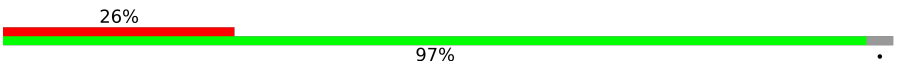
Chain b:

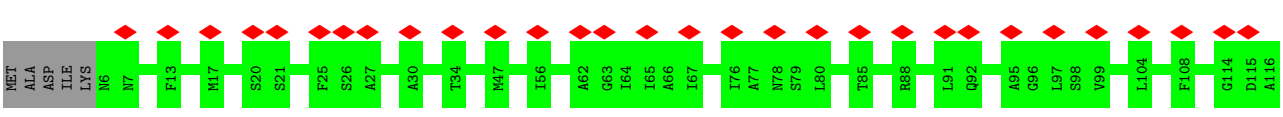


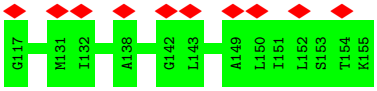


• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

Chain g:

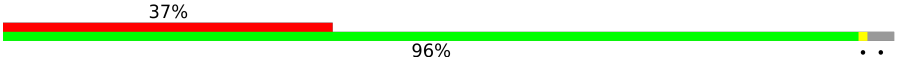


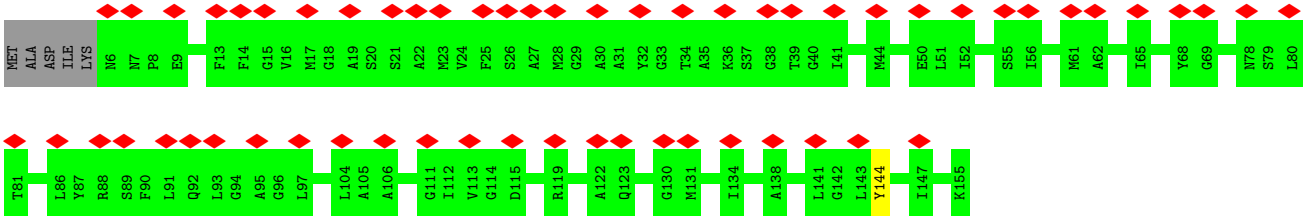




• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

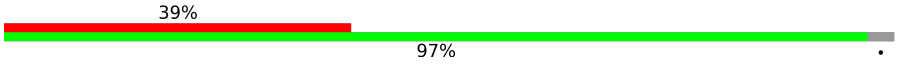
Chain h:

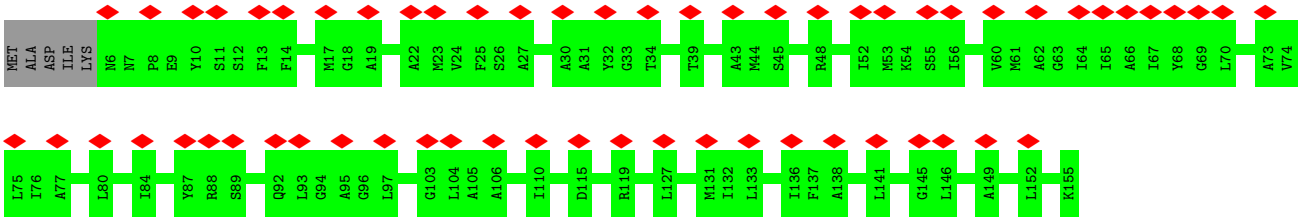




• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

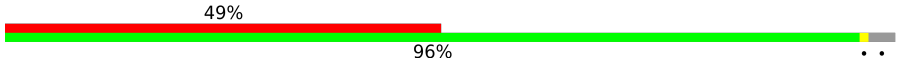
Chain i:

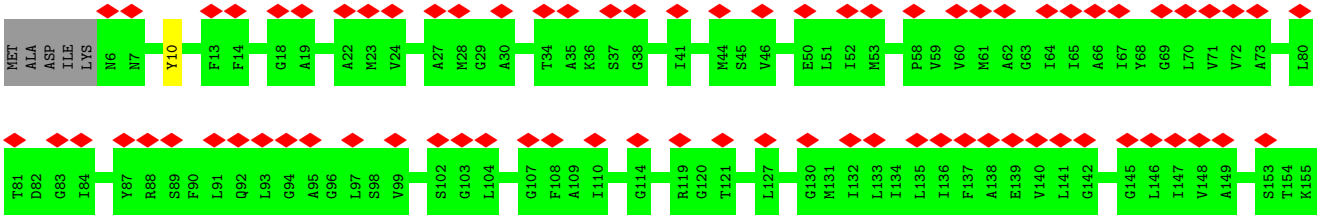




• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

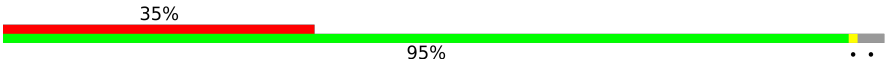
Chain j:

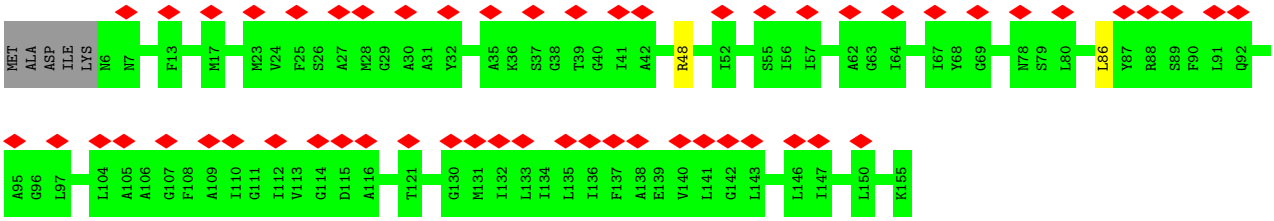




• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

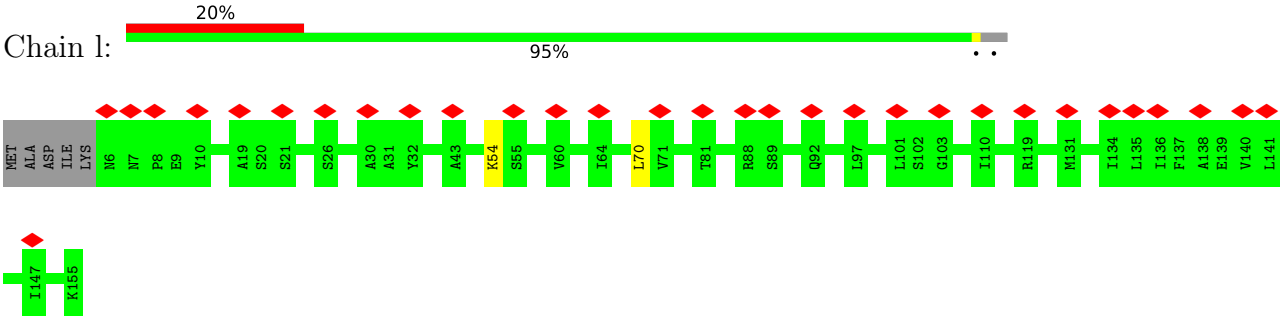
Chain k:





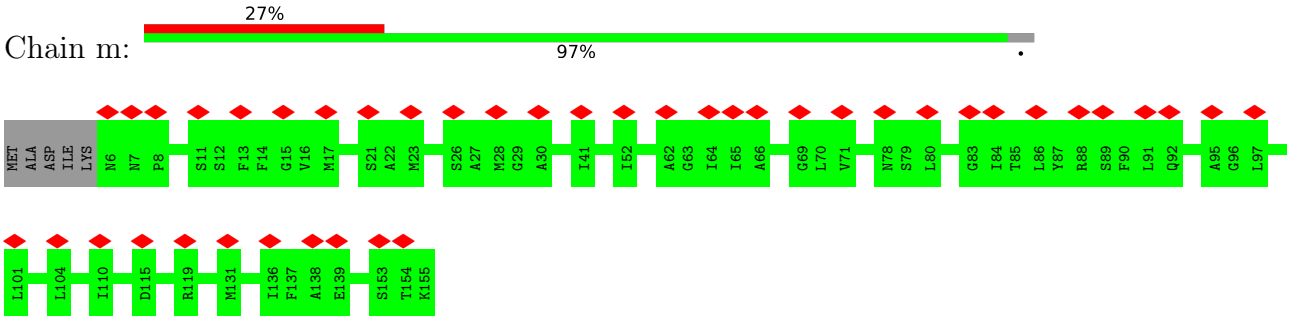
• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

Chain l:



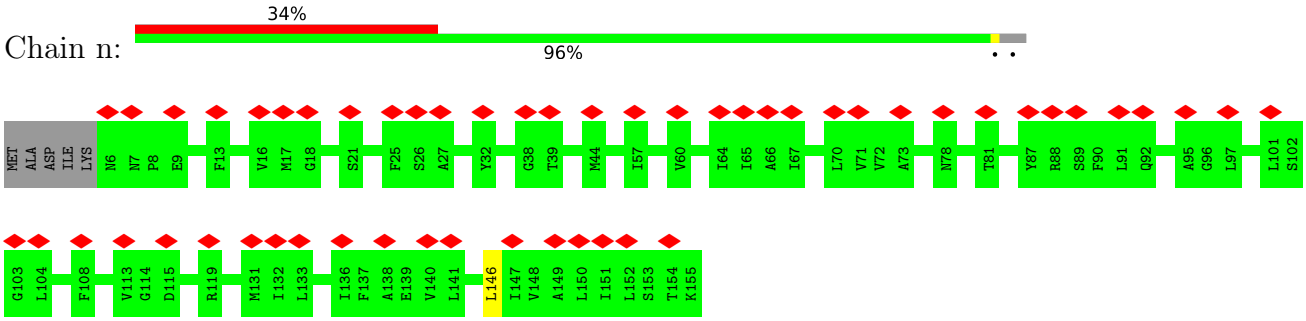
• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

Chain m:



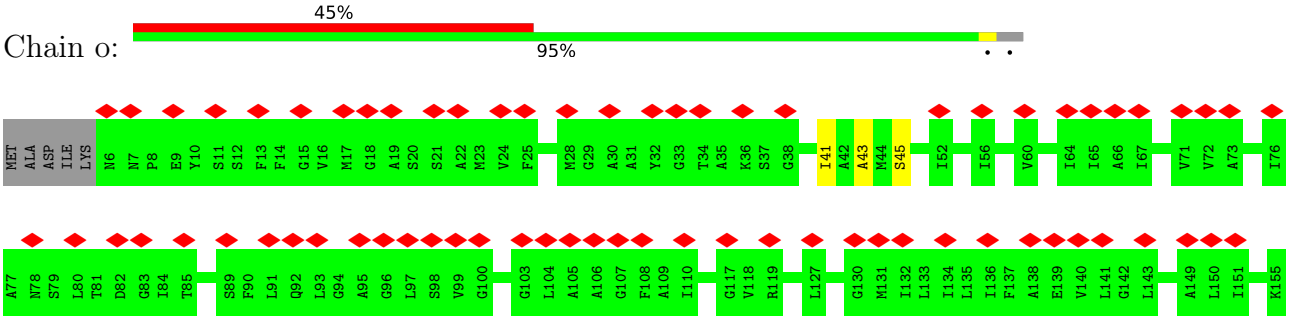
• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

