Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 01:43 PM EST

PDB ID	:	6VQ7
EMDB ID	:	EMD-21318
Title	:	Mammalian V-ATPase from rat brain - composite model of rotational state 2 bound to ADP and SidK (built from focused refinement models)
Authors	:	Abbas, Y.M.; Rubinstein, J.L.
Deposited on	:	2020-02-04
Resolution	:	4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

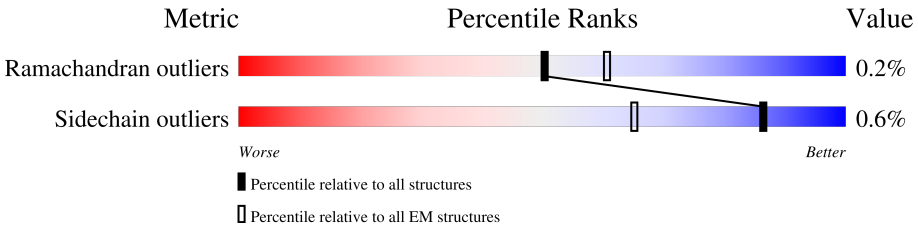
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.00 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	617	97%
1	B	617	97%
1	C	617	97%
2	D	511	90% 10%
2	E	511	89% 10%
2	F	511	89% 10%
3	G	382	18% 94% 6%
4	H	247	85% 13%
5	I	226	12% 100%

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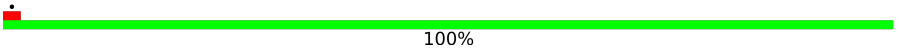
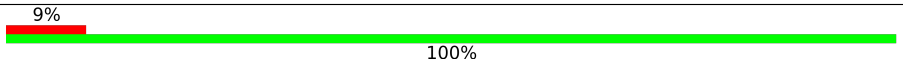
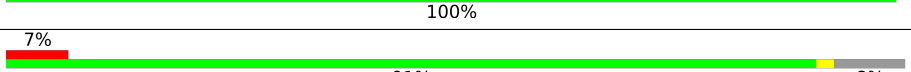
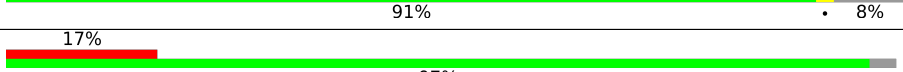
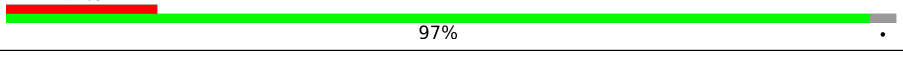
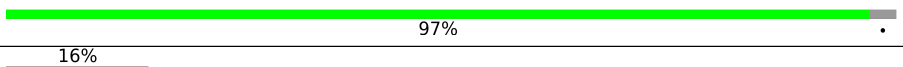
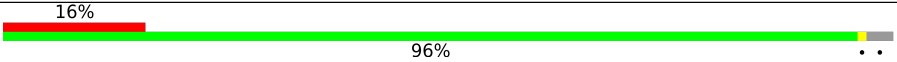
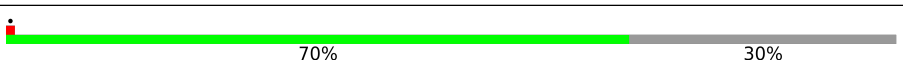
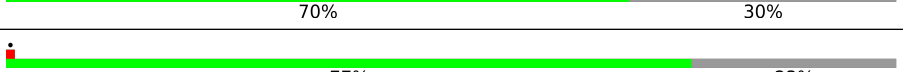
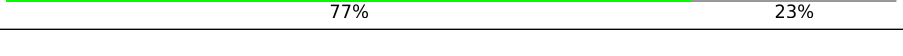
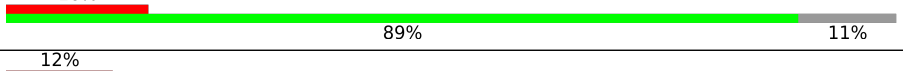
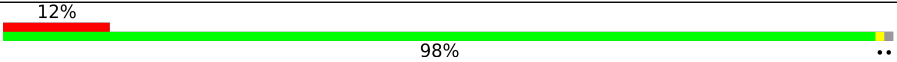
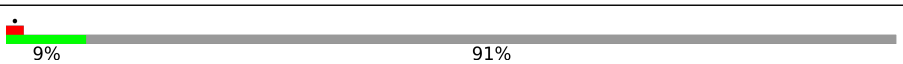
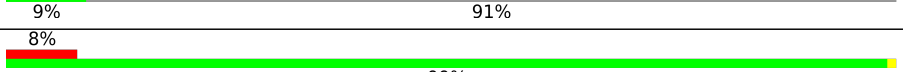
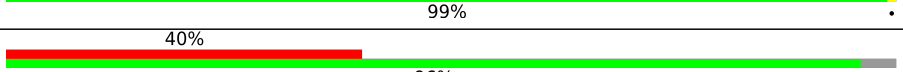
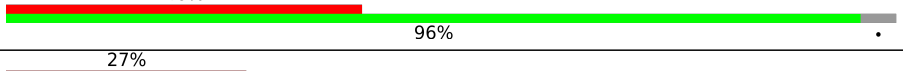
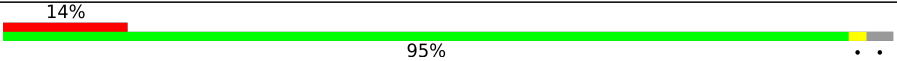
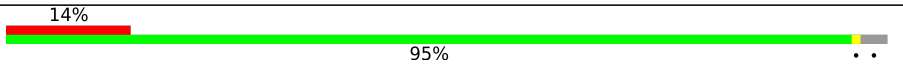
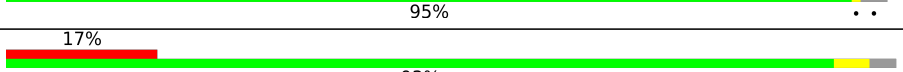
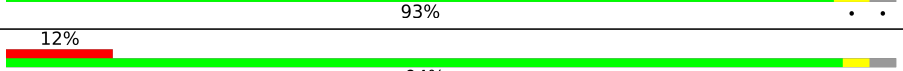
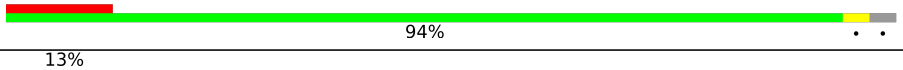
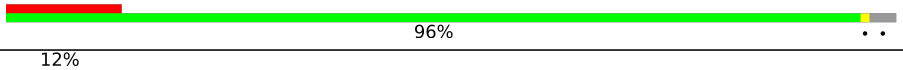
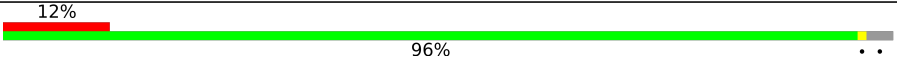
Mol	Chain	Length	Quality of chain
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	Q	301	
8	R	301	
8	S	301	
9	a	838	
10	b	205	
11	c	463	
12	d	351	
13	e	81	
14	f	98	
15	g	155	
15	h	155	
15	i	155	
15	j	155	
15	k	155	
15	l	155	
15	m	155	
15	n	155	
15	o	155	
16	p	350	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 62325 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 ATPase H+-transporting V1 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	B	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	C	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	E	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	F	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	360	Total	C	N	O	0	0
			1790	1070	360	360		

- Molecule 4 is a protein called ATPase H+-transporting V1 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	214	Total	C	N	O	S	0	0
			1716	1086	310	315	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	225	Total	C	N	O	S	0	0
			1607	1005	296	299	7		
5	J	225	Total	C	N	O	S	0	0
			1607	1005	296	299	7		
5	K	225	Total	C	N	O	S	0	0
			1607	1005	296	299	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	110	Total	C	N	O	S	0	0
			866	548	154	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	114	Total	C	N	O	S	0	0
			714	426	147	138	3		
7	N	114	Total	C	N	O	S	0	0
			714	426	147	138	3		
7	O	114	Total	C	N	O	S	0	0
			714	426	147	138	3		

