



Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 03:52 PM EST

PDB ID : 7UZF
EMDB ID : EMD-26909
Title : Rat Kidney V-ATPase with SidK, State 1
Authors : Rubinstein, J.L.; Abbas, Y.M.
Deposited on : 2022-05-09
Resolution : 3.80 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

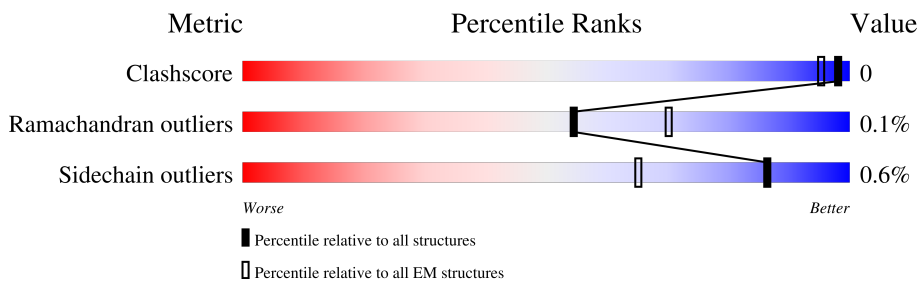
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	

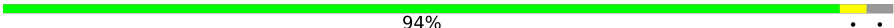

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Mol	Chain	Length	Quality of chain
5	I	226	93% 5%
5	J	226	94% 5%
5	K	226	18% 95%
6	L	119	89% 8%
7	M	118	88% 7% 5%
7	N	118	90% 7%
7	O	118	25% 92%
8	P	483	87% 11%
9	Q	280	91% 6%
9	R	280	92% 6%
9	S	280	93% 5%
10	a	838	88% 10%
11	b	205	94%
12	c	463	43% 56%
13	d	351	94%
14	e	81	6% 95% 5%
15	f	98	7% 85% 14%
16	g	155	94%
16	h	155	94%
16	i	155	94%
16	j	155	94%
16	k	155	96%
16	l	155	95%
16	m	155	94%
16	n	155	95%

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Mol	Chain	Length	Quality of chain
16	o	155	 94%
17	p	350	 14% 85%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 71930 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	597	Total	C	N	O	S	0	0
			4632	2936	783	887	26		
1	B	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	C	602	Total	C	N	O	S	0	0
			4666	2957	788	894	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
			3604	2287	614	683	20		
2	E	460	Total	C	N	O	S	0	0
			3603	2286	615	682	20		
2	F	457	Total	C	N	O	S	0	0
			3576	2269	610	677	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	P	431	Total	C	N	O	S	0	0
			3537	2243	610	658	26		

- Molecule 9 is a protein called Effector SidK.

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

- 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

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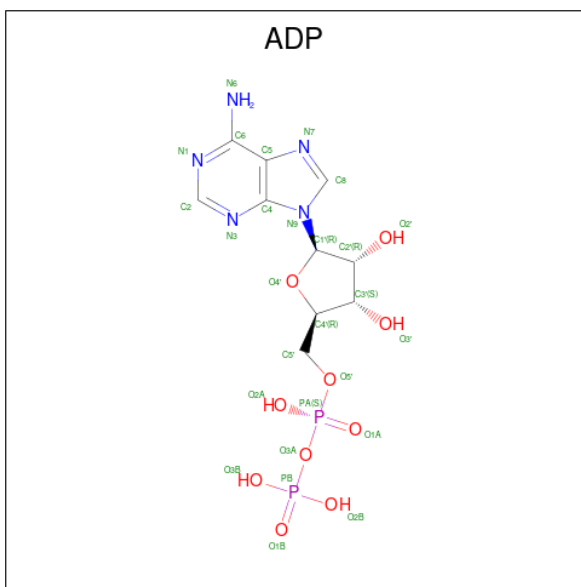
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	i	150	Total 1069	C 699	N 171	O 191	S 8	0	0
16	j	150	Total 1069	C 699	N 171	O 191	S 8	0	0
16	k	150	Total 1069	C 699	N 171	O 191	S 8	0	0
16	l	150	Total 1069	C 699	N 171	O 191	S 8	0	0
16	m	150	Total 1069	C 699	N 171	O 191	S 8	0	0
16	n	150	Total 1069	C 699	N 171	O 191	S 8	0	0
16	o	150	Total 1069	C 699	N 171	O 191	S 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	Total 423	C 284	N 62	O 75	S 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).

