



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:10 PM UTC

PDB ID : 9BRR / pdb_00009brr
EMDB ID : EMD-44841
Title : Intact V-ATPase State 3 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 : 4.50 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:

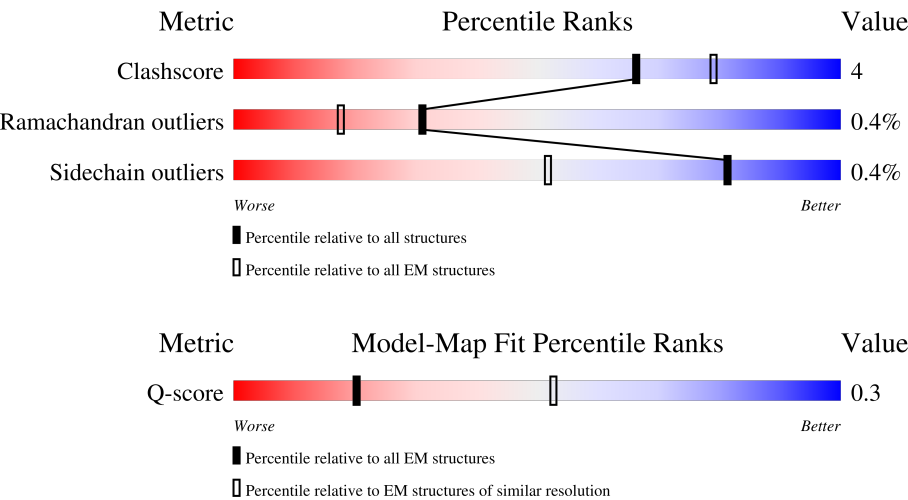
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.50 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	2937 (4.00 - 5.00)

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	b	205	
2	g	155	
2	h	155	
2	i	155	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	j	155	35% 89% 8% .
2	k	155	34% 81% 15% . .
2	l	155	30% 90% 7% .
2	m	155	33% 79% 15% . .
2	n	155	38% 91% 6% .
2	o	155	25% 81% 16% .
3	0	617	11% 92% 5% .
3	1	617	. 93% 5% .
3	2	617	9% 91% 6% .
4	3	511	. 84% 6% 10%
4	4	511	. 85% 7% 8%
4	5	511	. 88% . 8%
5	7	247	8% 83% . 14%
6	8	226	. 94% 5%
6	9	226	. 99% .
6	Q	226	8% 93% 6%
7	R	118	. 87% 9% .
7	T	118	. 94% . .
7	V	118	14% 89% 8% .
8	X	119	5% 90% . 8%
9	6	382	23% 88% 5% . 5%
10	U	483	21% 78% 9% . 12%
11	d	351	20% 87% 11% .
12	a	838	15% 83% 6% 10%
13	e	81	25% 80% 7% 7% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	f	98	32% 83% 13%
15	c	463	14% 40% 56%
16	p	350	7% 13% 86%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 65594 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 21 kDa proteolipid subunit c".

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

- Molecule 2 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

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

- Molecule 3 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	600	Total	C	N	O	S	0	0
			4656	2953	787	889	27		
3	0	602	Total	C	N	O	S	0	0
			4671	2961	789	894	27		
3	2	600	Total	C	N	O	S	0	0
			4656	2953	787	889	27		

- Molecule 4 is a protein called V-type proton ATPase subunit B, brain isoform.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	213	Total	C	N	O	S	0	0
			1722	1096	310	311	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
6	9	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
6	Q	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		

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

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

- 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 C 1.

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

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

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

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

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

- Molecule 12 is a protein called V-type proton ATPase 116 kDa subunit a 1.

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

- Molecule 13 is a protein called V-type proton ATPase subunit e 2.

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

- Molecule 14 is a protein called Ribonuclease kappa.

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

- Molecule 15 is a protein called V-type proton ATPase subunit S1.

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

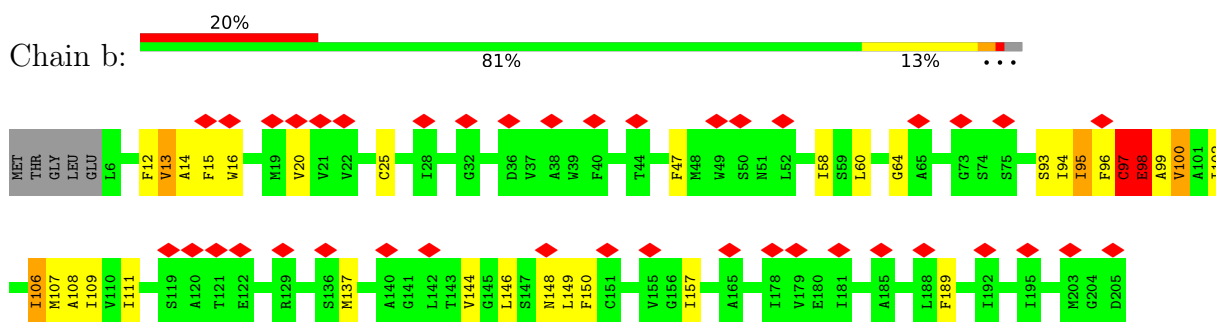
- Molecule 16 is a protein called Renin receptor cytoplasmic fragment.

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

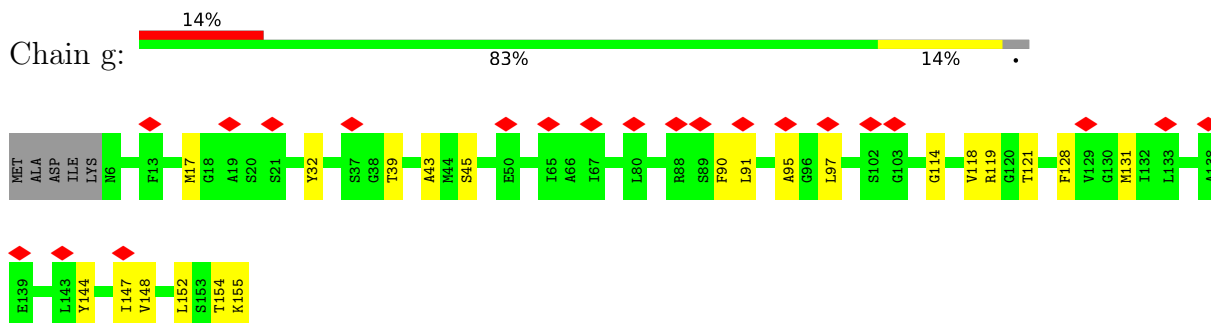
3 Residue-property plots [i](#)

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.

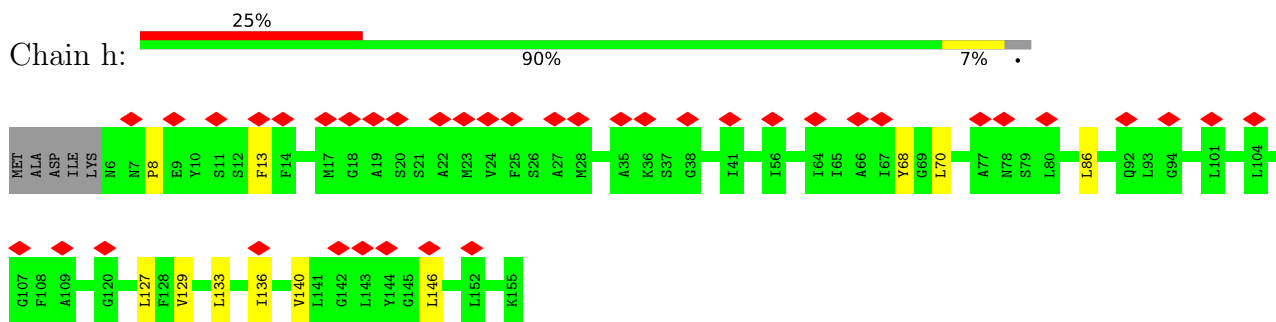
- Molecule 1: V-type proton ATPase 21 kDa proteolipid subunit c''



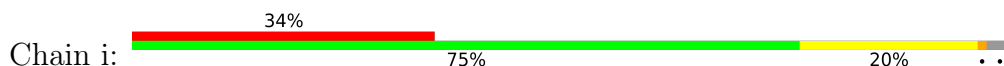
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

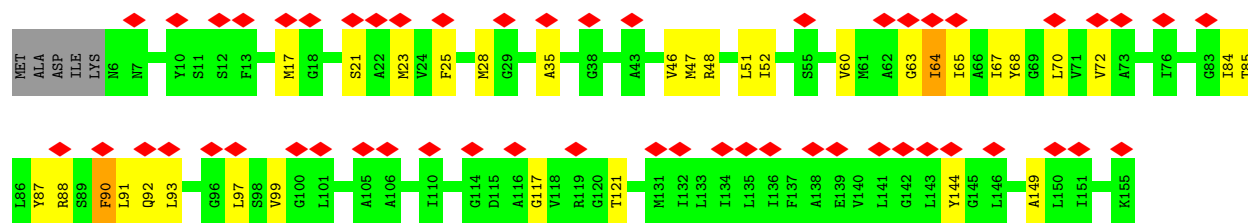


- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

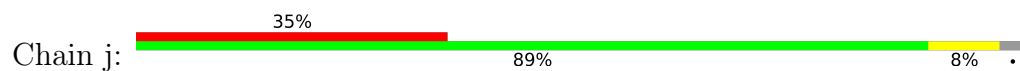


- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

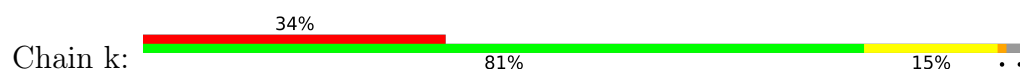




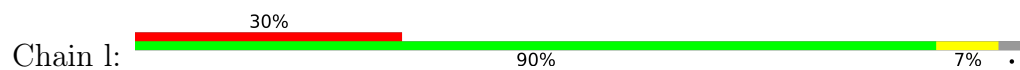
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c



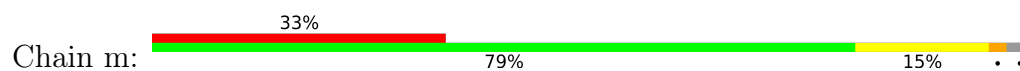
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

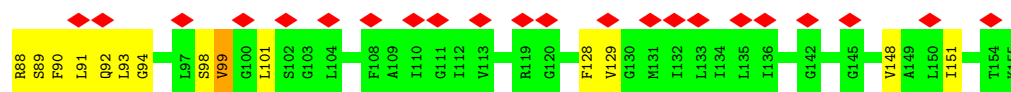


- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

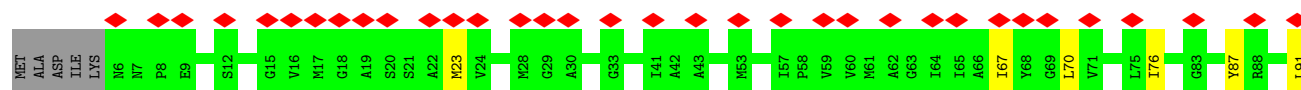
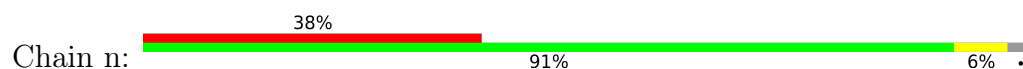


- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

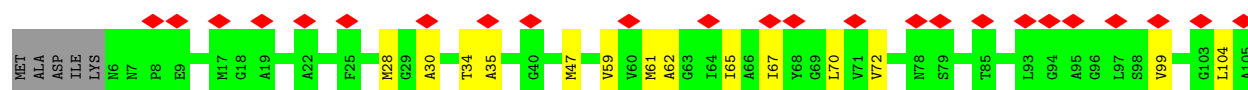
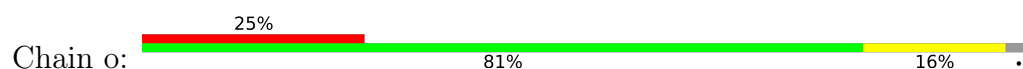




- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c



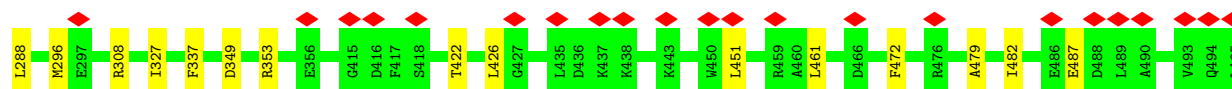
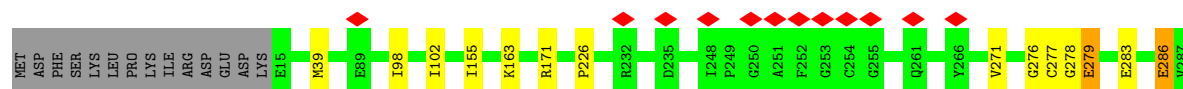
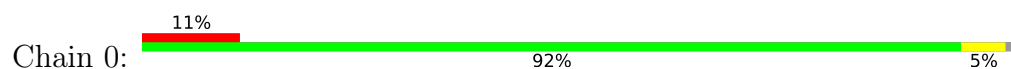
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

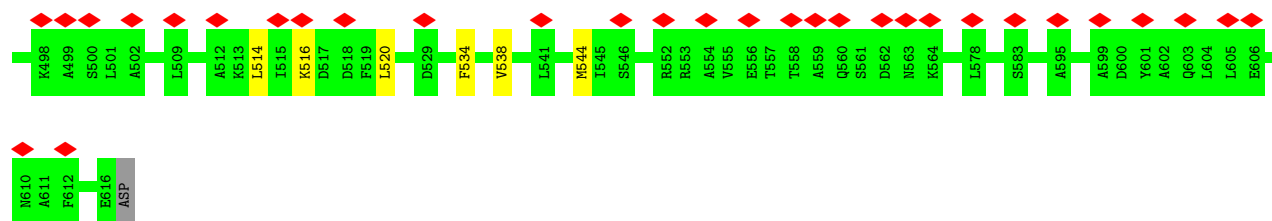


- Molecule 3: V-type proton ATPase catalytic subunit A

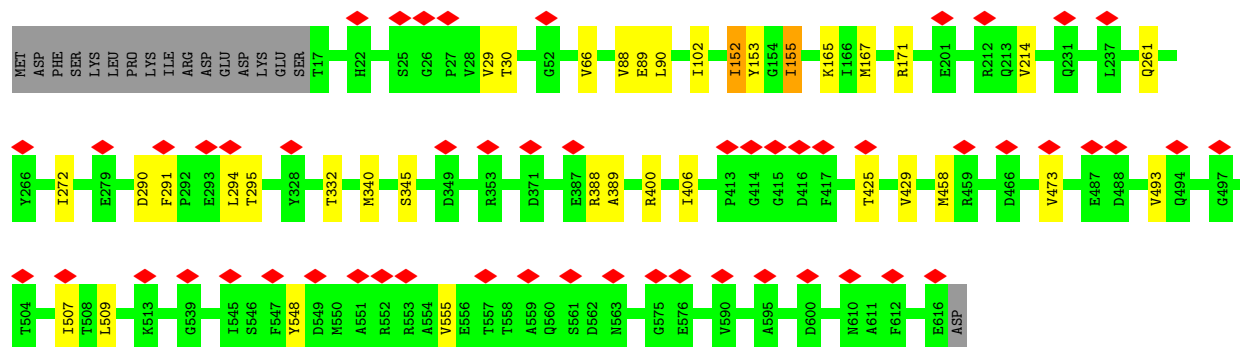
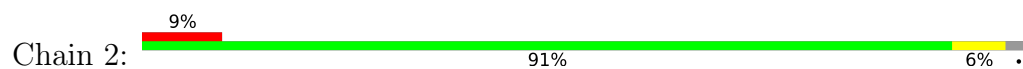