- Molecule 8 is a protein called Effector protein SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	212	Total	C	N	O	S	0	0
			1722	1096	292	325	9		
8	R	232	Total	C	N	O	S	0	0
			1878	1197	316	354	11		
8	S	224	Total	C	N	O	S	0	0
			1824	1162	306	346	10		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	GLY	-	expression tag	UNP Q5ZWW6
Q	279	ASP	-	expression tag	UNP Q5ZWW6
Q	280	TYR	-	expression tag	UNP Q5ZWW6
Q	281	LYS	-	expression tag	UNP Q5ZWW6
Q	282	ASP	-	expression tag	UNP Q5ZWW6
Q	283	HIS	-	expression tag	UNP Q5ZWW6
Q	284	ASP	-	expression tag	UNP Q5ZWW6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	285	GLY	-	expression tag	UNP Q5ZWW6
Q	286	ASP	-	expression tag	UNP Q5ZWW6
Q	287	TYR	-	expression tag	UNP Q5ZWW6
Q	288	LYS	-	expression tag	UNP Q5ZWW6
Q	289	ASP	-	expression tag	UNP Q5ZWW6
Q	290	HIS	-	expression tag	UNP Q5ZWW6
Q	291	ASP	-	expression tag	UNP Q5ZWW6
Q	292	ILE	-	expression tag	UNP Q5ZWW6
Q	293	ASP	-	expression tag	UNP Q5ZWW6
Q	294	TYR	-	expression tag	UNP Q5ZWW6
Q	295	LYS	-	expression tag	UNP Q5ZWW6
Q	296	ASP	-	expression tag	UNP Q5ZWW6
Q	297	ASP	-	expression tag	UNP Q5ZWW6
Q	298	ASP	-	expression tag	UNP Q5ZWW6
Q	299	ASP	-	expression tag	UNP Q5ZWW6
Q	300	LYS	-	expression tag	UNP Q5ZWW6
R	0	GLY	-	expression tag	UNP Q5ZWW6
R	279	ASP	-	expression tag	UNP Q5ZWW6
R	280	TYR	-	expression tag	UNP Q5ZWW6
R	281	LYS	-	expression tag	UNP Q5ZWW6
R	282	ASP	-	expression tag	UNP Q5ZWW6
R	283	HIS	-	expression tag	UNP Q5ZWW6
R	284	ASP	-	expression tag	UNP Q5ZWW6
R	285	GLY	-	expression tag	UNP Q5ZWW6
R	286	ASP	-	expression tag	UNP Q5ZWW6
R	287	TYR	-	expression tag	UNP Q5ZWW6
R	288	LYS	-	expression tag	UNP Q5ZWW6
R	289	ASP	-	expression tag	UNP Q5ZWW6
R	290	HIS	-	expression tag	UNP Q5ZWW6
R	291	ASP	-	expression tag	UNP Q5ZWW6
R	292	ILE	-	expression tag	UNP Q5ZWW6
R	293	ASP	-	expression tag	UNP Q5ZWW6
R	294	TYR	-	expression tag	UNP Q5ZWW6
R	295	LYS	-	expression tag	UNP Q5ZWW6
R	296	ASP	-	expression tag	UNP Q5ZWW6
R	297	ASP	-	expression tag	UNP Q5ZWW6
R	298	ASP	-	expression tag	UNP Q5ZWW6
R	299	ASP	-	expression tag	UNP Q5ZWW6
R	300	LYS	-	expression tag	UNP Q5ZWW6
S	0	GLY	-	expression tag	UNP Q5ZWW6
S	279	ASP	-	expression tag	UNP Q5ZWW6
S	280	TYR	-	expression tag	UNP Q5ZWW6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	281	LYS	-	expression tag	UNP Q5ZWW6
S	282	ASP	-	expression tag	UNP Q5ZWW6
S	283	HIS	-	expression tag	UNP Q5ZWW6
S	284	ASP	-	expression tag	UNP Q5ZWW6
S	285	GLY	-	expression tag	UNP Q5ZWW6
S	286	ASP	-	expression tag	UNP Q5ZWW6
S	287	TYR	-	expression tag	UNP Q5ZWW6
S	288	LYS	-	expression tag	UNP Q5ZWW6
S	289	ASP	-	expression tag	UNP Q5ZWW6
S	290	HIS	-	expression tag	UNP Q5ZWW6
S	291	ASP	-	expression tag	UNP Q5ZWW6
S	292	ILE	-	expression tag	UNP Q5ZWW6
S	293	ASP	-	expression tag	UNP Q5ZWW6
S	294	TYR	-	expression tag	UNP Q5ZWW6
S	295	LYS	-	expression tag	UNP Q5ZWW6
S	296	ASP	-	expression tag	UNP Q5ZWW6
S	297	ASP	-	expression tag	UNP Q5ZWW6
S	298	ASP	-	expression tag	UNP Q5ZWW6
S	299	ASP	-	expression tag	UNP Q5ZWW6
S	300	LYS	-	expression tag	UNP Q5ZWW6

- Molecule 9 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	750	Total	C	N	O	S	0	0
			5009	3241	864	883	21		

- Molecule 10 is a protein called ATPase, H+ transporting, V0 subunit B (Predicted), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

- Molecule 11 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	41	Total	C	N	O	S	0	0
			337	228	51	54	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	350	Total	C	N	O	S	0	0
			2833	1829	460	530	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	78	Total	C	N	O	S	0	0
			622	428	98	93	3		

- Molecule 14 is a protein called Ribonuclease K.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	84	Total	C	N	O	0	0
			452	282	85	85		

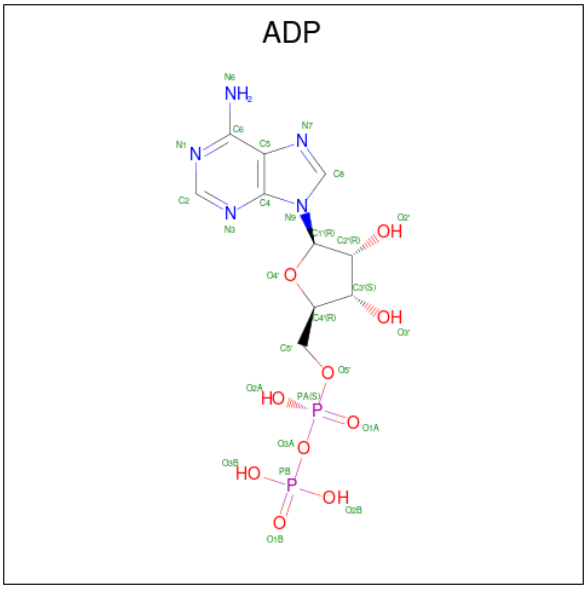
- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	h	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	i	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	j	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	k	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	l	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	m	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	n	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
15	o	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

- Molecule 16 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	52	Total	C	N	O	S	0	0
			432	290	63	76	3		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

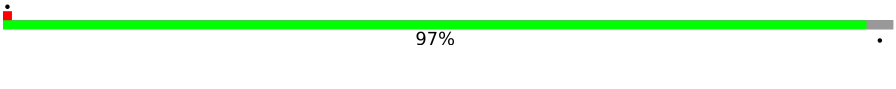
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Mg	0
			1	1	

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.

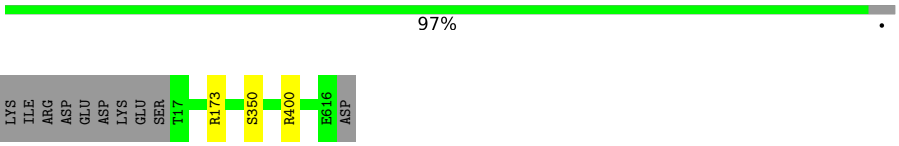
• Molecule 1: ATPase H+-transporting V1 subunit A

Chain A:



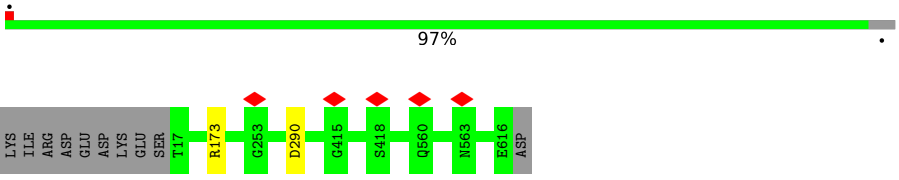
• Molecule 1: ATPase H+-transporting V1 subunit A

Chain B:



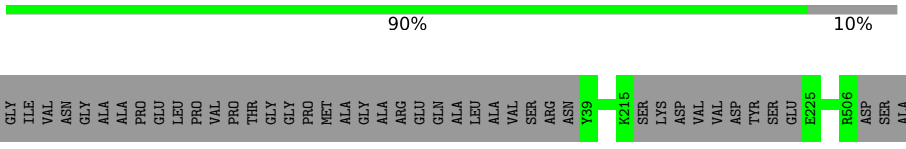
• Molecule 1: ATPase H+-transporting V1 subunit A

Chain C:



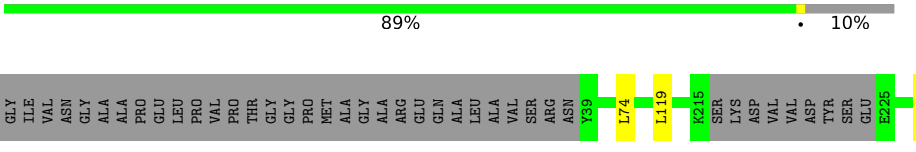
• Molecule 2: V-type proton ATPase subunit B, brain isoform

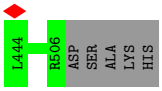
Chain D:



• Molecule 2: V-type proton ATPase subunit B, brain isoform

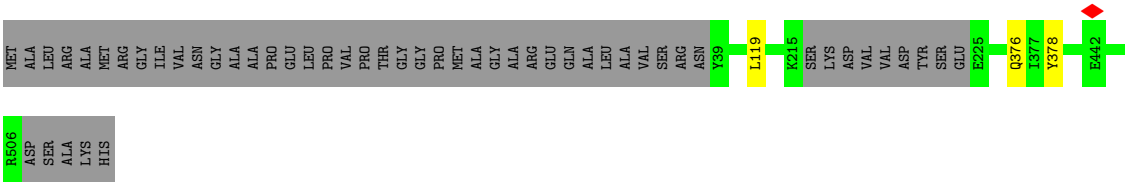
Chain E:





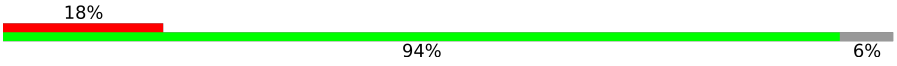
• Molecule 2: V-type proton ATPase subunit B, brain isoform

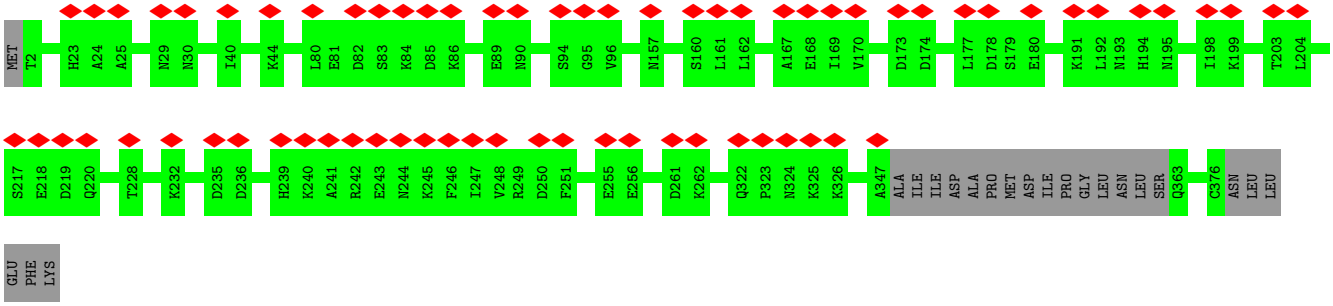
Chain F:



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

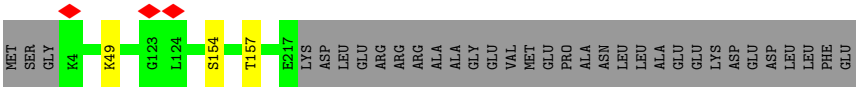
Chain G:





