



Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 03:20 PM EST

PDB ID : 7UZI
EMDB ID : EMD-26912
Title : Rat Kidney V-ATPase lacking subunit H, with SidK and NCOA7B, State 2
Authors : Rubinstein, J.L.; Abbas, Y.M.
Deposited on : 2022-05-09
Resolution : 3.90 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.dev70
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) : 2.36

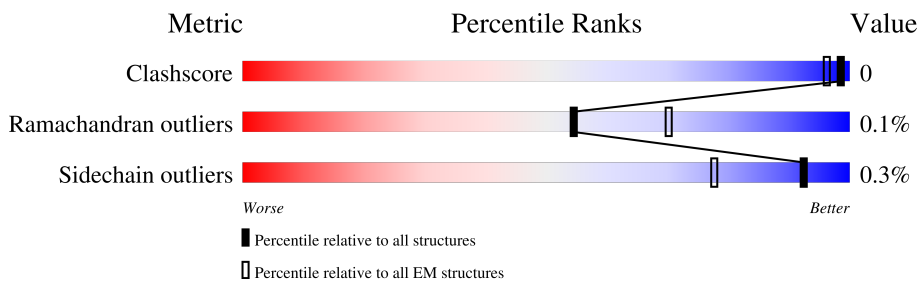
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	617	
1	B	617	
1	C	617	
2	D	511	
2	E	511	
2	F	511	
3	G	382	
4	H	247	

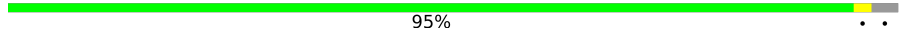
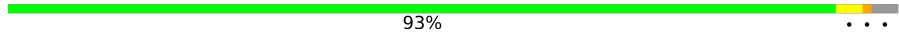

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Mol	Chain	Length	Quality of chain
5	I	226	9% 96% ..
5	J	226	95% ..
5	K	226	8% 95% ..
6	L	119	87% 5% 8%
7	M	118	13% 88% 7% 5%
7	N	118	90% 6% ..
7	O	118	91% 6% .
8	Q	301	86% 12%
8	R	301	86% 11%
8	S	301	85% 13%
9	T	171	95% 5% .
9	U	171	25% 93% 6% .
10	a	838	6% 88% 10%
11	b	205	96% ..
12	c	463	43% 56%
13	d	351	96% ..
14	e	81	95% 5%
15	f	98	85% 14%
16	g	155	95% ..
16	h	155	95% ..
16	i	155	96% ..
16	j	155	96% ..
16	k	155	94% ..
16	l	155	96% ..
16	m	155	94% ..

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Mol	Chain	Length	Quality of chain
16	n	155	 95% . .
16	o	155	 93% . . .
17	p	350	 14% 85% . .

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 71172 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
			Total	C	N	O	S		
1	A	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	B	602	Total	C	N	O	S	0	0
			4666	2957	788	894	27		
1	C	601	Total	C	N	O	S	0	0
			4657	2952	787	891	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	460	Total	C	N	O	S	0	0
			3603	2286	615	682	20		
2	E	457	Total	C	N	O	S	0	0
			3576	2269	610	677	20		
2	F	460	Total	C	N	O	S	0	0
			3604	2287	614	683	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	358	Total	C	N	O	S	0	0
			2919	1873	492	545	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	218	Total	C	N	O	S	0	0
			1760	1116	316	323	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	223	Total	C	N	O	S	0	0
			1808	1137	319	342	10		
5	J	223	Total	C	N	O	S	0	0
			1808	1137	319	342	10		
5	K	223	Total	C	N	O	S	0	0
			1808	1137	319	342	10		

- 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
			875	553	157	163	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	112	Total	C	N	O	S	0	0
			920	563	173	181	3		
7	N	114	Total	C	N	O	S	0	0
			935	571	176	185	3		
7	O	114	Total	C	N	O	S	0	0
			935	571	176	185	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	264	Total	C	N	O	S	0	0
			2130	1352	358	410	10		
8	R	267	Total	C	N	O	S	0	0
			2155	1369	362	413	11		
8	S	263	Total	C	N	O	S	0	0
			2126	1350	357	409	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 Nuclear receptor coactivator 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	T	170	1377	887	230	257	3	0	0
9	U	170	1377	887	230	257	3	0	0

- Molecule 10 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	a	757	6164	4025	1032	1066	41	0	0

- Molecule 11 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

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

- Molecule 12 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	c	204	1652	1087	259	297	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	d	348	2817	1817	458	528	14	0	0

- Molecule 14 is a protein called V-type proton ATPase subunit e 2.

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

- Molecule 15 is a protein called Ribonuclease K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	f	84	652	431	101	114	6	0	0

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

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

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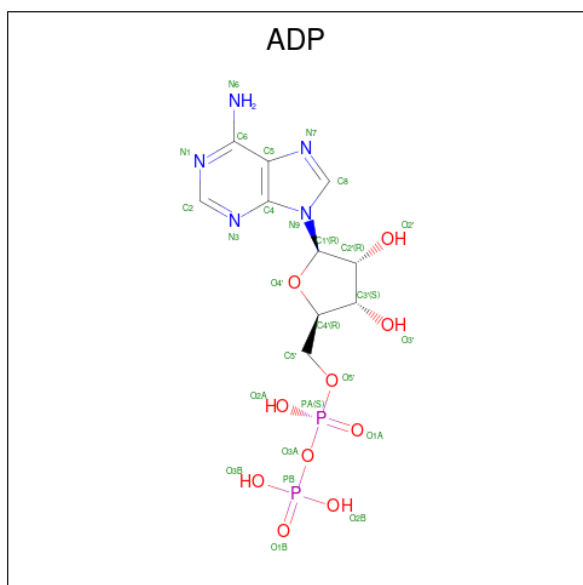
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	o	150	1069	699	171	191	8	0	0

- Molecule 17 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	p	51	423	284	62	75	2	0	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

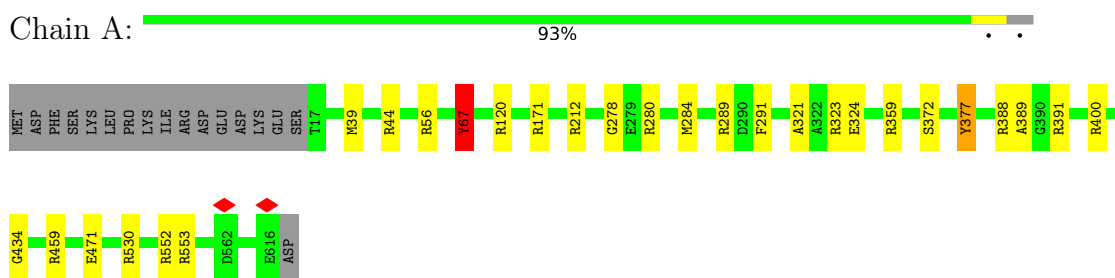


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	B	1	27	10	5	10	2	0

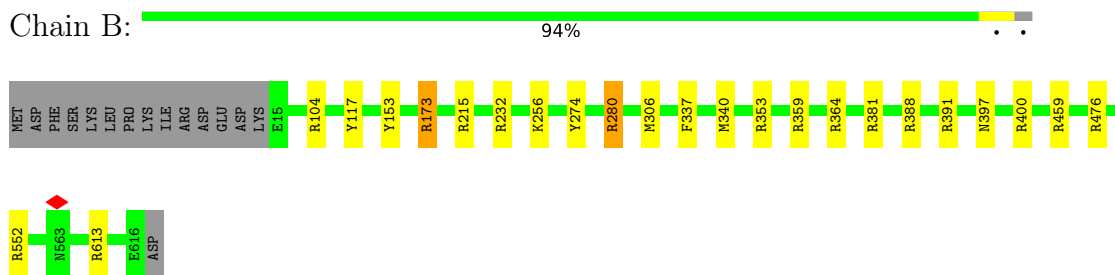
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

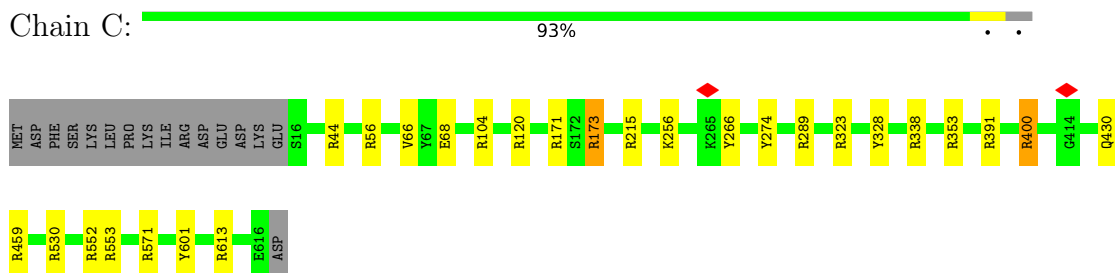
- Molecule 1: ATPase H⁺-transporting V1 subunit A



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

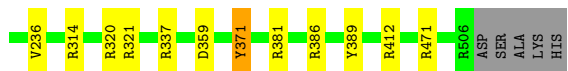
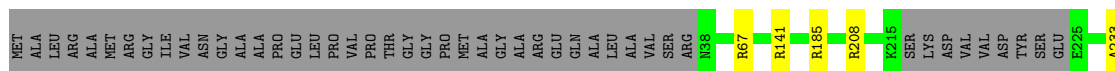


- Molecule 1: ATPase H⁺-transporting V1 subunit A

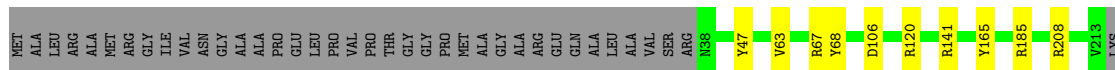
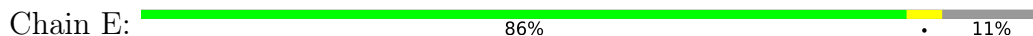