- Molecule 3: V-type proton ATPase catalytic subunit A

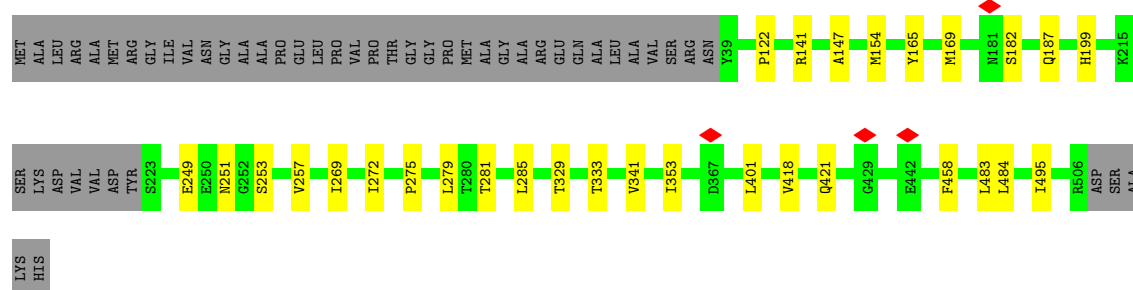
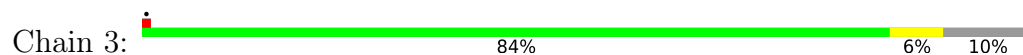




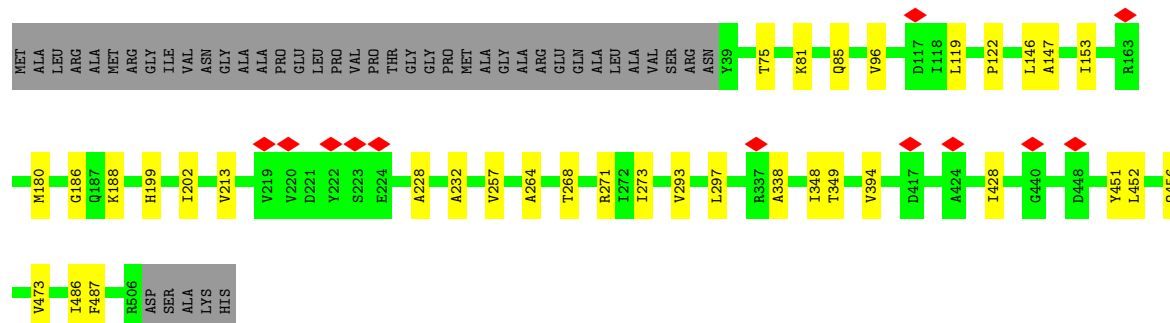
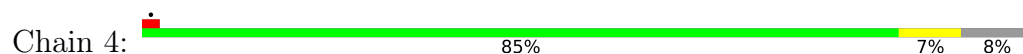
• Molecule 3: V-type proton ATPase catalytic subunit A



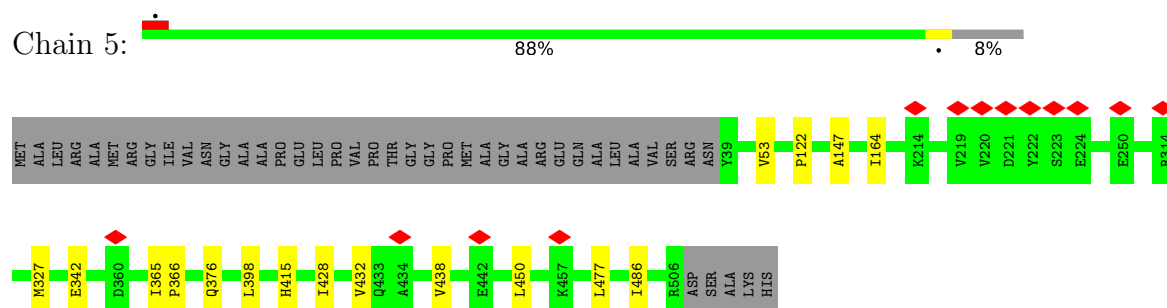
• Molecule 4: V-type proton ATPase subunit B, brain isoform



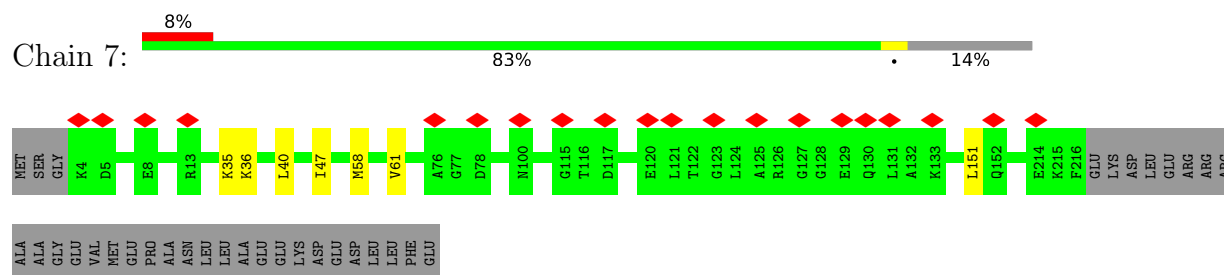
• Molecule 4: V-type proton ATPase subunit B, brain isoform



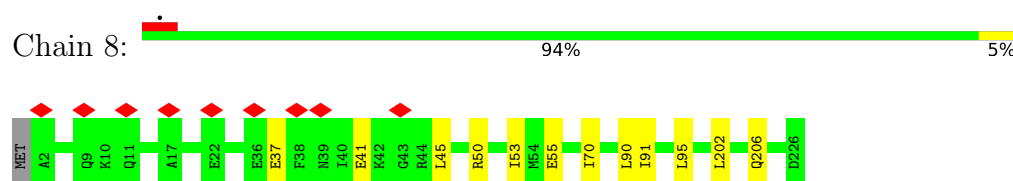
- Molecule 4: V-type proton ATPase subunit B, brain isoform



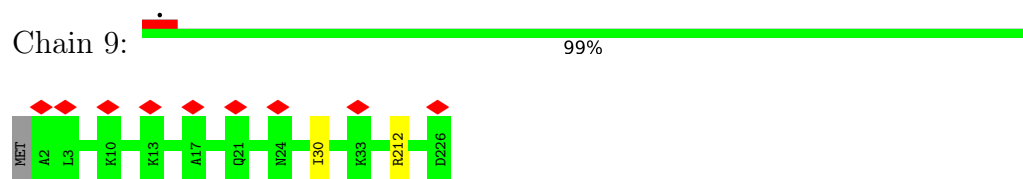
- Molecule 5: V-type proton ATPase subunit D



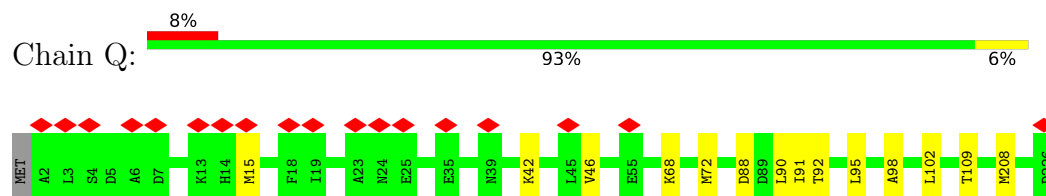
- Molecule 6: V-type proton ATPase subunit E 1



- Molecule 6: V-type proton ATPase subunit E 1



- Molecule 6: V-type proton ATPase subunit E 1



- Molecule 7: V-type proton ATPase subunit G 2





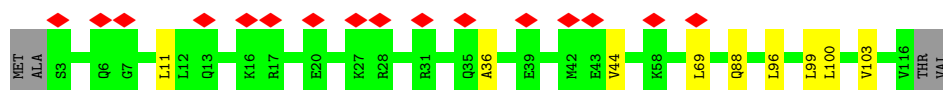
- Molecule 7: V-type proton ATPase subunit G 2

Chain T: 94%



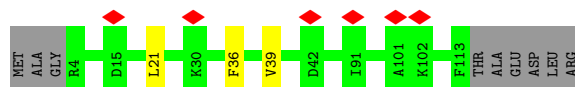
- Molecule 7: V-type proton ATPase subunit G 2

Chain V: 14% 89% 8%



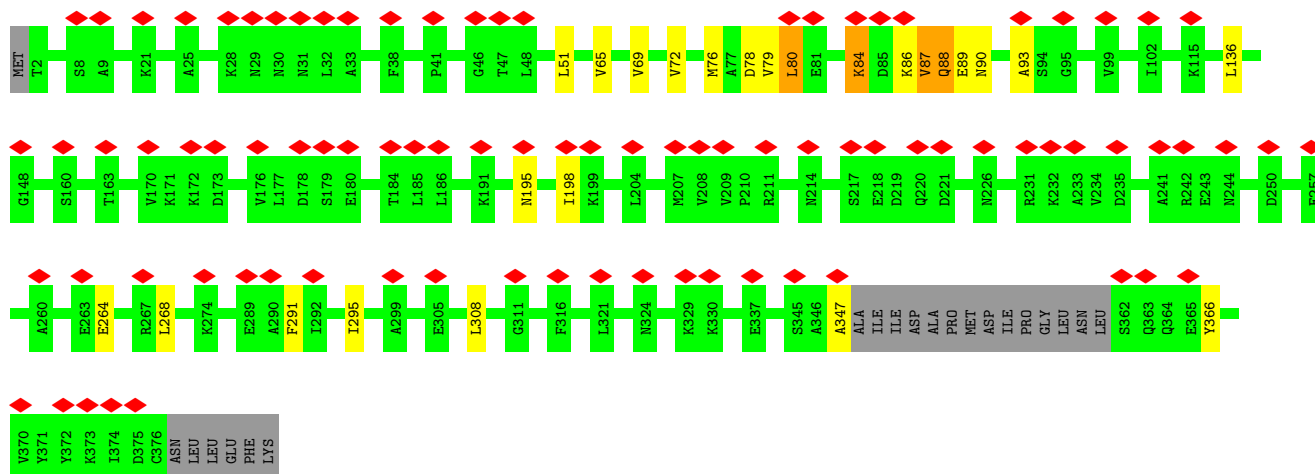
- Molecule 8: V-type proton ATPase subunit F

Chain X: 5% 90% 8%



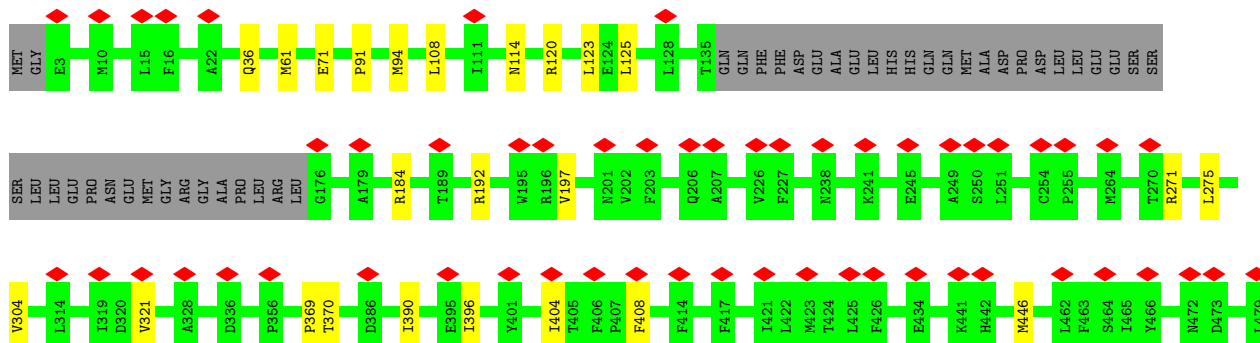
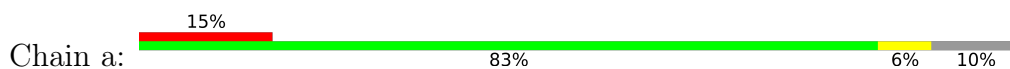
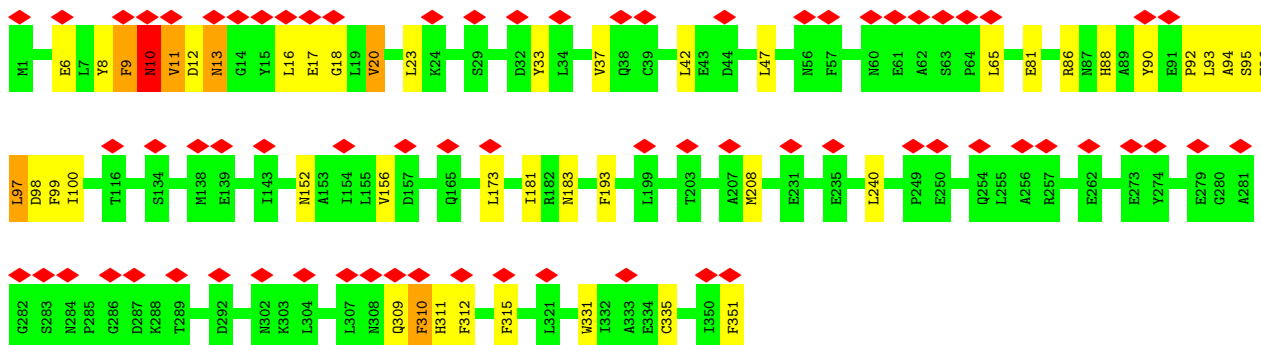
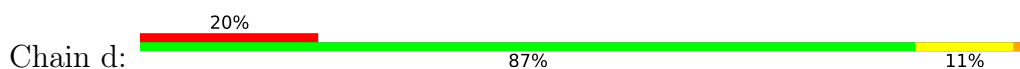
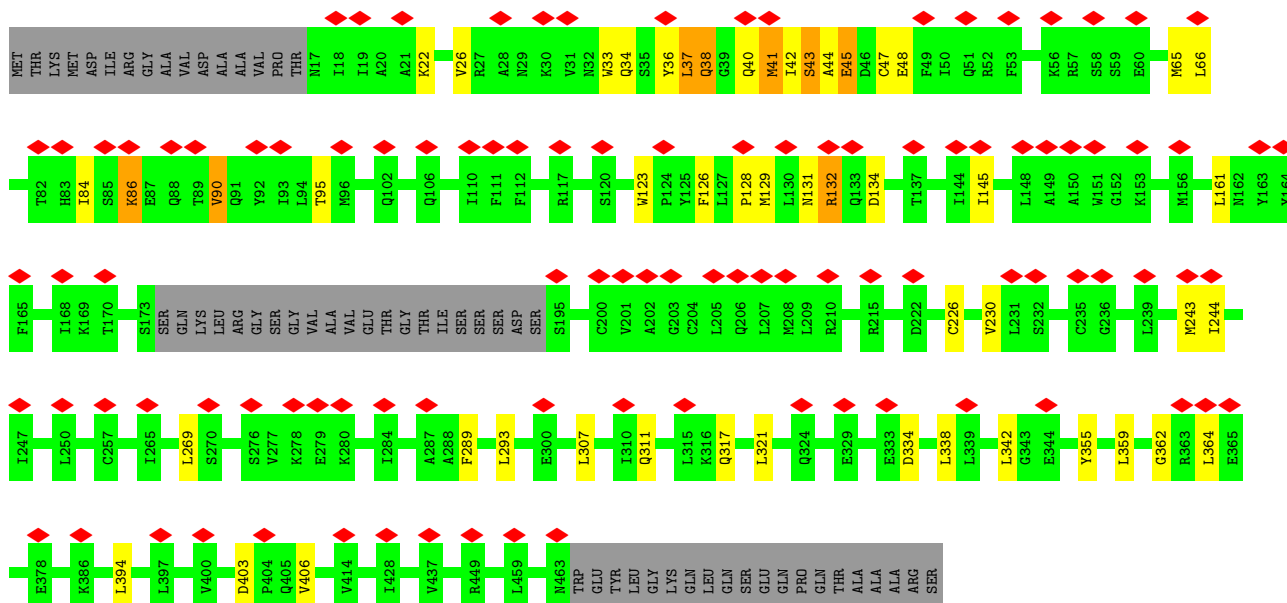
- Molecule 9: V-type proton ATPase subunit C 1

Chain 6: 23% 88% 5% 5%

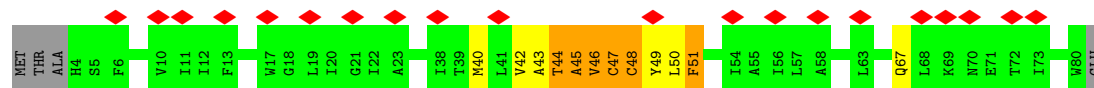
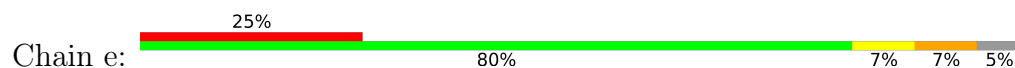