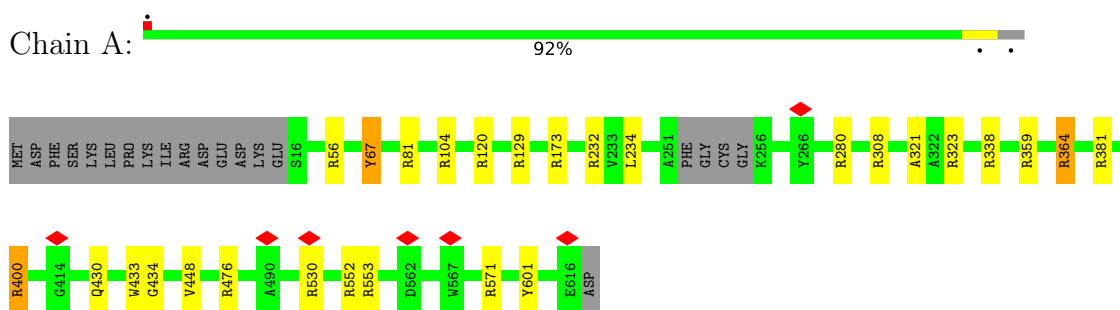


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	C	1	Total 27	C 10	N 5	O 10	P 2	0

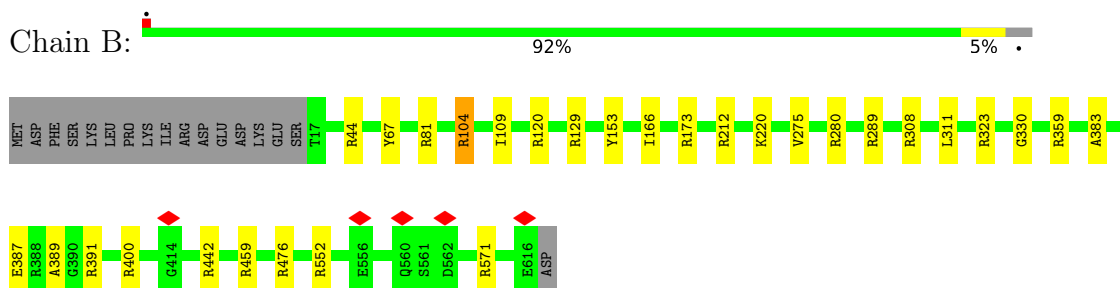
3 Residue-property plots [i](#)

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.

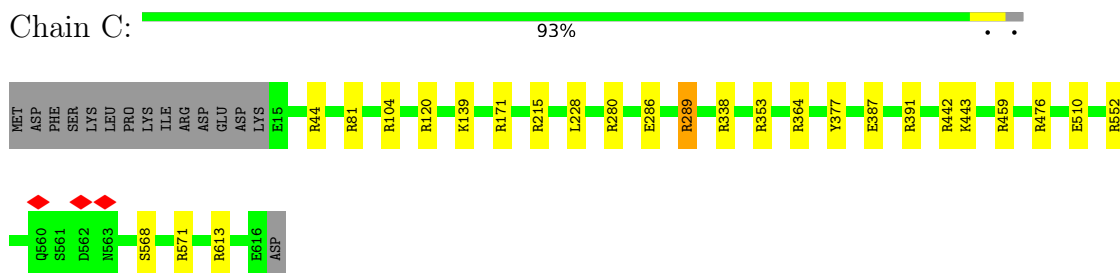
- Molecule 1: ATPase H⁺-transporting V1 subunit A