Chain n:



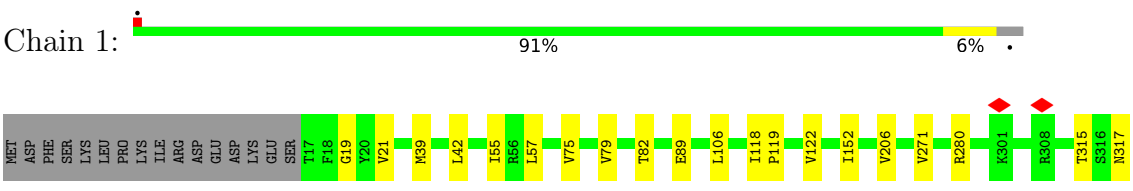
• Molecule 13: V-type proton ATPase 16 kDa proteolipid subunit c

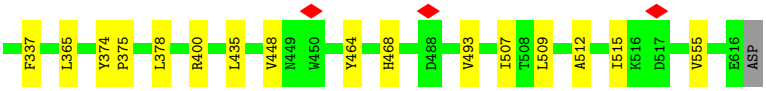
Chain o:



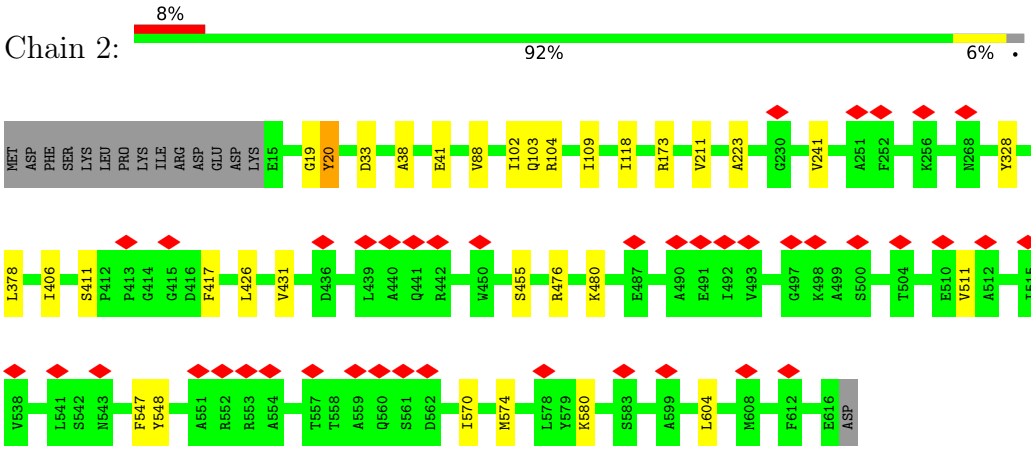
• Molecule 14: V-type proton ATPase catalytic subunit A

Chain 1:

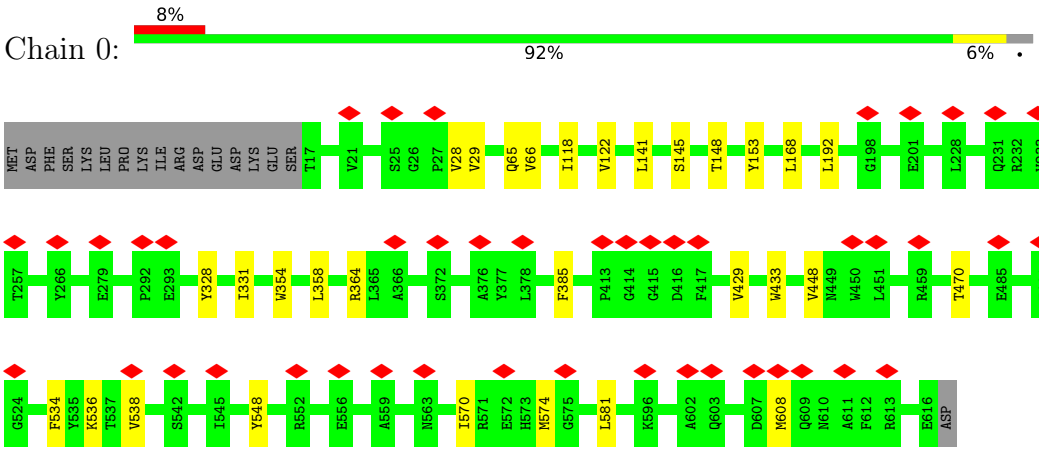




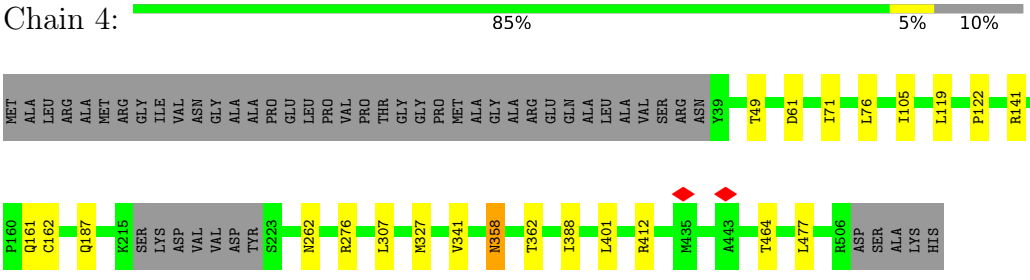
• Molecule 14: V-type proton ATPase catalytic subunit A



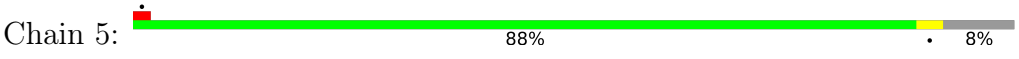
• Molecule 14: V-type proton ATPase catalytic subunit A

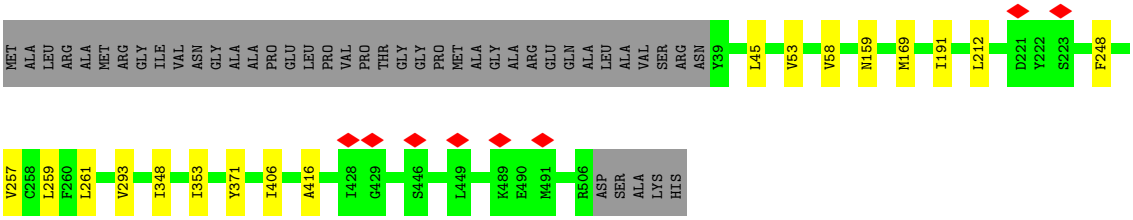


• Molecule 15: V-type proton ATPase subunit B, brain isoform

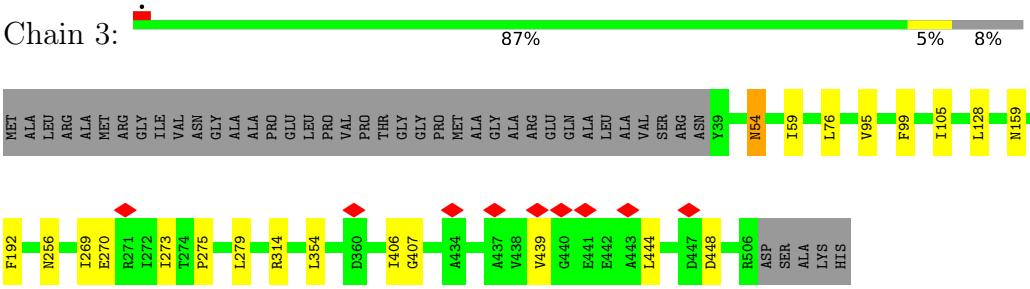


• Molecule 15: V-type proton ATPase subunit B, brain isoform

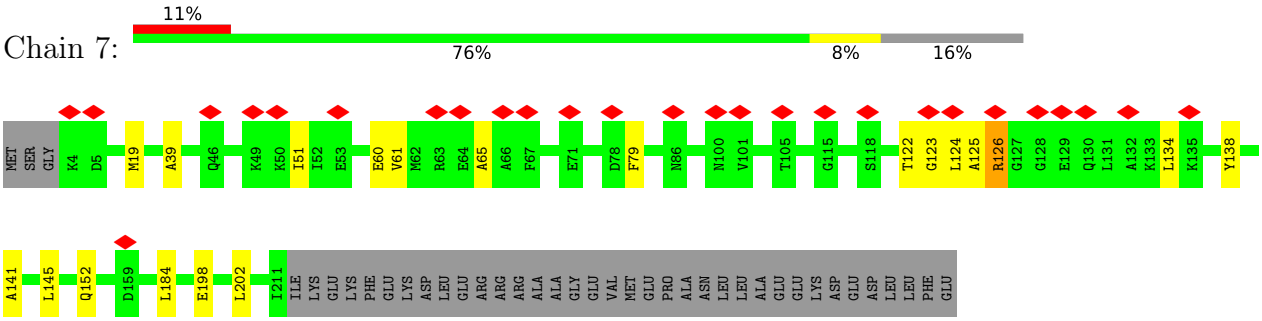




• Molecule 15: V-type proton ATPase subunit B, brain isoform



• Molecule 16: V-type proton ATPase subunit D



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30487	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 ($e^-/Å^2$)	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	0.028	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	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	8	0.32	0/1840	0.59	1/2462 (0.0%)
1	9	0.35	0/1840	0.61	1/2462 (0.0%)
1	Q	0.31	0/1840	0.56	0/2462
2	R	0.32	0/930	0.64	0/1237
2	T	0.33	0/930	0.68	0/1237
2	V	0.30	0/930	0.65	0/1237
3	6	0.29	0/2985	0.55	0/4032
4	U	0.29	0/3568	0.56	0/4806
5	a	0.30	0/6274	0.55	0/8486
6	e	0.32	0/648	0.47	0/891
7	f	0.28	0/674	0.49	0/915
8	X	0.27	0/889	0.56	0/1199
9	d	0.30	0/2908	0.54	0/3937
10	c	0.29	0/1697	0.56	0/2311
11	p	0.27	0/420	0.46	0/576
12	b	0.34	0/1518	0.55	0/2061
13	g	0.36	0/1084	0.63	0/1466
13	h	0.37	0/1084	0.64	1/1466 (0.1%)
13	i	0.30	0/1084	0.55	0/1466
13	j	0.38	1/1084 (0.1%)	0.57	0/1466
13	k	0.32	0/1084	0.71	1/1466 (0.1%)
13	l	0.34	0/1084	0.61	2/1466 (0.1%)
13	m	0.34	0/1084	0.61	0/1466
13	n	0.36	0/1084	0.60	1/1466 (0.1%)
13	o	0.32	0/1084	0.58	0/1466
14	0	0.33	0/4752	0.57	0/6433
14	1	0.35	0/4752	0.56	0/6433
14	2	0.34	0/4767	0.59	2/6453 (0.0%)
15	3	0.36	0/3740	0.58	0/5069
15	4	0.39	0/3681	0.59	0/4987
15	5	0.36	0/3740	0.57	0/5069
16	7	0.32	0/1694	0.62	0/2267
All	All	0.33	1/66773 (0.0%)	0.58	9/90216 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	9	0	1
5	a	0	1
9	d	0	1
13	k	0	1
15	4	0	1
16	7	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	j	10	TYR	CE2-CZ	-5.72	1.31	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	k	86	LEU	CB-CG-CD2	9.45	127.06	111.00
13	l	70	LEU	CA-CB-CG	6.54	130.34	115.30
1	9	89	ASP	CB-CG-OD1	6.04	123.73	118.30
14	2	20	TYR	N-CA-CB	-5.87	100.04	110.60
13	l	70	LEU	CB-CG-CD1	-5.86	101.04	111.00
13	n	146	LEU	CB-CG-CD2	-5.79	101.15	111.00
14	2	33	ASP	CB-CG-OD2	5.26	123.03	118.30
1	8	45	LEU	CB-CG-CD1	-5.11	102.31	111.00
13	h	144	TYR	CA-CB-CG	5.05	123.00	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	4	141	ARG	Sidechain
16	7	126	ARG	Sidechain
1	9	212	ARG	Sidechain
5	a	489	ARG	Sidechain
9	d	21	ARG	Sidechain
13	k	48	ARG	Sidechain