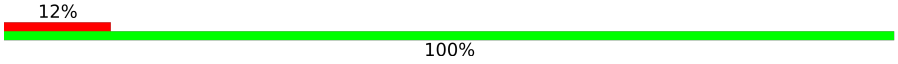
• Molecule 4: ATPase H+-transporting V1 subunit D

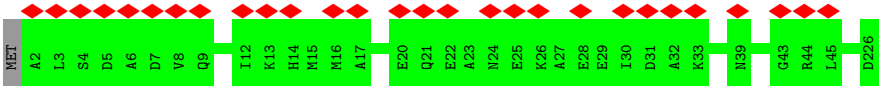
Chain H:



• Molecule 5: V-type proton ATPase subunit E 1

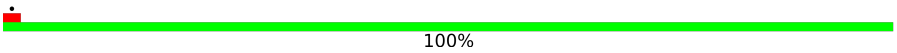
Chain I:

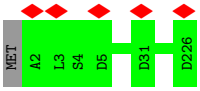




• Molecule 5: V-type proton ATPase subunit E 1

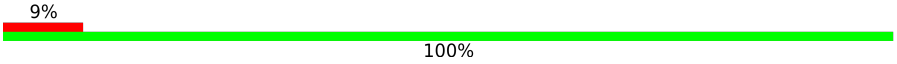
Chain J:

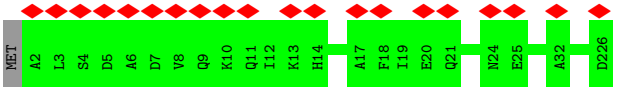




• Molecule 5: V-type proton ATPase subunit E 1

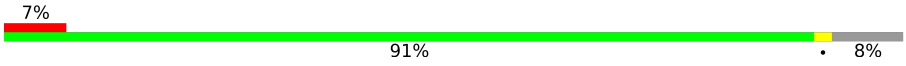
Chain K:

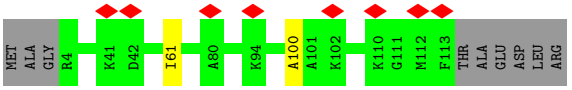




• Molecule 6: V-type proton ATPase subunit F

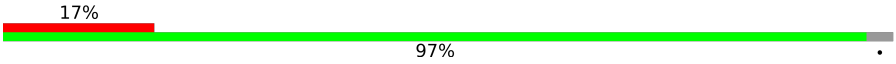
Chain L:

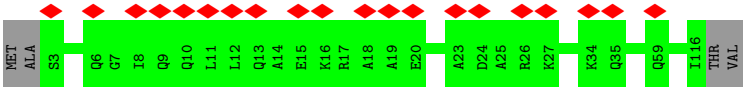




• Molecule 7: V-type proton ATPase subunit G

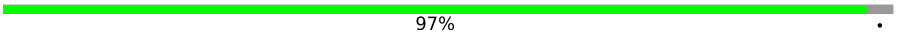
Chain M:

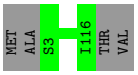




• Molecule 7: V-type proton ATPase subunit G

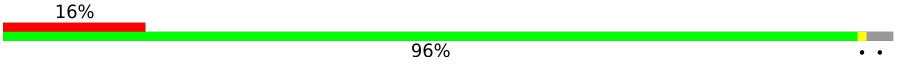
Chain N:

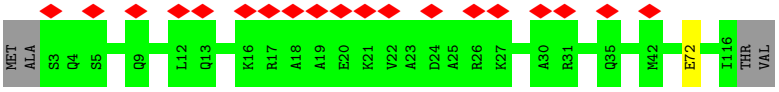




• Molecule 7: V-type proton ATPase subunit G

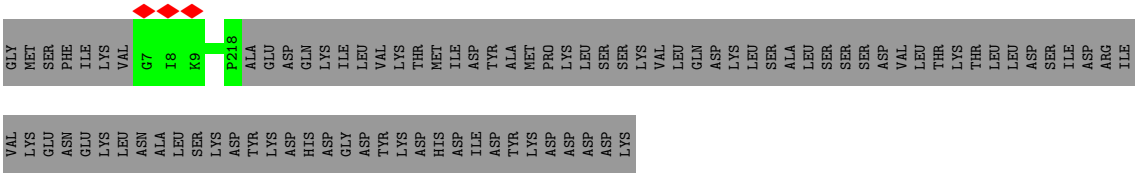
Chain O:





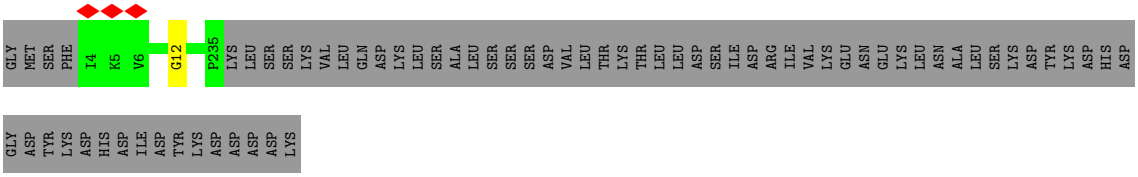
• Molecule 8: Effector protein SidK

Chain Q:



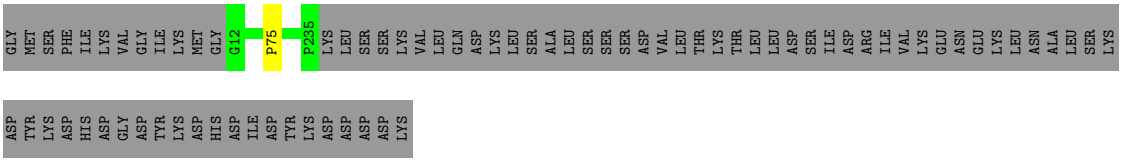
• Molecule 8: Effector protein SidK

Chain R:



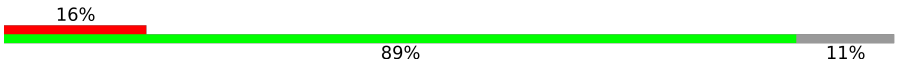
• Molecule 8: Effector protein SidK

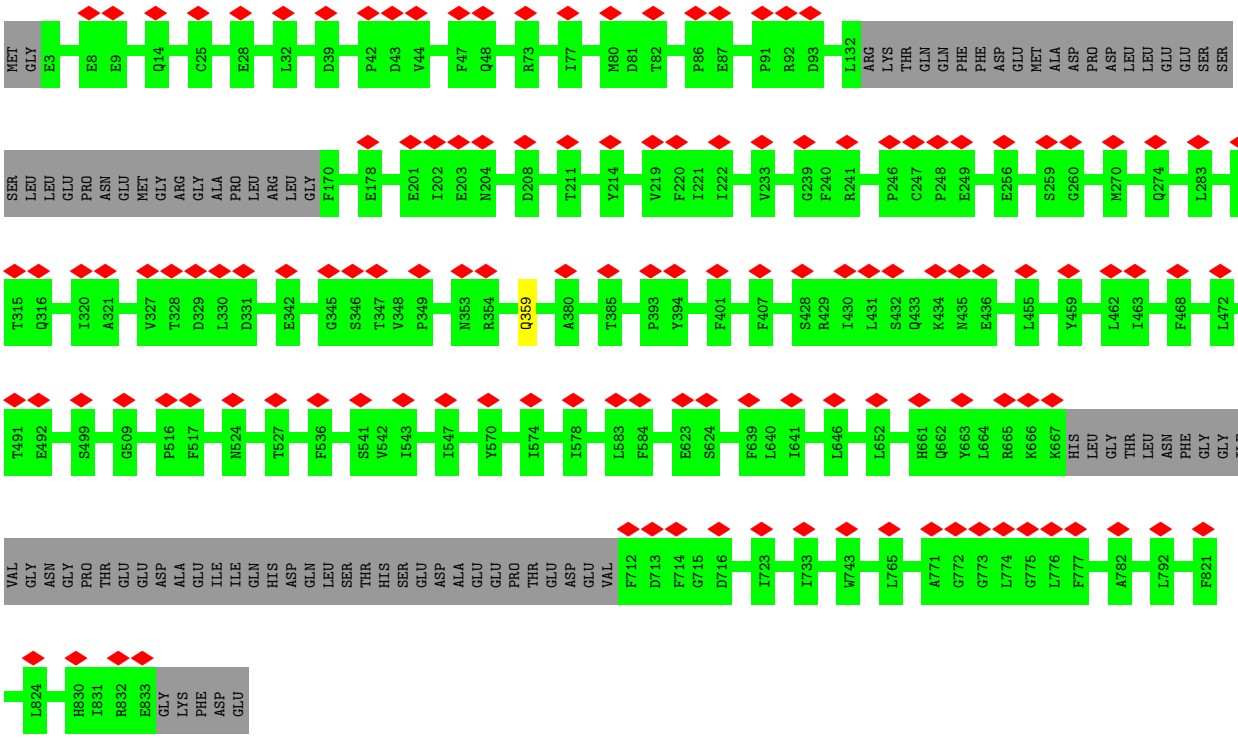
Chain S:



• Molecule 9: V-type proton ATPase 116 kDa subunit a isoform 1

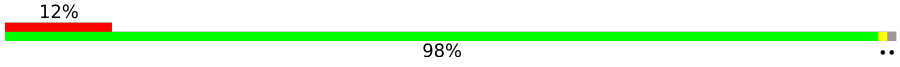
Chain a:

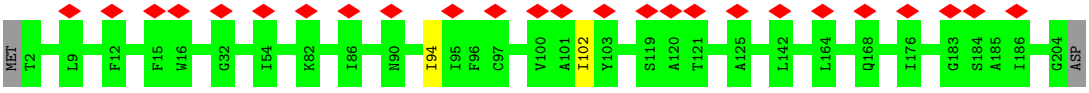




• Molecule 10: ATPase, H+ transporting, V0 subunit B (Predicted), isoform CRA_a

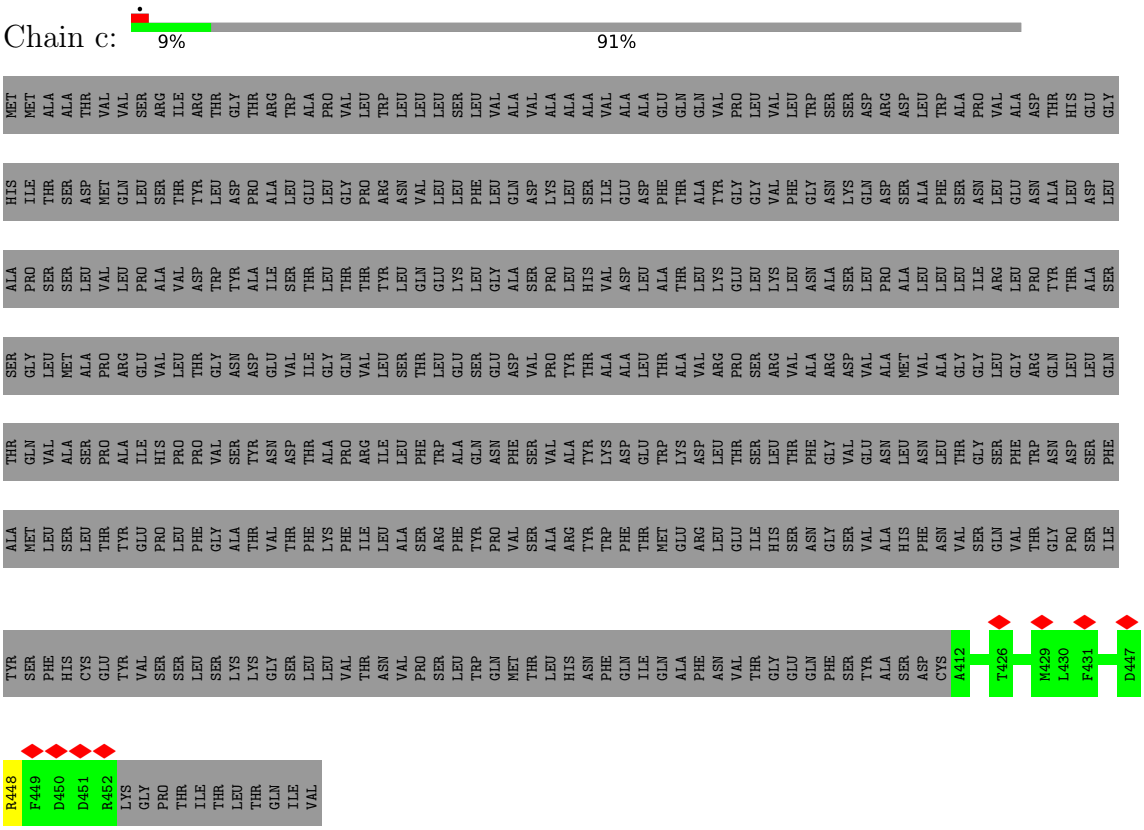
Chain b:





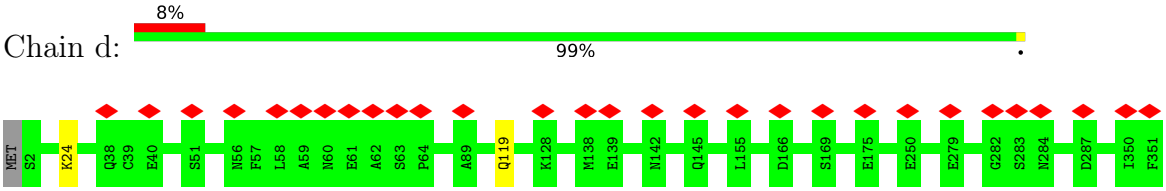
• Molecule 11: V-type proton ATPase subunit S1

Chain c:



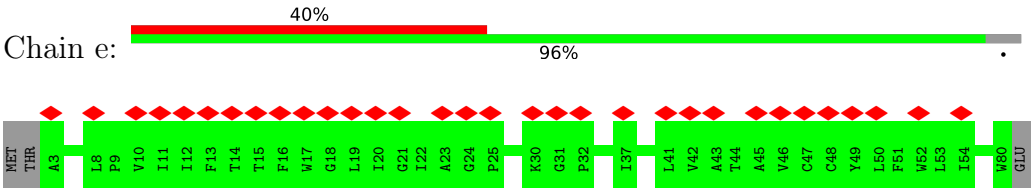
- Molecule 12: V-type proton ATPase subunit

Chain d:



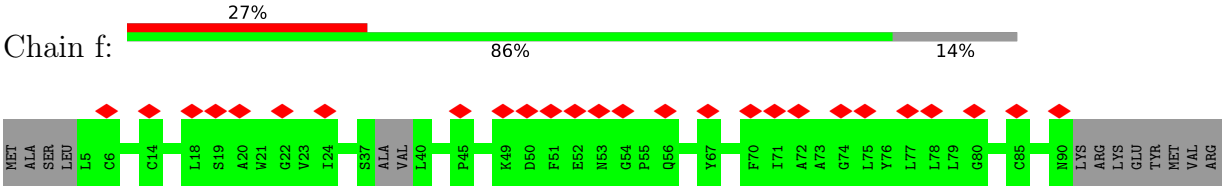
- Molecule 13: V-type proton ATPase subunit e 2

Chain e:



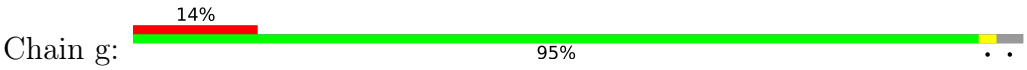
- Molecule 14: Ribonuclease K

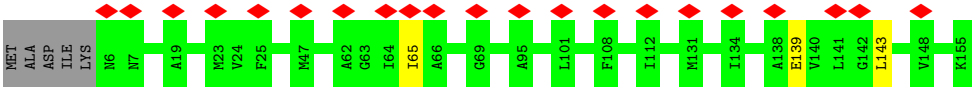
Chain f:



- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

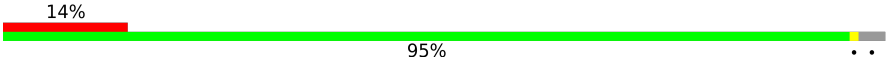
Chain g:

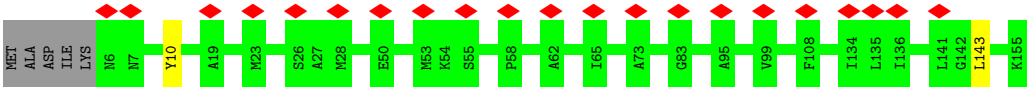




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

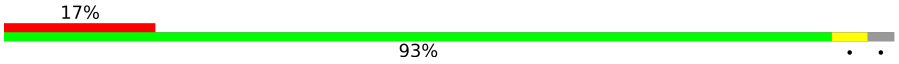
Chain h:

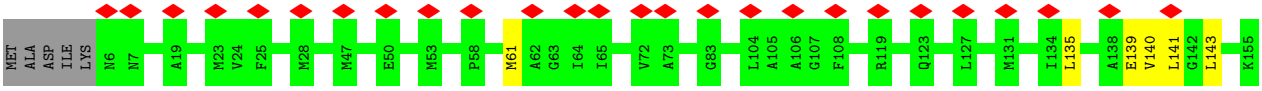




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

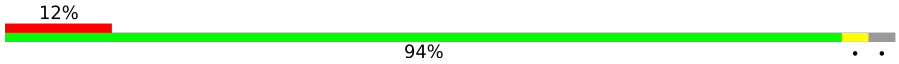
Chain i:

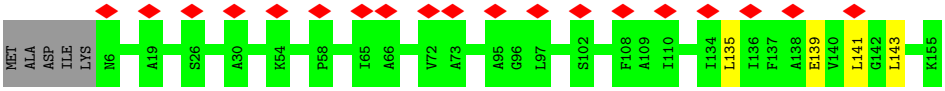




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

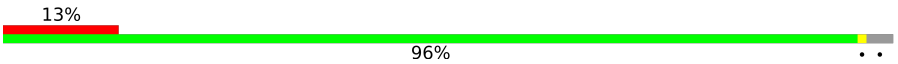
Chain j:

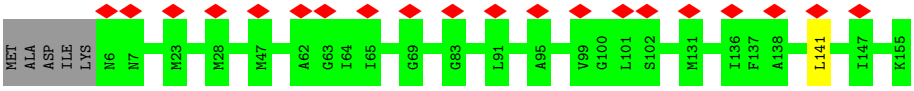




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

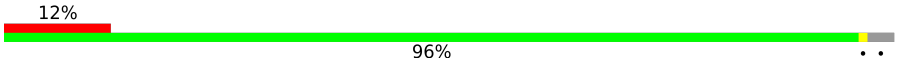
Chain k:

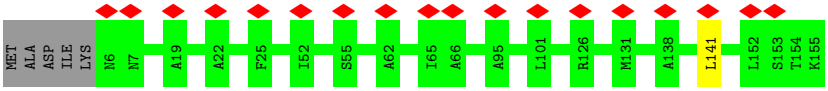




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

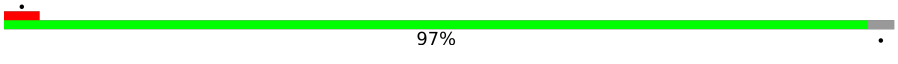
Chain l:

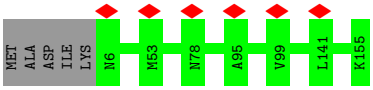




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

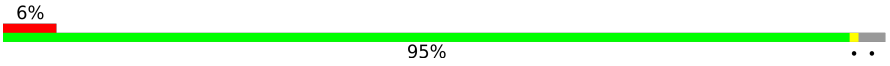
Chain m:

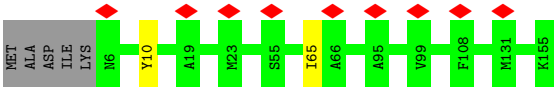




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

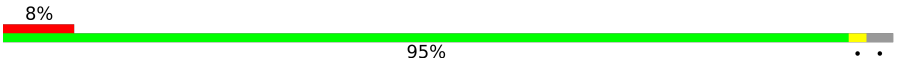
Chain n:

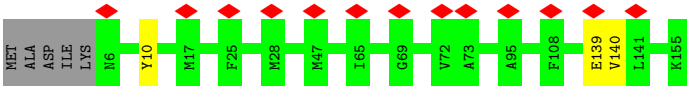




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

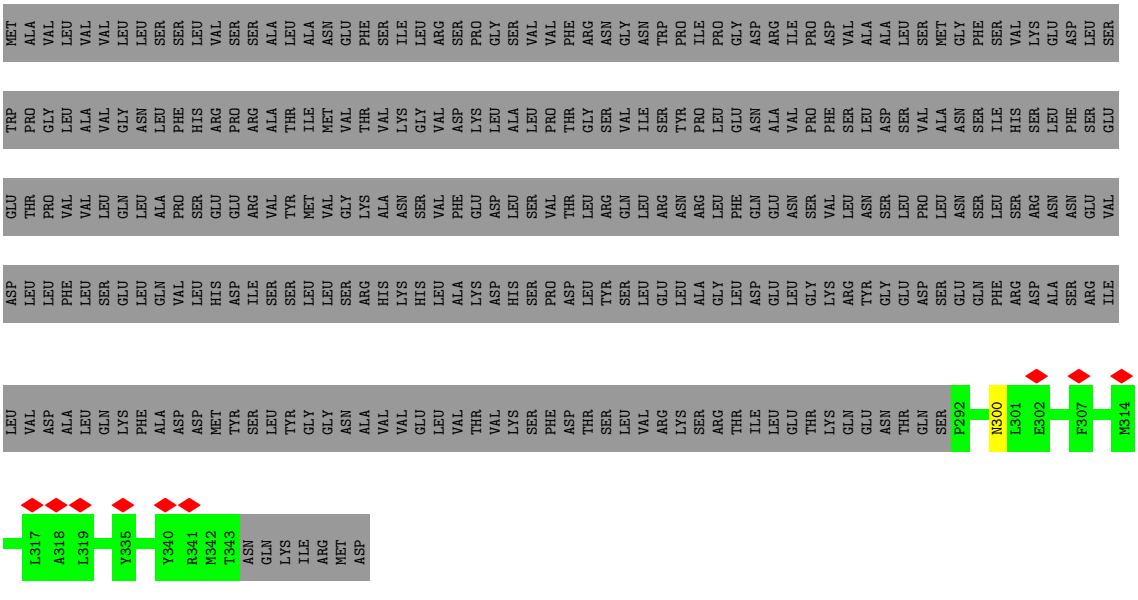
Chain o:





• Molecule 16: Renin receptor

Chain p:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.387	Depositor
Minimum map value	-0.610	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	0/4746	0.53	0/6425
1	B	0.72	0/4746	0.53	0/6425
1	C	0.73	1/4746 (0.0%)	0.55	0/6425
2	D	0.70	0/3666	0.53	0/4967
2	E	0.70	0/3666	0.52	0/4967
2	F	0.68	0/3666	0.52	0/4967
3	G	0.38	0/1788	0.67	0/2494
4	H	0.81	0/1733	0.58	0/2319
5	I	0.58	0/1619	0.52	0/2192
5	J	0.58	0/1619	0.53	0/2192
5	K	0.57	0/1619	0.54	0/2192
6	L	0.80	0/880	0.75	0/1189
7	M	0.53	0/717	0.51	0/980
7	N	0.53	0/717	0.52	0/980
7	O	0.54	0/717	0.53	0/980
8	Q	0.69	0/1754	0.49	0/2362
8	R	0.69	0/1912	0.51	0/2575
8	S	0.70	0/1858	0.51	0/2505
9	a	0.50	0/5117	0.55	0/7008
10	b	0.51	0/1537	0.49	0/2088
11	c	0.53	0/347	0.56	0/466
12	d	0.73	0/2899	0.53	0/3927
13	e	0.46	0/646	0.46	0/889
14	f	0.40	0/459	0.49	0/635
15	g	0.50	0/1083	0.53	0/1466
15	h	0.48	0/1083	0.53	0/1466
15	i	0.49	0/1083	0.52	0/1466
15	j	0.48	0/1083	0.51	0/1466
15	k	0.49	0/1083	0.53	0/1466
15	l	0.48	0/1083	0.52	0/1466
15	m	0.53	0/1083	0.60	0/1466
15	n	0.47	0/1083	0.51	0/1466

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
15	o	0.49	0/1083	0.51	0/1466
16	p	0.50	0/445	0.60	0/609
All	All	0.63	1/63366 (0.0%)	0.54	0/85952

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	ASP	C-N	-5.22	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/617 (97%)	574 (96%)	23 (4%)	1 (0%)	47	79
1	B	598/617 (97%)	573 (96%)	24 (4%)	1 (0%)	47	79
1	C	598/617 (97%)	579 (97%)	19 (3%)	0	100	100
2	D	455/511 (89%)	443 (97%)	12 (3%)	0	100	100
2	E	455/511 (89%)	443 (97%)	9 (2%)	3 (1%)	22	61
2	F	455/511 (89%)	441 (97%)	12 (3%)	2 (0%)	34	71
3	G	356/382 (93%)	355 (100%)	1 (0%)	0	100	100
4	H	212/247 (86%)	207 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	223/226 (99%)	221 (99%)	2 (1%)	0	100	100
5	J	223/226 (99%)	221 (99%)	2 (1%)	0	100	100
5	K	223/226 (99%)	223 (100%)	0	0	100	100
6	L	108/119 (91%)	101 (94%)	5 (5%)	2 (2%)	8	40
7	M	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	N	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	O	112/118 (95%)	112 (100%)	0	0	100	100
8	Q	210/301 (70%)	204 (97%)	6 (3%)	0	100	100
8	R	230/301 (76%)	223 (97%)	6 (3%)	1 (0%)	34	71
8	S	222/301 (74%)	215 (97%)	6 (3%)	1 (0%)	29	67
9	a	744/838 (89%)	722 (97%)	21 (3%)	1 (0%)	51	84
10	b	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
11	c	39/463 (8%)	39 (100%)	0	0	100	100
12	d	348/351 (99%)	330 (95%)	17 (5%)	1 (0%)	41	75
13	e	76/81 (94%)	74 (97%)	2 (3%)	0	100	100
14	f	80/98 (82%)	77 (96%)	3 (4%)	0	100	100
15	g	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	h	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	22	61
15	i	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	j	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	k	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	l	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	m	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	n	148/155 (96%)	144 (97%)	3 (2%)	1 (1%)	22	61
15	o	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	22	61
16	p	50/350 (14%)	47 (94%)	2 (4%)	1 (2%)	7	40
All	All	8372/9848 (85%)	8149 (97%)	206 (2%)	17 (0%)	50	79

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	p	300	ASN
2	E	299	ASP

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Mol	Chain	Res	Type
2	F	119	LEU
15	n	10	TYR
15	o	10	TYR
1	B	350	SER
2	E	119	LEU
2	E	378	TYR
6	L	100	ALA
8	R	12	GLY
12	d	119	GLN
1	A	278	GLY
2	F	378	TYR
6	L	61	ILE
9	a	359	GLN
15	h	10	TYR
8	S	75	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	507/524 (97%)	505 (100%)	2 (0%)	91	94
1	B	507/524 (97%)	505 (100%)	2 (0%)	91	94
1	C	507/524 (97%)	506 (100%)	1 (0%)	93	96
2	D	393/431 (91%)	393 (100%)	0	100	100
2	E	393/431 (91%)	392 (100%)	1 (0%)	92	95
2	F	393/431 (91%)	392 (100%)	1 (0%)	92	95
4	H	183/212 (86%)	180 (98%)	3 (2%)	62	79
5	I	141/198 (71%)	141 (100%)	0	100	100
5	J	141/198 (71%)	141 (100%)	0	100	100
5	K	141/198 (71%)	141 (100%)	0	100	100
6	L	92/100 (92%)	92 (100%)	0	100	100
7	M	43/100 (43%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	N	43/100 (43%)	43 (100%)	0	100 100
7	O	43/100 (43%)	42 (98%)	1 (2%)	50 70
8	Q	191/274 (70%)	191 (100%)	0	100 100
8	R	208/274 (76%)	208 (100%)	0	100 100
8	S	203/274 (74%)	203 (100%)	0	100 100
9	a	354/743 (48%)	354 (100%)	0	100 100
10	b	156/158 (99%)	154 (99%)	2 (1%)	69 82
11	c	36/395 (9%)	35 (97%)	1 (3%)	43 65
12	d	305/306 (100%)	304 (100%)	1 (0%)	92 95
13	e	64/68 (94%)	64 (100%)	0	100 100
14	f	8/83 (10%)	8 (100%)	0	100 100
15	g	109/113 (96%)	106 (97%)	3 (3%)	43 65
15	h	109/113 (96%)	108 (99%)	1 (1%)	78 88
15	i	109/113 (96%)	103 (94%)	6 (6%)	21 50
15	j	109/113 (96%)	105 (96%)	4 (4%)	34 60
15	k	109/113 (96%)	108 (99%)	1 (1%)	78 88
15	l	109/113 (96%)	108 (99%)	1 (1%)	78 88
15	m	109/113 (96%)	109 (100%)	0	100 100
15	n	109/113 (96%)	108 (99%)	1 (1%)	78 88
15	o	109/113 (96%)	107 (98%)	2 (2%)	59 77
16	p	47/313 (15%)	47 (100%)	0	100 100
All	All	6080/7976 (76%)	6046 (99%)	34 (1%)	86 92

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	296	MET
1	B	173	ARG
1	B	400	ARG
1	C	173	ARG
2	E	74	LEU
2	F	376	GLN
4	H	49	LYS
4	H	154	SER

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Mol	Chain	Res	Type
4	H	157	THR
7	O	72	GLU
10	b	94	ILE
10	b	102	ILE
11	c	448	ARG
12	d	24	LYS
15	g	65	ILE
15	g	139	GLU
15	g	143	LEU
15	h	143	LEU
15	i	61	MET
15	i	135	LEU
15	i	139	GLU
15	i	140	VAL
15	i	141	LEU
15	i	143	LEU
15	j	135	LEU
15	j	139	GLU
15	j	141	LEU
15	j	143	LEU
15	k	141	LEU
15	l	141	LEU
15	n	65	ILE
15	o	139	GLU
15	o	140	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	B	22	HIS
1	C	22	HIS
1	C	103	GLN
1	C	268	ASN
2	D	181	ASN
4	H	137	ASN
5	J	66	GLN
8	R	184	HIS
9	a	548	HIS
9	a	762	HIS
12	d	297	HIS
15	m	78	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	ADP	B	701	18	24,29,29	0.67	0	29,45,45	0.70	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	B	701	18	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	701	ADP	C5-C6-N6	2.25	123.78	120.35

There are no chirality outliers.