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

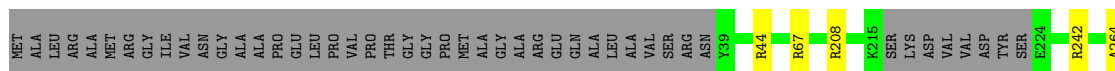


- Molecule 1: ATPase H⁺-transporting V1 subunit A

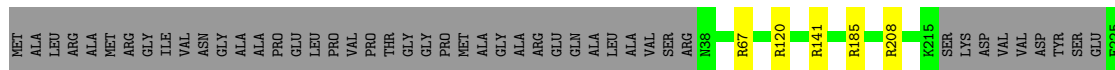


- Molecule 2: V-type proton ATPase subunit B, brain isoform

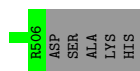
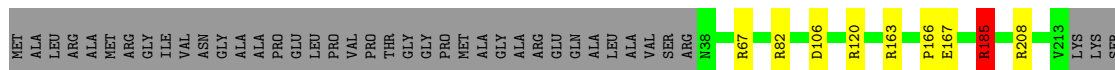
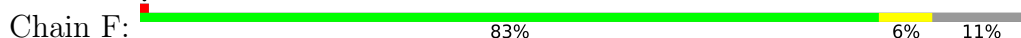




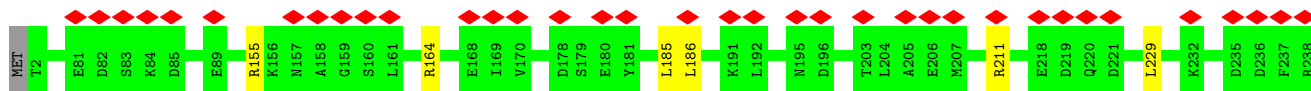
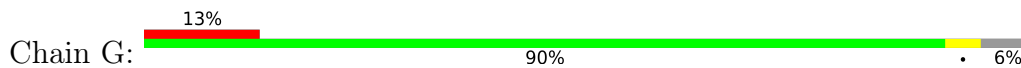
• Molecule 2: V-type proton ATPase subunit B, brain isoform



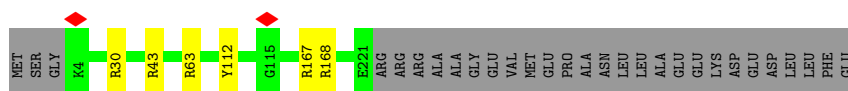
• Molecule 2: V-type proton ATPase subunit B, brain isoform



• 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:  93% 5%



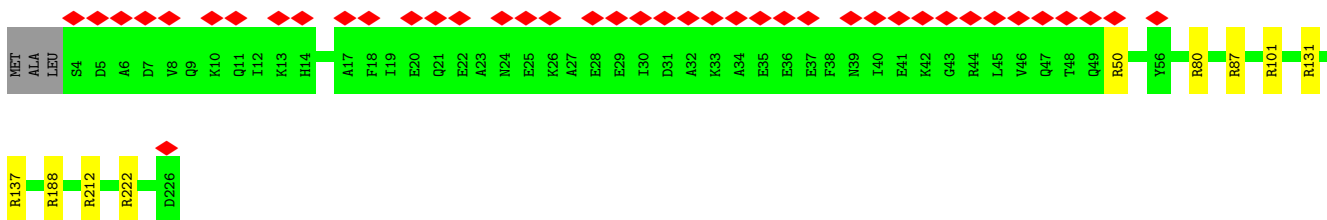
• Molecule 5: V-type proton ATPase subunit E 1

Chain J:  94% 5%



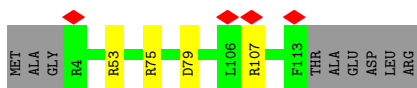
• Molecule 5: V-type proton ATPase subunit E 1

Chain K:  18% 95%




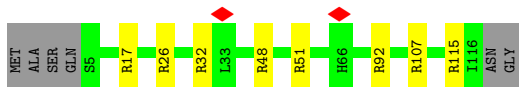
• Molecule 6: V-type proton ATPase subunit F