- Molecule 10: V-type proton ATPase subunit H

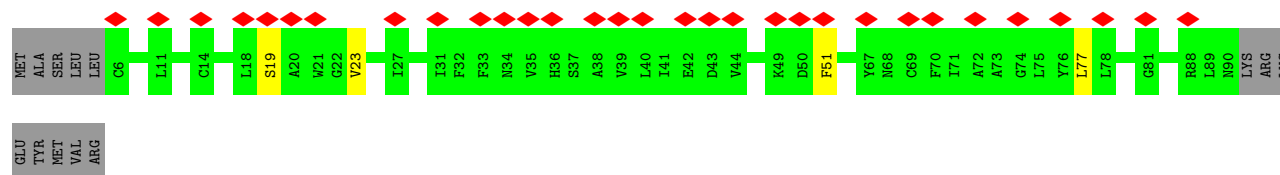
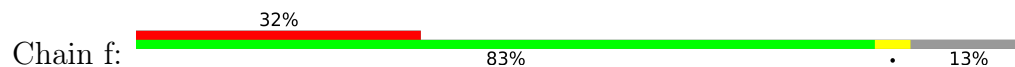
Chain U: 21% 78% 9% 12%



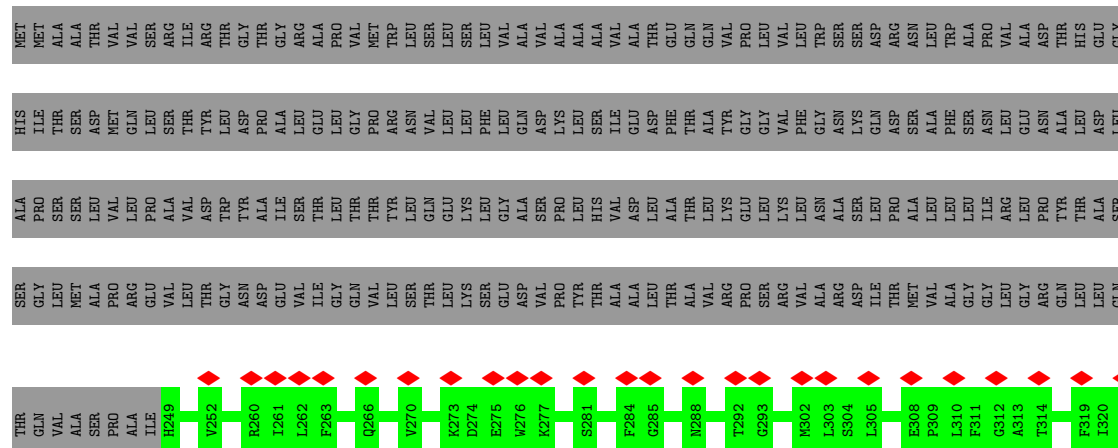
- Molecule 13: V-type proton ATPase subunit e 2



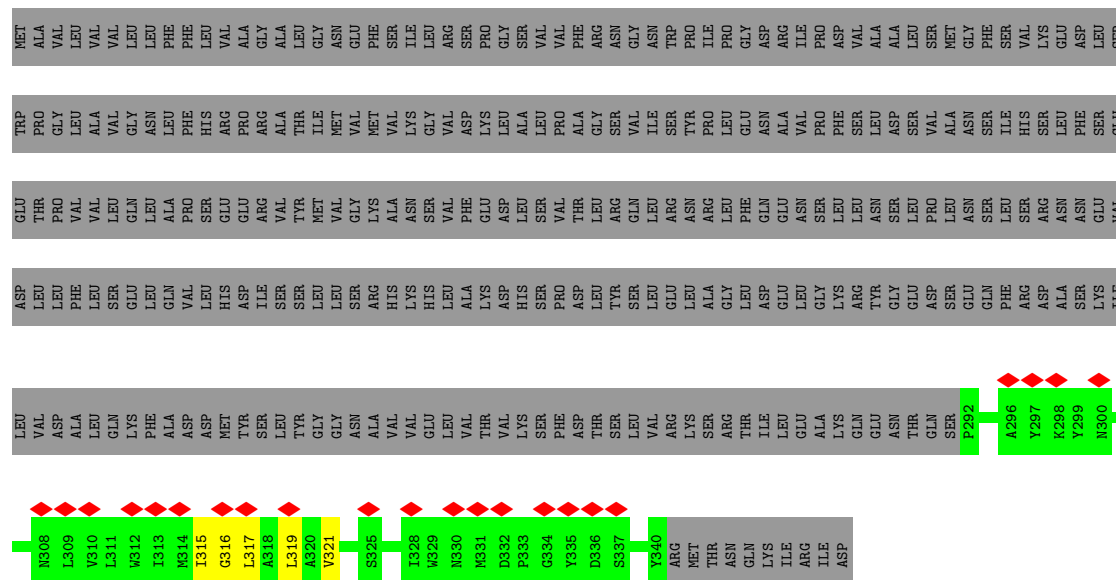
- Molecule 14: Ribonuclease kappa



- Molecule 15: V-type proton ATPase subunit S1



- Molecule 16: Renin receptor cytoplasmic fragment



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22018	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	-0.020	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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	b	0.47	0/1518	0.72	2/2061 (0.1%)
2	g	0.21	0/1084	0.48	0/1466
2	h	0.20	0/1084	0.46	0/1466
2	i	0.54	0/1084	0.82	2/1466 (0.1%)
2	j	0.20	0/1084	0.43	0/1466
2	k	0.47	1/1084 (0.1%)	0.68	2/1466 (0.1%)
2	l	0.21	0/1084	0.43	0/1466
2	m	0.55	0/1084	0.82	2/1466 (0.1%)
2	n	0.23	0/1084	0.47	0/1466
2	o	0.24	0/1084	0.47	0/1466
3	0	0.20	0/4767	0.44	1/6453 (0.0%)
3	1	0.19	0/4752	0.42	0/6433
3	2	0.22	0/4752	0.48	0/6433
4	3	0.20	0/3681	0.44	0/4987
4	4	0.20	0/3740	0.42	0/5069
4	5	0.19	0/3740	0.43	0/5069
5	7	0.22	0/1741	0.45	0/2328
6	8	0.22	0/1840	0.46	1/2462 (0.0%)
6	9	0.18	0/1840	0.39	0/2462
6	Q	0.20	0/1840	0.44	0/2462
7	R	0.28	0/930	0.50	0/1237
7	T	0.20	0/930	0.46	0/1237
7	V	0.21	0/930	0.41	0/1237
8	X	0.20	0/889	0.45	0/1199
9	6	0.25	0/2985	0.48	2/4032 (0.0%)
10	U	0.32	0/3568	0.57	2/4806 (0.0%)
11	d	0.34	1/2908 (0.0%)	0.58	5/3937 (0.1%)
12	a	0.23	0/6274	0.46	2/8486 (0.0%)
13	e	0.43	0/648	0.79	1/891 (0.1%)
14	f	0.20	0/674	0.39	0/915
15	c	0.32	1/1697 (0.1%)	0.58	0/2311
16	p	0.44	0/420	0.80	0/576
All	All	0.26	3/66820 (0.0%)	0.50	22/90277 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	d	10	ASN	C-O	-5.58	1.17	1.24
2	k	87	TYR	C-O	5.17	1.30	1.24
15	c	446	MET	N-CA	5.01	1.49	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	13	VAL	N-CA-C	-8.16	102.39	110.30
1	b	13	VAL	N-CA-CB	7.83	119.16	110.62
10	U	38	GLN	N-CA-C	-6.85	100.15	109.54
2	k	87	TYR	N-CA-C	-6.74	103.02	111.11
2	m	87	TYR	N-CA-C	-6.54	104.14	111.28
11	d	310	PHE	CA-CB-CG	-6.35	107.45	113.80
3	0	286	GLU	N-CA-CB	6.24	119.29	110.12
2	m	99	VAL	N-CA-CB	6.19	117.38	110.51
10	U	128	PRO	N-CA-C	-6.08	105.25	113.40
2	i	87	TYR	CB-CA-C	-6.03	101.31	110.83
9	6	89	GLU	N-CA-C	-5.91	104.18	111.75
12	a	501	THR	CA-C-O	-5.90	115.94	120.19
11	d	97	LEU	N-CA-CB	-5.80	101.44	109.91
11	d	20	VAL	CA-C-O	-5.72	115.10	121.05
13	e	51	PHE	N-CA-CB	5.67	118.23	110.01
9	6	88	GLN	N-CA-C	-5.64	105.70	112.58
12	a	491	MET	N-CA-C	-5.23	105.70	111.71
2	i	90	PHE	CB-CA-C	5.22	119.45	110.79
11	d	9	PHE	CA-C-O	-5.18	115.12	120.92
11	d	310	PHE	N-CA-CB	-5.14	101.81	110.49
2	k	102	SER	CA-C-O	-5.10	115.64	120.90
6	8	55	GLU	N-CA-CB	5.08	117.37	110.01