- Molecule 2: V-type proton ATPase subunit B, brain isoform

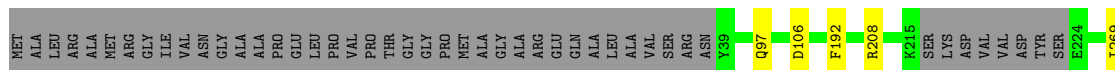
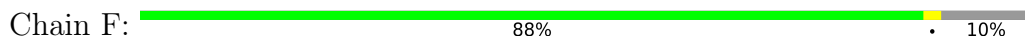




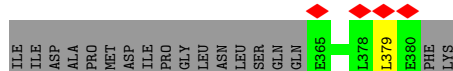
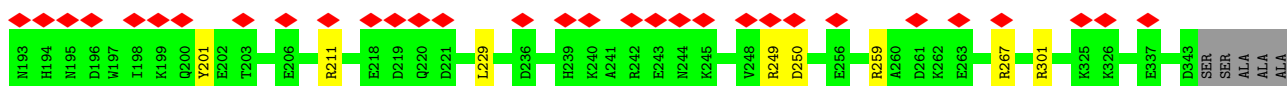
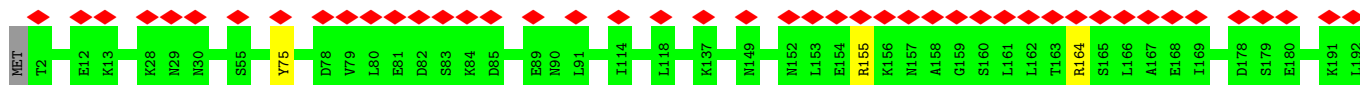
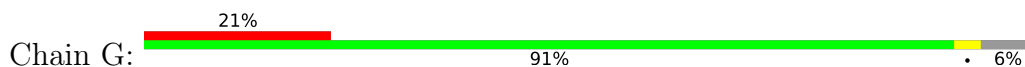
- Molecule 2: V-type proton ATPase subunit B, brain isoform



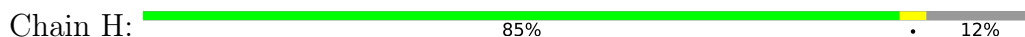
- Molecule 2: V-type proton ATPase subunit B, brain isoform



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

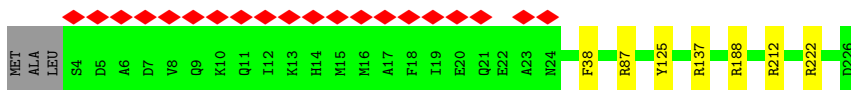


- Molecule 4: ATPase H⁺-transporting V1 subunit D



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

Chain I:  9% 96%



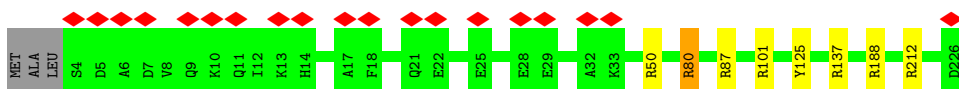
• Molecule 5: V-type proton ATPase subunit E 1

Chain J:  95%




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

Chain K:  8% 95%

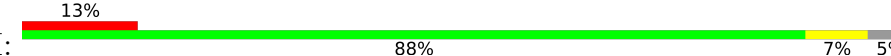


• Molecule 6: V-type proton ATPase subunit F

Chain L:  87% 5% 8%

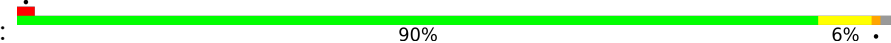


• Molecule 7: V-type proton ATPase subunit G

Chain M:  13% 88% 7% 5%



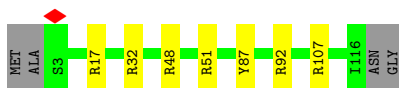
• Molecule 7: V-type proton ATPase subunit G

Chain N:  90% 6%

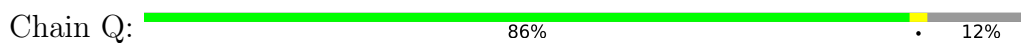


• Molecule 7: V-type proton ATPase subunit G

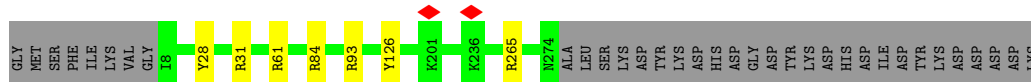
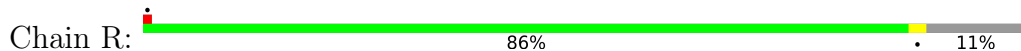
Chain O:  91% 6%



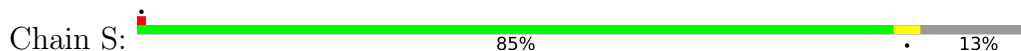
• Molecule 8: V-type proton ATPase subunit H



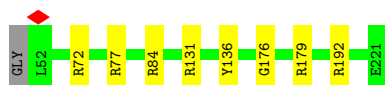
• Molecule 8: V-type proton ATPase subunit H



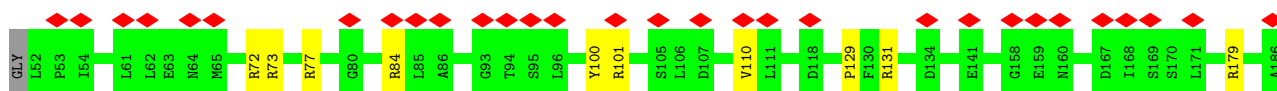
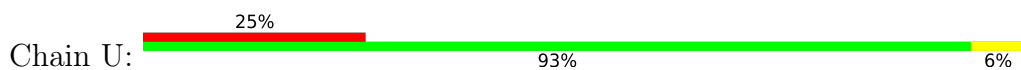
• Molecule 8: V-type proton ATPase subunit H



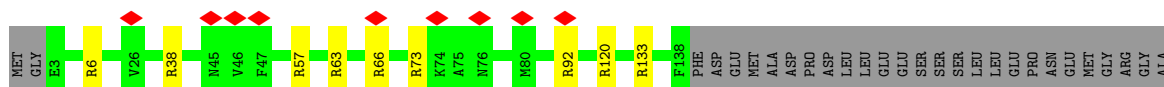
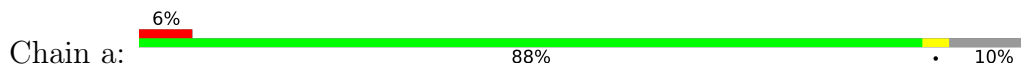
• Molecule 9: Nuclear receptor coactivator 7

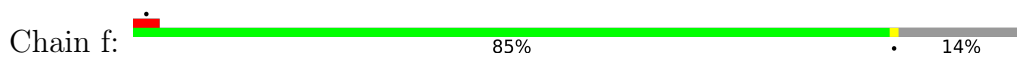


• Molecule 9: Nuclear receptor coactivator 7

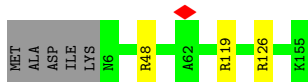


• Molecule 10: V-type proton ATPase 116 kDa subunit a isoform 1





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



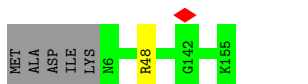
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



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



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



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



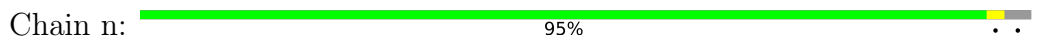
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



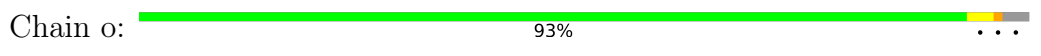
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



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



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



- Molecule 17: Renin receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32453	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.825	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	58.541	Depositor
Minimum map value	-38.914	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.222	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	449.65, 449.65, 449.65	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3225, 1.3225, 1.3225	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: 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	0.66	0/4746	0.99	21/6425 (0.3%)
1	B	0.65	0/4761	0.99	19/6445 (0.3%)
1	C	0.65	0/4752	0.99	25/6433 (0.4%)
2	D	0.67	0/3674	1.02	15/4978 (0.3%)
2	E	0.65	0/3647	0.97	15/4944 (0.3%)
2	F	0.66	0/3675	0.95	8/4979 (0.2%)
3	G	0.66	0/2973	0.93	9/4016 (0.2%)
4	H	0.61	0/1778	0.90	7/2377 (0.3%)
5	I	0.61	0/1825	0.90	6/2442 (0.2%)
5	J	0.62	0/1825	0.92	10/2442 (0.4%)
5	K	0.60	0/1825	0.90	8/2442 (0.3%)
6	L	0.64	0/889	1.02	6/1199 (0.5%)
7	M	0.66	0/928	0.98	7/1236 (0.6%)
7	N	0.65	0/943	0.96	8/1256 (0.6%)
7	O	0.65	0/943	0.93	7/1256 (0.6%)
8	Q	0.60	0/2164	0.86	5/2915 (0.2%)
8	R	0.61	0/2189	0.87	5/2947 (0.2%)
8	S	0.61	0/2160	0.86	4/2910 (0.1%)
9	T	0.71	0/1417	0.95	6/1919 (0.3%)
9	U	0.73	0/1417	0.97	8/1919 (0.4%)
10	a	0.70	0/6322	0.92	19/8551 (0.2%)
11	b	0.62	0/1537	0.91	5/2088 (0.2%)
12	c	0.68	0/1707	0.92	3/2324 (0.1%)
13	d	0.65	0/2882	0.95	10/3903 (0.3%)
14	e	0.73	0/648	0.92	0/891
15	f	0.69	0/668	0.89	2/907 (0.2%)
16	g	0.58	0/1084	0.87	3/1466 (0.2%)
16	h	0.60	0/1084	0.82	2/1466 (0.1%)
16	i	0.59	0/1084	0.84	1/1466 (0.1%)
16	j	0.59	0/1084	0.83	2/1466 (0.1%)
16	k	0.59	0/1084	0.85	3/1466 (0.2%)
16	l	0.60	0/1084	0.86	0/1466

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	m	0.61	0/1084	0.88	5/1466 (0.3%)
16	n	0.60	0/1084	0.91	4/1466 (0.3%)
16	o	0.59	0/1084	0.91	5/1466 (0.3%)
17	p	0.72	0/436	0.93	0/598
All	All	0.65	0/72487	0.94	263/97936 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	1
2	D	0	2
2	E	0	3
2	F	0	1
5	K	0	1
7	N	0	1
8	R	0	1
8	S	0	1
9	T	0	1
11	b	0	1
13	d	0	1
16	g	0	1
16	k	0	1
16	o	0	2
17	p	0	1
All	All	0	23

There are no bond length outliers.