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	8	1823	0	1895	15	0
1	9	1823	0	1895	40	0
1	Q	1823	0	1895	14	0
2	R	925	0	935	8	0
2	T	925	0	935	11	0
2	V	925	0	935	9	0
3	6	2931	0	2969	7	0
4	U	3501	0	3481	18	0
5	a	6117	0	6154	0	0
6	e	623	0	641	0	0
7	f	658	0	652	0	0
8	X	875	0	883	5	0
9	d	2842	0	2782	0	0
10	c	1642	0	1568	0	0
11	p	407	0	403	0	0
12	b	1484	0	1528	0	0
13	g	1069	0	1136	0	0
13	h	1069	0	1136	0	0
13	i	1069	0	1136	0	0
13	j	1069	0	1136	0	0
13	k	1069	0	1136	0	0
13	l	1069	0	1136	0	0
13	m	1069	0	1136	0	0
13	n	1069	0	1136	0	0
13	o	1069	0	1136	0	0
14	0	4656	0	4643	26	0
14	1	4656	0	4643	23	0
14	2	4671	0	4654	25	0
15	3	3667	0	3667	14	0
15	4	3610	0	3613	27	0
15	5	3667	0	3667	13	0
16	7	1676	0	1781	16	0
All	All	65548	0	66443	225	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 4.