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	b	1484	0	1528	43	0
2	g	1069	0	1136	22	0
2	h	1069	0	1136	9	0
2	i	1069	0	1136	28	0
2	j	1069	0	1136	15	0
2	k	1069	0	1136	24	0
2	l	1069	0	1136	13	0
2	m	1069	0	1136	20	0
2	n	1069	0	1136	12	0
2	o	1069	0	1136	27	0
3	0	4671	0	4654	23	0
3	1	4656	0	4643	20	0
3	2	4656	0	4643	25	0
4	3	3610	0	3613	19	0
4	4	3667	0	3667	24	0
4	5	3667	0	3667	13	0
5	7	1722	0	1833	4	0
6	8	1823	0	1895	10	0
6	9	1823	0	1895	2	0
6	Q	1823	0	1895	12	0
7	R	925	0	935	17	0
7	T	925	0	935	2	0
7	V	925	0	935	8	0
8	X	875	0	883	2	0
9	6	2931	0	2969	15	0
10	U	3501	0	3481	46	0
11	d	2842	0	2782	46	0
12	a	6117	0	6154	60	0
13	e	623	0	641	13	0
14	f	658	0	652	7	0
15	c	1642	0	1568	22	0
16	p	407	0	403	4	0
All	All	65594	0	66495	509	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 (509) 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)
3:0:277:CYS:SG	3:0:327:ILE:HD11	1.78	1.22
12:a:497:TRP:CZ2	12:a:508:LEU:HD22	1.80	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:86:ARG:HH12	11:d:97:LEU:HB3	1.17	1.09
10:U:38:GLN:NE2	10:U:48:GLU:HG3	1.68	1.06
12:a:498:THR:HG22	12:a:499:GLU:HG2	1.39	1.04
11:d:86:ARG:NH1	11:d:97:LEU:HB3	1.75	1.02
12:a:497:TRP:HZ2	12:a:508:LEU:HD22	1.18	0.99
1:b:12:PHE:HZ	1:b:16:TRP:CZ3	1.84	0.94
11:d:12:ASP:O	11:d:16:LEU:HD13	1.67	0.94
10:U:38:GLN:CG	10:U:45:GLU:HA	1.97	0.93
1:b:12:PHE:CZ	1:b:16:TRP:CZ3	2.56	0.93
2:j:24:VAL:HG22	2:k:101:LEU:HD11	1.51	0.91
12:a:502:LEU:HD21	14:f:51:PHE:HD2	1.38	0.89
10:U:38:GLN:HG3	10:U:45:GLU:HA	1.56	0.87
10:U:38:GLN:HG3	10:U:45:GLU:CA	2.06	0.86
3:0:277:CYS:HG	3:0:327:ILE:HD11	1.39	0.84
11:d:17:GLU:HA	11:d:20:VAL:HG22	1.60	0.83
12:a:497:TRP:HE1	12:a:508:LEU:HD13	1.43	0.83
3:0:277:CYS:SG	3:0:327:ILE:CD1	2.65	0.83
2:g:119:ARG:HH22	15:c:446:MET:HE3	1.43	0.82
4:4:180:MET:HE3	4:4:394:VAL:HG21	1.62	0.82
12:a:502:LEU:HD21	14:f:51:PHE:CD2	2.14	0.82
2:j:24:VAL:HG22	2:k:101:LEU:CD1	2.10	0.81
12:a:502:LEU:CD2	14:f:51:PHE:CD2	2.64	0.79
10:U:38:GLN:HE22	10:U:48:GLU:HG3	1.46	0.79
10:U:40:GLN:HG2	10:U:41:MET:H	1.48	0.77
10:U:359:LEU:HD12	10:U:394:LEU:HD21	1.65	0.77
2:o:131:MET:HE1	2:o:135:LEU:HD11	1.68	0.76
11:d:16:LEU:HD23	11:d:93:LEU:HD22	1.67	0.75
2:k:80:LEU:HD21	2:l:91:LEU:HD11	1.69	0.75
6:8:41:GLU:OE2	7:R:29:LYS:HE3	1.87	0.75
1:b:12:PHE:CZ	1:b:16:TRP:CE3	2.74	0.74
12:a:498:THR:CG2	12:a:499:GLU:HG2	2.16	0.74
2:i:28:MET:HE2	2:j:105:ALA:HB2	1.68	0.74
9:6:80:LEU:HD23	9:6:84:LYS:HG2	1.70	0.74
10:U:38:GLN:HG2	10:U:45:GLU:HA	1.68	0.73
12:a:492:PHE:CD2	12:a:498:THR:HA	2.22	0.73
10:U:38:GLN:HE21	10:U:48:GLU:HG3	1.53	0.72
16:p:315:ILE:O	16:p:319:LEU:HG	1.89	0.72
12:a:497:TRP:HZ2	12:a:508:LEU:CD2	2.00	0.72
2:n:67:ILE:HA	2:n:70:LEU:HD12	1.71	0.72
11:d:16:LEU:HD23	11:d:93:LEU:CD2	2.20	0.72
11:d:12:ASP:O	11:d:16:LEU:CD1	2.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:449:PHE:HD1	15:c:450:ASP:H	1.38	0.71
3:1:95:MET:HE3	3:1:337:PHE:CZ	2.26	0.70
2:i:28:MET:CE	2:j:105:ALA:HB2	2.20	0.69
12:a:497:TRP:HE1	12:a:508:LEU:CD1	2.05	0.69
10:U:36:TYR:O	10:U:37:LEU:C	2.34	0.69
7:R:11:LEU:HD11	12:a:321:VAL:CG1	2.23	0.69
2:n:70:LEU:HD21	2:o:144:TYR:HB3	1.74	0.68
7:R:24:ASP:O	7:R:28:ARG:HG3	1.93	0.68
6:Q:68:LYS:HE3	6:Q:72:MET:HE3	1.74	0.68
1:b:60:LEU:HD13	1:b:146:LEU:HD22	1.75	0.67
2:j:20:SER:O	2:j:24:VAL:HG23	1.94	0.67
12:a:497:TRP:NE1	12:a:508:LEU:HD13	2.09	0.67
4:4:486:ILE:HG23	4:4:487:PHE:HD1	1.59	0.67
2:g:121:THR:OG1	2:g:131:MET:HE1	1.93	0.67
13:e:43:ALA:O	13:e:44:THR:C	2.37	0.67
2:g:17:MET:HE1	15:c:425:THR:HG21	1.75	0.67
13:e:45:ALA:O	13:e:46:VAL:C	2.37	0.67
2:o:28:MET:HA	2:o:28:MET:HE2	1.77	0.67
3:0:278:GLY:O	3:0:353:ARG:NH1	2.28	0.66
1:b:97:CYS:O	1:b:99:ALA:N	2.29	0.66
2:k:23:MET:HE3	2:k:70:LEU:CD2	2.25	0.65
10:U:145:ILE:HG23	10:U:161:LEU:HD23	1.77	0.65
4:3:329:THR:O	4:3:333:THR:HG23	1.96	0.64
10:U:40:GLN:HG2	10:U:41:MET:N	2.13	0.64
11:d:97:LEU:O	11:d:100:ILE:HG12	1.97	0.64
12:a:408:PHE:CE1	13:e:47:CYS:HB3	2.31	0.64
2:k:22:ALA:HA	2:k:100:GLY:HA3	1.80	0.63
4:3:122:PRO:HB3	4:3:147:ALA:HB2	1.80	0.63
3:2:290:ASP:OD1	3:2:294:LEU:HD12	1.98	0.63
2:g:39:THR:HG22	2:g:119:ARG:HH21	1.64	0.63
1:b:189:PHE:CD2	2:o:70:LEU:HD11	2.34	0.62
7:R:11:LEU:HD11	12:a:321:VAL:HG11	1.80	0.62
1:b:58:ILE:HD12	2:g:148:VAL:HG21	1.81	0.62
2:i:35:ALA:HB1	2:j:112:ILE:HG21	1.82	0.61
6:Q:90:LEU:HD11	7:V:88:GLN:HG2	1.82	0.61
7:V:99:LEU:O	7:V:103:VAL:HG23	2.01	0.61
9:6:291:PHE:CZ	9:6:295:ILE:HD11	2.36	0.61
1:b:100:VAL:HG23	1:b:148:ASN:HB3	1.82	0.61
2:g:119:ARG:HH22	15:c:446:MET:CE	2.14	0.61
1:b:102:ILE:HD11	12:a:742:ARG:HH21	1.65	0.60
3:2:458:MET:HE2	3:2:473:VAL:HG13	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:125:LEU:HD11	12:a:275:LEU:HD12	1.83	0.60
1:b:97:CYS:O	1:b:98:GLU:C	2.44	0.60
11:d:10:ASN:O	11:d:11:VAL:C	2.45	0.60
2:g:147:ILE:HD11	12:a:745:ALA:HB1	1.84	0.60
2:i:72:VAL:HG21	2:i:99:VAL:HG11	1.84	0.59
4:4:186:GLY:H	4:4:349:THR:HG22	1.67	0.59
9:6:87:VAL:HG23	9:6:88:GLN:HE21	1.67	0.59
10:U:40:GLN:CG	10:U:41:MET:H	2.15	0.59
2:l:87:TYR:O	2:l:91:LEU:HD23	2.03	0.59
4:4:119:LEU:HD23	4:4:153:ILE:HG21	1.84	0.59
10:U:38:GLN:HA	10:U:44:ALA:HA	1.85	0.59
6:8:37:GLU:OE1	7:R:29:LYS:HB2	2.03	0.59
2:m:89:SER:HA	2:m:92:GLN:HE21	1.68	0.59
10:U:244:ILE:HD13	10:U:269:LEU:HD22	1.85	0.59
2:g:154:THR:HG21	12:a:537:LEU:HD11	1.85	0.58
2:l:23:MET:HE3	2:m:98:SER:HB3	1.85	0.58
6:Q:15:MET:HE2	7:V:11:LEU:HD13	1.85	0.58
11:d:12:ASP:C	11:d:16:LEU:HD13	2.29	0.58
3:0:514:LEU:HD22	3:0:544:MET:HE2	1.85	0.58
4:5:450:LEU:HD22	4:5:486:ILE:HG22	1.86	0.58
4:4:186:GLY:N	4:4:349:THR:HG22	2.19	0.57
1:b:98:GLU:O	1:b:99:ALA:C	2.47	0.57
2:m:85:THR:CG2	2:m:88:ARG:HG3	2.34	0.57
2:m:14:PHE:HB3	2:m:93:LEU:HB2	1.85	0.57
11:d:99:PHE:CG	11:d:193:PHE:HD1	2.21	0.57
13:e:46:VAL:O	13:e:50:LEU:HG	2.04	0.57
3:2:261:GLN:NE2	3:2:294:LEU:HD13	2.19	0.57
13:e:47:CYS:O	13:e:50:LEU:N	2.37	0.57
10:U:226:CYS:O	10:U:230:VAL:HG23	2.05	0.57
1:b:149:LEU:HD22	1:b:150:PHE:CE1	2.40	0.57
2:m:59:VAL:HG11	2:n:134:ILE:CD1	2.35	0.57
2:l:51:LEU:HD23	2:l:54:LYS:HD3	1.86	0.57
3:0:472:PHE:CD1	3:0:538:VAL:HG22	2.39	0.57
4:5:415:HIS:NE2	4:5:477:LEU:HD11	2.20	0.57
2:j:68:TYR:CD1	2:j:146:LEU:HD22	2.40	0.57
2:h:129:VAL:O	2:h:133:LEU:HD13	2.05	0.57
2:g:39:THR:HG22	2:g:119:ARG:NH2	2.19	0.56
2:k:23:MET:SD	2:l:148:VAL:HG11	2.45	0.56
3:0:39:MET:SD	4:5:53:VAL:HG21	2.44	0.56
2:i:99:VAL:HB	2:i:149:ALA:HB2	1.86	0.56
4:4:146:LEU:HD22	6:9:212:ARG:HD3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:21:LEU:HD21	8:X:36:PHE:CD2	2.41	0.56
1:b:95:ILE:C	1:b:97:CYS:N	2.60	0.55
3:1:534:PHE:O	3:1:538:VAL:HG23	2.06	0.55
4:3:253:SER:O	4:3:257:VAL:HG23	2.06	0.55
1:b:150:PHE:CG	2:o:28:MET:HE1	2.41	0.55
2:i:52:ILE:HD11	2:j:127:LEU:CD2	2.36	0.55
11:d:97:LEU:O	11:d:98:ASP:C	2.49	0.55
12:a:527:ASP:OD2	12:a:529:ILE:HG22	2.06	0.55
4:3:169:MET:HE3	4:3:182:SER:OG	2.07	0.55
11:d:92:PRO:O	11:d:93:LEU:C	2.48	0.55
4:5:365:ILE:HB	4:5:366:PRO:HD3	1.88	0.55
12:a:493:THR:O	12:a:494:GLN:C	2.49	0.55
11:d:96:PHE:CE2	11:d:208:MET:HE2	2.42	0.54
1:b:95:ILE:O	1:b:96:PHE:C	2.50	0.54
2:g:32:TYR:CD2	15:c:443:LEU:HD11	2.41	0.54
2:o:107:GLY:HA2	2:o:110:ILE:HG22	1.88	0.54
3:2:152:ILE:HG23	3:2:400:ARG:NH1	2.23	0.54
3:0:102:ILE:O	3:0:102:ILE:HG22	2.07	0.54
3:0:534:PHE:O	3:0:538:VAL:HG23	2.08	0.54
10:U:230:VAL:HG12	10:U:243:MET:SD	2.47	0.54
12:a:497:TRP:CE2	12:a:508:LEU:HD22	2.38	0.54
1:b:150:PHE:CD2	2:o:28:MET:HE1	2.43	0.54
11:d:92:PRO:O	11:d:95:SER:N	2.40	0.54
12:a:492:PHE:HB2	12:a:496:ASN:O	2.08	0.54
12:a:494:GLN:HE21	12:a:514:ILE:CG2	2.21	0.54
15:c:447:ASP:O	15:c:448:ARG:C	2.50	0.54
11:d:17:GLU:HA	11:d:20:VAL:CG2	2.34	0.54
10:U:131:ASN:O	10:U:132:ARG:C	2.51	0.54
2:n:23:MET:CE	2:o:148:VAL:HG21	2.38	0.54
13:e:45:ALA:O	13:e:47:CYS:N	2.41	0.54
3:2:507:ILE:HG22	3:2:548:TYR:CE1	2.43	0.54
11:d:88:HIS:NE2	15:c:450:ASP:OD2	2.40	0.54
3:1:118:ILE:HG23	3:1:118:ILE:O	2.08	0.53
12:a:492:PHE:HD1	12:a:493:THR:H	1.55	0.53
7:R:24:ASP:OD2	7:R:28:ARG:NE	2.41	0.53
11:d:16:LEU:CD2	11:d:93:LEU:HD22	2.38	0.53
11:d:23:LEU:HD22	11:d:81:GLU:OE2	2.08	0.53
16:p:316:GLY:HA2	16:p:319:LEU:HD12	1.90	0.53
2:i:88:ARG:HA	2:i:91:LEU:HB3	1.90	0.53
2:k:23:MET:HE3	2:k:70:LEU:HD22	1.88	0.53
2:m:72:VAL:HG11	2:m:99:VAL:HG11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:516:LYS:HA	3:0:520:LEU:HD12	1.91	0.53
4:4:268:THR:HG22	4:4:271:ARG:NH2	2.24	0.53
4:4:228:ALA:HB3	4:4:293:VAL:HG12	1.89	0.53
4:5:164:ILE:HD11	4:5:342:GLU:HB3	1.90	0.53
2:k:34:THR:HG22	2:l:113:VAL:HG21	1.89	0.53
2:m:61:MET:O	2:m:64:ILE:HG22	2.08	0.53
3:2:214:VAL:HG22	3:2:388:ARG:HD3	1.90	0.53
10:U:37:LEU:HA	10:U:47:CYS:CB	2.39	0.53
12:a:120:ARG:HA	12:a:123:LEU:HD12	1.89	0.53
7:V:96:LEU:O	7:V:100:LEU:HD23	2.08	0.53
11:d:97:LEU:O	11:d:100:ILE:N	2.42	0.53
3:0:98:ILE:HD13	3:0:288:LEU:HD21	1.91	0.53
12:a:502:LEU:CD2	14:f:51:PHE:CE2	2.92	0.53
2:i:46:VAL:HG12	2:i:47:MET:HE2	1.91	0.52
4:5:415:HIS:HE2	4:5:477:LEU:HD11	1.73	0.52
7:R:24:ASP:OD2	7:R:28:ARG:NH2	2.41	0.52
2:i:67:ILE:O	2:i:68:TYR:C	2.50	0.52
2:j:51:LEU:HD12	2:j:51:LEU:O	2.09	0.52
2:k:56:ILE:O	2:k:56:ILE:HG22	2.10	0.52
9:6:347:ALA:HB2	12:a:192:ARG:NH2	2.25	0.52
12:a:271:ARG:CZ	12:a:275:LEU:HD21	2.38	0.52
2:n:23:MET:HE1	2:n:70:LEU:HD23	1.91	0.52
4:3:249:GLU:OE1	6:8:70:ILE:HD12	2.09	0.52
10:U:26:VAL:HG23	10:U:95:THR:HG21	1.91	0.52
2:o:28:MET:HB2	2:o:104:LEU:HD13	1.91	0.52
4:5:327:MET:HE1	4:5:365:ILE:CD1	2.40	0.52
4:5:376:GLN:OE1	4:5:398:LEU:HD12	2.10	0.52
1:b:13:VAL:O	1:b:14:ALA:C	2.52	0.52
2:g:128:PHE:HA	2:g:131:MET:HE3	1.91	0.52
3:0:451:LEU:HD21	3:0:487:GLU:HG3	1.92	0.52
12:a:501:THR:HG23	12:a:502:LEU:HG	1.92	0.52
1:b:107:MET:HG2	1:b:144:VAL:HG11	1.92	0.52
2:k:72:VAL:HG11	2:k:99:VAL:HG11	1.91	0.52
2:k:99:VAL:HB	2:k:149:ALA:HB2	1.92	0.52
6:8:90:LEU:HD21	7:R:88:GLN:HG3	1.92	0.52
11:d:6:GLU:HA	11:d:10:ASN:HB2	1.92	0.52
1:b:189:PHE:CG	2:o:70:LEU:HD11	2.46	0.51
4:4:199:HIS:HA	4:4:202:ILE:HG22	1.91	0.51
3:1:387:GLU:OE1	4:4:264:ALA:HB3	2.10	0.51
4:4:75:THR:HG23	4:4:81:LYS:NZ	2.25	0.51
2:g:154:THR:OG1	12:a:537:LEU:HD21	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:17:MET:HE1	2:m:94:GLY:HA2	1.92	0.51
3:2:272:ILE:HD13	3:2:345:SER:HB3	1.92	0.51
15:c:442:SER:O	15:c:443:LEU:C	2.53	0.51
1:b:106:ILE:C	1:b:108:ALA:N	2.68	0.51
10:U:38:GLN:HA	10:U:44:ALA:C	2.36	0.51
2:k:28:MET:HE2	2:k:104:LEU:HD11	1.92	0.51
3:1:257:THR:HG21	3:1:283:GLU:OE1	2.11	0.51
3:2:458:MET:HE3	3:2:473:VAL:HG22	1.93	0.51
4:5:438:VAL:HG12	5:7:35:LYS:NZ	2.25	0.51
13:e:47:CYS:O	13:e:48:CYS:C	2.53	0.51
7:R:29:LYS:O	7:R:30:ALA:C	2.53	0.51
12:a:494:GLN:O	12:a:495:GLY:C	2.54	0.51
1:b:106:ILE:O	1:b:109:ILE:N	2.44	0.51
2:m:85:THR:HG22	2:m:88:ARG:HG3	1.93	0.51
12:a:502:LEU:HD23	14:f:51:PHE:CE2	2.46	0.51
1:b:95:ILE:O	1:b:97:CYS:N	2.44	0.50
1:b:98:GLU:HG2	1:b:99:ALA:N	2.27	0.50
2:n:70:LEU:HD11	2:o:144:TYR:HB3	1.93	0.50
4:3:275:PRO:O	4:3:279:LEU:HD23	2.12	0.50
4:4:213:VAL:HG23	4:4:473:VAL:HG21	1.94	0.50
13:e:40:MET:O	13:e:43:ALA:HB3	2.11	0.50
4:4:188:LYS:HD2	4:4:338:ALA:HB3	1.93	0.50
10:U:42:ILE:HG23	10:U:84:ILE:HD11	1.93	0.50
2:j:16:VAL:CG1	2:k:90:PHE:CE2	2.95	0.50
1:b:157:ILE:HG21	2:o:35:ALA:HB1	1.94	0.50
2:j:16:VAL:HG12	2:k:90:PHE:CE2	2.46	0.50
2:k:86:LEU:HA	2:k:89:SER:HB2	1.93	0.50
4:3:165:TYR:OH	4:3:401:LEU:HD22	2.12	0.50
11:d:99:PHE:CG	11:d:193:PHE:CD1	3.00	0.49
15:c:418:GLY:HA2	15:c:421:MET:HE2	1.94	0.49
3:2:214:VAL:HG22	3:2:388:ARG:CD	2.42	0.49
2:i:63:GLY:HA3	2:j:137:PHE:CZ	2.47	0.49
2:o:142:GLY:O	2:o:146:LEU:HD23	2.12	0.49
3:1:233:VAL:HG11	3:1:520:LEU:HD13	1.94	0.49
10:U:307:LEU:O	10:U:311:GLN:HG2	2.12	0.49
11:d:97:LEU:HD23	11:d:100:ILE:HD11	1.93	0.49
2:g:95:ALA:HB2	2:g:152:LEU:HB2	1.94	0.49
11:d:152:ASN:O	11:d:156:VAL:HG23	2.12	0.49
3:0:296:MET:HE1	3:0:308:ARG:CZ	2.43	0.49
15:c:429:MET:HA	15:c:429:MET:HE3	1.95	0.49
1:b:58:ILE:HD12	2:g:148:VAL:CG2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:98:ALA:O	6:Q:102:LEU:HD23	2.13	0.49
9:6:76:MET:HA	9:6:79:VAL:HG23	1.94	0.49
11:d:16:LEU:HB3	11:d:315:PHE:CZ	2.48	0.49
2:m:148:VAL:HA	2:m:151:ILE:HG22	1.95	0.49
6:9:30:ILE:HG21	7:T:25:ALA:HB1	1.95	0.49
3:1:34:MET:SD	3:1:62:ALA:HB3	2.53	0.49
7:R:11:LEU:HD11	12:a:321:VAL:HG13	1.92	0.49
2:i:21:SER:CB	2:i:97:LEU:HD23	2.42	0.48
2:k:22:ALA:HA	2:k:100:GLY:CA	2.42	0.48
3:0:155:ILE:HD11	3:0:163:LYS:HB3	1.94	0.48
7:R:28:ARG:O	7:R:31:ARG:HG2	2.12	0.48
10:U:22:LYS:O	10:U:26:VAL:HG22	2.13	0.48
12:a:404:ILE:HG21	13:e:43:ALA:HB1	1.94	0.48
3:2:458:MET:CE	3:2:473:VAL:HG22	2.43	0.48
11:d:16:LEU:CD2	11:d:93:LEU:CD2	2.90	0.48
1:b:111:ILE:HG23	1:b:137:MET:SD	2.53	0.48