Chain L:  89% 8%



• Molecule 7: V-type proton ATPase subunit G

Chain M:  88% 7% 5%

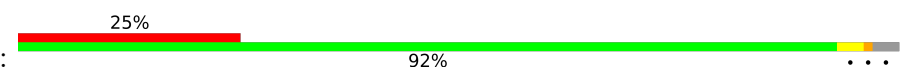


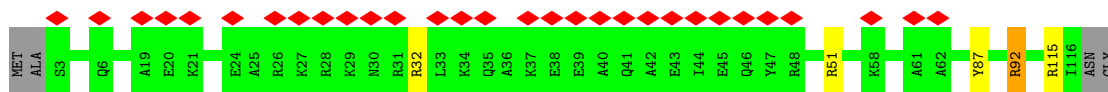
• Molecule 7: V-type proton ATPase subunit G

Chain N:  90% 7%

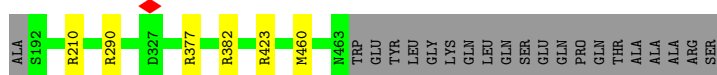
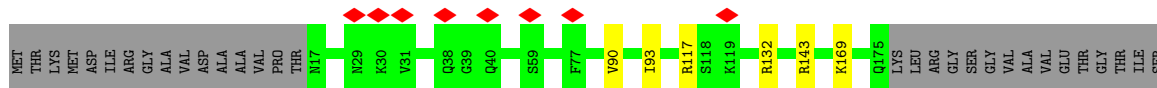
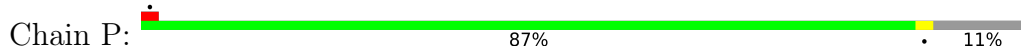


• Molecule 7: V-type proton ATPase subunit G

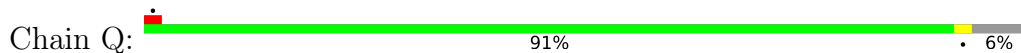
Chain O:  25% 92%



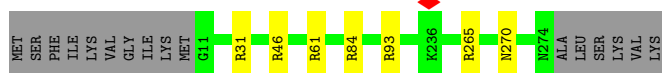
• Molecule 8: V-type proton ATPase subunit H



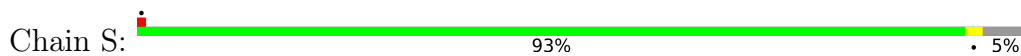
• Molecule 9: Effector SidK



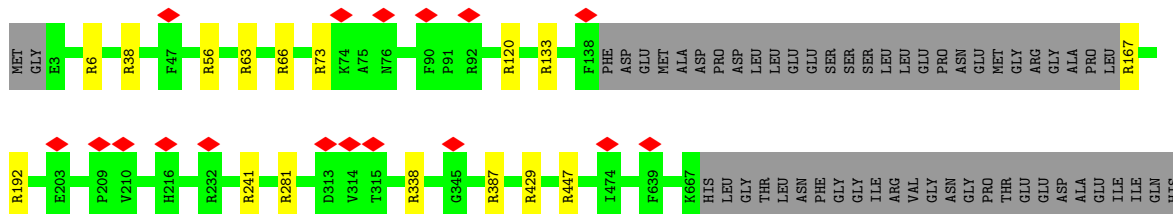
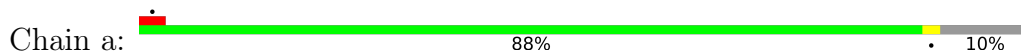
• Molecule 9: Effector SidK



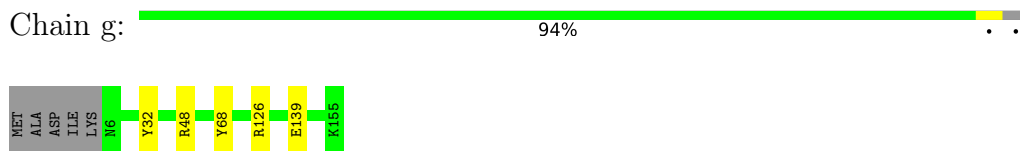
• Molecule 9: Effector SidK



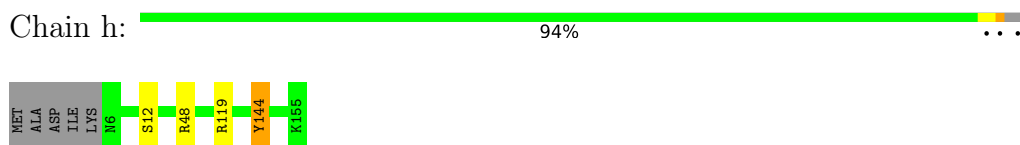
• Molecule 10: V-type proton ATPase 116 kDa subunit a isoform 1