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ARG	NE-CZ-NH1	11.13	125.87	120.30
1	C	353	ARG	NE-CZ-NH1	10.50	125.55	120.30
2	D	141	ARG	NE-CZ-NH1	9.64	125.12	120.30
8	R	93	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	B	353	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	D	321	ARG	NE-CZ-NH1	8.28	124.44	120.30
8	S	93	ARG	NE-CZ-NH1	8.27	124.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	108	ARG	NE-CZ-NH1	8.18	124.39	120.30
15	f	62	TYR	CB-CG-CD2	-8.15	116.11	121.00
7	M	51	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	C	459	ARG	NE-CZ-NH1	8.03	124.31	120.30
16	j	48	ARG	NE-CZ-NH1	7.98	124.29	120.30
10	a	447	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	C	613	ARG	NE-CZ-NH1	7.85	124.22	120.30
13	d	186	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	B	391	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	D	208	ARG	NE-CZ-NH1	7.67	124.13	120.30
4	H	201	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	400	ARG	NE-CZ-NH2	7.57	124.08	120.30
5	K	188	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	476	ARG	NE-CZ-NH1	7.53	124.07	120.30
2	E	400	ARG	NE-CZ-NH1	7.53	124.06	120.30
7	N	48	ARG	NE-CZ-NH1	7.51	124.05	120.30
10	a	133	ARG	NE-CZ-NH1	7.40	124.00	120.30
8	R	84	ARG	NE-CZ-NH1	7.29	123.94	120.30
3	G	155	ARG	NE-CZ-NH1	7.24	123.92	120.30
3	G	211	ARG	NE-CZ-NH1	7.20	123.90	120.30
6	L	75	ARG	NE-CZ-NH1	7.19	123.89	120.30
5	I	188	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	E	386	ARG	NE-CZ-NH1	7.17	123.89	120.30
6	L	4	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	67	TYR	CB-CG-CD1	-7.16	116.70	121.00
2	D	320	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	289	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	364	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	553	ARG	NE-CZ-NH1	7.04	123.82	120.30
11	b	103	TYR	CB-CG-CD2	-7.03	116.78	121.00
6	L	107	ARG	NE-CZ-NH1	6.99	123.80	120.30
2	D	412	ARG	NE-CZ-NH1	6.99	123.79	120.30
16	g	48	ARG	NE-CZ-NH1	6.99	123.79	120.30
13	d	341	ARG	NE-CZ-NH1	6.96	123.78	120.30
7	N	115	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	530	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	D	371	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	B	364	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	C	56	ARG	NE-CZ-NH1	6.82	123.71	120.30
7	O	51	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	B	173	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	C	391	ARG	NE-CZ-NH1	6.78	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	44	ARG	NE-CZ-NH1	6.77	123.68	120.30
10	a	57	ARG	NE-CZ-NH1	6.76	123.68	120.30
13	d	182	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	104	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	E	320	ARG	NE-CZ-NH1	6.74	123.67	120.30
10	a	6	ARG	NE-CZ-NH1	6.71	123.66	120.30
16	o	48	ARG	NE-CZ-NH1	6.71	123.66	120.30
16	n	48	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	171	ARG	NE-CZ-NH1	6.68	123.64	120.30
13	d	246	ARG	NE-CZ-NH1	6.67	123.64	120.30
9	T	77	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	E	120	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	C	120	ARG	NE-CZ-NH1	6.60	123.60	120.30
5	K	125	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	B	613	ARG	NE-CZ-NH1	6.57	123.59	120.30
5	J	101	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	459	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	E	208	ARG	NE-CZ-NH1	6.54	123.57	120.30
7	O	48	ARG	NE-CZ-NH1	6.53	123.57	120.30
13	d	21	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	44	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	C	552	ARG	NE-CZ-NH1	6.49	123.55	120.30
5	K	101	ARG	NE-CZ-NH1	6.48	123.54	120.30
7	M	17	ARG	NE-CZ-NH1	6.47	123.53	120.30
5	K	80	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	280	ARG	NE-CZ-NH1	6.43	123.51	120.30
9	U	131	ARG	NE-CZ-NH1	6.42	123.51	120.30
8	S	265	ARG	NE-CZ-NH1	6.41	123.50	120.30
16	k	48	ARG	NE-CZ-NH1	6.41	123.50	120.30
2	E	485	ARG	NE-CZ-NH1	6.38	123.49	120.30
16	o	144	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	B	459	ARG	NE-CZ-NH1	6.35	123.48	120.30
5	K	137	ARG	NE-CZ-NH1	6.35	123.47	120.30
2	F	485	ARG	NE-CZ-NH1	6.34	123.47	120.30
10	a	339	ARG	NE-CZ-NH1	6.34	123.47	120.30
16	h	48	ARG	NE-CZ-NH1	6.33	123.47	120.30
8	Q	46	ARG	NE-CZ-NH1	6.32	123.46	120.30
7	M	92	ARG	NE-CZ-NH1	6.32	123.46	120.30
6	L	53	ARG	NE-CZ-NH1	6.31	123.45	120.30
9	U	73	ARG	NE-CZ-NH1	6.31	123.45	120.30
16	n	88	ARG	NE-CZ-NH1	6.29	123.45	120.30
16	m	88	ARG	NE-CZ-NH1	6.29	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	281	ARG	NE-CZ-NH1	6.27	123.44	120.30
9	U	84	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	552	ARG	NE-CZ-NH1	6.23	123.42	120.30
10	a	241	ARG	NE-CZ-NH1	6.23	123.41	120.30
8	S	84	ARG	NE-CZ-NH1	6.22	123.41	120.30
16	m	48	ARG	NE-CZ-NH1	6.21	123.41	120.30
3	G	267	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	117	TYR	CB-CG-CD2	-6.20	117.28	121.00
10	a	179	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	C	338	ARG	NE-CZ-NH1	-6.18	117.21	120.30
13	d	293	ARG	NE-CZ-NH1	6.15	123.37	120.30
10	a	120	ARG	NE-CZ-NH1	6.14	123.37	120.30
11	b	200	ARG	NE-CZ-NH1	6.13	123.37	120.30
8	Q	93	ARG	NE-CZ-NH1	6.13	123.36	120.30
10	a	768	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	F	287	TYR	CB-CG-CD2	-6.12	117.33	121.00
11	b	129	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	323	ARG	NE-CZ-NH1	6.09	123.35	120.30
3	G	259	ARG	NE-CZ-NH1	6.09	123.34	120.30
2	F	506	ARG	NE-CZ-NH1	6.07	123.34	120.30
10	a	279	ARG	NE-CZ-NH1	6.07	123.34	120.30
10	a	66	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	571	ARG	NE-CZ-NH1	6.04	123.32	120.30
7	N	32	ARG	NE-CZ-NH1	6.04	123.32	120.30
3	G	164	ARG	NE-CZ-NH1	6.04	123.32	120.30
5	J	222	ARG	NE-CZ-NH2	-6.02	117.29	120.30
5	J	135	ARG	NE-CZ-NH1	6.01	123.31	120.30
10	a	63	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	377	TYR	CB-CG-CD2	-6.00	117.40	121.00
2	D	314	ARG	NE-CZ-NH1	6.00	123.30	120.30
5	J	212	ARG	NE-CZ-NH1	6.00	123.30	120.30
9	U	100	TYR	CB-CG-CD2	-5.99	117.41	121.00
2	F	320	ARG	NE-CZ-NH1	5.98	123.29	120.30
8	R	265	ARG	NE-CZ-NH1	5.96	123.28	120.30
5	I	87	ARG	NE-CZ-NH1	5.95	123.28	120.30
12	c	448	ARG	NE-CZ-NH1	5.95	123.28	120.30
8	Q	265	ARG	NE-CZ-NH1	5.95	123.27	120.30
8	Q	84	ARG	NE-CZ-NH1	5.93	123.27	120.30
12	c	338	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	D	67	ARG	NE-CZ-NH1	5.93	123.27	120.30
9	T	72	ARG	NE-CZ-NH1	5.92	123.26	120.30
5	J	131	ARG	NE-CZ-NH1	5.91	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	87	ARG	NE-CZ-NH1	5.91	123.26	120.30
3	G	301	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	388	ARG	NE-CZ-NH2	5.89	123.25	120.30
9	T	192	ARG	NE-CZ-NH1	5.89	123.24	120.30
2	E	67	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	F	208	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	104	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	120	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	359	ARG	NE-CZ-NH1	5.82	123.21	120.30
10	a	73	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	232	ARG	NE-CZ-NH1	5.81	123.20	120.30
5	J	199	ARG	NE-CZ-NH1	5.81	123.20	120.30
16	n	48	ARG	NE-CZ-NH2	-5.80	117.40	120.30
5	I	212	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	553	ARG	NE-CZ-NH1	5.79	123.19	120.30
5	J	50	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	359	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	391	ARG	NE-CZ-NH1	5.77	123.18	120.30
2	F	308	ARG	NE-CZ-NH1	5.76	123.18	120.30
9	U	77	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	D	386	ARG	NE-CZ-NH1	5.75	123.17	120.30
6	L	79	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	215	ARG	NE-CZ-NH1	5.75	123.17	120.30
16	g	126	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	280	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	552	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	291	PHE	CB-CG-CD2	-5.73	116.79	120.80
9	T	179	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	E	185	ARG	NE-CZ-NH1	5.70	123.15	120.30
8	R	61	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	E	337	ARG	NE-CZ-NH1	5.68	123.14	120.30
13	d	102	TYR	CB-CG-CD2	-5.67	117.60	121.00
4	H	179	ARG	NE-CZ-NH1	5.66	123.13	120.30
7	O	92	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	323	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
2	E	276	ARG	NE-CZ-NH1	5.65	123.12	120.30
16	g	48	ARG	NE-CZ-NH2	-5.64	117.48	120.30
7	O	17	ARG	NE-CZ-NH1	5.63	123.11	120.30
7	M	107	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	552	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	338	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	56	ARG	NE-CZ-NH1	5.60	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	61	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	D	185	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	A	552	ARG	NE-CZ-NH2	-5.59	117.51	120.30
12	c	260	ARG	NE-CZ-NH1	5.58	123.09	120.30
16	m	144	TYR	CB-CG-CD2	-5.57	117.66	121.00
2	F	271	ARG	NE-CZ-NH1	5.56	123.08	120.30
11	b	34	ARG	NE-CZ-NH1	5.55	123.07	120.30
16	j	48	ARG	NE-CZ-NH2	-5.54	117.53	120.30
9	U	101	ARG	NE-CZ-NH1	5.53	123.06	120.30
5	K	50	ARG	NE-CZ-NH1	5.52	123.06	120.30
7	N	51	ARG	NE-CZ-NH1	5.52	123.06	120.30
13	d	218	ARG	NE-CZ-NH1	5.50	123.05	120.30
5	J	222	ARG	NE-CZ-NH1	5.49	123.04	120.30
3	G	249	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	400	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	E	412	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	215	ARG	NE-CZ-NH2	-5.47	117.57	120.30
11	b	135	TYR	CB-CG-CD2	-5.47	117.72	121.00
16	n	126	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	289	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	530	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	E	165	TYR	CB-CG-CD2	-5.44	117.73	121.00
3	G	201	TYR	CB-CG-CD1	-5.44	117.73	121.00
8	Q	61	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	D	381	ARG	NE-CZ-NH1	5.43	123.02	120.30
3	G	75	TYR	CB-CG-CD2	-5.42	117.75	121.00
5	K	212	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	388	ARG	NE-CZ-NH2	5.42	123.01	120.30
16	k	119	ARG	NE-CZ-NH1	5.42	123.01	120.30
10	a	177	ARG	NE-CZ-NH1	5.39	123.00	120.30
13	d	237	ARG	NE-CZ-NH1	5.39	122.99	120.30
7	M	115	ARG	NE-CZ-NH1	5.38	122.99	120.30
10	a	38	ARG	NE-CZ-NH1	5.37	122.99	120.30
7	N	87	TYR	CB-CG-CD2	-5.37	117.78	121.00
7	O	87	TYR	CB-CG-CD2	-5.35	117.79	121.00
7	O	107	ARG	NE-CZ-NH1	5.35	122.97	120.30
5	I	222	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	212	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	E	141	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	D	386	ARG	NE-CZ-NH2	5.31	122.95	120.30
2	D	471	ARG	NE-CZ-NH1	5.30	122.95	120.30
7	N	107	ARG	NE-CZ-NH1	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	242	ARG	NE-CZ-NH1	5.28	122.94	120.30
7	N	17	ARG	NE-CZ-NH1	5.27	122.94	120.30
5	J	80	ARG	NE-CZ-NH1	5.27	122.94	120.30
16	k	68	TYR	CB-CG-CD2	-5.26	117.84	121.00
16	h	68	TYR	CB-CG-CD2	-5.25	117.85	121.00
16	m	119	ARG	NE-CZ-NH1	5.25	122.92	120.30
16	i	119	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	215	ARG	NE-CZ-NH1	5.23	122.92	120.30
5	I	125	TYR	CB-CG-CD2	-5.23	117.86	121.00
9	U	72	ARG	NE-CZ-NH1	5.22	122.91	120.30
9	U	179	ARG	NE-CZ-NH1	5.22	122.91	120.30
10	a	741	ARG	NE-CZ-NH1	5.22	122.91	120.30
4	H	13	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	274	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	B	274	TYR	CB-CG-CD1	-5.20	117.88	121.00
7	N	92	ARG	NE-CZ-NH1	5.20	122.90	120.30
9	T	84	ARG	NE-CZ-NH1	5.19	122.89	120.30
16	o	119	ARG	NE-CZ-NH1	5.19	122.89	120.30
9	T	131	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	328	TYR	CB-CG-CD2	-5.18	117.89	121.00
16	m	126	ARG	NE-CZ-NH1	5.17	122.89	120.30
13	d	327	ARG	NE-CZ-NH1	5.16	122.88	120.30
4	H	126	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	552	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	400	ARG	NE-CZ-NH1	5.13	122.86	120.30
4	H	30	ARG	NE-CZ-NH1	5.13	122.86	120.30
7	M	87	TYR	CB-CG-CD2	-5.13	117.92	121.00
7	M	26	ARG	NE-CZ-NH1	5.12	122.86	120.30
16	o	126	ARG	NE-CZ-NH1	5.11	122.85	120.30
15	f	62	TYR	CB-CG-CD1	5.10	124.06	121.00
2	D	337	ARG	NE-CZ-NH1	5.10	122.85	120.30
8	R	126	TYR	CB-CG-CD2	-5.09	117.94	121.00
4	H	6	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	F	192	PHE	CB-CG-CD2	-5.08	117.24	120.80
16	o	48	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	601	TYR	CB-CG-CD2	-5.07	117.96	121.00
5	I	137	ARG	NE-CZ-NH1	5.07	122.84	120.30
10	a	291	ARG	NE-CZ-NH1	5.07	122.83	120.30
7	O	32	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	D	386	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
10	a	660	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	171	ARG	NE-CZ-NH1	5.05	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	167	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	44	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	E	120	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	173	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	TYR	Sidechain
1	A	67	TYR	Sidechain
1	B	153	TYR	Sidechain
1	B	280	ARG	Sidechain
1	C	266	TYR	Sidechain
2	D	371	TYR	Sidechain
2	D	389	TYR	Sidechain
2	E	314	ARG	Sidechain
2	E	389	TYR	Sidechain
2	E	68	TYR	Sidechain
2	F	271	ARG	Sidechain
5	K	80	ARG	Sidechain
7	N	92	ARG	Sidechain
8	R	31	ARG	Sidechain
8	S	28	TYR	Sidechain
9	T	136	TYR	Sidechain
11	b	26	TYR	Sidechain
13	d	104	TYR	Sidechain
16	g	119	ARG	Sidechain
16	k	10	TYR	Sidechain
16	o	119	ARG	Sidechain
16	o	88	ARG	Sidechain
17	p	297	TYR	Sidechain