2:l:24:VAL:HG21	2:m:101:LEU:HD13	1.94	0.48
11:d:16:LEU:HB3	11:d:315:PHE:HZ	1.78	0.48
2:k:92:GLN:O	2:k:93:LEU:C	2.57	0.48
2:m:20:SER:O	2:m:24:VAL:HG23	2.13	0.48
2:o:67:ILE:HA	2:o:70:LEU:HD12	1.96	0.48
12:a:114:ASN:C	12:a:114:ASN:HD22	2.21	0.48
2:o:47:MET:HE1	11:d:351:PHE:CE1	2.49	0.48
11:d:99:PHE:CD2	11:d:193:PHE:HD1	2.31	0.48
12:a:71:GLU:HG2	12:a:108:LEU:HD21	1.94	0.48
16:p:317:LEU:O	16:p:321:VAL:HG23	2.13	0.48
1:b:98:GLU:CD	12:a:742:ARG:HH22	2.20	0.48
2:g:45:SER:HB3	2:h:127:LEU:HD13	1.95	0.48
3:2:167:MET:HE1	3:2:340:MET:HE2	1.96	0.48
11:d:13:ASN:HD22	11:d:16:LEU:HD22	1.78	0.48
2:g:91:LEU:HD23	2:g:155:LYS:HB2	1.95	0.48
3:1:95:MET:HE3	3:1:337:PHE:CE2	2.49	0.48
2:i:60:VAL:O	2:i:64:ILE:HG23	2.14	0.48
2:i:90:PHE:O	2:i:91:LEU:C	2.56	0.48
3:0:277:CYS:HB2	3:0:349:ASP:O	2.14	0.48
11:d:92:PRO:C	11:d:94:ALA:N	2.70	0.48
11:d:331:TRP:CD1	11:d:335:CYS:HG	2.32	0.48
3:1:116:ILE:HD11	4:3:341:VAL:CG2	2.43	0.47
3:2:102:ILE:O	3:2:102:ILE:HG22	2.14	0.47
12:a:125:LEU:CD1	12:a:275:LEU:HD12	2.43	0.47
6:8:202:LEU:O	6:8:206:GLN:NE2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:23:MET:HE1	2:i:70:LEU:HD13	1.97	0.47
10:U:403:ASP:HB3	10:U:406:VAL:HG22	1.96	0.47
2:i:21:SER:HB2	2:i:97:LEU:HD23	1.96	0.47
6:Q:109:THR:HG22	6:Q:109:THR:O	2.15	0.47
8:X:39:VAL:O	8:X:39:VAL:HG13	2.15	0.47
1:b:16:TRP:O	1:b:20:VAL:HG23	2.14	0.47
12:a:501:THR:HG23	12:a:502:LEU:N	2.30	0.47
3:0:296:MET:HE1	3:0:308:ARG:NH2	2.29	0.47
10:U:38:GLN:HA	10:U:45:GLU:N	2.30	0.47
11:d:92:PRO:O	11:d:95:SER:OG	2.32	0.47
3:1:102:ILE:O	3:1:102:ILE:HG13	2.15	0.47
3:2:389:ALA:HB2	3:2:406:ILE:HD13	1.97	0.47
11:d:8:TYR:O	11:d:9:PHE:C	2.57	0.47
2:l:23:MET:SD	2:m:148:VAL:HG11	2.55	0.46
4:4:119:LEU:HD21	4:4:273:ILE:HD11	1.97	0.46
10:U:355:TYR:O	10:U:359:LEU:HD23	2.14	0.46
2:k:91:LEU:HD22	2:k:152:LEU:HD22	1.98	0.46
4:4:486:ILE:HG23	4:4:487:PHE:CD1	2.47	0.46
2:i:25:PHE:HZ	16:p:317:LEU:HD12	1.81	0.46
4:3:251:ASN:O	4:3:251:ASN:ND2	2.44	0.46
9:6:195:ASN:HA	9:6:198:ILE:HG22	1.97	0.46
12:a:806:ARG:NH2	12:a:810:VAL:HG11	2.30	0.46
3:0:422:THR:O	3:0:426:LEU:HD23	2.16	0.46
11:d:17:GLU:O	11:d:18:GLY:C	2.57	0.46
2:k:109:ALA:O	2:k:113:VAL:HG23	2.15	0.46
6:Q:102:LEU:HD22	7:V:100:LEU:HD11	1.98	0.46
10:U:38:GLN:HG3	10:U:45:GLU:N	2.31	0.46
1:b:150:PHE:HB3	2:o:28:MET:HE1	1.96	0.46
4:4:293:VAL:CG2	4:4:348:ILE:HD13	2.46	0.46
3:0:283:GLU:HA	3:0:286:GLU:OE1	2.15	0.46
2:h:136:ILE:O	2:h:140:VAL:HG23	2.16	0.46
2:m:98:SER:O	2:m:99:VAL:C	2.58	0.46
2:o:30:ALA:HA	2:o:62:ALA:HB1	1.97	0.46
6:8:50:ARG:HA	6:8:53:ILE:HD12	1.98	0.46
10:U:37:LEU:HA	10:U:47:CYS:SG	2.56	0.46
10:U:334:ASP:O	10:U:338:LEU:HD23	2.16	0.46
6:Q:42:LYS:HG3	7:V:36:ALA:HB1	1.97	0.46
11:d:23:LEU:HD13	11:d:81:GLU:OE2	2.15	0.46
11:d:309:GLN:O	11:d:311:HIS:N	2.49	0.46
2:k:70:LEU:HD11	2:l:144:TYR:CG	2.50	0.46
3:2:507:ILE:HD11	3:2:555:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:338:LEU:O	10:U:342:LEU:HD13	2.17	0.45
1:b:95:ILE:HG22	1:b:96:PHE:N	2.30	0.45
2:h:70:LEU:HD11	2:i:144:TYR:CD1	2.52	0.45
6:Q:72:MET:HE2	7:V:69:LEU:HD13	1.98	0.45
11:d:33:TYR:O	11:d:37:VAL:HG23	2.17	0.45
3:1:256:LYS:HD3	3:1:409:ALA:HB1	1.97	0.45
6:Q:88:ASP:O	6:Q:92:THR:HG23	2.17	0.45
12:a:491:MET:HE2	12:a:491:MET:HB2	1.81	0.45
15:c:437:LEU:O	15:c:437:LEU:HD23	2.17	0.45
7:R:41:GLN:HA	7:R:44:VAL:HG12	1.98	0.45
10:U:145:ILE:HG23	10:U:161:LEU:CD2	2.47	0.45
10:U:289:PHE:O	10:U:293:LEU:HD23	2.16	0.45
11:d:183:ASN:HB3	11:d:240:LEU:HD22	1.98	0.45
2:o:28:MET:HE2	2:o:28:MET:CA	2.45	0.45
9:6:65:VAL:O	9:6:69:VAL:HG22	2.17	0.45
1:b:150:PHE:CB	2:o:28:MET:HE1	2.47	0.45
1:b:98:GLU:O	1:b:100:VAL:N	2.49	0.45
3:2:291:PHE:O	3:2:295:THR:HG22	2.17	0.45
4:3:199:HIS:HB2	4:3:353:ILE:HD11	1.98	0.45
4:5:428:ILE:O	4:5:432:VAL:HG23	2.17	0.45
12:a:408:PHE:CE1	13:e:51:PHE:CE2	3.05	0.45
2:g:144:TYR:HA	2:g:147:ILE:HD12	1.99	0.45
2:k:14:PHE:HB3	2:k:93:LEU:HB2	1.97	0.45
2:m:90:PHE:O	2:m:91:LEU:C	2.60	0.45
6:Q:91:ILE:O	6:Q:95:LEU:HD23	2.16	0.45
9:6:72:VAL:HG22	9:6:136:LEU:HD22	1.99	0.45
12:a:507:VAL:HG13	13:e:67:GLN:OE1	2.17	0.45
12:a:603:THR:HG22	12:a:603:THR:O	2.17	0.45
3:1:338:ARG:HG3	3:1:404:VAL:HG23	1.98	0.44
5:7:47:ILE:HD11	5:7:151:LEU:HD22	1.99	0.44
2:i:17:MET:HB2	2:i:93:LEU:HD13	1.98	0.44
3:2:171:ARG:HD2	3:2:171:ARG:O	2.17	0.44
10:U:38:GLN:HA	10:U:44:ALA:CA	2.47	0.44
15:c:371:VAL:HG12	15:c:372:SER:N	2.32	0.44
2:n:70:LEU:HD11	2:o:144:TYR:CG	2.52	0.44
4:3:187:GLN:HG2	4:3:401:LEU:HD12	1.98	0.44
4:4:232:ALA:HB3	4:4:297:LEU:HD23	2.00	0.44
9:6:264:GLU:O	9:6:268:LEU:HD13	2.17	0.44
2:g:43:ALA:HA	15:c:449:PHE:CZ	2.53	0.44
2:h:13:PHE:CE2	2:i:90:PHE:CZ	3.05	0.44
3:1:380:ALA:CB	4:4:268:THR:HG21	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:281:THR:O	4:3:285:LEU:HD23	2.18	0.44
2:i:92:GLN:O	2:i:93:LEU:C	2.60	0.44
3:2:89:GLU:C	3:2:90:LEU:HD22	2.43	0.44
12:a:370:THR:OG1	12:a:390:ILE:HG21	2.18	0.44
12:a:446:MET:N	12:a:446:MET:HE2	2.33	0.44
12:a:492:PHE:HB3	12:a:497:TRP:HB2	2.00	0.44
3:0:271:VAL:HG11	3:0:337:PHE:CD2	2.53	0.44
12:a:573:PRO:HA	12:a:576:ILE:HG22	2.00	0.44
1:b:149:LEU:HD22	1:b:150:PHE:CD1	2.53	0.43
2:i:28:MET:HE1	2:j:105:ALA:HB2	1.99	0.43
2:m:59:VAL:HG12	2:n:137:PHE:CE2	2.53	0.43
3:2:88:VAL:HG11	3:2:332:THR:HG21	2.00	0.43
9:6:366:TYR:OH	12:a:197:VAL:HG22	2.17	0.43
11:d:94:ALA:HA	11:d:97:LEU:HD12	1.99	0.43
2:m:59:VAL:HG12	2:n:137:PHE:CD2	2.54	0.43
4:3:421:GLN:HB2	4:3:495:ILE:HD11	2.00	0.43
10:U:126:PHE:HA	10:U:129:MET:HB2	1.99	0.43
12:a:755:GLU:O	12:a:759:THR:HG23	2.18	0.43
1:b:111:ILE:HD12	1:b:137:MET:SD	2.57	0.43
3:1:286:GLU:OE2	4:3:165:TYR:CD1	2.72	0.43
3:0:171:ARG:O	3:0:171:ARG:HG3	2.18	0.43
4:3:458:PHE:HD1	4:3:483:LEU:HD13	1.83	0.43
4:4:122:PRO:HB3	4:4:147:ALA:HB2	2.01	0.43
15:c:450:ASP:O	15:c:451:ASP:O	2.37	0.43
2:h:13:PHE:CZ	2:i:90:PHE:CE2	3.07	0.43
2:i:48:ARG:CG	2:i:51:LEU:HD12	2.48	0.43
2:i:85:THR:HG22	2:i:85:THR:O	2.17	0.43
9:6:93:ALA:HB1	9:6:291:PHE:CE2	2.54	0.43
10:U:36:TYR:CZ	10:U:41:MET:HB2	2.54	0.43
11:d:47:LEU:O	11:d:47:LEU:HD23	2.18	0.43
2:j:61:MET:HE1	2:j:110:ILE:HD13	2.01	0.43
6:Q:46:VAL:HG12	7:V:44:VAL:HG21	2.00	0.43
9:6:88:GLN:C	9:6:90:ASN:N	2.74	0.43
2:o:34:THR:HG23	2:o:59:VAL:HG13	2.01	0.43
2:o:137:PHE:O	2:o:141:LEU:HD23	2.19	0.43
4:4:428:ILE:HG21	4:4:451:TYR:CZ	2.53	0.43
10:U:90:VAL:O	10:U:90:VAL:HG13	2.19	0.43
10:U:317:GLN:O	10:U:321:LEU:HD23	2.18	0.43
12:a:61:MET:SD	12:a:304:VAL:HG23	2.59	0.43
12:a:508:LEU:HD23	12:a:509:GLN:O	2.18	0.43
1:b:150:PHE:CD2	2:o:28:MET:CE	3.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:114:GLY:O	2:g:118:VAL:HG13	2.18	0.42
3:2:152:ILE:H	3:2:152:ILE:HG13	1.56	0.42
13:e:45:ALA:C	13:e:47:CYS:N	2.77	0.42
2:k:87:TYR:CZ	2:k:91:LEU:HD11	2.54	0.42
2:o:61:MET:O	2:o:65:ILE:HD12	2.19	0.42
3:0:479:ALA:O	3:0:482:ILE:HG22	2.18	0.42
4:5:147:ALA:H	6:Q:208:MET:HE3	1.83	0.42
6:8:53:ILE:HD11	7:R:44:VAL:CG2	2.50	0.42
11:d:173:LEU:HD23	11:d:181:ILE:HD13	2.00	0.42
15:c:365:CYS:HG	15:c:393:PHE:HE2	1.66	0.42
2:o:72:VAL:HG11	2:o:99:VAL:HG11	1.99	0.42
3:2:507:ILE:CD1	3:2:555:VAL:HG21	2.48	0.42
11:d:42:LEU:HD12	11:d:65:LEU:HB3	2.01	0.42
2:h:8:PRO:HD2	2:h:86:LEU:HD22	2.00	0.42
1:b:60:LEU:HD13	1:b:146:LEU:CD2	2.45	0.42
4:3:418:VAL:HG23	4:3:484:LEU:HD11	2.00	0.42
7:R:29:LYS:O	7:R:32:ARG:N	2.53	0.42
1:b:93:SER:O	1:b:94:ILE:C	2.62	0.42
6:8:91:ILE:O	6:8:95:LEU:HD23	2.19	0.42
9:6:78:ASP:O	9:6:79:VAL:C	2.63	0.42
2:h:13:PHE:CZ	2:i:90:PHE:CZ	3.08	0.42
3:1:380:ALA:HB2	4:4:268:THR:HG21	2.02	0.42
11:d:86:ARG:HG3	11:d:97:LEU:HD13	2.01	0.42
2:h:68:TYR:CD1	2:h:146:LEU:HD11	2.55	0.42
2:i:35:ALA:HB1	2:j:112:ILE:CG2	2.47	0.42
3:1:327:ILE:HG22	3:1:385:PHE:CE1	2.54	0.42
6:8:45:LEU:HD21	7:R:37:LYS:HZ2	1.85	0.42
12:a:396:ILE:HD11	12:a:565:PHE:HB2	2.01	0.42
1:b:106:ILE:O	1:b:108:ALA:N	2.53	0.42
2:k:80:LEU:HD21	2:l:91:LEU:CD1	2.46	0.42
2:o:99:VAL:HG23	2:o:146:LEU:HD13	2.01	0.42
3:0:226:PRO:HG3	3:0:461:LEU:HD22	2.01	0.42
3:0:276:GLY:HA3	3:0:279:GLU:CD	2.44	0.42
4:5:327:MET:HE1	4:5:365:ILE:HD13	2.01	0.42
10:U:34:GLN:HA	10:U:37:LEU:HG	2.01	0.42
3:1:374:TYR:HB3	3:1:378:LEU:HD12	2.02	0.42
4:4:452:LEU:HD21	4:4:456:GLN:OE1	2.20	0.42
11:d:9:PHE:HE2	11:d:312:PHE:CE1	2.38	0.42
12:a:36:GLN:OE1	12:a:369:PRO:HG3	2.20	0.42
2:n:76:ILE:HD12	2:n:92:GLN:HB3	2.01	0.41
3:2:493:VAL:HG11	3:2:509:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:425:THR:O	3:2:429:VAL:HG22	2.20	0.41
4:5:122:PRO:HB2	4:5:147:ALA:HB2	2.02	0.41
11:d:16:LEU:HD22	11:d:90:TYR:HE1	1.85	0.41
12:a:369:PRO:HB3	12:a:822:PHE:HB2	2.01	0.41
2:l:23:MET:CE	2:m:98:SER:HB3	2.49	0.41
3:2:29:VAL:HG12	3:2:66:VAL:HG12	2.01	0.41
9:6:84:LYS:HB2	9:6:87:VAL:CG1	2.50	0.41
2:k:90:PHE:O	2:k:91:LEU:C	2.63	0.41
2:m:16:VAL:HG22	2:n:91:LEU:HD23	2.02	0.41
10:U:37:LEU:CA	10:U:47:CYS:HB2	2.51	0.41
2:g:97:LEU:HD21	15:c:429:MET:SD	2.60	0.41
2:i:84:ILE:HD11	2:i:88:ARG:HB2	2.02	0.41
3:1:507:ILE:HD11	3:1:555:VAL:HG21	2.02	0.41
4:4:85:GLN:C	4:4:96:VAL:HG23	2.46	0.41
5:7:36:LYS:O	5:7:40:LEU:HD23	2.21	0.41
1:b:95:ILE:HD12	1:b:95:ILE:HA	1.83	0.41
3:1:220:LYS:HD3	3:1:220:LYS:N	2.35	0.41
10:U:33:TRP:CZ3	10:U:37:LEU:CD2	3.03	0.41
10:U:129:MET:HA	10:U:129:MET:HE3	2.02	0.41
15:c:450:ASP:O	15:c:451:ASP:C	2.63	0.41
1:b:47:PHE:HB2	2:g:90:PHE:HD2	1.86	0.41
2:o:140:VAL:HG12	2:o:144:TYR:CE2	2.56	0.41
14:f:23:VAL:HG11	14:f:77:LEU:HD21	2.03	0.41
1:b:93:SER:OG	1:b:94:ILE:N	2.53	0.41
2:g:32:TYR:CZ	15:c:443:LEU:HD21	2.55	0.41
2:n:87:TYR:CE2	2:n:91:LEU:HD11	2.56	0.41
3:1:69:GLU:HG2	4:3:154:MET:HE1	2.03	0.41
3:2:165:LYS:O	3:2:340:MET:HE1	2.21	0.41
4:3:269:ILE:O	4:3:272:ILE:HG22	2.21	0.41
4:4:257:VAL:HG13	4:4:257:VAL:O	2.21	0.41
7:R:24:ASP:OD2	7:R:28:ARG:CZ	2.68	0.41
10:U:37:LEU:HA	10:U:47:CYS:HB2	2.02	0.41
12:a:91:PRO:O	12:a:94:MET:HE1	2.21	0.41
13:e:47:CYS:C	13:e:49:TYR:N	2.76	0.41
14:f:19:SER:O	14:f:23:VAL:HG23	2.20	0.41
15:c:447:ASP:O	15:c:449:PHE:N	2.53	0.41
5:7:58:MET:HA	5:7:61:VAL:HG12	2.03	0.41
12:a:494:GLN:HE21	12:a:514:ILE:HG23	1.86	0.41
6:8:45:LEU:CD2	7:R:37:LYS:HD3	2.51	0.40
10:U:65:MET:SD	10:U:66:LEU:HD23	2.61	0.40
15:c:354:GLN:O	15:c:354:GLN:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:117:GLY:O	2:i:121:THR:HG23	2.22	0.40
4:3:141:ARG:HD3	4:3:141:ARG:O	2.21	0.40
7:T:35:GLN:O	7:T:39:GLU:OE1	2.38	0.40
9:6:51:LEU:HD23	9:6:308:LEU:HD21	2.02	0.40
15:c:450:ASP:C	15:c:451:ASP:O	2.64	0.40
10:U:362:GLY:O	10:U:364:LEU:HD12	2.22	0.40
2:m:128:PHE:CD1	2:m:129:VAL:HG23	2.57	0.40
3:2:29:VAL:HG22	3:2:30:THR:H	1.87	0.40
1:b:12:PHE:O	1:b:13:VAL:C	2.64	0.40
1:b:64:GLY:HA3	1:b:149:LEU:HA	2.02	0.40
2:l:145:GLY:O	2:l:148:VAL:HG12	2.22	0.40
10:U:86:LYS:O	10:U:90:VAL:HG12	2.21	0.40
12:a:492:PHE:H	12:a:493:THR:HG23	1.87	0.40
12:a:514:ILE:O	12:a:517:VAL:HG22	2.21	0.40
15:c:368:VAL:O	15:c:368:VAL:HG13	2.22	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	b	198/205 (97%)	178 (90%)	16 (8%)	4 (2%)	6	31
2	g	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
2	h	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
2	i	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
2	j	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
2	k	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
2	l	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
2	m	148/155 (96%)	135 (91%)	12 (8%)	1 (1%)	18	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	n	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
2	o	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
3	0	600/617 (97%)	580 (97%)	20 (3%)	0	100	100
3	1	598/617 (97%)	561 (94%)	37 (6%)	0	100	100
3	2	598/617 (97%)	562 (94%)	35 (6%)	1 (0%)	43	77
4	3	457/511 (89%)	436 (95%)	21 (5%)	0	100	100
4	4	466/511 (91%)	444 (95%)	22 (5%)	0	100	100
4	5	466/511 (91%)	452 (97%)	14 (3%)	0	100	100
5	7	211/247 (85%)	208 (99%)	3 (1%)	0	100	100
6	8	223/226 (99%)	216 (97%)	7 (3%)	0	100	100
6	9	223/226 (99%)	219 (98%)	4 (2%)	0	100	100
6	Q	223/226 (99%)	219 (98%)	4 (2%)	0	100	100
7	R	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
7	T	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
7	V	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
8	X	108/119 (91%)	99 (92%)	9 (8%)	0	100	100
9	6	357/382 (94%)	337 (94%)	18 (5%)	2 (1%)	21	58
10	U	422/483 (87%)	383 (91%)	32 (8%)	7 (2%)	7	35
11	d	349/351 (99%)	326 (93%)	20 (6%)	3 (1%)	14	49
12	a	746/838 (89%)	701 (94%)	40 (5%)	5 (1%)	18	55
13	e	75/81 (93%)	66 (88%)	6 (8%)	3 (4%)	2	18
14	f	83/98 (85%)	77 (93%)	6 (7%)	0	100	100
15	c	201/463 (43%)	170 (85%)	27 (13%)	4 (2%)	6	31
16	p	47/350 (13%)	44 (94%)	3 (6%)	0	100	100
All	All	8319/9428 (88%)	7877 (95%)	412 (5%)	30 (0%)	31	67