All (225) 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)
1:9:91:ILE:HD11	1:9:212:ARG:NH1	1.56	1.20
1:9:212:ARG:HE	15:4:146:LEU:CD2	1.54	1.19
1:9:91:ILE:HD11	1:9:212:ARG:CZ	1.75	1.15
1:9:212:ARG:HE	15:4:146:LEU:HD23	1.05	1.11
1:9:212:ARG:NH1	1:9:216:PHE:HE1	1.54	1.05
1:9:212:ARG:NE	15:4:146:LEU:HD23	1.84	0.93
1:9:91:ILE:HG12	1:9:212:ARG:NH2	1.85	0.92
1:9:91:ILE:CG1	1:9:212:ARG:NH2	2.33	0.91
1:9:212:ARG:NE	15:4:146:LEU:CD2	2.34	0.90
1:9:212:ARG:NH1	1:9:216:PHE:CE1	2.40	0.88
1:9:91:ILE:CD1	1:9:212:ARG:NH1	2.38	0.86
1:9:212:ARG:HH11	1:9:216:PHE:HE1	1.22	0.85
1:9:91:ILE:CD1	1:9:212:ARG:CZ	2.54	0.84
3:6:72:VAL:HG12	3:6:136:LEU:HD22	1.60	0.83
1:9:91:ILE:HG12	1:9:212:ARG:HH22	1.43	0.82
1:9:212:ARG:HD2	1:9:216:PHE:CD1	2.14	0.82
1:9:212:ARG:HD2	1:9:216:PHE:CE1	2.16	0.81
1:9:212:ARG:HE	15:4:146:LEU:HD21	1.48	0.78
4:U:26:VAL:HG21	4:U:95:THR:HG21	1.68	0.74
1:Q:215:LEU:HD11	2:V:95:VAL:HG21	1.69	0.73
1:9:212:ARG:CD	1:9:216:PHE:CE1	2.73	0.71
14:1:55:ILE:HD12	14:1:365:LEU:HD21	1.72	0.70
14:1:57:LEU:HD21	15:5:53:VAL:HG22	1.74	0.69
1:9:212:ARG:NE	15:4:146:LEU:HD21	2.07	0.69
1:8:67:GLN:O	1:8:70:ILE:HG22	1.93	0.69
15:3:54:ASN:O	15:3:54:ASN:ND2	2.27	0.68
1:Q:46:VAL:HG21	2:V:40:ALA:HB1	1.74	0.68
16:7:122:THR:O	16:7:126:ARG:NH1	2.26	0.67
15:3:439:VAL:HG22	16:7:39:ALA:HB2	1.77	0.66
1:8:53:ILE:HD11	2:R:44:VAL:HG22	1.77	0.66
4:U:349:LEU:HD13	4:U:368:PRO:HG3	1.78	0.66
1:9:91:ILE:CG1	1:9:212:ARG:CZ	2.76	0.64
1:9:87:ARG:HG2	1:9:212:ARG:NH2	2.13	0.64
1:9:49:GLN:CD	2:T:44:VAL:HG11	2.20	0.62
4:U:260:LEU:HD23	4:U:265:ILE:HD11	1.81	0.62
14:1:39:MET:CE	14:1:57:LEU:HD22	2.30	0.61
14:0:29:VAL:HG12	14:0:66:VAL:CG2	2.31	0.61
4:U:260:LEU:HD23	4:U:265:ILE:CD1	2.31	0.61
2:T:30:ALA:HB1	2:T:34:LYS:NZ	2.17	0.60
4:U:289:PHE:HB3	4:U:338:LEU:HD21	1.84	0.60
14:1:507:ILE:HD11	14:1:555:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:493:VAL:HG11	14:1:509:LEU:HD11	1.84	0.59
4:U:87:GLU:HA	4:U:90:VAL:HG12	1.84	0.59
1:8:102:LEU:HD12	1:8:200:LEU:HD12	1.85	0.58
1:9:212:ARG:CZ	1:9:216:PHE:CE1	2.85	0.58
14:1:315:THR:HG23	14:1:317:ASN:OD1	2.03	0.58
14:2:417:PHE:CE1	14:2:426:LEU:HD22	2.38	0.58
1:9:212:ARG:HH21	15:4:146:LEU:CD2	2.16	0.58
8:X:8:ILE:HG13	8:X:63:ILE:HG23	1.85	0.57
14:1:106:LEU:HD21	15:4:159:ASN:OD1	2.04	0.57
15:5:53:VAL:HG12	15:5:58:VAL:HG22	1.87	0.57
14:2:346:MET:SD	14:2:406:ILE:HD13	2.45	0.57
16:7:141:ALA:O	16:7:145:LEU:HD23	2.06	0.56
1:Q:27:ALA:HB3	2:V:21:LYS:HE3	1.87	0.56
1:9:91:ILE:HG13	1:9:212:ARG:NH2	2.17	0.56
1:9:38:PHE:CE1	2:T:36:ALA:HB2	2.41	0.56
2:T:30:ALA:HB1	2:T:34:LYS:HZ1	1.70	0.56
14:2:88:VAL:HG23	14:2:211:VAL:HG22	1.88	0.56
14:2:570:ILE:HG23	14:2:574:MET:CE	2.36	0.56
1:9:212:ARG:CZ	1:9:216:PHE:HE1	2.18	0.55
1:Q:8:VAL:HG13	2:V:3:SER:OG	2.06	0.55
14:0:331:ILE:HD11	14:0:385:PHE:HD1	1.71	0.55
15:5:259:LEU:HD12	15:5:261:LEU:HD21	1.89	0.55
14:0:534:PHE:O	14:0:538:VAL:HG23	2.08	0.54
14:0:29:VAL:HG12	14:0:66:VAL:HG22	1.88	0.54
1:9:212:ARG:CD	1:9:216:PHE:CD1	2.89	0.54
1:Q:192:VAL:HG22	15:5:45:LEU:HD23	1.90	0.53
4:U:314:VAL:HG12	4:U:318:LEU:HG	1.91	0.53
14:2:102:ILE:O	14:2:102:ILE:HG22	2.08	0.53
14:2:19:GLY:C	14:2:20:TYR:CG	2.81	0.53
1:8:120:VAL:O	1:8:124:LEU:HD23	2.09	0.53
14:1:118:ILE:HD11	15:4:159:ASN:HA	1.91	0.53
14:2:570:ILE:HG23	14:2:574:MET:HE3	1.91	0.53
14:2:88:VAL:HG13	14:2:103:GLN:OE1	2.09	0.52
16:7:122:THR:CB	16:7:126:ARG:HH12	2.23	0.52
2:R:96:LEU:O	2:R:100:LEU:HD23	2.09	0.52
4:U:349:LEU:HD13	4:U:368:PRO:CG	2.40	0.52
16:7:198:GLU:O	16:7:202:LEU:HD23	2.09	0.52
14:2:358:LEU:HD23	14:2:378:LEU:HD22	1.92	0.52
1:8:42:LYS:O	1:8:46:VAL:HG23	2.10	0.51
1:9:212:ARG:NH2	15:4:146:LEU:CD2	2.73	0.51
3:6:273:LYS:HA	3:6:276:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:0:118:ILE:HD11	15:3:159:ASN:HA	1.93	0.51
15:4:71:ILE:HD11	15:4:119:LEU:HB2	1.92	0.51
1:9:212:ARG:CZ	15:4:146:LEU:CD2	2.89	0.51
1:Q:127:LEU:HD23	1:Q:132:MET:HG2	1.93	0.51
15:5:191:ILE:HB	15:5:353:ILE:HG22	1.91	0.51
14:2:223:ALA:HB1	14:2:241:VAL:HG21	1.93	0.51
14:2:511:VAL:HG21	14:2:548:TYR:HD1	1.76	0.51
16:7:123:GLY:O	16:7:125:ALA:N	2.44	0.51
3:6:266:THR:O	3:6:270:THR:HG23	2.10	0.51
14:2:104:ARG:HG2	14:2:109:ILE:HD11	1.93	0.50
1:9:212:ARG:CZ	15:4:146:LEU:HD21	2.41	0.50
14:1:375:PRO:HD2	14:1:378:LEU:HD11	1.93	0.50
14:2:368:MET:SD	16:7:202:LEU:HD12	2.51	0.50
1:9:91:ILE:HG13	15:4:146:LEU:HD21	1.93	0.50
4:U:245:PHE:CE2	4:U:249:LEU:HD11	2.46	0.50
14:1:152:ILE:HD11	14:1:400:ARG:HH12	1.77	0.50
15:5:169:MET:O	15:5:212:LEU:HD23	2.12	0.50
14:1:435:LEU:CD2	14:1:448:VAL:HG22	2.42	0.49
1:8:53:ILE:HD11	2:R:44:VAL:CG2	2.39	0.49
1:9:211:VAL:O	1:9:215:LEU:HD23	2.12	0.49
1:Q:27:ALA:HB1	2:V:25:ALA:HB2	1.92	0.49
14:0:28:VAL:HG22	14:0:65:GLN:HG3	1.95	0.49
14:0:122:VAL:O	14:0:122:VAL:HG13	2.13	0.49
1:Q:37:GLU:OE1	2:V:33:LEU:HD11	2.12	0.49
14:1:464:TYR:CE1	14:1:468:HIS:CE1	3.01	0.49
14:0:28:VAL:HG21	14:0:364:ARG:HG2	1.94	0.48
14:2:88:VAL:HG23	14:2:211:VAL:CG2	2.43	0.48
4:U:245:PHE:CZ	4:U:249:LEU:HD11	2.48	0.48
15:3:99:PHE:HD2	15:3:269:ILE:HG21	1.78	0.48
15:3:275:PRO:O	15:3:279:LEU:HD23	2.14	0.48
14:2:511:VAL:HG22	14:2:547:PHE:CE2	2.49	0.48
14:0:364:ARG:O	14:0:364:ARG:HG3	2.14	0.48
15:4:187:GLN:CD	15:4:401:LEU:HD12	2.34	0.47
15:4:262:ASN:O	15:4:262:ASN:ND2	2.47	0.47
16:7:122:THR:CB	16:7:126:ARG:NH1	2.77	0.47
14:1:374:TYR:HB3	14:1:378:LEU:HD12	1.95	0.47
14:0:354:TRP:CZ2	14:0:358:LEU:HD11	2.50	0.47
14:0:496:VAL:HG11	14:0:500:SER:O	2.14	0.47
3:6:205:ALA:O	3:6:208:VAL:HG23	2.15	0.47
14:2:19:GLY:C	14:2:20:TYR:CD2	2.88	0.47
4:U:43:SER:OG	4:U:80:LEU:HD11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:170:THR:OG1	4:U:198:VAL:HG22	2.14	0.47
1:8:45:LEU:HD13	2:R:37:LYS:HA	1.97	0.47
14:0:234:LEU:HD21	14:0:448:VAL:HG11	1.95	0.47
14:2:103:GLN:O	14:2:103:GLN:HG2	2.15	0.47
14:2:211:VAL:HG12	14:2:328:TYR:HB3	1.97	0.47
14:2:476:ARG:HG3	14:2:480:LYS:NZ	2.29	0.47
15:3:59:ILE:HG22	15:3:95:VAL:HG22	1.97	0.47
2:R:103:VAL:HG12	2:R:103:VAL:O	2.14	0.47
1:Q:50:ARG:CZ	1:Q:53:ILE:HD11	2.45	0.47
8:X:22:LEU:CD2	16:7:134:LEU:HD23	2.45	0.47
14:1:21:VAL:O	14:1:75:VAL:HG23	2.14	0.47
2:T:33:LEU:O	2:T:36:ALA:HB3	2.16	0.46
14:0:29:VAL:HG12	14:0:66:VAL:HG21	1.98	0.46
1:8:102:LEU:O	1:8:106:VAL:HG23	2.16	0.46
15:4:358:ASN:O	15:4:358:ASN:ND2	2.48	0.46
14:0:141:LEU:HD12	14:0:145:SER:OG	2.15	0.46
15:4:76:LEU:HD22	15:4:105:ILE:HD13	1.98	0.46
15:5:293:VAL:CG1	15:5:348:ILE:HD13	2.46	0.46
2:T:29:LYS:O	2:T:33:LEU:HD23	2.15	0.46
14:2:38:ALA:HB3	14:2:41:GLU:OE2	2.16	0.46
14:2:431:VAL:HG13	14:2:455:SER:HB3	1.97	0.46
4:U:230:VAL:HG12	4:U:243:MET:HE3	1.97	0.46
2:T:88:GLN:OE1	2:T:88:GLN:HA	2.16	0.45
1:9:38:PHE:HE1	2:T:36:ALA:HB2	1.81	0.45
4:U:258:GLU:OE2	4:U:297:THR:HG22	2.16	0.45
8:X:13:ASP:O	8:X:17:VAL:HG23	2.16	0.45
1:8:30:ILE:HG22	2:R:25:ALA:HB2	1.99	0.45
16:7:19:MET:HB2	16:7:184:LEU:HD21	1.99	0.45
15:4:307:LEU:HD23	15:4:327:MET:HG3	1.98	0.45
1:Q:8:VAL:HG22	2:V:3:SER:OG	2.17	0.45
14:1:19:GLY:C	14:1:79:VAL:HG12	2.37	0.45
14:0:148:THR:O	14:0:168:LEU:HD12	2.16	0.45
15:3:314:ARG:O	15:3:314:ARG:HG2	2.16	0.45
1:Q:75:LEU:HD21	2:V:73:VAL:HG21	1.97	0.45
14:0:470:THR:O	14:0:470:THR:HG22	2.16	0.45
15:4:388:ILE:HG23	15:4:464:THR:HG22	1.98	0.45
15:5:259:LEU:HD12	15:5:261:LEU:CD2	2.47	0.45
4:U:46:ASP:OD2	4:U:80:LEU:HD12	2.17	0.44
14:1:271:VAL:HG21	14:1:337:PHE:HD1	1.80	0.44
16:7:65:ALA:HB1	16:7:138:TYR:CZ	2.51	0.44
15:3:270:GLU:HA	15:3:273:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:136:CYS:SG	1:8:181:VAL:HG23	2.57	0.44
14:1:89:GLU:HG3	14:1:206:VAL:HG13	1.99	0.44
14:0:331:ILE:HD11	14:0:385:PHE:CD1	2.52	0.44
1:8:90:LEU:HD11	2:R:88:GLN:OE1	2.18	0.44
14:1:106:LEU:HD22	15:4:161:GLN:HB2	2.00	0.44
15:4:362:THR:O	15:4:362:THR:HG22	2.18	0.44
14:1:42:LEU:O	14:1:82:THR:HG22	2.18	0.44
15:5:248:PHE:CD1	15:5:257:VAL:HG21	2.53	0.44
15:5:406:ILE:HD11	15:5:416:ALA:HB2	2.00	0.44
16:7:51:ILE:HD11	16:7:152:GLN:OE1	2.18	0.43
2:T:29:LYS:N	2:T:29:LYS:HD3	2.33	0.43
15:3:192:PHE:CD1	15:3:354:LEU:HD21	2.53	0.43
15:3:128:LEU:HD12	15:3:256:ASN:C	2.38	0.43
1:9:146:ALA:HB1	1:9:150:LYS:NZ	2.34	0.43
1:8:45:LEU:HD13	2:R:37:LYS:CA	2.49	0.43
14:2:118:ILE:HD11	15:5:159:ASN:HA	2.00	0.43
14:0:328:TYR:HA	14:0:331:ILE:HD12	2.01	0.43
1:8:128:LEU:HD23	1:8:128:LEU:O	2.19	0.42
3:6:54:LEU:HD22	3:6:119:LYS:HE3	2.01	0.42
14:2:411:SER:HG	15:5:371:TYR:HE2	1.64	0.42
2:T:70:SER:O	2:T:73:VAL:HG22	2.19	0.42
14:0:581:LEU:HD11	14:0:608:MET:HE1	1.99	0.42
1:8:127:LEU:HD23	1:8:132:MET:HE3	2.01	0.42
15:3:76:LEU:HD11	15:3:105:ILE:HG13	2.00	0.42
14:1:57:LEU:CD2	15:5:53:VAL:HG22	2.47	0.42
14:0:153:TYR:CE2	14:0:192:LEU:HD22	2.55	0.42
14:0:511:VAL:HG21	14:0:548:TYR:HB2	2.02	0.42
15:4:122:PRO:HB2	15:4:147:ALA:HB2	2.01	0.42
14:0:234:LEU:HD21	14:0:448:VAL:CG1	2.50	0.42
4:U:398:LEU:HD21	4:U:410:ALA:HB3	2.02	0.42
14:2:511:VAL:HG22	14:2:547:PHE:HE2	1.85	0.42
15:3:444:LEU:HD13	15:3:448:ASP:OD2	2.20	0.42
1:Q:101:ARG:HG3	2:V:96:LEU:HD21	2.02	0.41
15:3:174:ILE:HD12	15:3:177:ILE:HD12	2.02	0.41
15:3:406:ILE:HG22	15:3:407:GLY:N	2.35	0.41
8:X:105:ILE:HG21	16:7:152:GLN:NE2	2.35	0.41
1:9:38:PHE:CE1	2:T:32:ARG:O	2.73	0.41
1:9:87:ARG:CG	1:9:212:ARG:NH2	2.82	0.41
14:0:153:TYR:CZ	14:0:192:LEU:HD22	2.55	0.41
15:4:49:THR:HG21	15:4:61:ASP:O	2.19	0.41
15:4:162:CYS:O	15:4:341:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:0:570:ILE:HG23	14:0:574:MET:HE2	2.02	0.41
1:9:18:PHE:CG	3:6:48:LEU:HD23	2.56	0.41
4:U:398:LEU:HD23	4:U:407:LEU:HD23	2.02	0.41
1:9:17:ALA:HB3	3:6:312:LEU:HD22	2.02	0.41
15:4:412:ARG:HD2	15:4:477:LEU:HD13	2.01	0.41
1:Q:44:ARG:O	1:Q:48:THR:HG23	2.21	0.41
14:2:580:LYS:HB3	14:2:604:LEU:HD13	2.02	0.41
16:7:60:GLU:OE2	16:7:61:VAL:HG23	2.20	0.41
16:7:122:THR:OG1	16:7:126:ARG:NH1	2.54	0.41
14:1:79:VAL:HG13	14:1:79:VAL:O	2.21	0.41
14:0:234:LEU:HD22	14:0:433:TRP:CD1	2.56	0.41
1:8:67:GLN:O	1:8:71:GLN:OE1	2.38	0.40
4:U:74:ALA:HB3	4:U:113:ASP:HB2	2.04	0.40
14:1:512:ALA:HA	14:1:515:ILE:HG22	2.02	0.40
14:0:245:THR:HG22	14:0:429:VAL:HG12	2.03	0.40
1:9:201:ASP:O	1:9:205:GLN:OE1	2.40	0.40
14:1:119:PRO:O	14:1:122:VAL:HG13	2.22	0.40
1:Q:112:TYR:O	1:Q:116:LEU:HD23	2.21	0.40
8:X:18:THR:HG21	16:7:79:PHE:HE2	1.86	0.40
15:4:76:LEU:CD2	15:4:105:ILE:HD13	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	223/226 (99%)	219 (98%)	4 (2%)	0	100	100
1	9	223/226 (99%)	221 (99%)	2 (1%)	0	100	100
1	Q	223/226 (99%)	214 (96%)	9 (4%)	0	100	100
2	R	112/118 (95%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
2	V	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
3	6	357/382 (94%)	336 (94%)	21 (6%)	0	100	100
4	U	422/483 (87%)	388 (92%)	31 (7%)	3 (1%)	22	62
5	a	746/838 (89%)	701 (94%)	44 (6%)	1 (0%)	51	85
6	e	75/81 (93%)	71 (95%)	4 (5%)	0	100	100
7	f	83/98 (85%)	74 (89%)	9 (11%)	0	100	100
8	X	108/119 (91%)	97 (90%)	11 (10%)	0	100	100
9	d	349/351 (99%)	333 (95%)	16 (5%)	0	100	100
10	c	201/463 (43%)	168 (84%)	33 (16%)	0	100	100
11	p	47/350 (13%)	45 (96%)	2 (4%)	0	100	100
12	b	198/205 (97%)	186 (94%)	12 (6%)	0	100	100
13	g	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
13	h	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
13	i	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
13	j	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
13	k	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
13	l	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
13	m	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
13	n	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
13	o	148/155 (96%)	142 (96%)	4 (3%)	2 (1%)	11	47
14	0	598/617 (97%)	549 (92%)	49 (8%)	0	100	100
14	1	598/617 (97%)	551 (92%)	47 (8%)	0	100	100
14	2	600/617 (97%)	565 (94%)	35 (6%)	0	100	100
15	3	466/511 (91%)	445 (96%)	21 (4%)	0	100	100
15	4	457/511 (89%)	419 (92%)	38 (8%)	0	100	100
15	5	466/511 (91%)	439 (94%)	27 (6%)	0	100	100
16	7	206/247 (83%)	196 (95%)	9 (4%)	1 (0%)	29	68
All	All	8314/9428 (88%)	7818 (94%)	489 (6%)	7 (0%)	54	85