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	A	4651	0	4644	1	0
1	B	4666	0	4655	2	0
1	C	4657	0	4649	1	0
2	D	3603	0	3608	1	0
2	E	3576	0	3576	1	0
2	F	3604	0	3608	1	0
3	G	2919	0	2961	0	0
4	H	1760	0	1869	0	0
5	I	1808	0	1880	1	0
5	J	1808	0	1880	0	0
5	K	1808	0	1880	0	0
6	L	875	0	883	0	0
7	M	920	0	918	1	0
7	N	935	0	931	0	0
7	O	935	0	931	0	0
8	Q	2130	0	2168	0	0
8	R	2155	0	2201	1	0
8	S	2126	0	2165	2	0
9	T	1377	0	1315	0	0
9	U	1377	0	1315	1	0
10	a	6164	0	6197	0	0
11	b	1503	0	1551	0	0
12	c	1652	0	1584	0	0
13	d	2817	0	2756	0	0
14	e	623	0	641	0	0
15	f	652	0	647	0	0
16	g	1069	0	1136	0	0
16	h	1069	0	1136	0	0
16	i	1069	0	1136	0	0
16	j	1069	0	1136	0	0
16	k	1069	0	1136	0	0
16	l	1069	0	1136	0	0
16	m	1069	0	1136	0	0
16	n	1069	0	1136	0	0
16	o	1069	0	1136	0	0
17	p	423	0	416	0	0
18	B	27	0	12	0	0
All	All	71172	0	72065	11	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 0.