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	98	GLU
10	U	41	MET
10	U	134	ASP
11	d	10	ASN
11	d	11	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	a	498	THR
9	6	84	LYS
10	U	43	SER
10	U	45	GLU
10	U	132	ARG
12	a	502	LEU
13	e	45	ALA
15	c	447	ASP
1	b	106	ILE
2	m	86	LEU
9	6	80	LEU
10	U	123	TRP
11	d	310	PHE
15	c	448	ARG
1	b	15	PHE
10	U	37	LEU
12	a	492	PHE
15	c	449	PHE
1	b	97	CYS
12	a	184	ARG
12	a	493	THR
13	e	47	CYS
15	c	385	VAL
3	2	155	ILE
13	e	46	VAL

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	b	154/158 (98%)	149 (97%)	5 (3%)	34	55
2	g	109/113 (96%)	109 (100%)	0	100	100
2	h	109/113 (96%)	109 (100%)	0	100	100
2	i	109/113 (96%)	107 (98%)	2 (2%)	51	67
2	j	109/113 (96%)	109 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	k	109/113 (96%)	108 (99%)	1 (1%)	70	76
2	l	109/113 (96%)	109 (100%)	0	100	100
2	m	109/113 (96%)	105 (96%)	4 (4%)	30	51
2	n	109/113 (96%)	109 (100%)	0	100	100
2	o	109/113 (96%)	109 (100%)	0	100	100
3	0	509/524 (97%)	508 (100%)	1 (0%)	87	85
3	1	507/524 (97%)	507 (100%)	0	100	100
3	2	507/524 (97%)	504 (99%)	3 (1%)	78	80
4	3	395/431 (92%)	395 (100%)	0	100	100
4	4	402/431 (93%)	402 (100%)	0	100	100
4	5	402/431 (93%)	402 (100%)	0	100	100
5	7	184/212 (87%)	184 (100%)	0	100	100
6	8	197/198 (100%)	197 (100%)	0	100	100
6	9	197/198 (100%)	197 (100%)	0	100	100
6	Q	197/198 (100%)	197 (100%)	0	100	100
7	R	96/99 (97%)	96 (100%)	0	100	100
7	T	96/99 (97%)	96 (100%)	0	100	100
7	V	96/99 (97%)	96 (100%)	0	100	100
8	X	94/100 (94%)	94 (100%)	0	100	100
9	6	326/344 (95%)	324 (99%)	2 (1%)	78	80
10	U	384/429 (90%)	381 (99%)	3 (1%)	73	77
11	d	306/306 (100%)	304 (99%)	2 (1%)	76	79
12	a	669/741 (90%)	667 (100%)	2 (0%)	86	84
13	e	65/68 (96%)	62 (95%)	3 (5%)	24	46
14	f	71/83 (86%)	71 (100%)	0	100	100
15	c	180/395 (46%)	178 (99%)	2 (1%)	65	74
16	p	44/309 (14%)	44 (100%)	0	100	100
All	All	7059/7918 (89%)	7029 (100%)	30 (0%)	81	82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	25	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	95	ILE
1	b	97	CYS
1	b	98	GLU
1	b	100	VAL
2	i	64	ILE
2	i	65	ILE
2	k	89	SER
2	m	16	VAL
2	m	20	SER
2	m	21	SER
2	m	26	SER
3	0	279	GLU
3	2	152	ILE
3	2	153	TYR
3	2	155	ILE
9	6	86	LYS
9	6	87	VAL
10	U	43	SER
10	U	86	LYS
10	U	90	VAL
11	d	10	ASN
11	d	13	ASN
12	a	492	PHE
12	a	498	THR
13	e	42	VAL
13	e	44	THR
13	e	48	CYS
15	c	447	ASP
15	c	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	197	GLN
2	h	6	ASN
2	k	7	ASN
2	k	92	GLN
2	m	92	GLN
3	1	47	HIS
3	1	146	HIS
3	1	563	ASN
3	2	172	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3	209	GLN
4	3	256	ASN
4	5	42	GLN
5	7	16	GLN
6	8	49	GLN
6	8	169	GLN
6	Q	77	ASN
7	R	66	GLN
7	V	56	GLN
8	X	96	HIS
9	6	16	GLN
9	6	88	GLN
10	U	83	HIS
10	U	91	GLN
10	U	240	GLN
10	U	440	HIS
11	d	10	ASN
11	d	13	ASN
11	d	309	GLN
12	a	18	GLN
12	a	53	ASN
12	a	318	ASN
12	a	372	ASN
12	a	419	HIS
12	a	494	GLN
12	a	511	ASN
12	a	668	HIS
12	a	669	GLN
14	f	64	GLN
15	c	392	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

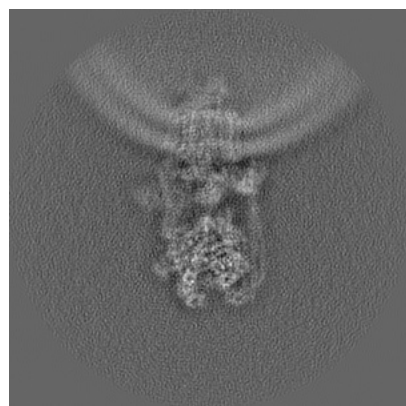
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44841. These allow visual inspection of the internal detail of the map and identification of artifacts.

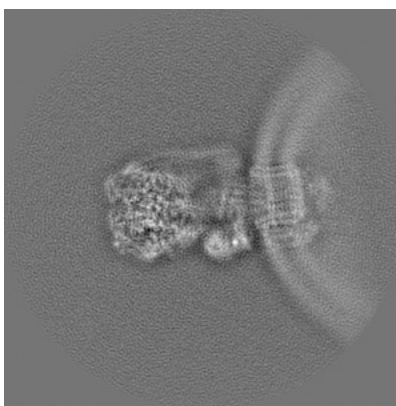
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

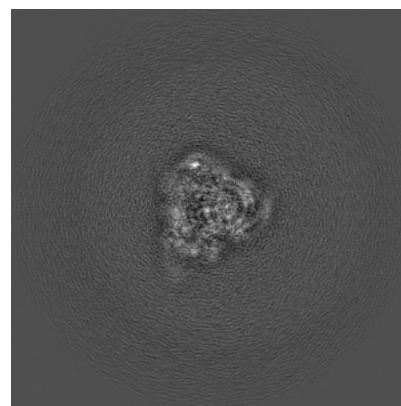
6.1.1 Primary map



X

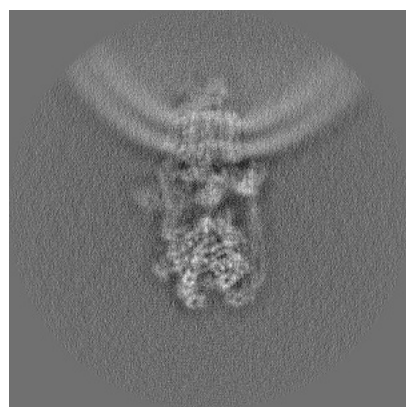


Y

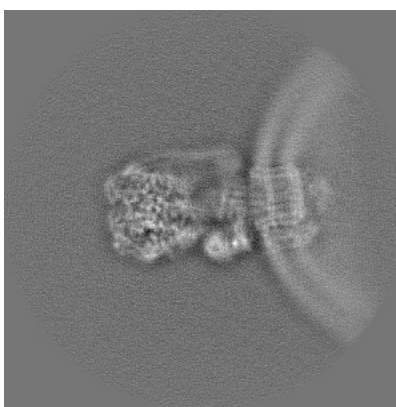


Z

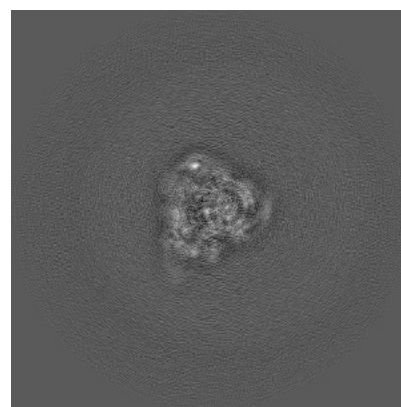
6.1.2 Raw map



X



Y

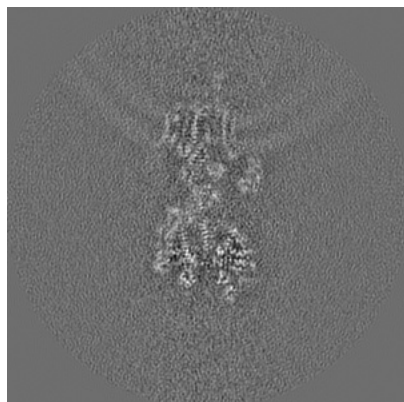


Z

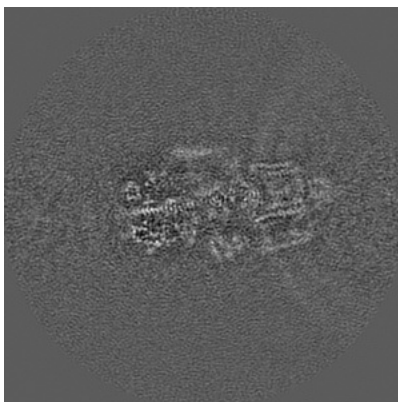
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

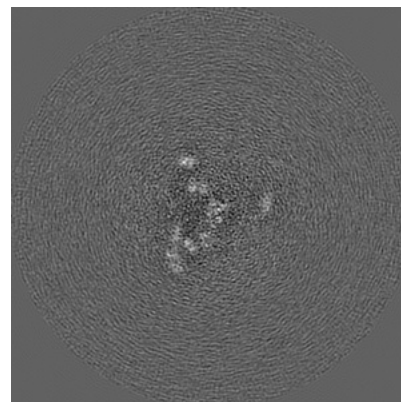
6.2.1 Primary map



X Index: 224

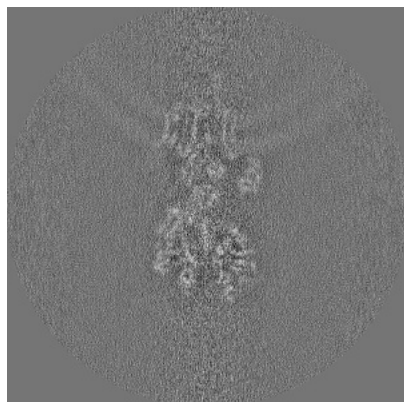


Y Index: 224

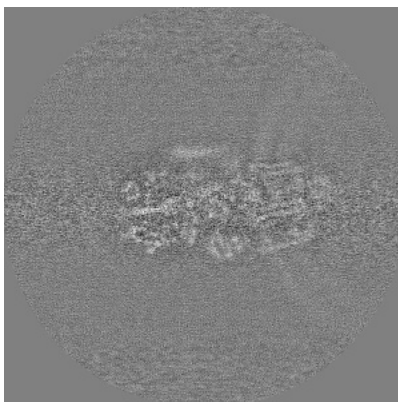


Z Index: 224

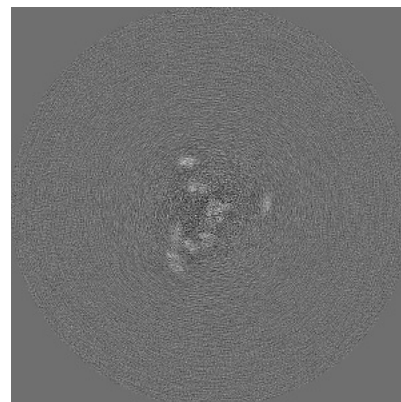
6.2.2 Raw map



X Index: 224



Y Index: 224

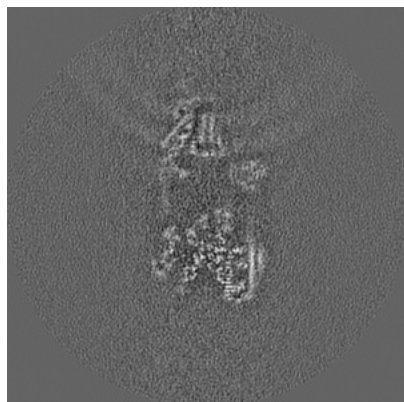


Z Index: 224

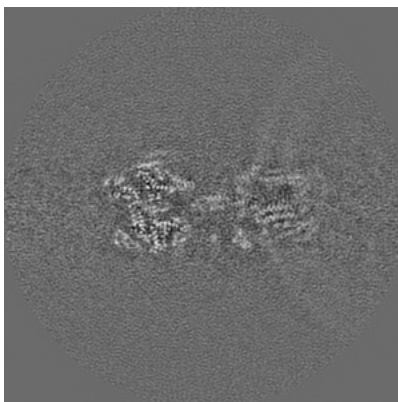
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