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	U	123	TRP
13	o	45	SER
4	U	134	ASP
13	o	43	ALA
4	U	279	GLU
5	a	502	LEU
16	7	124	LEU

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	8	197/198 (100%)	196 (100%)	1 (0%)	88 93
1	9	197/198 (100%)	196 (100%)	1 (0%)	88 93
1	Q	197/198 (100%)	197 (100%)	0	100 100
2	R	96/99 (97%)	96 (100%)	0	100 100
2	T	96/99 (97%)	95 (99%)	1 (1%)	76 86
2	V	96/99 (97%)	96 (100%)	0	100 100
3	6	326/344 (95%)	325 (100%)	1 (0%)	92 95
4	U	384/429 (90%)	384 (100%)	0	100 100
5	a	669/741 (90%)	669 (100%)	0	100 100
6	e	65/68 (96%)	65 (100%)	0	100 100
7	f	71/83 (86%)	71 (100%)	0	100 100
8	X	94/100 (94%)	94 (100%)	0	100 100
9	d	306/306 (100%)	306 (100%)	0	100 100
10	c	180/395 (46%)	180 (100%)	0	100 100
11	p	44/309 (14%)	44 (100%)	0	100 100
12	b	154/158 (98%)	154 (100%)	0	100 100
13	g	109/113 (96%)	109 (100%)	0	100 100
13	h	109/113 (96%)	109 (100%)	0	100 100
13	i	109/113 (96%)	109 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	j	109/113 (96%)	109 (100%)	0	100	100
13	k	109/113 (96%)	109 (100%)	0	100	100
13	l	109/113 (96%)	108 (99%)	1 (1%)	78	88
13	m	109/113 (96%)	109 (100%)	0	100	100
13	n	109/113 (96%)	109 (100%)	0	100	100
13	o	109/113 (96%)	108 (99%)	1 (1%)	78	88
14	0	507/524 (97%)	506 (100%)	1 (0%)	93	96
14	1	507/524 (97%)	506 (100%)	1 (0%)	93	96
14	2	509/524 (97%)	508 (100%)	1 (0%)	93	96
15	3	402/431 (93%)	401 (100%)	1 (0%)	93	96
15	4	395/431 (92%)	393 (100%)	2 (0%)	88	93
15	5	402/431 (93%)	402 (100%)	0	100	100
16	7	179/212 (84%)	179 (100%)	0	100	100
All	All	7054/7918 (89%)	7042 (100%)	12 (0%)	93	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	8	62	LYS
1	9	26	LYS
2	T	115	ARG
3	6	267	ARG
13	l	54	LYS
13	o	41	ILE
14	1	280	ARG
14	2	173	ARG
14	0	536	LYS
15	4	276	ARG
15	4	358	ASN
15	3	54	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	a	803	HIS
10	c	364	HIS

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Mol	Chain	Res	Type
14	1	468	HIS
14	2	22	HIS
15	3	54	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

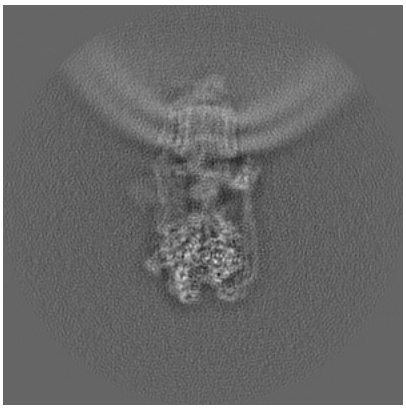
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44842. These allow visual inspection of the internal detail of the map and identification of artifacts.

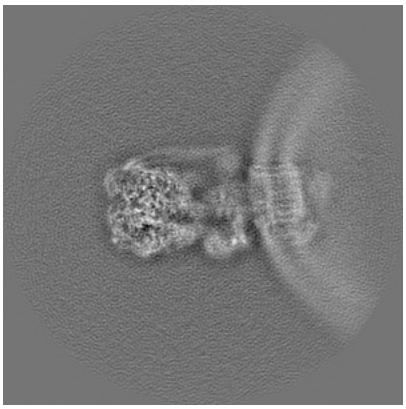
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

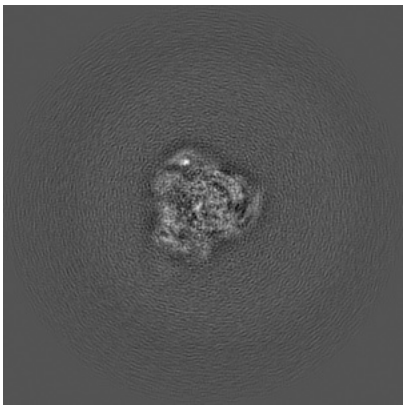
6.1.1 Primary map



X

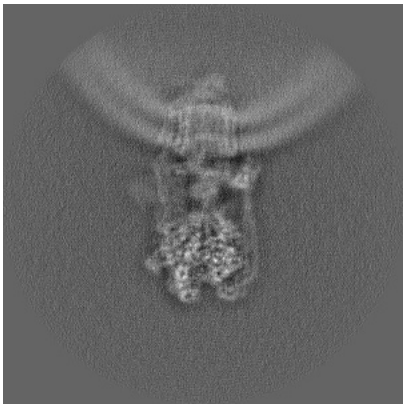


Y

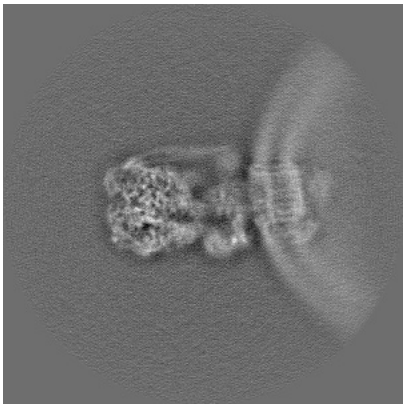


Z

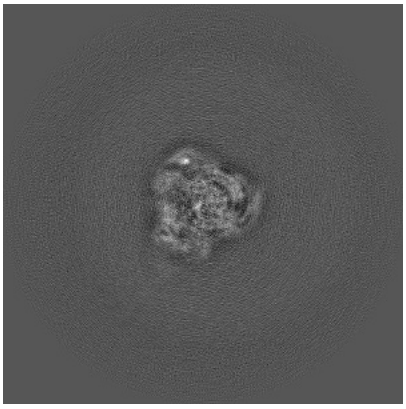
6.1.2 Raw map



X



Y

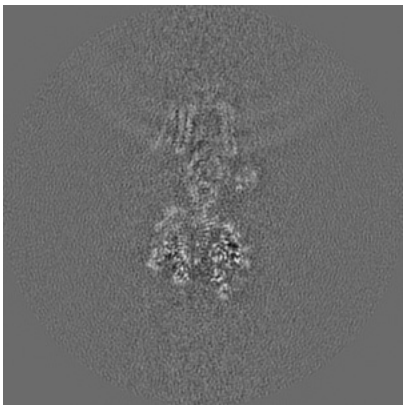


Z

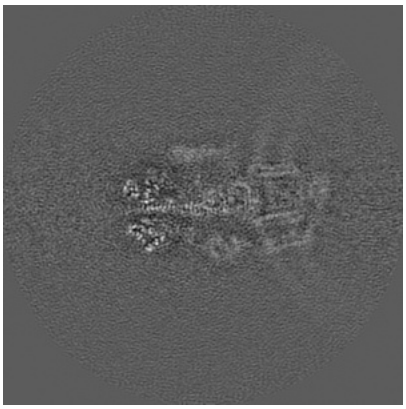
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

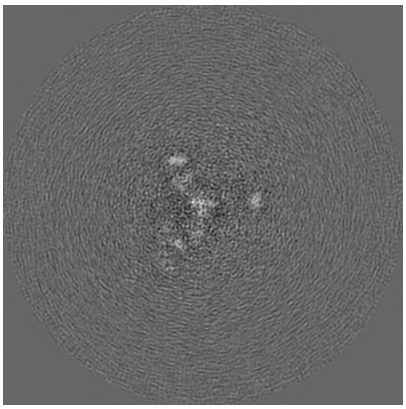
6.2.1 Primary map



X Index: 224

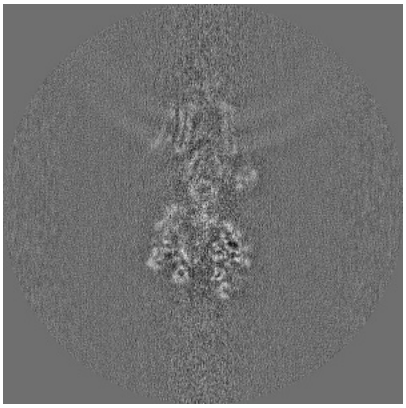


Y Index: 224

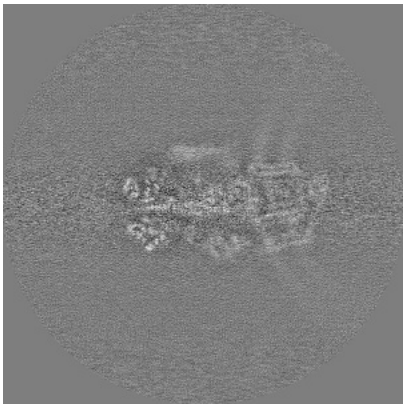


Z Index: 224

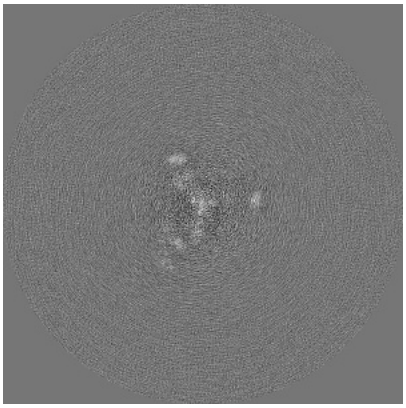
6.2.2 Raw map



X Index: 224



Y Index: 224

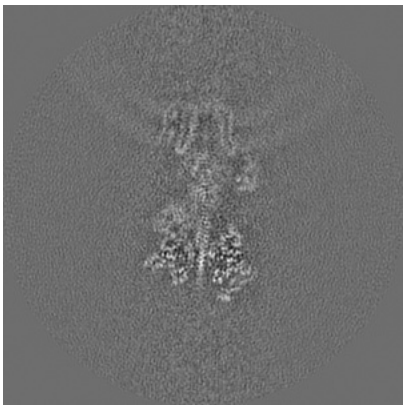


Z Index: 224

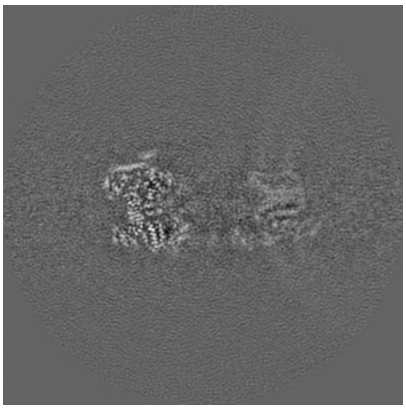
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