All (11) 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)
5:I:38:PHE:CD1	7:M:36:ALA:HB2	2.44	0.53
1:C:66:VAL:HG12	1:C:68:GLU:H	1.76	0.50
1:B:397:ASN:HB3	8:R:28:TYR:CG	2.52	0.44
2:D:233:ALA:HB1	2:D:236:VAL:HG21	2.02	0.42
9:U:110:VAL:HG21	9:U:129:PRO:HA	2.02	0.41
1:A:67:TYR:CE2	1:A:321:ALA:CB	3.02	0.41
2:F:97:GLN:HG2	2:F:269:ILE:HG21	2.03	0.41
1:B:337:PHE:CD2	1:B:340:MET:HE3	2.55	0.41
2:E:47:TYR:CE2	2:E:63:VAL:HA	2.55	0.40
8:S:151:PHE:CZ	8:S:200:PHE:HA	2.56	0.40
8:S:94:LEU:HD23	8:S:94:LEU:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/617 (97%)	562 (94%)	32 (5%)	4 (1%)	22	60
1	B	600/617 (97%)	563 (94%)	37 (6%)	0	100	100
1	C	599/617 (97%)	572 (96%)	27 (4%)	0	100	100
2	D	456/511 (89%)	423 (93%)	33 (7%)	0	100	100
2	E	453/511 (89%)	430 (95%)	23 (5%)	0	100	100
2	F	456/511 (89%)	438 (96%)	18 (4%)	0	100	100
3	G	354/382 (93%)	341 (96%)	12 (3%)	1 (0%)	41	75
4	H	216/247 (87%)	210 (97%)	6 (3%)	0	100	100
5	I	221/226 (98%)	217 (98%)	4 (2%)	0	100	100
5	J	221/226 (98%)	214 (97%)	7 (3%)	0	100	100
5	K	221/226 (98%)	215 (97%)	6 (3%)	0	100	100
6	L	108/119 (91%)	102 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	110/118 (93%)	110 (100%)	0	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	262/301 (87%)	254 (97%)	8 (3%)	0	100	100
8	R	265/301 (88%)	257 (97%)	8 (3%)	0	100	100
8	S	261/301 (87%)	254 (97%)	7 (3%)	0	100	100
9	T	168/171 (98%)	159 (95%)	8 (5%)	1 (1%)	25	63
9	U	168/171 (98%)	159 (95%)	8 (5%)	1 (1%)	25	63
10	a	751/838 (90%)	709 (94%)	39 (5%)	3 (0%)	34	71
11	b	201/205 (98%)	194 (96%)	7 (4%)	0	100	100
12	c	202/463 (44%)	189 (94%)	11 (5%)	2 (1%)	15	52
13	d	346/351 (99%)	336 (97%)	10 (3%)	0	100	100
14	e	75/81 (93%)	75 (100%)	0	0	100	100
15	f	82/98 (84%)	80 (98%)	2 (2%)	0	100	100
16	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	h	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	i	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
16	j	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	k	148/155 (96%)	148 (100%)	0	0	100	100
16	l	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	m	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
16	n	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	o	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
17	p	49/350 (14%)	48 (98%)	1 (2%)	0	100	100
All	All	8999/10190 (88%)	8646 (96%)	341 (4%)	12 (0%)	54	84

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	a	487	ILE
1	A	389	ALA
3	G	250	ASP
12	c	353	SER
10	a	619	PHE

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Mol	Chain	Res	Type
1	A	372	SER
9	T	176	GLY
9	U	204	LEU
10	a	92	ARG
12	c	345	GLY
1	A	278	GLY
1	A	434	GLY

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%)	503 (99%)	4 (1%)	81	89
1	B	509/524 (97%)	505 (99%)	4 (1%)	81	89
1	C	508/524 (97%)	504 (99%)	4 (1%)	81	89
2	D	394/431 (91%)	393 (100%)	1 (0%)	92	95
2	E	391/431 (91%)	390 (100%)	1 (0%)	92	95
2	F	394/431 (91%)	392 (100%)	2 (0%)	88	93
3	G	325/344 (94%)	323 (99%)	2 (1%)	86	91
4	H	189/212 (89%)	189 (100%)	0	100	100
5	I	196/198 (99%)	196 (100%)	0	100	100
5	J	196/198 (99%)	196 (100%)	0	100	100
5	K	196/198 (99%)	196 (100%)	0	100	100
6	L	94/100 (94%)	94 (100%)	0	100	100
7	M	97/101 (96%)	97 (100%)	0	100	100
7	N	99/101 (98%)	99 (100%)	0	100	100
7	O	99/101 (98%)	99 (100%)	0	100	100
8	Q	241/274 (88%)	241 (100%)	0	100	100
8	R	244/274 (89%)	244 (100%)	0	100	100
8	S	241/274 (88%)	241 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	T	148/148 (100%)	148 (100%)	0	100	100
9	U	148/148 (100%)	148 (100%)	0	100	100
10	a	674/743 (91%)	674 (100%)	0	100	100
11	b	156/158 (99%)	156 (100%)	0	100	100
12	c	182/395 (46%)	181 (100%)	1 (0%)	88	93
13	d	303/306 (99%)	302 (100%)	1 (0%)	92	95
14	e	65/68 (96%)	65 (100%)	0	100	100
15	f	70/83 (84%)	70 (100%)	0	100	100
16	g	109/113 (96%)	109 (100%)	0	100	100
16	h	109/113 (96%)	109 (100%)	0	100	100
16	i	109/113 (96%)	109 (100%)	0	100	100
16	j	109/113 (96%)	109 (100%)	0	100	100
16	k	109/113 (96%)	109 (100%)	0	100	100
16	l	109/113 (96%)	108 (99%)	1 (1%)	78	87
16	m	109/113 (96%)	109 (100%)	0	100	100
16	n	109/113 (96%)	109 (100%)	0	100	100
16	o	109/113 (96%)	108 (99%)	1 (1%)	78	87
17	p	46/313 (15%)	46 (100%)	0	100	100
All	All	7693/8619 (89%)	7671 (100%)	22 (0%)	92	95

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	MET
1	A	284	MET
1	A	324	GLU
1	A	471	GLU
1	B	173	ARG
1	B	256	LYS
1	B	306	MET
1	B	381	ARG
1	C	173	ARG
1	C	256	LYS
1	C	400	ARG
1	C	430	GLN
2	D	359	ASP

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Mol	Chain	Res	Type
2	E	106	ASP
2	F	106	ASP
2	F	359	ASP
3	G	229	LEU
3	G	379	LEU
12	c	298	ASP
13	d	24	LYS
16	l	139	GLU
16	o	61	MET

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

Mol	Chain	Res	Type
2	E	199	HIS
12	c	364	HIS
13	d	340	HIS
16	j	6	ASN
16	m	6	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
18	ADP	B	801	-	24,29,29	1.27	2 (8%)	29,45,45	1.50	5 (17%)

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
18	ADP	B	801	-	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	801	ADP	O4'-C1'	3.45	1.45	1.41
18	B	801	ADP	C5-C4	-2.17	1.35	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	801	ADP	C4-C5-N7	4.45	114.04	109.40
18	B	801	ADP	PA-O3A-PB	-2.75	123.40	132.83
18	B	801	ADP	O2B-PB-O3A	2.69	113.64	104.64
18	B	801	ADP	C2-N1-C6	-2.41	114.63	118.75
18	B	801	ADP	O3B-PB-O1B	-2.06	102.62	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

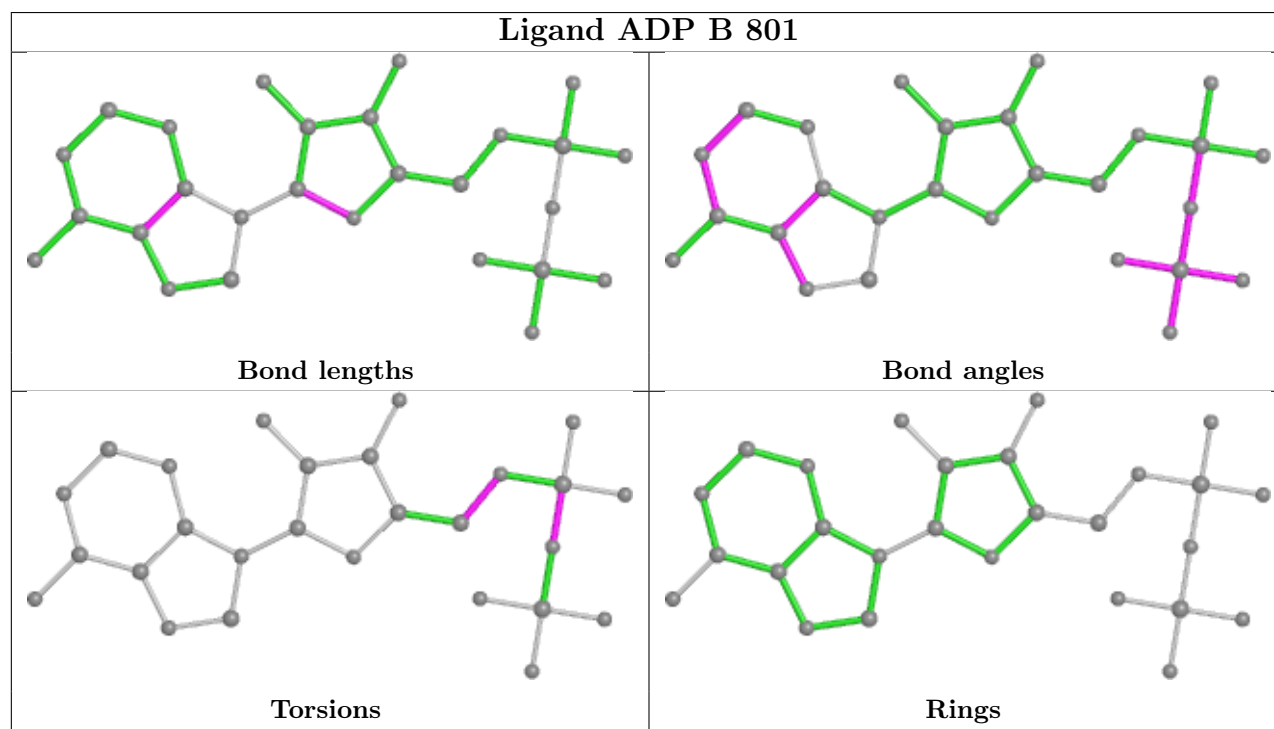
Mol	Chain	Res	Type	Atoms
18	B	801	ADP	PB-O3A-PA-O1A
18	B	801	ADP	C4'-C5'-O5'-PA
18	B	801	ADP	PB-O3A-PA-O2A

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 than 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.