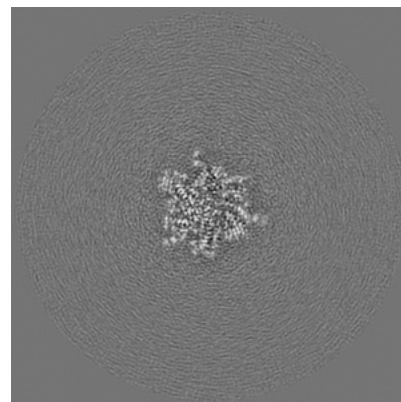
6.3.1 Primary map



X Index: 208

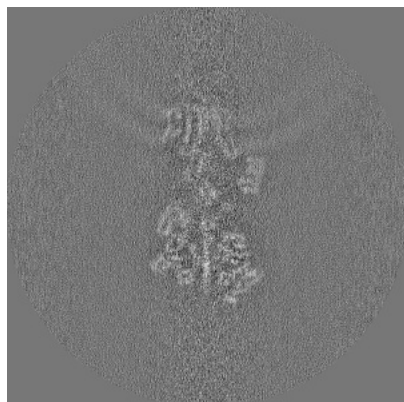


Y Index: 209

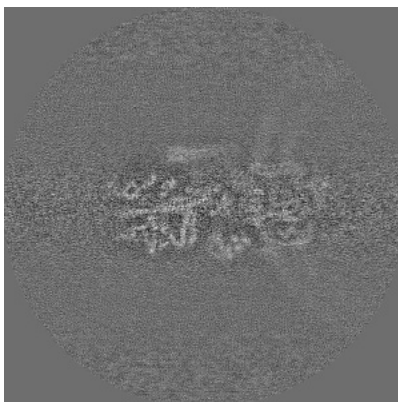


Z Index: 168

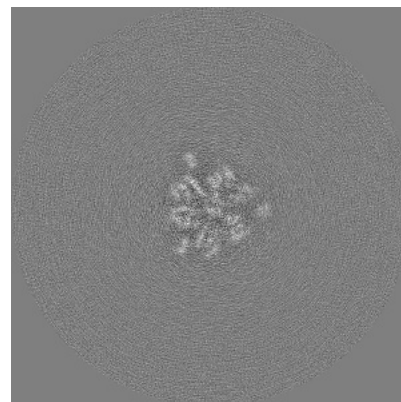
6.3.2 Raw map



X Index: 219



Y Index: 221

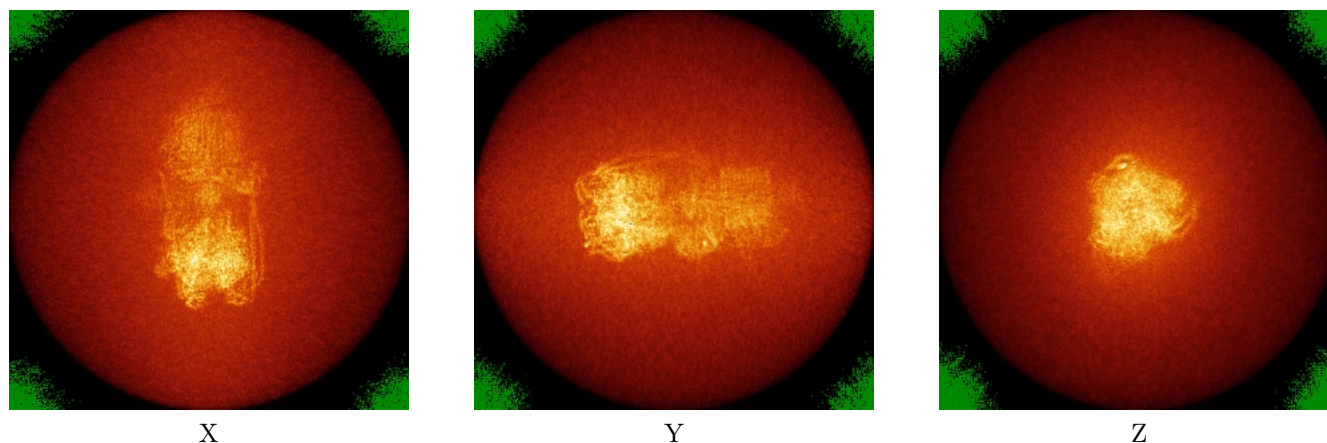


Z Index: 199

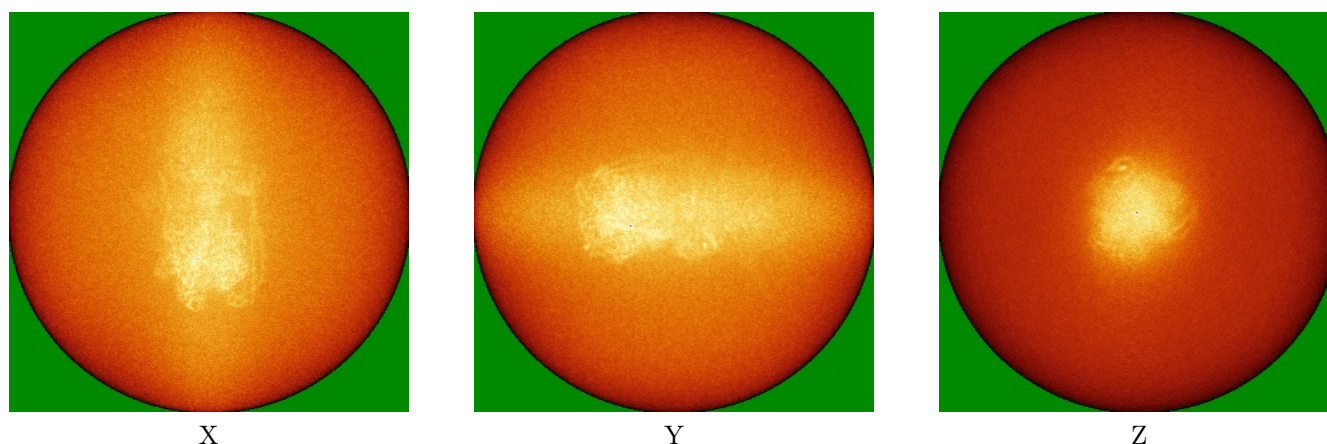
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

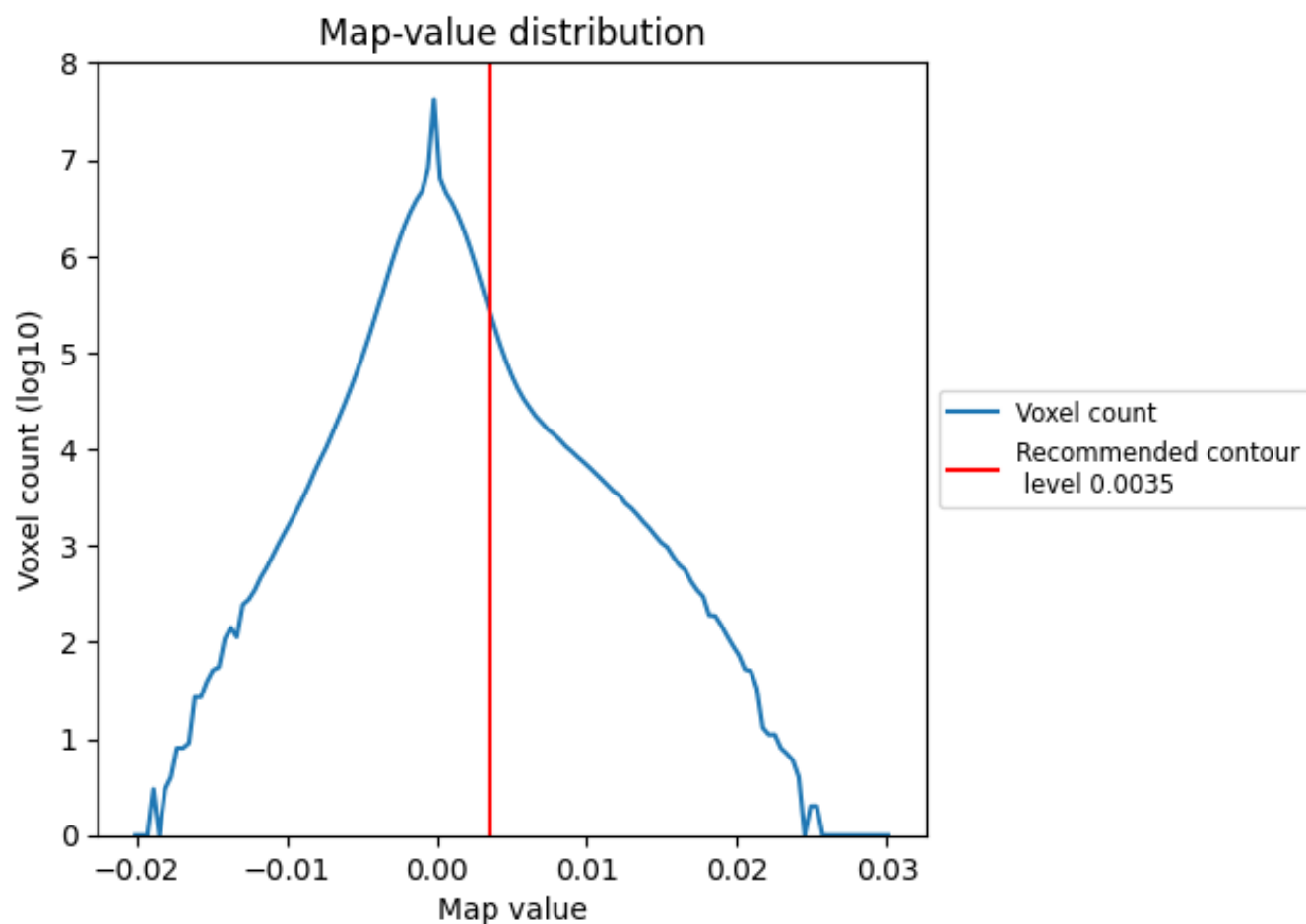
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

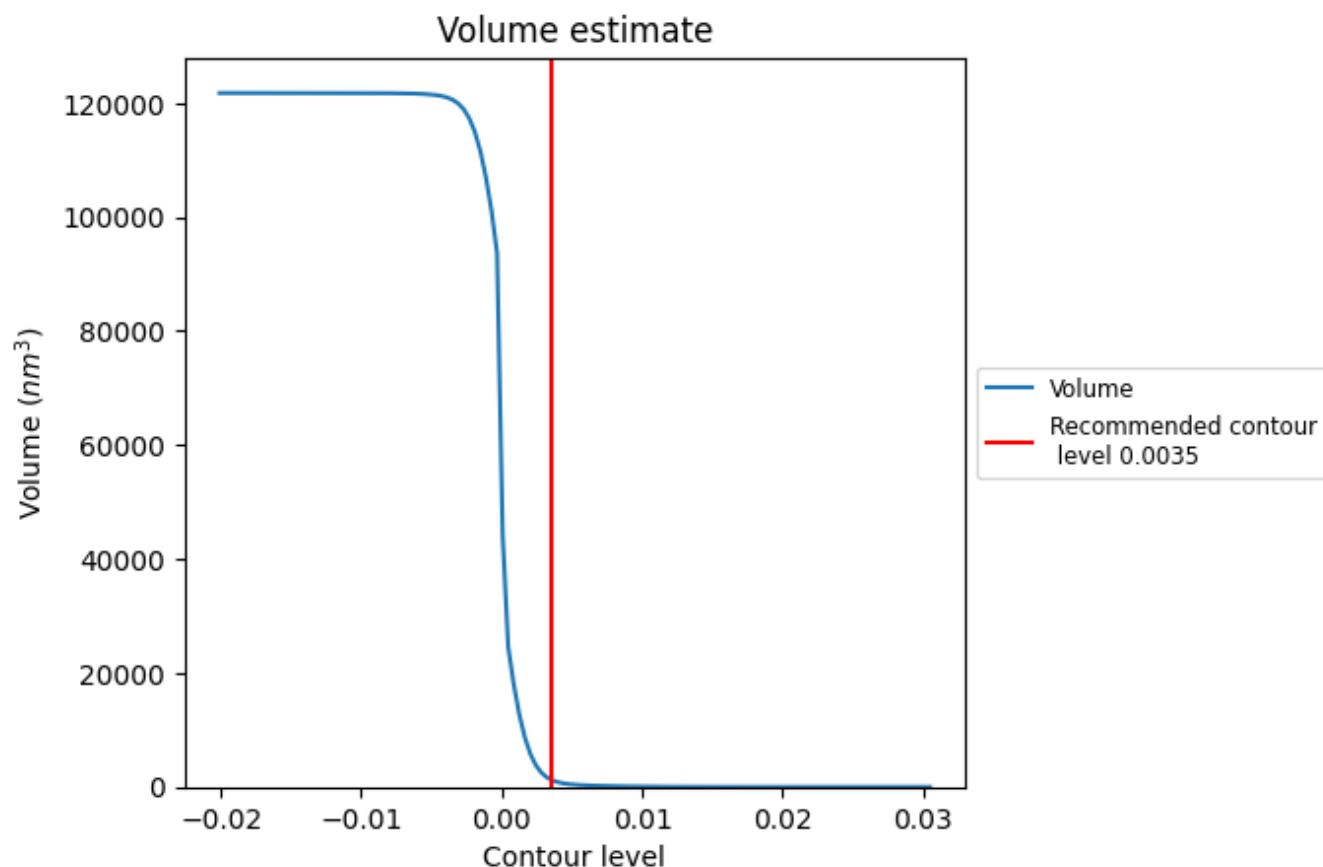
This section contains the results of statistical analysis of the map.

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.