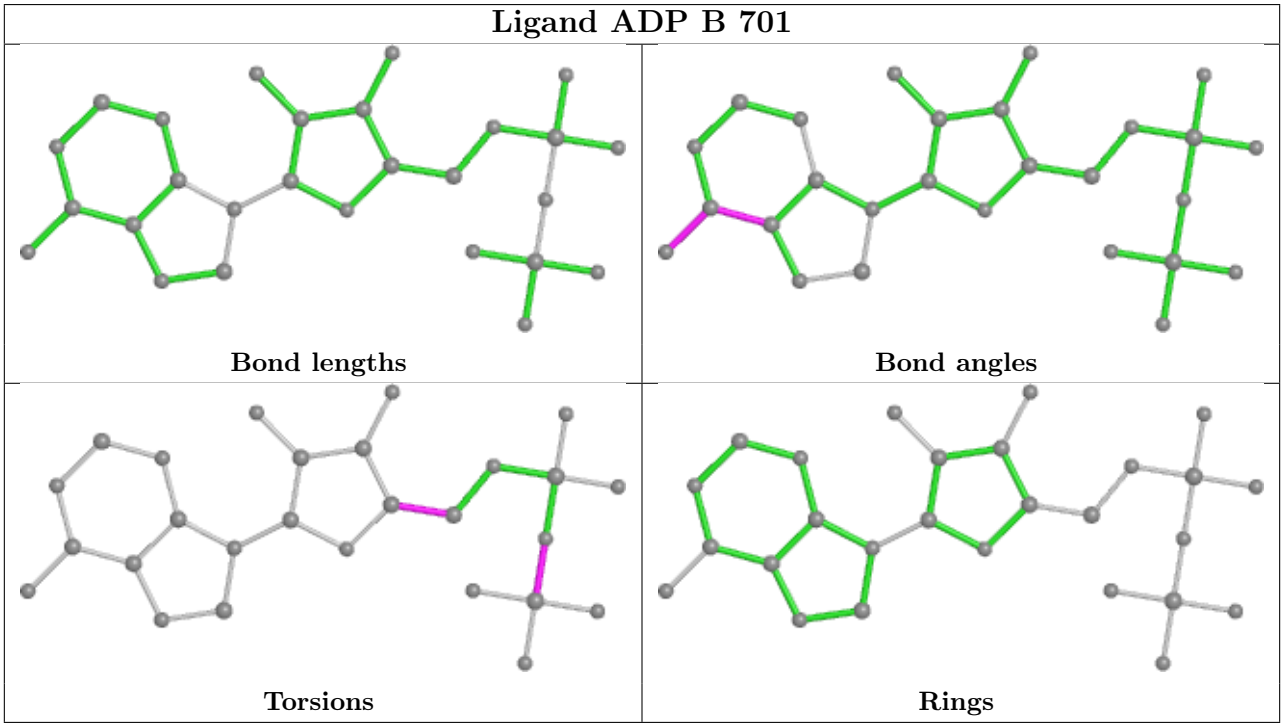
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	701	ADP	O4'-C4'-C5'-O5'
17	B	701	ADP	C3'-C4'-C5'-O5'
17	B	701	ADP	PA-O3A-PB-O1B
17	B	701	ADP	PA-O3A-PB-O2B
17	B	701	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

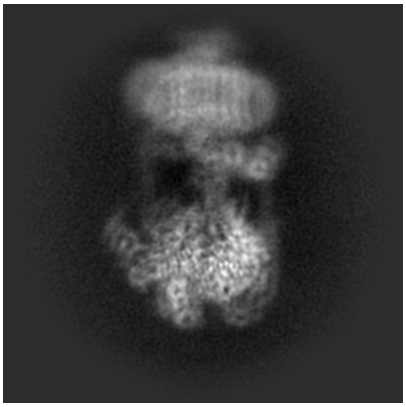
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21318. These allow visual inspection of the internal detail of the map and identification of artifacts.

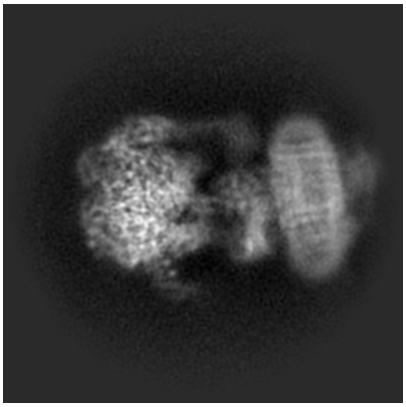
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

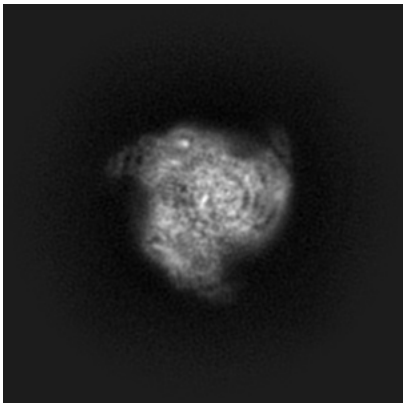
6.1.1 Primary map



X



Y

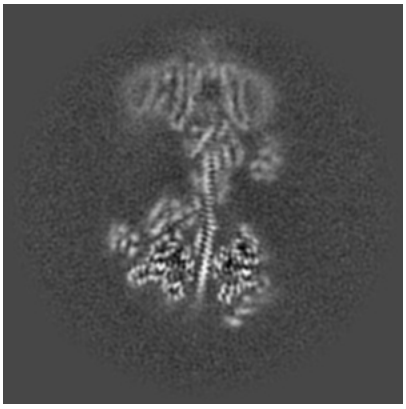


Z

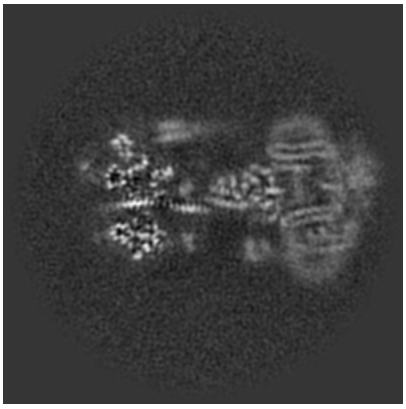
The images above show the map projected in three orthogonal directions.

6.2 Central slices

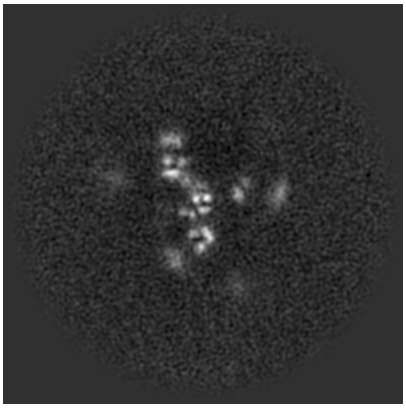
6.2.1 Primary map



X Index: 170



Y Index: 170

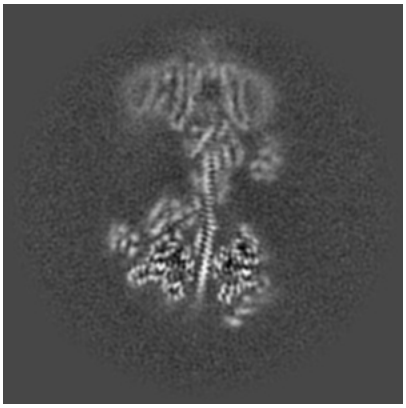


Z Index: 170

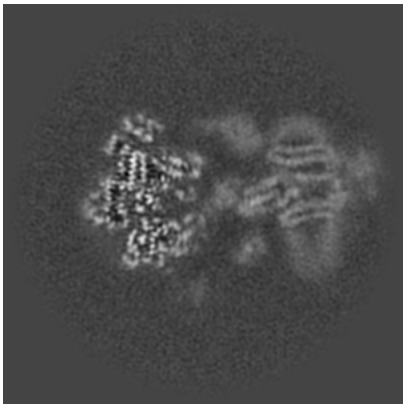
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

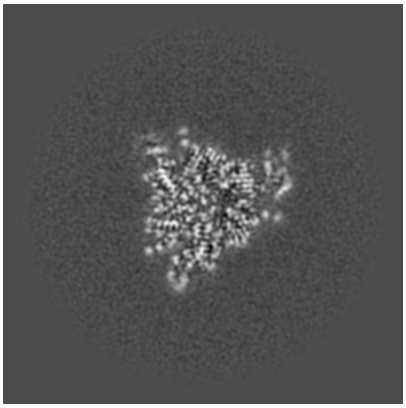
6.3.1 Primary map



X Index: 170



Y Index: 189



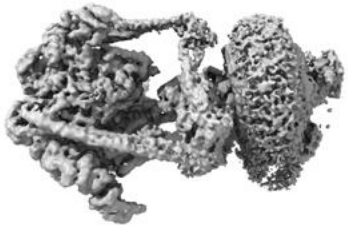
Z Index: 118

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

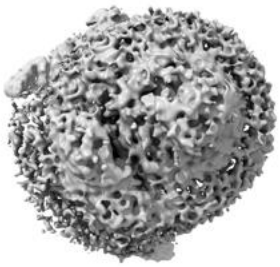
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