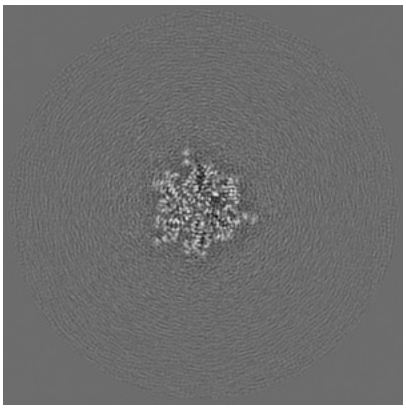
6.3.1 Primary map



X Index: 219

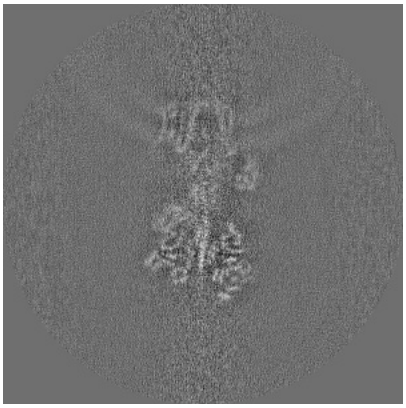


Y Index: 205

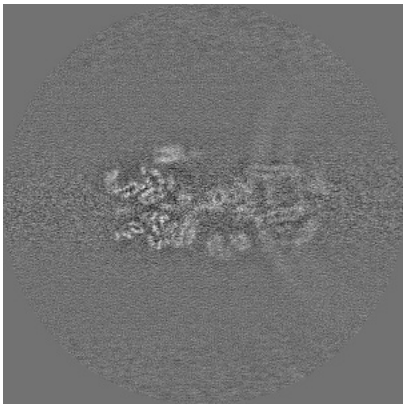


Z Index: 167

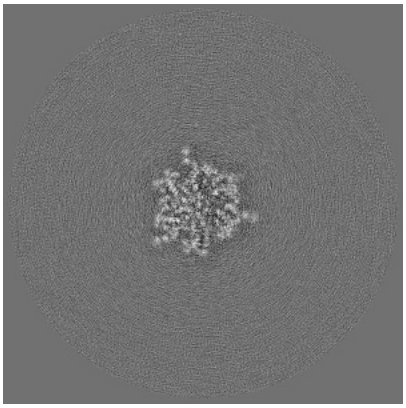
6.3.2 Raw map



X Index: 220



Y Index: 216

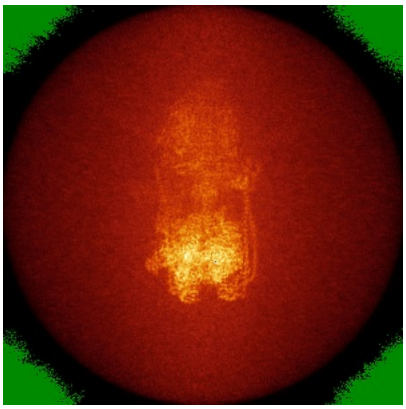


Z Index: 168

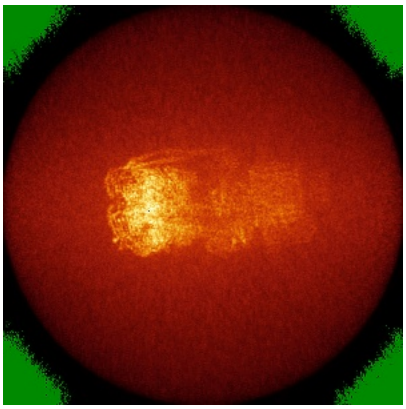
The images above show the largest variance slices of the map in three orthogonal directions.

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

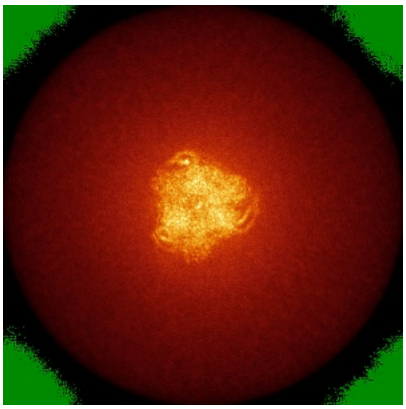
6.4.1 Primary map



X

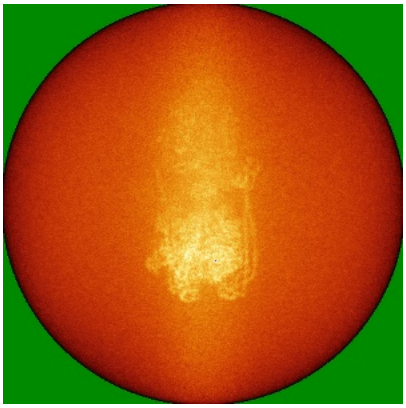


Y

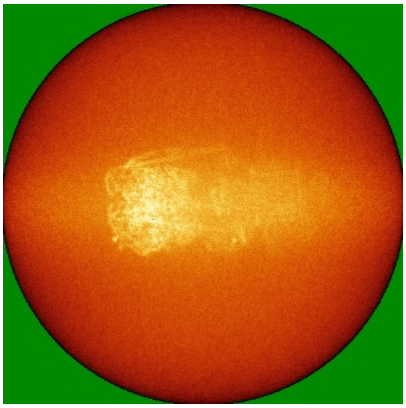


Z

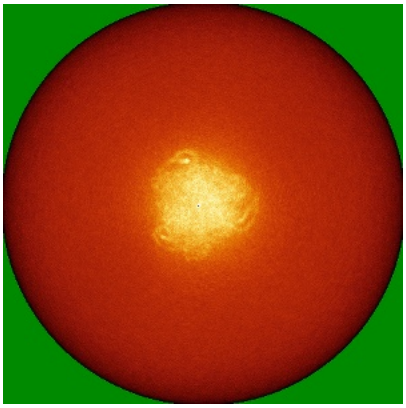
6.4.2 Raw map



X



Y

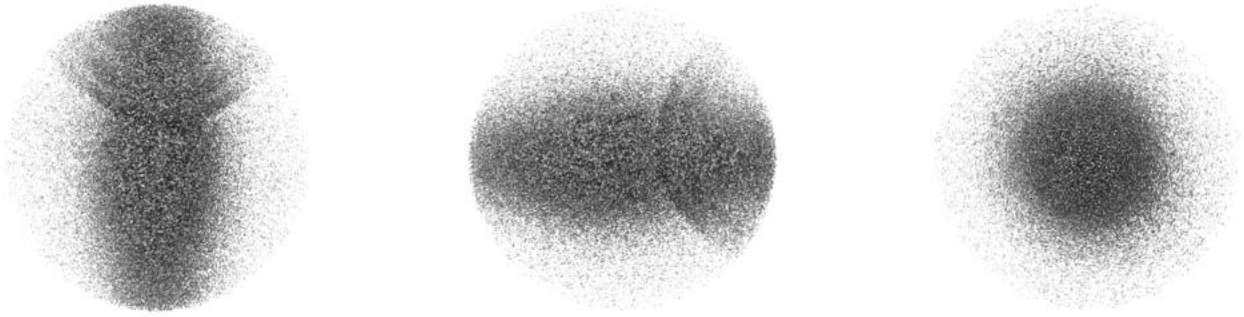


Z

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)

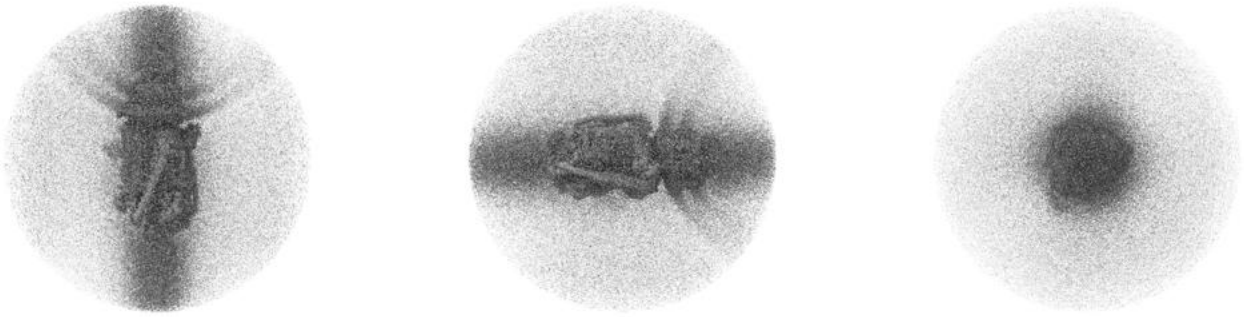
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. 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.