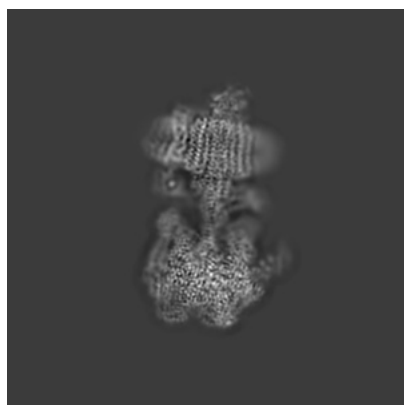
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26912. These allow visual inspection of the internal detail of the map and identification of artifacts.

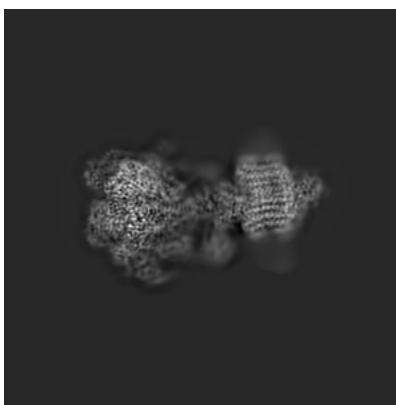
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

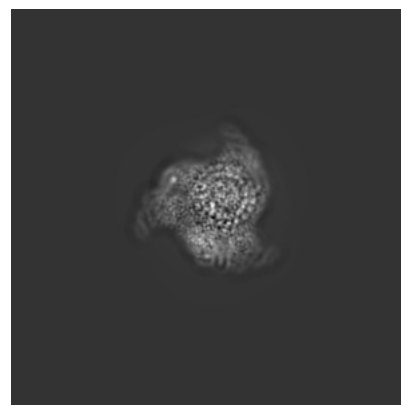
6.1.1 Primary map



X



Y



Z

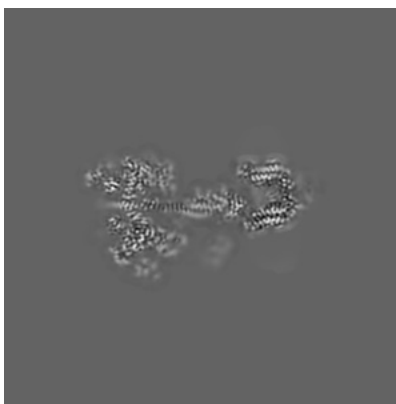
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

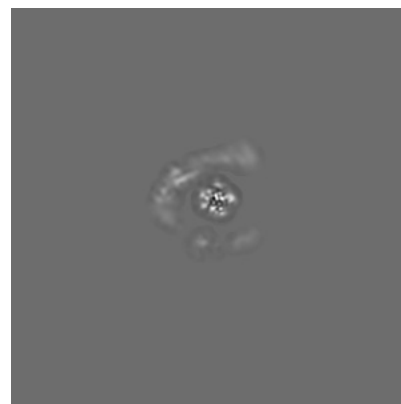
6.2.1 Primary map



X Index: 170



Y Index: 170

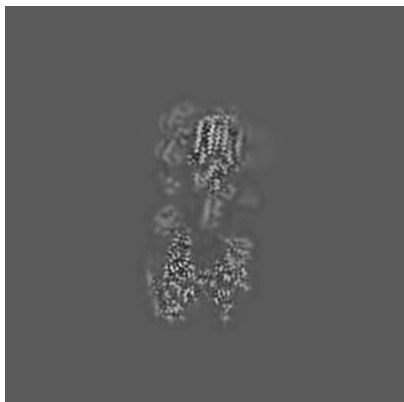


Z Index: 170

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

6.3 Largest variance slices [i](#)

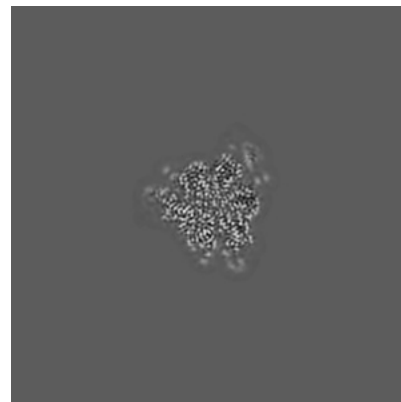
6.3.1 Primary map



X Index: 163



Y Index: 173

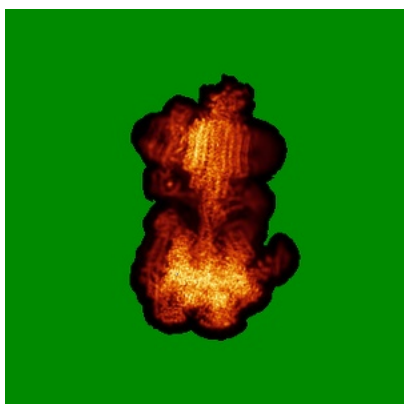


Z Index: 109

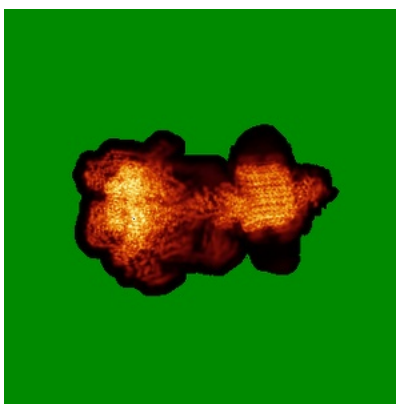
The images above show the largest variance slices of the map in three orthogonal directions.

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

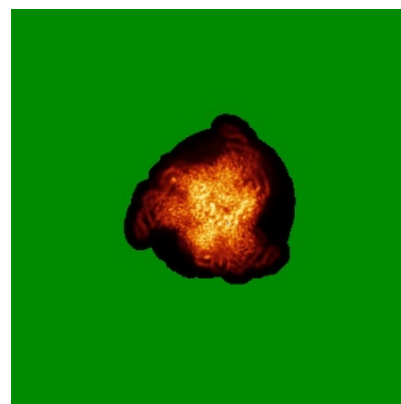
6.4.1 Primary map



X



Y



Z

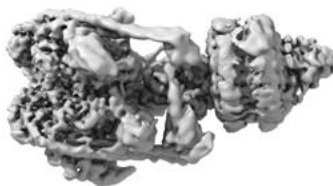
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

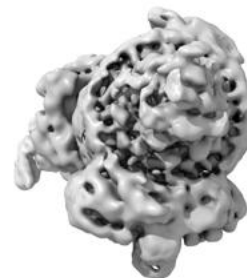
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

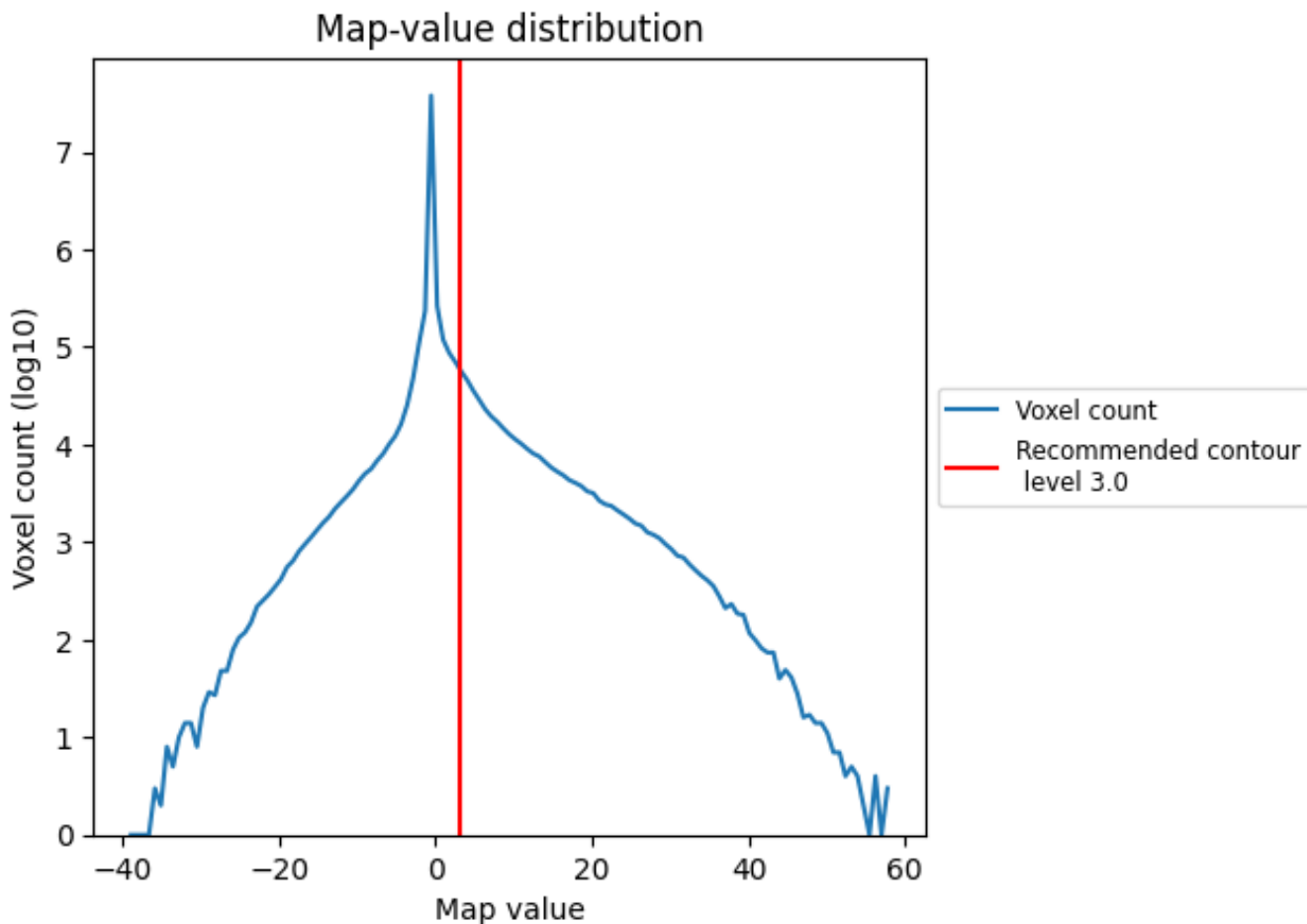
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