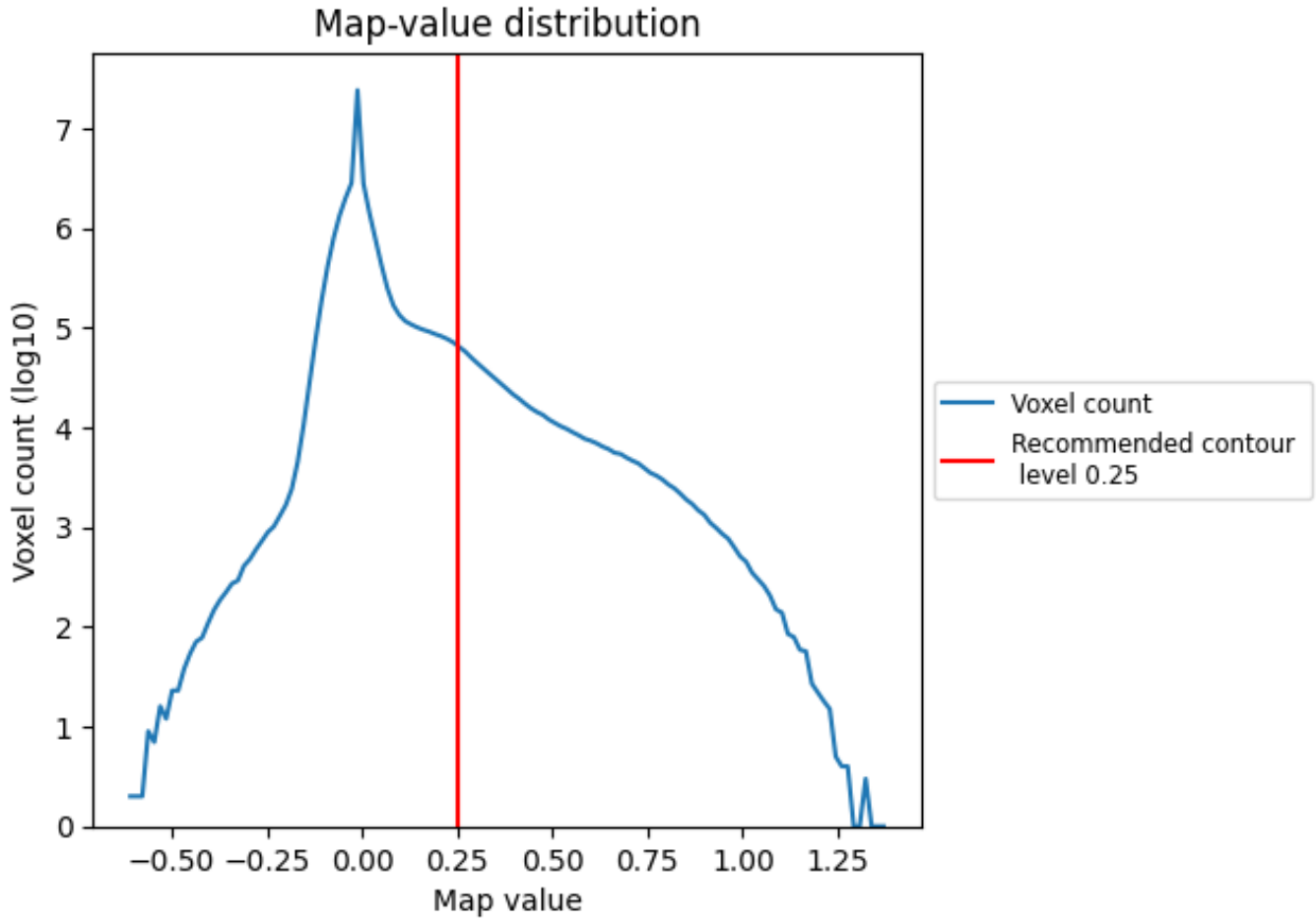
6.5 Mask visualisation (i)

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

7 Map analysis

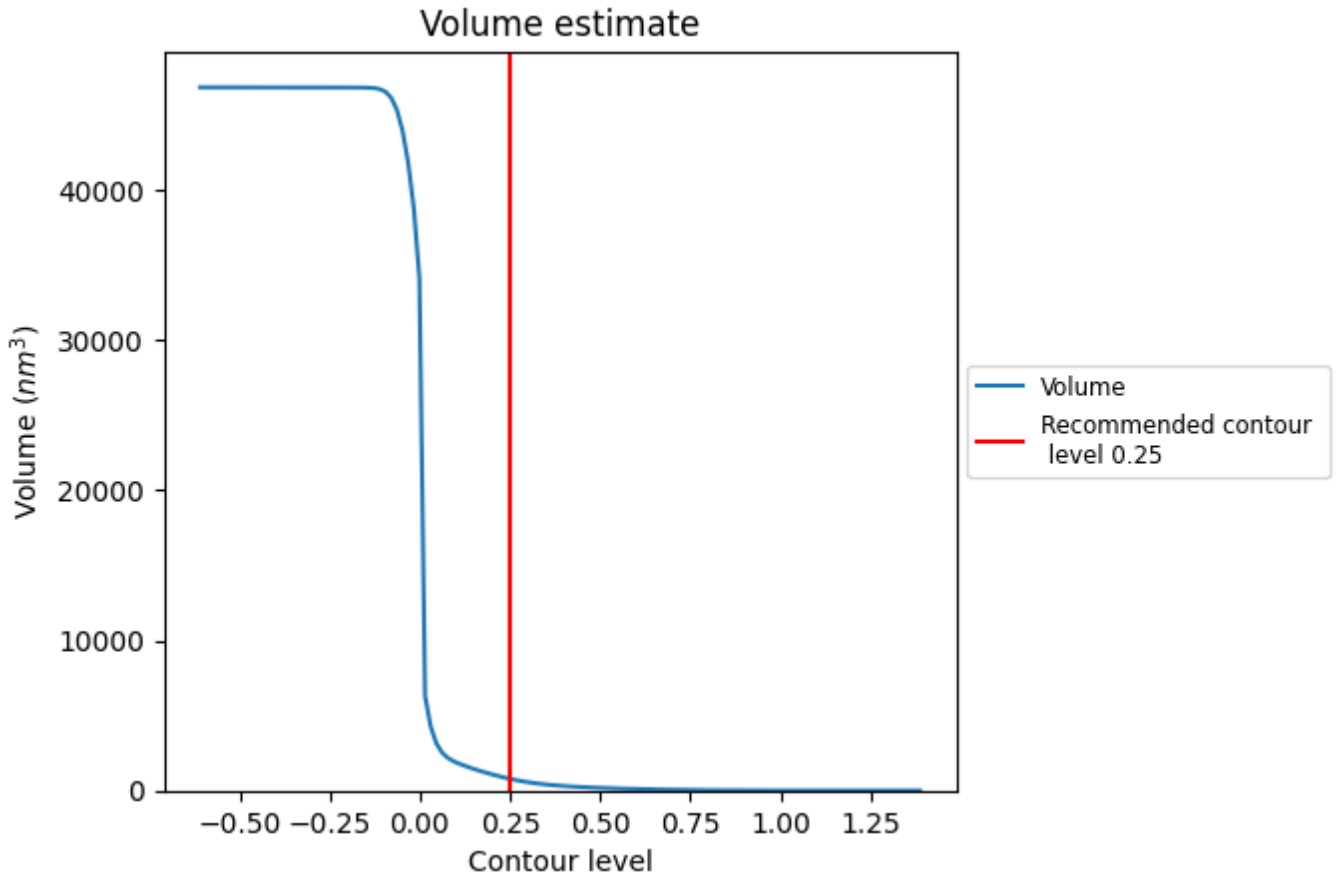
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

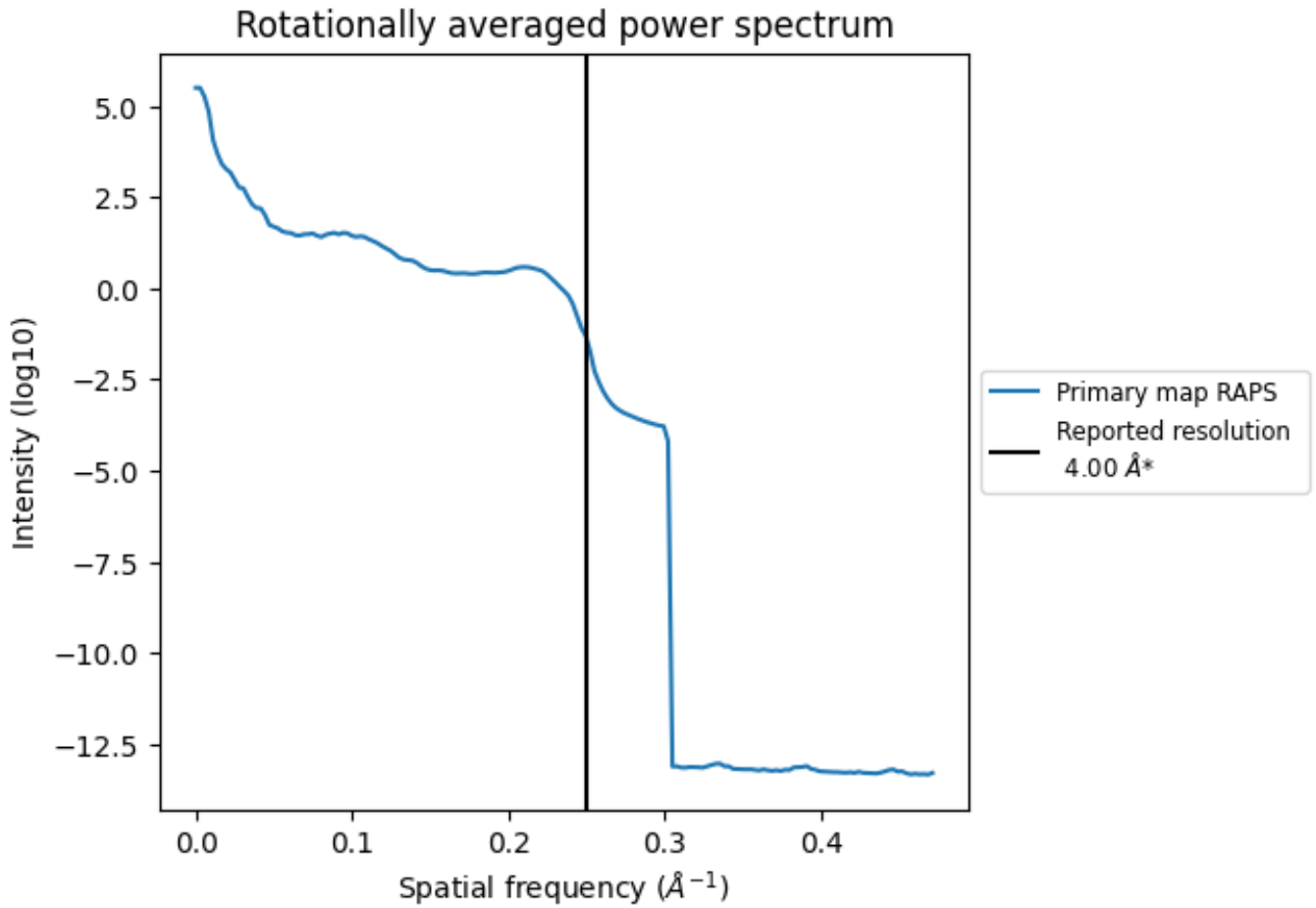
7.2 Volume estimate



The volume at the recommended contour level is 778 nm^3; this corresponds to an approximate mass of 703 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 0.250 $Å^{-1}$