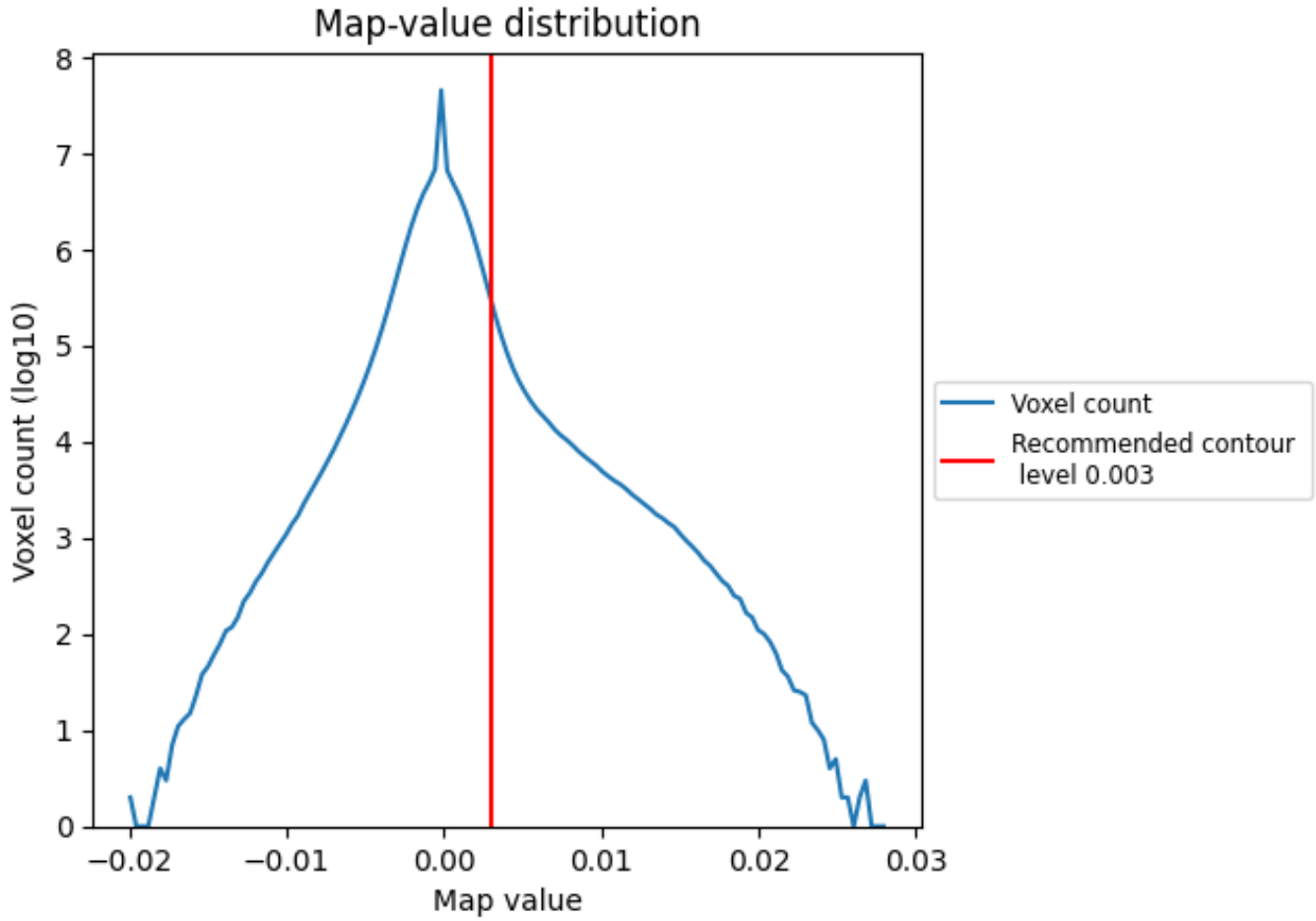
6.6 Mask visualisation (i)

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

7 Map analysis

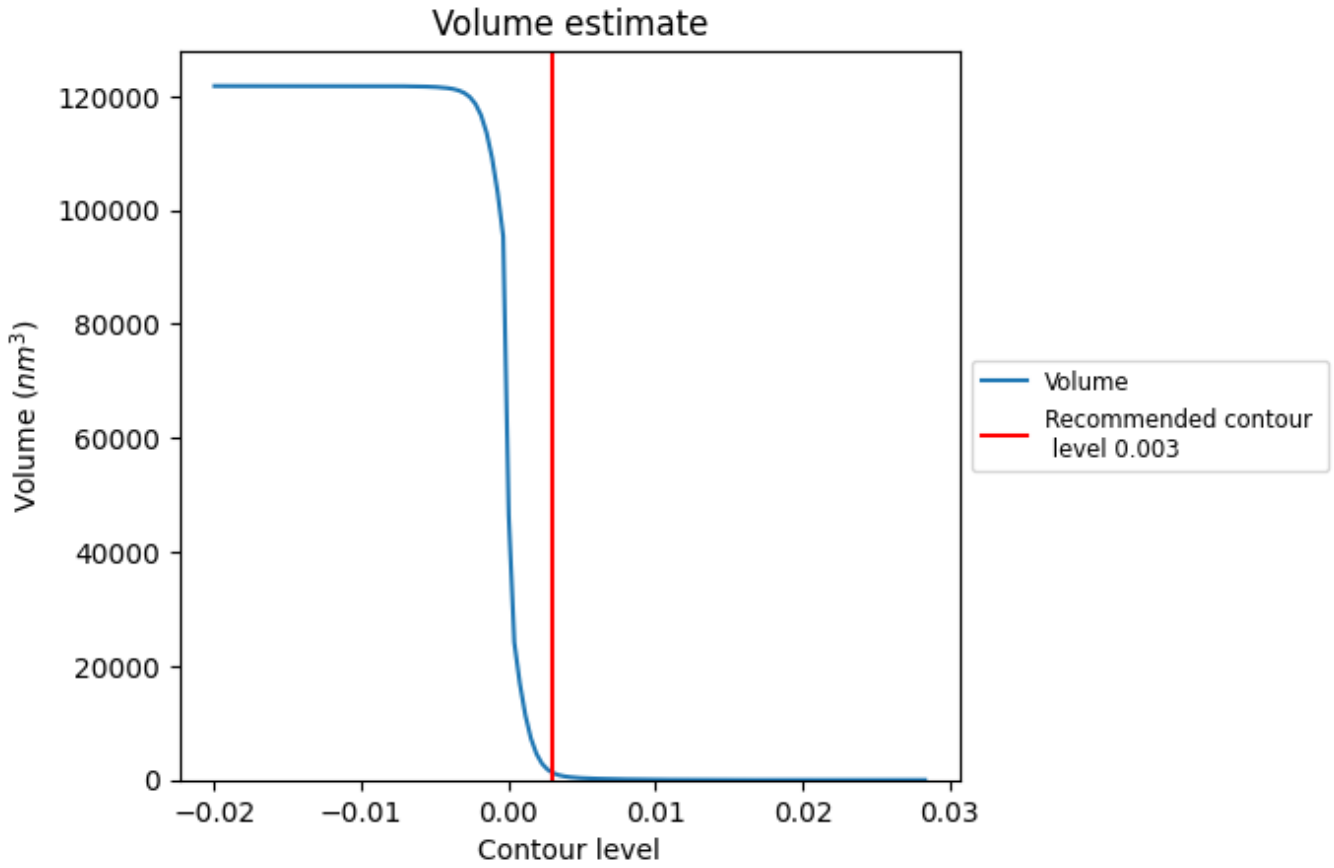
This section contains the results of statistical analysis of the map.

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.

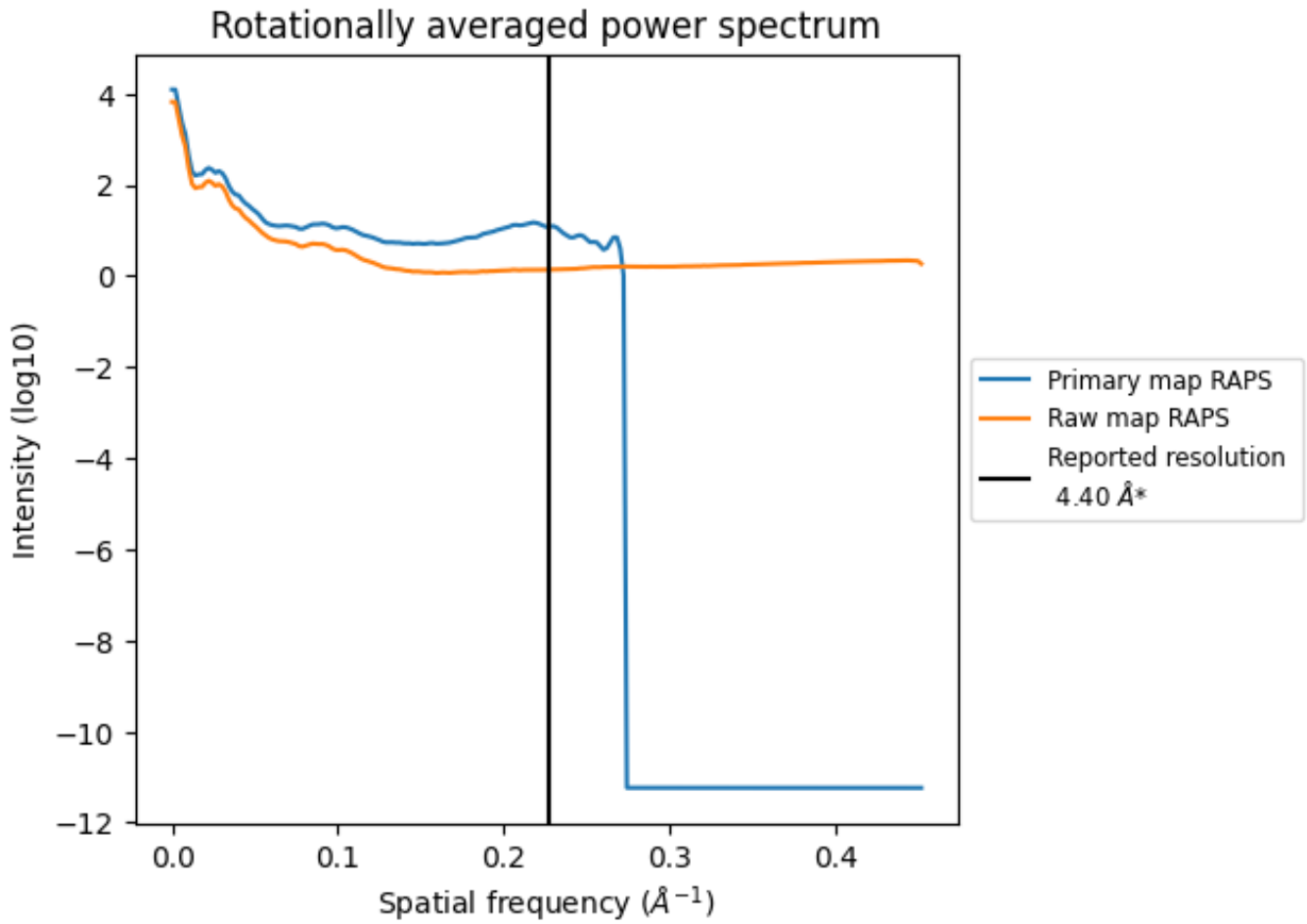
7.2 Volume estimate



The volume at the recommended contour level is 1305 nm^3; this corresponds to an approximate mass of 1179 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)