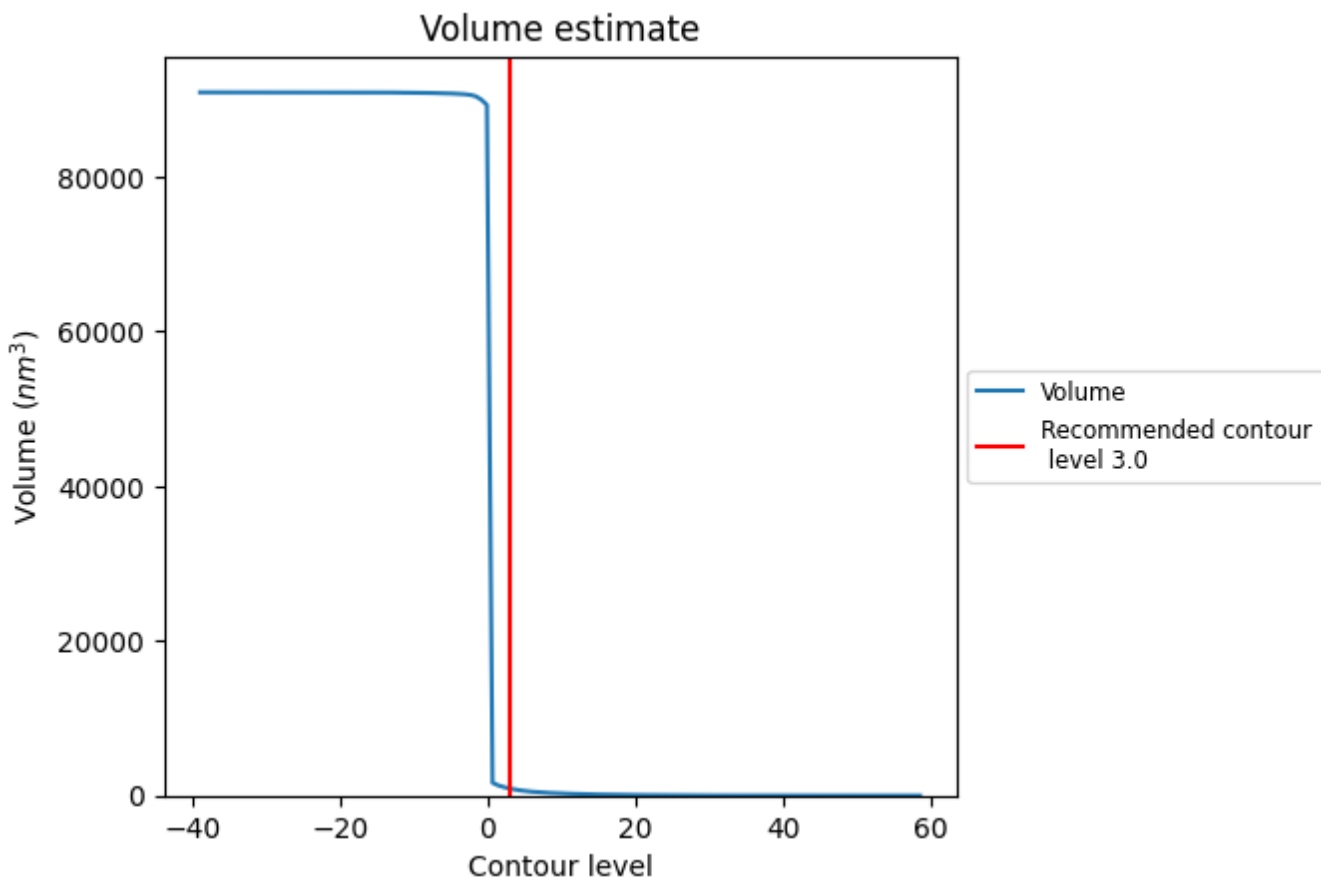
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

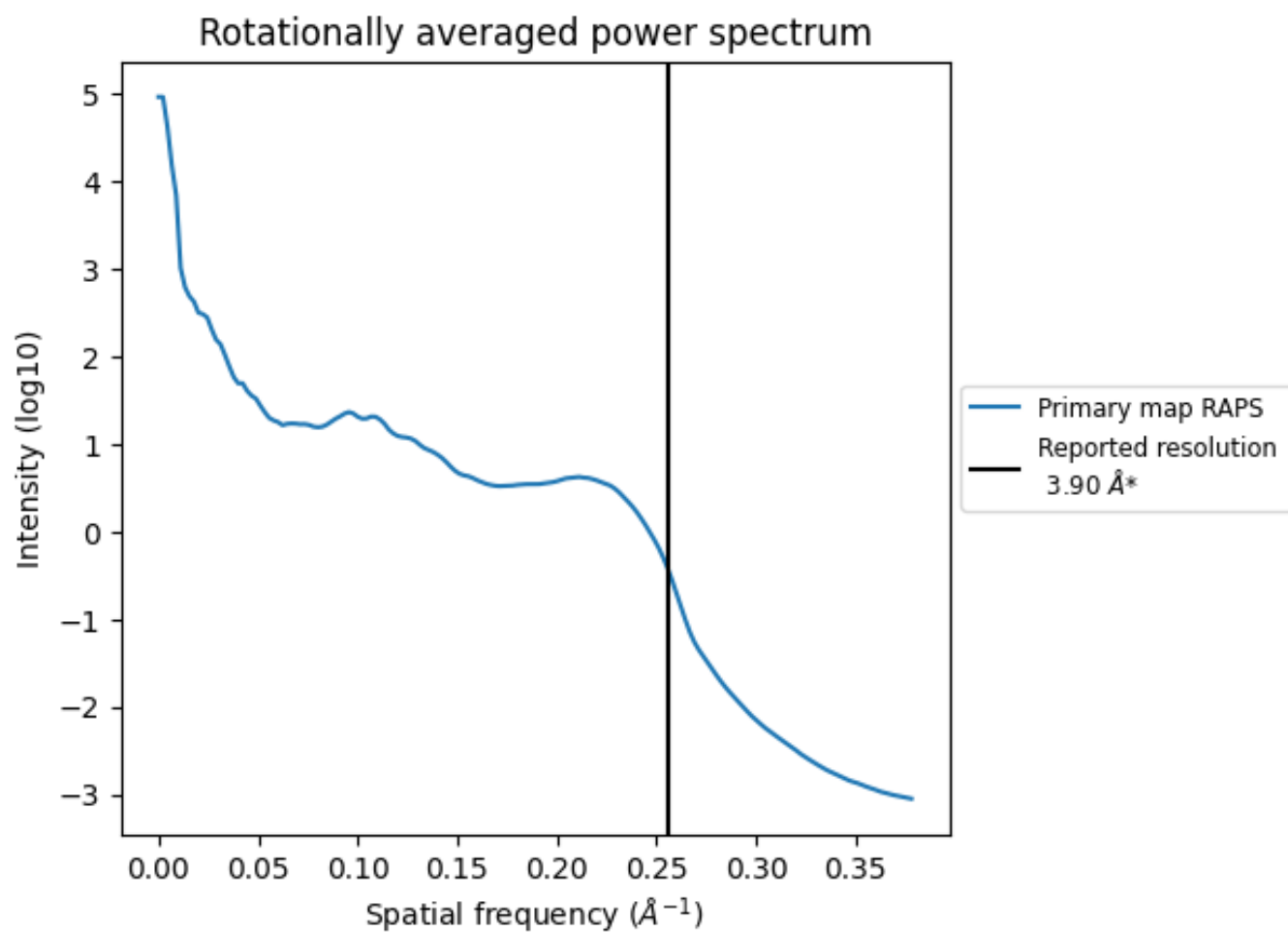
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 911 nm³; this corresponds to an approximate mass of 823 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 0.256 Å⁻¹