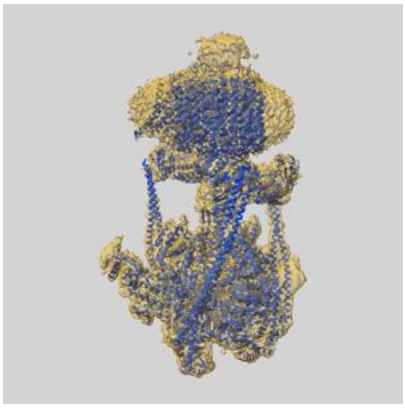
8 Fourier-Shell correlation (i)

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

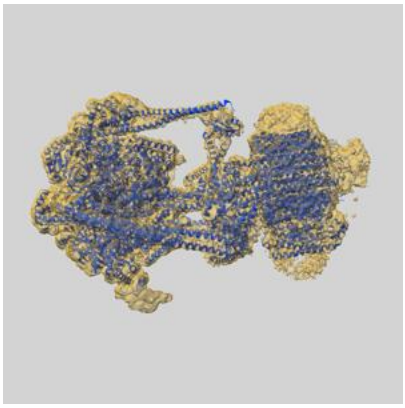
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21318 and PDB model 6VQ7. Per-residue inclusion information can be found in section 3 on page 10.

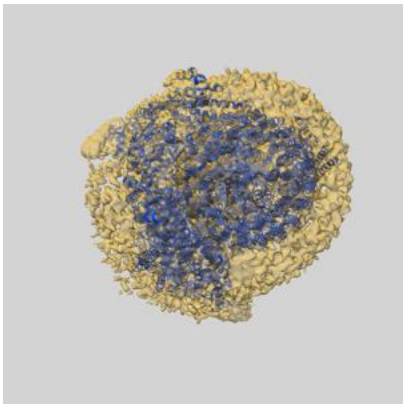
9.1 Map-model overlay



X



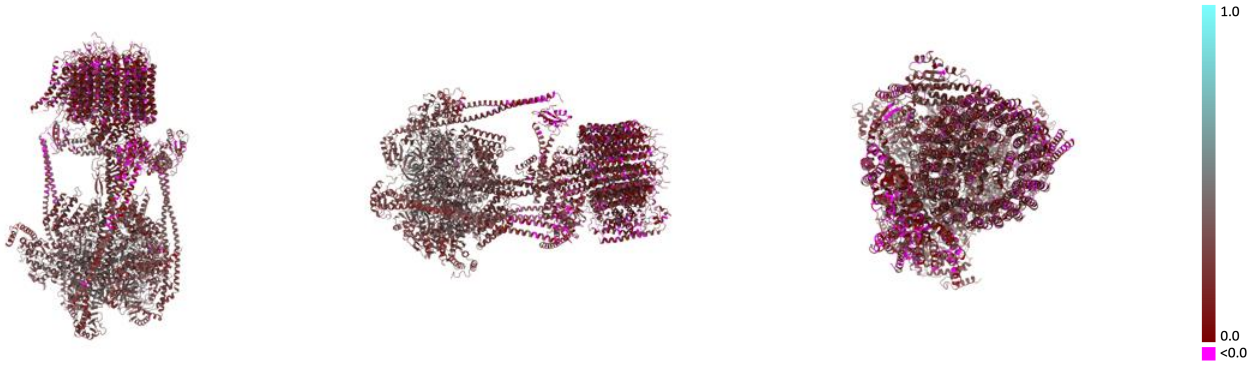
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

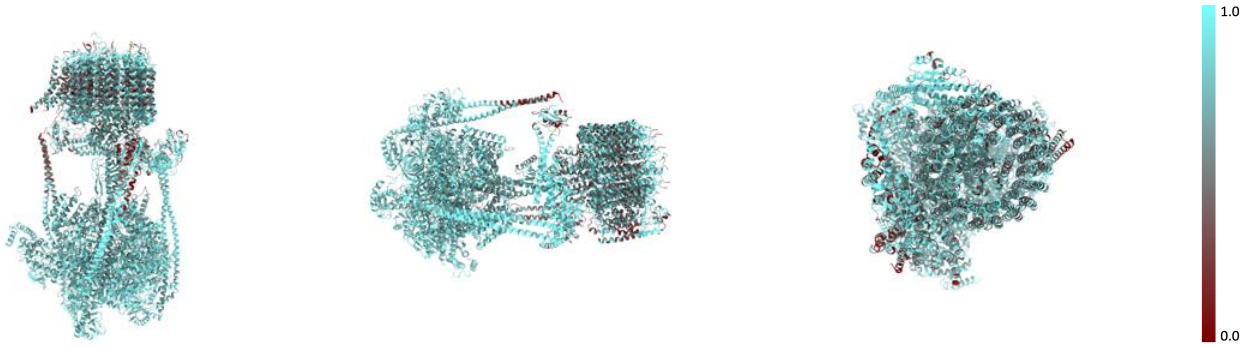
9.2 Q-score mapped to coordinate model



X Y Z

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

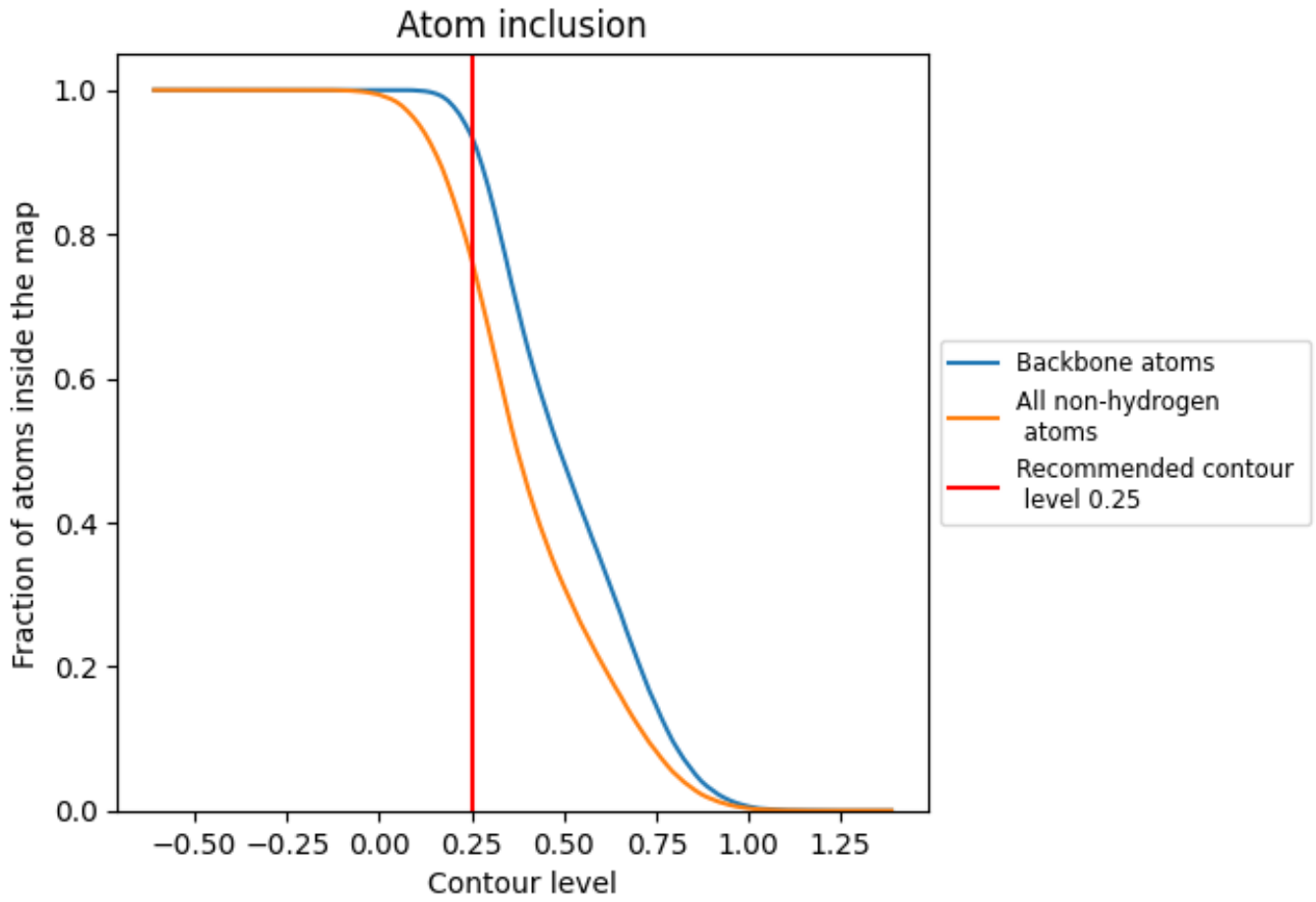
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 77% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.2580
A	0.8242	0.3340
B	0.8336	0.3510
C	0.8172	0.3300
D	0.8379	0.3640
E	0.8330	0.3510
F	0.8359	0.3630
G	0.7698	0.1760
H	0.7549	0.2730
I	0.7446	0.2520
J	0.8302	0.2660
K	0.7845	0.2530
L	0.7165	0.2080
M	0.7725	0.2260
N	0.8755	0.2450
O	0.7668	0.2230
Q	0.8007	0.2560
R	0.7974	0.2660
S	0.8097	0.2560
a	0.6851	0.1480
b	0.6828	0.1690
c	0.5770	0.1690
d	0.6741	0.2080
e	0.5385	0.1120
f	0.6378	0.1380
g	0.6844	0.1240
h	0.6938	0.1350
i	0.6815	0.1300
j	0.6730	0.1370
k	0.6616	0.1510
l	0.6682	0.1790
m	0.6863	0.1980
n	0.6777	0.1900
o	0.6844	0.1640
p	0.6295	0.1430