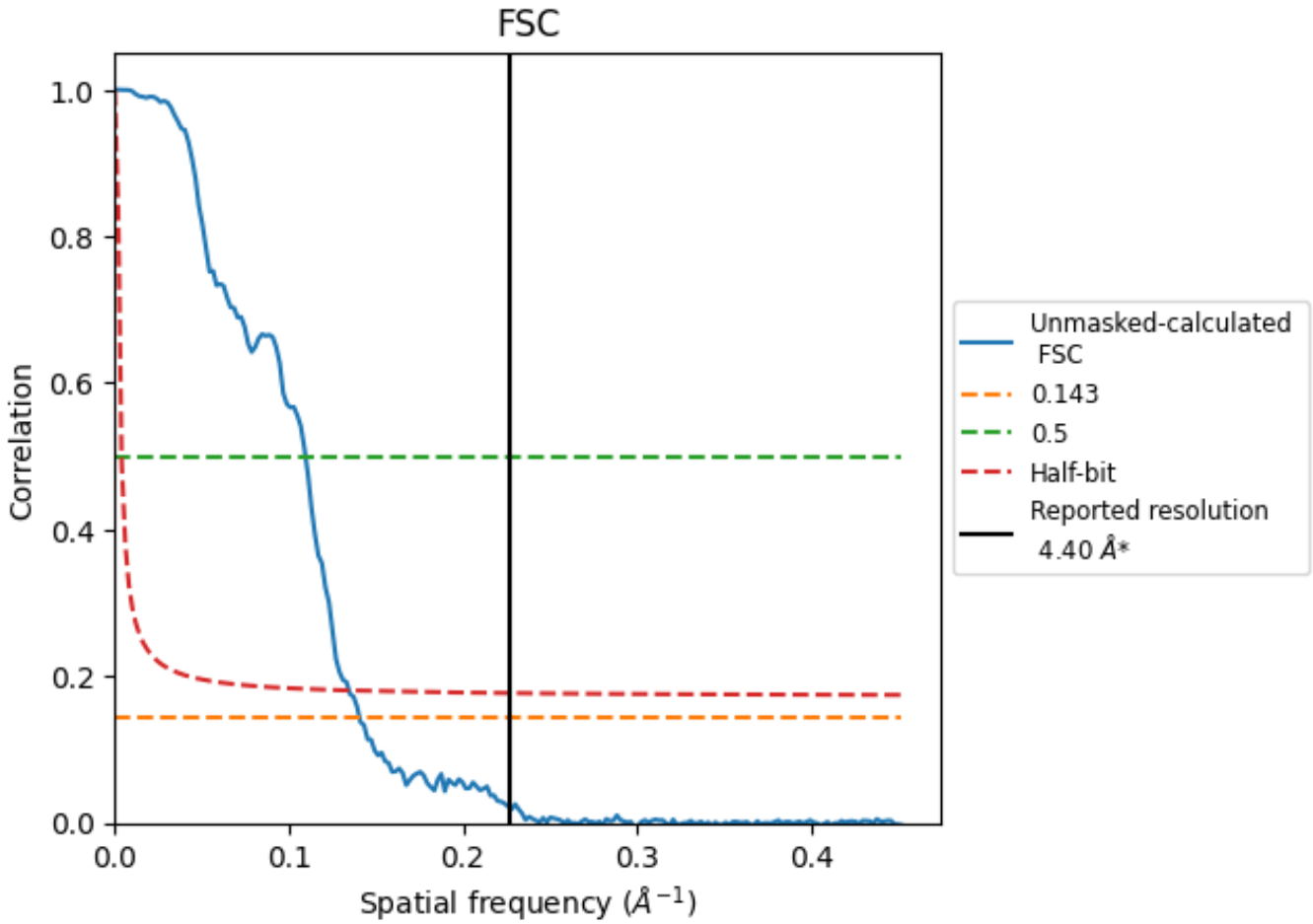


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

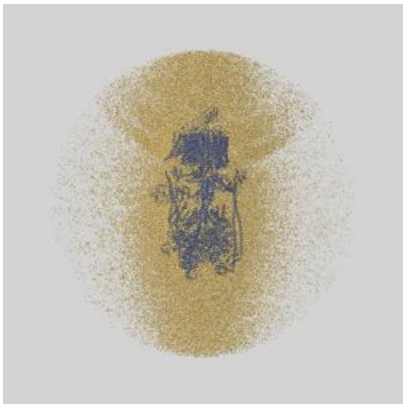
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.11	9.12	7.43

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

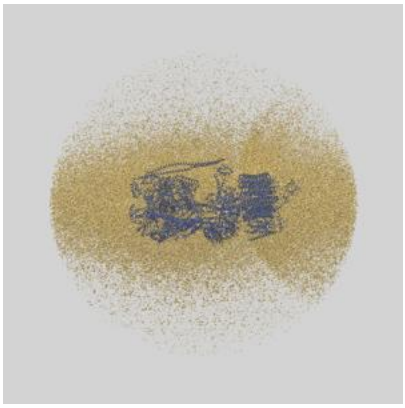
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44842 and PDB model 9BRS. Per-residue inclusion information can be found in section 3 on page 8.

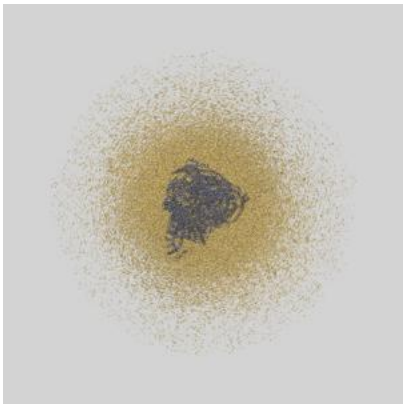
9.1 Map-model overlay



X



Y



Z

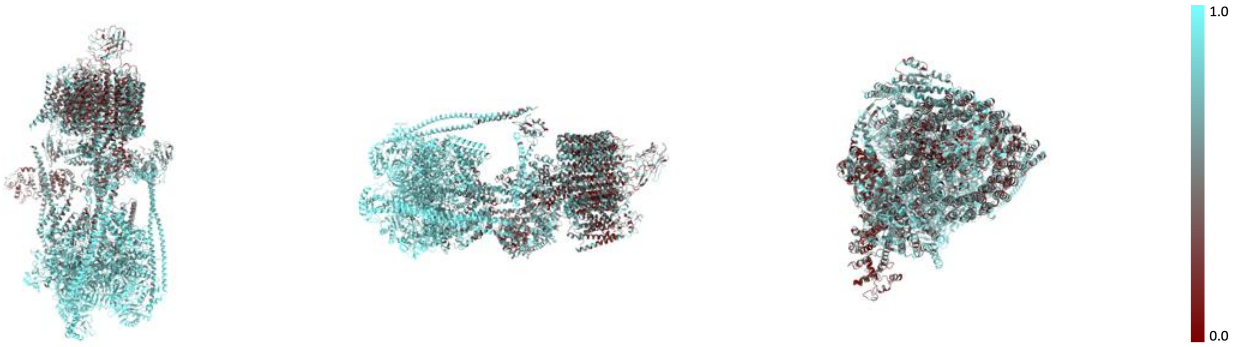
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

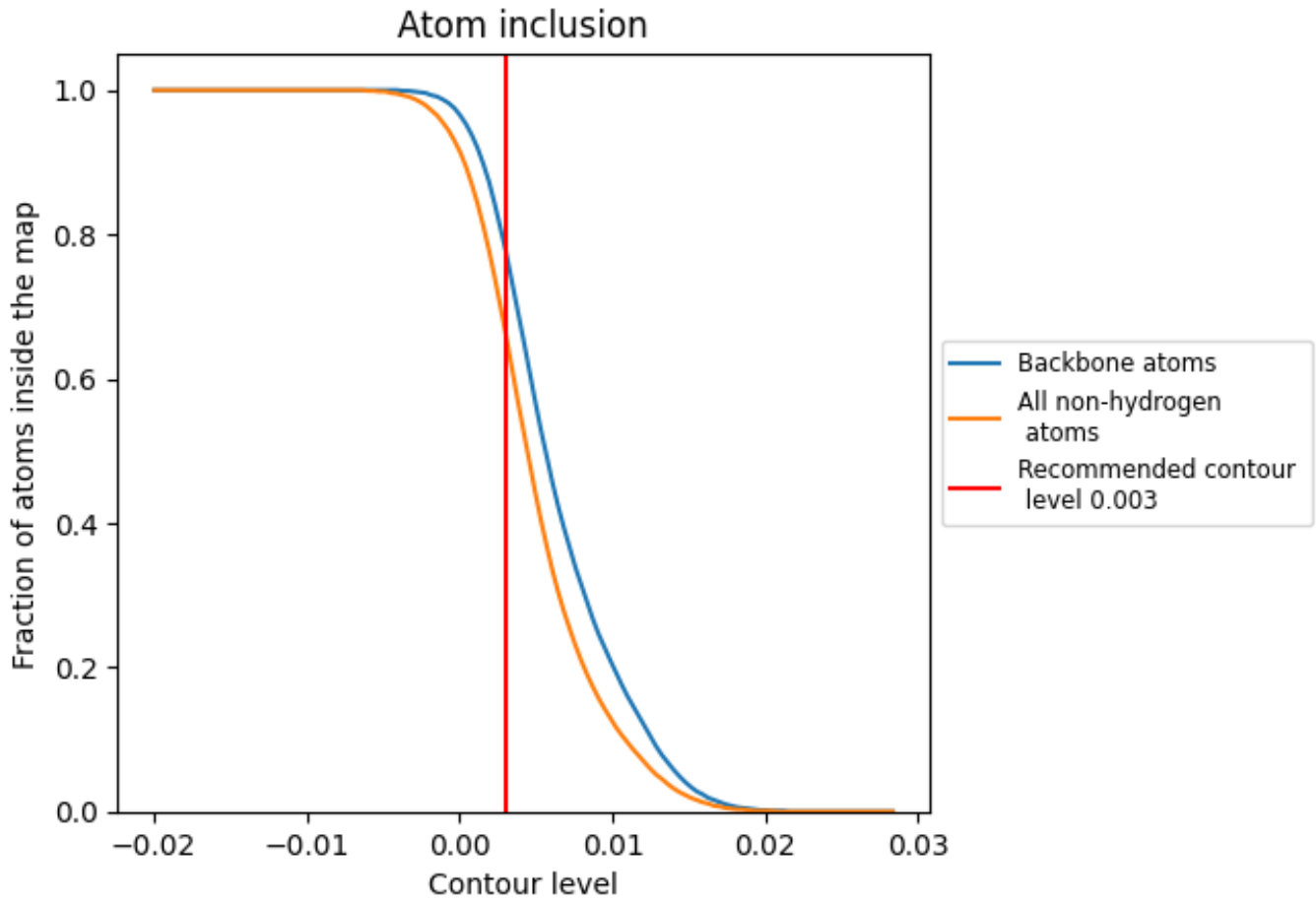
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6640	0.2770
0	0.7570	0.3260
1	0.8390	0.4030
2	0.7640	0.3520
3	0.8140	0.4020
4	0.8410	0.4220
5	0.8260	0.4140
6	0.6350	0.1920
7	0.6950	0.2920
8	0.8040	0.3220
9	0.8430	0.3220
Q	0.7950	0.2950
R	0.7680	0.2430
T	0.8480	0.2670
U	0.3860	0.1520
V	0.8330	0.2470
X	0.6590	0.2500
a	0.5820	0.2150
b	0.4670	0.1740
c	0.4390	0.1730
d	0.4480	0.1810
e	0.4710	0.1750
f	0.3950	0.1160
g	0.5690	0.1940
h	0.5080	0.1840
i	0.4610	0.1680
j	0.4170	0.1500
k	0.5000	0.1740
l	0.5830	0.2150
m	0.5570	0.2110
n	0.5030	0.1830
o	0.4780	0.1780
p	0.3840	0.1590