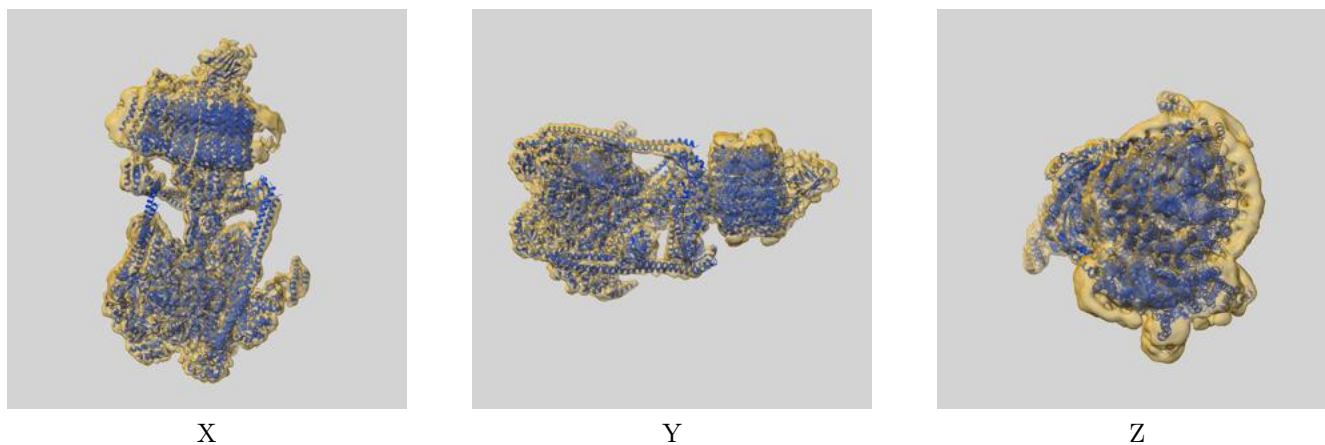
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

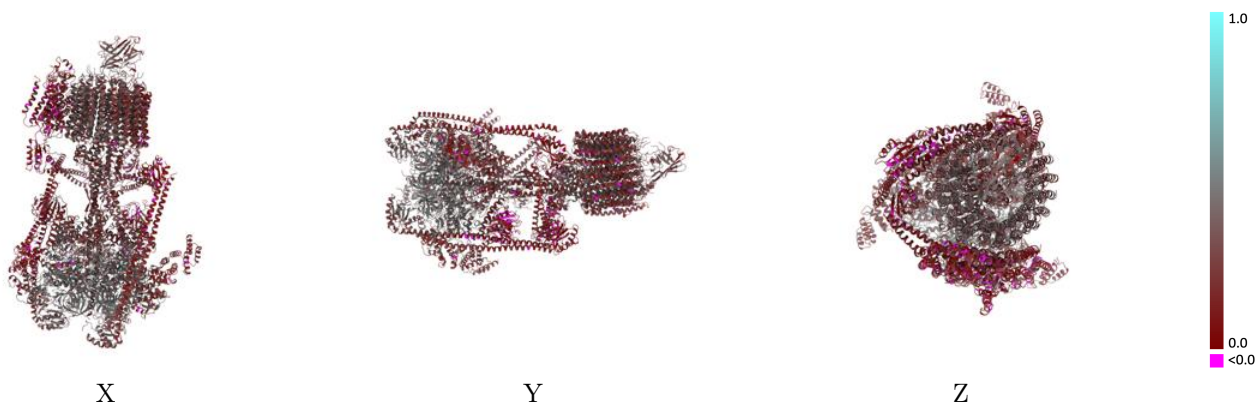
This section contains information regarding the fit between EMDB map EMD-26912 and PDB model 7UZI. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



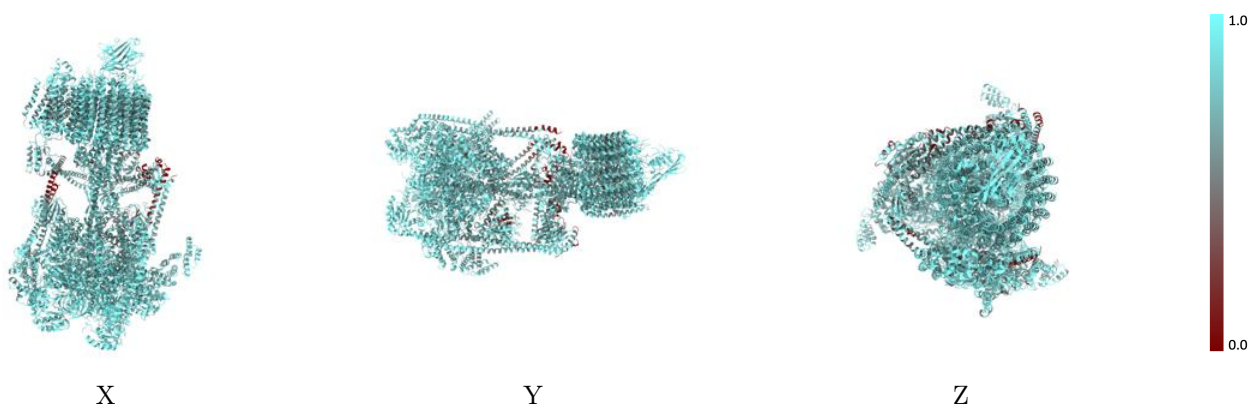
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



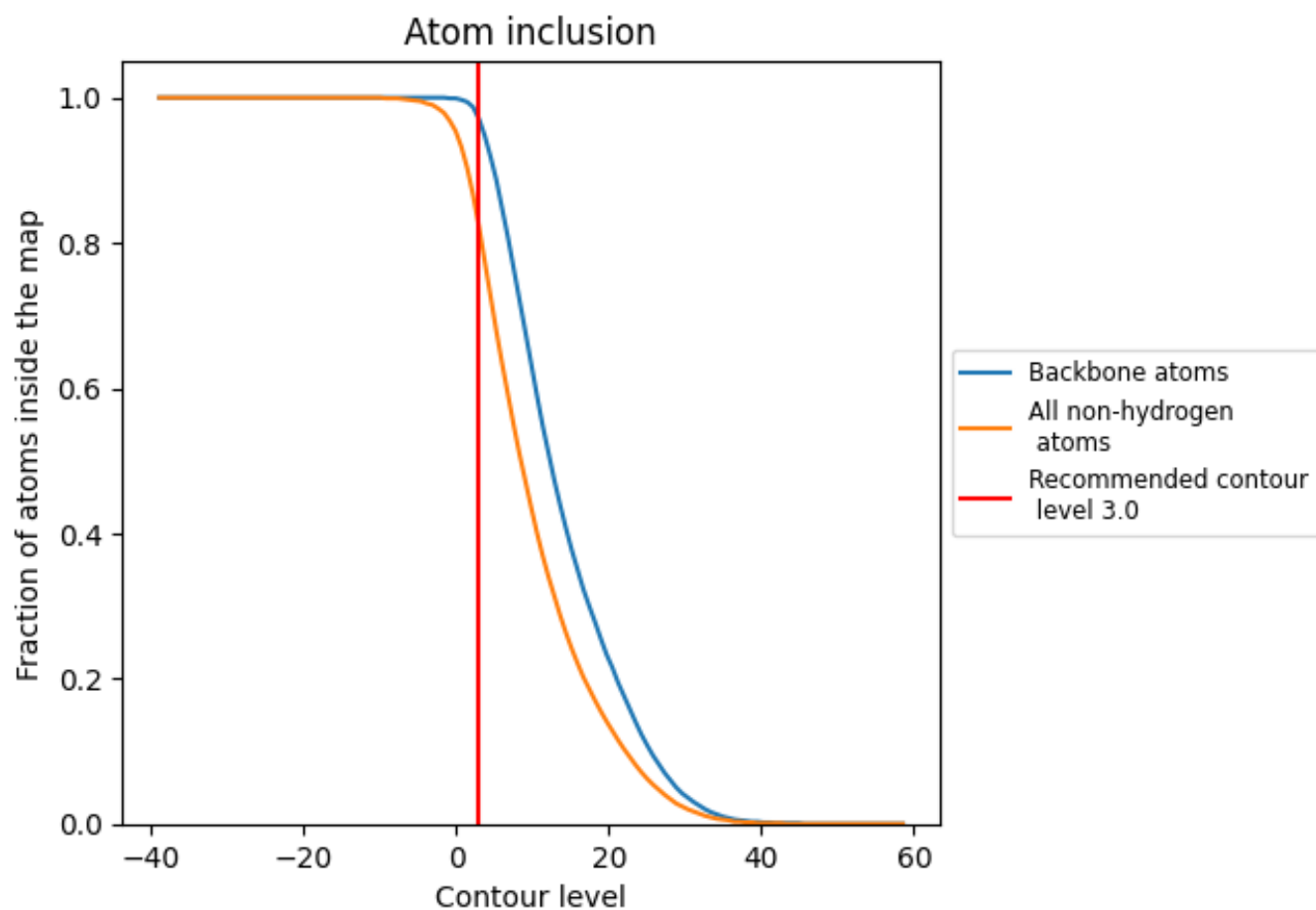
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 82% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.2930
A	 0.8570	 0.3600
B	 0.8770	 0.3880
C	 0.8740	 0.3770
D	 0.9030	 0.4380
E	 0.8750	 0.3930
F	 0.8810	 0.3930
G	 0.6200	 0.1280
H	 0.8240	 0.3060
I	 0.7650	 0.2780
J	 0.8250	 0.2680
K	 0.7840	 0.2670
L	 0.8190	 0.2660
M	 0.7170	 0.2070
N	 0.8160	 0.2120
O	 0.8030	 0.2190
Q	 0.8110	 0.2220
R	 0.8030	 0.2140
S	 0.7810	 0.2080
T	 0.8390	 0.2100
U	 0.6620	 0.1000
a	 0.7490	 0.1440
b	 0.8270	 0.3090
c	 0.8930	 0.3290
d	 0.8330	 0.3200
e	 0.7830	 0.1630
f	 0.8200	 0.1270
g	 0.7930	 0.2650
h	 0.7680	 0.2400
i	 0.7960	 0.2560
j	 0.8160	 0.2870
k	 0.8620	 0.3370
l	 0.8770	 0.3720
m	 0.8470	 0.3650
n	 0.8590	 0.3660



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Chain	Atom inclusion	Q-score
o	 0.8840	 0.3780
p	 0.8500	 0.3230