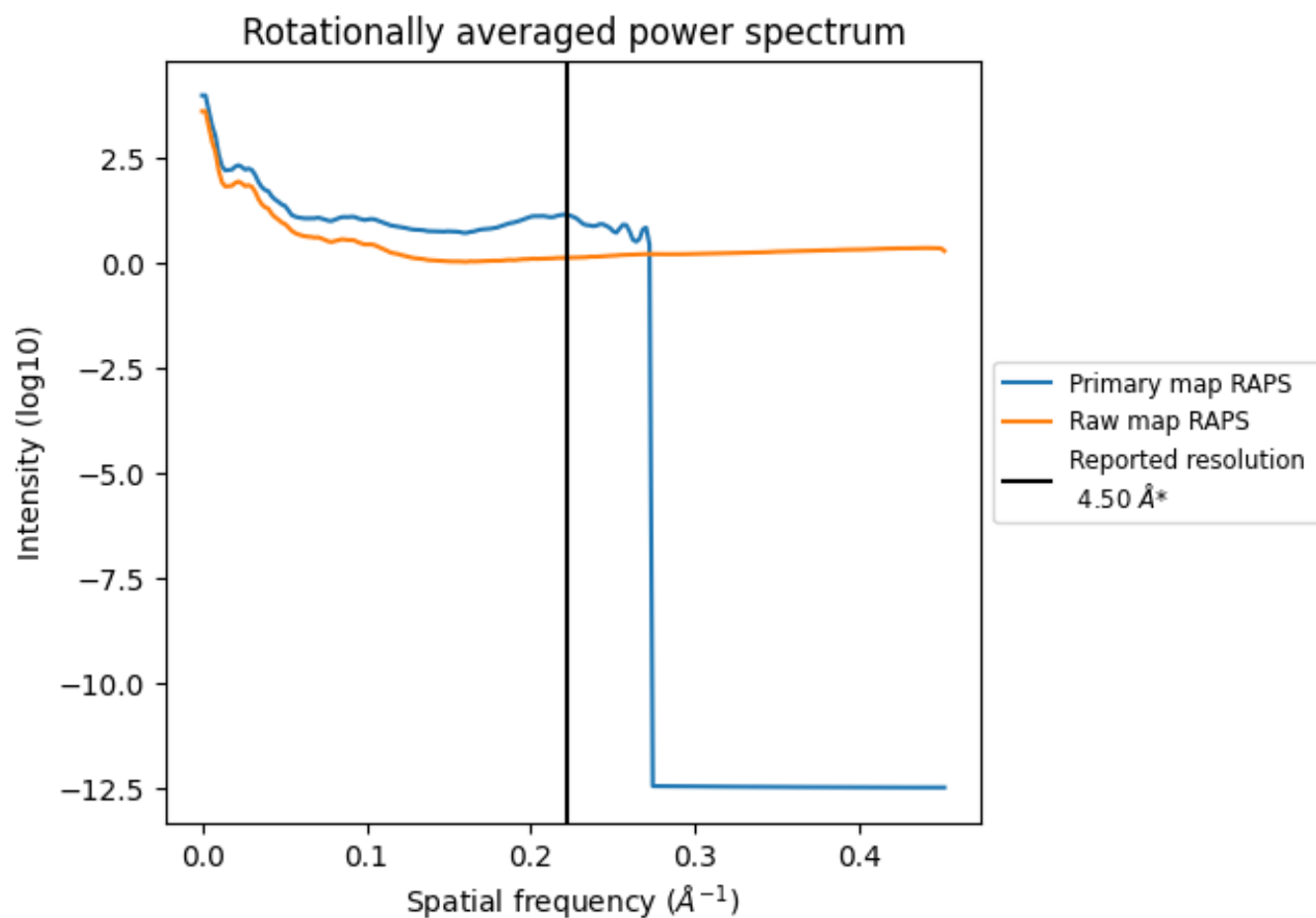
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1317 nm^3 ; this corresponds to an approximate mass of 1190 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 ⓘ

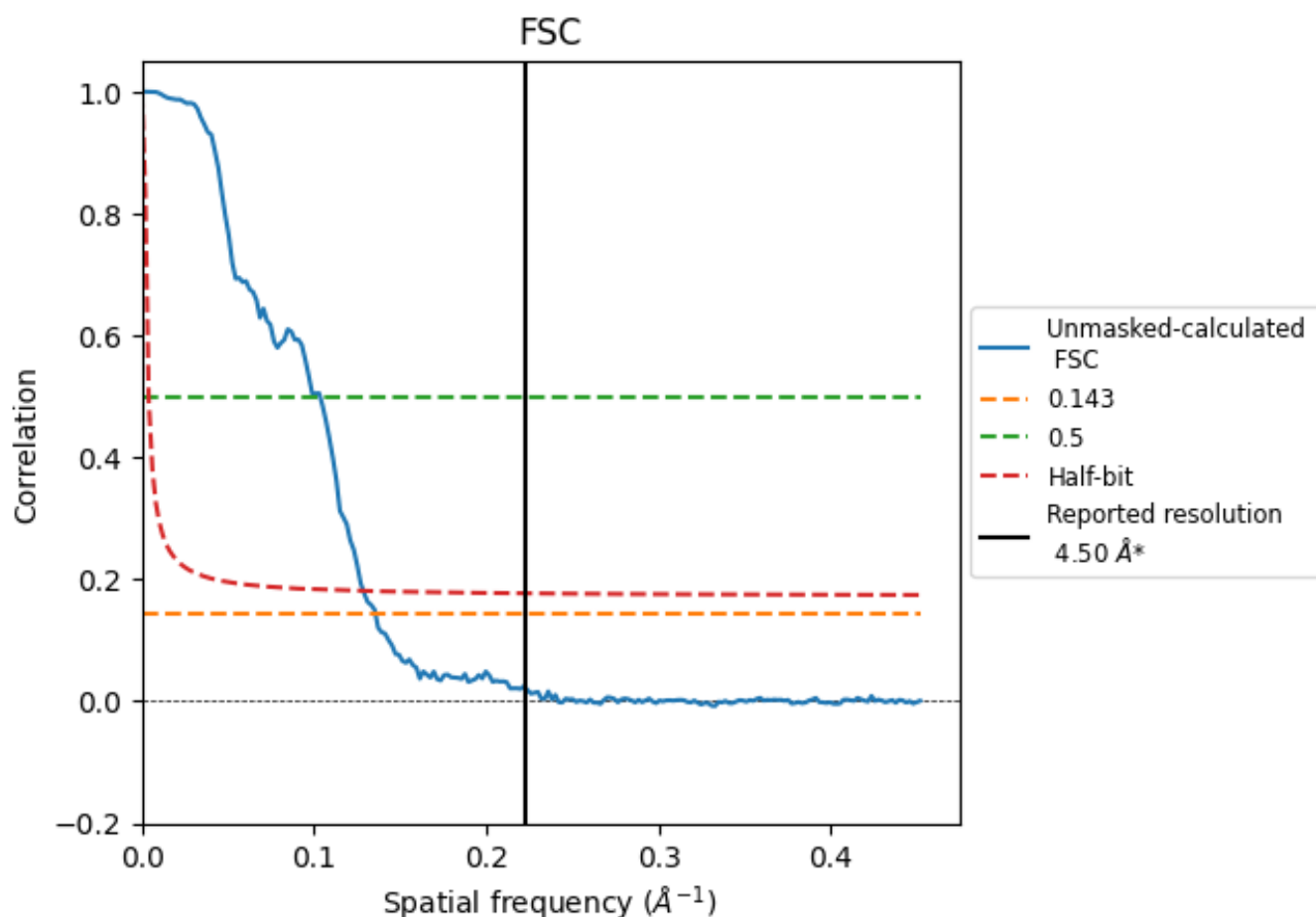


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

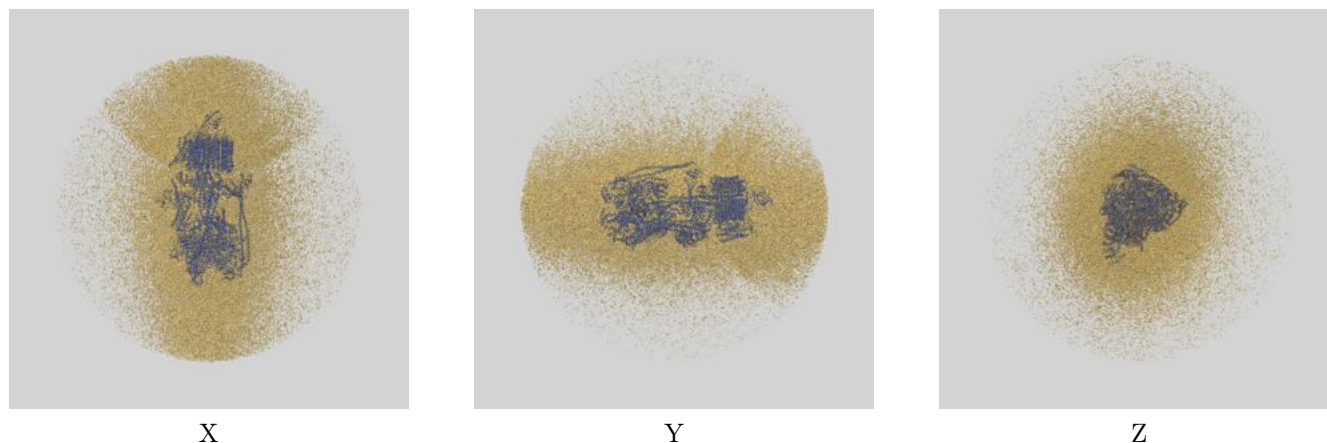
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.37	9.67	7.78

*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 7.37 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

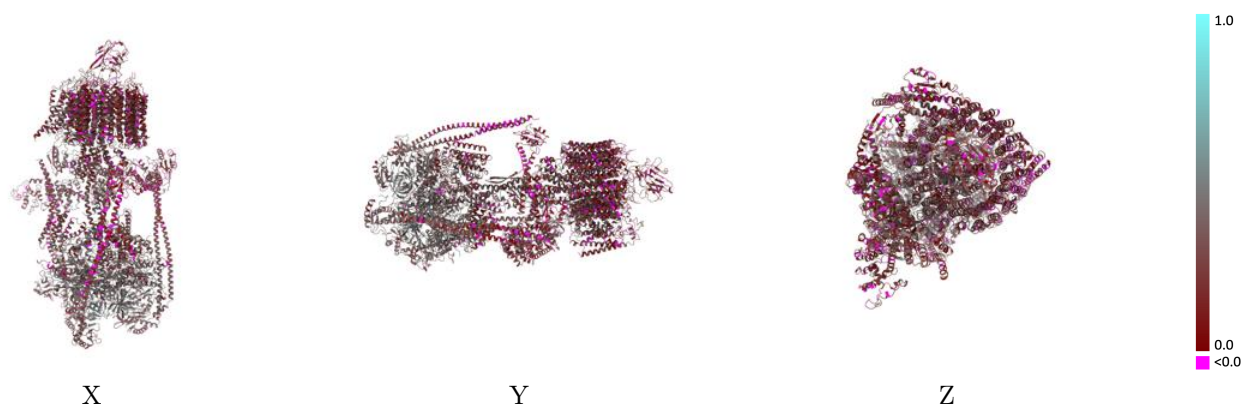
This section contains information regarding the fit between EMDB map EMD-44841 and PDB model 9BRR. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



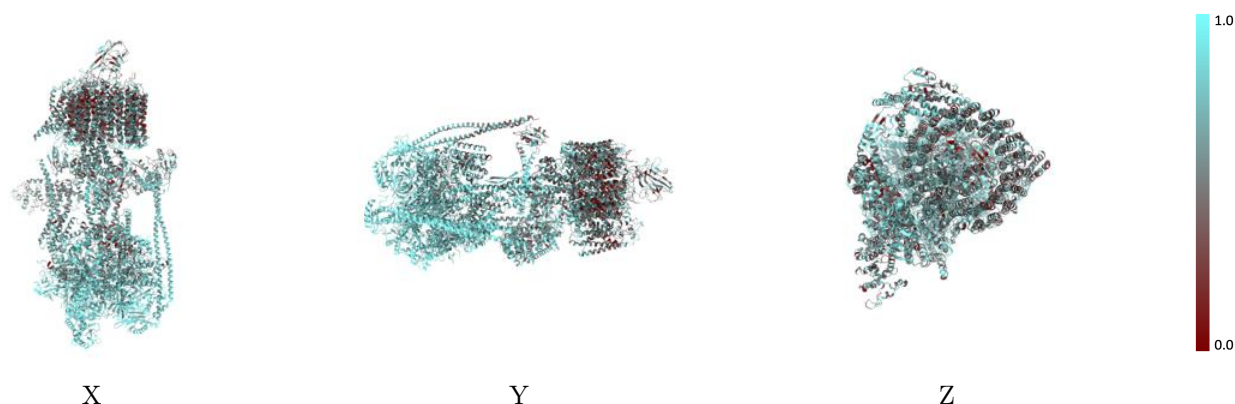
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



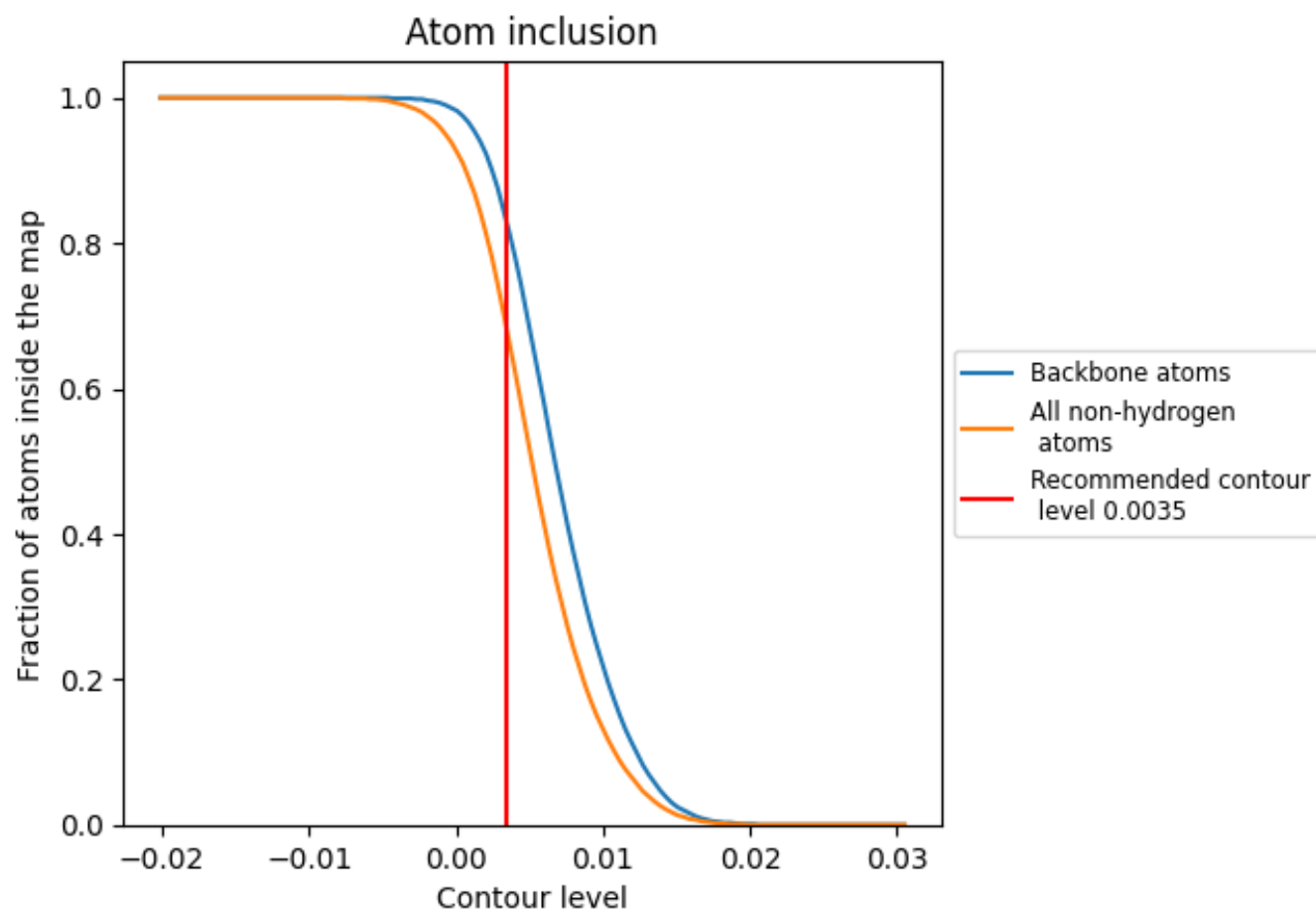
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 68% 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	 0.6780	 0.3000
0	 0.7070	 0.3390
1	 0.7920	 0.3800
2	 0.7170	 0.3250
3	 0.7980	 0.4080
4	 0.7830	 0.4000
5	 0.7810	 0.4000
6	 0.6030	 0.1810
7	 0.7070	 0.3330
8	 0.8000	 0.3220
9	 0.8090	 0.3210
Q	 0.7580	 0.2930
R	 0.7860	 0.2580
T	 0.8370	 0.2640
U	 0.5970	 0.2070
V	 0.7030	 0.2190
X	 0.7670	 0.3430
a	 0.6430	 0.2510
b	 0.5850	 0.2830
c	 0.5180	 0.2450
d	 0.5950	 0.2980
e	 0.5750	 0.2540
f	 0.4980	 0.1840
g	 0.6330	 0.2980
h	 0.5580	 0.2640
i	 0.5110	 0.2340
j	 0.4790	 0.2130
k	 0.5280	 0.2200
l	 0.5620	 0.2270
m	 0.5030	 0.2240
n	 0.4700	 0.2170
o	 0.5650	 0.2620
p	 0.4370	 0.2520