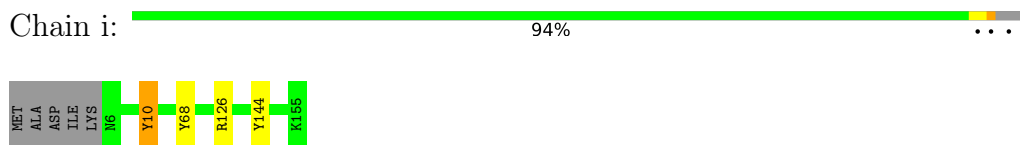
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



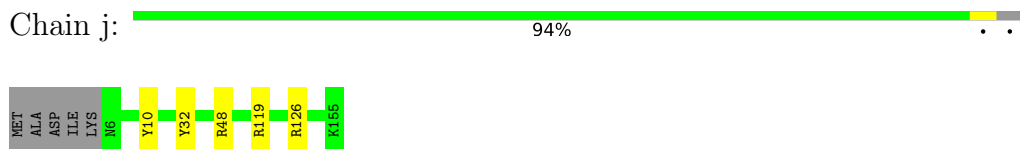
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



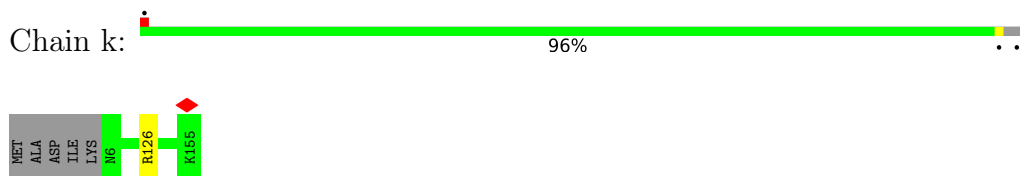
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



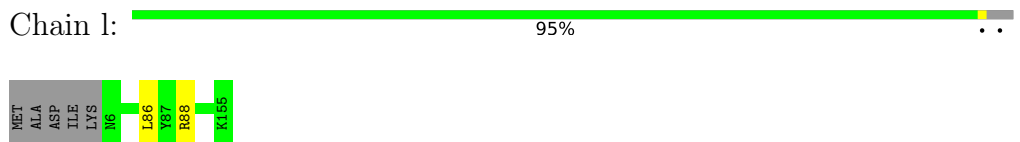
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



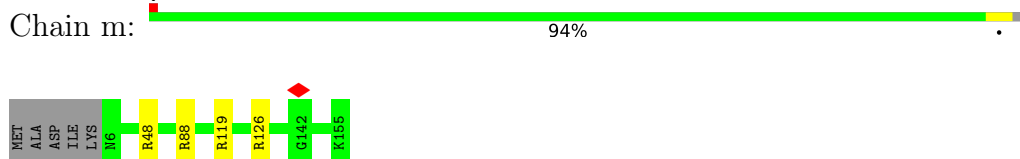
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45083	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	70.456	Depositor
Minimum map value	-45.496	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.338	Depositor
Recommended contour level	4.0	Depositor
Map size (\AA)	449.65, 449.65, 449.65	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.65	0/4725	0.98	19/6396 (0.3%)
1	B	0.65	0/4746	0.99	21/6425 (0.3%)
1	C	0.64	0/4761	0.97	17/6445 (0.3%)
2	D	0.65	0/3675	0.96	9/4979 (0.2%)
2	E	0.65	0/3674	1.01	18/4978 (0.4%)
2	F	0.65	0/3647	0.99	18/4944 (0.4%)
3	G	0.67	0/2973	0.92	9/4016 (0.2%)
4	H	0.62	0/1778	0.92	6/2377 (0.3%)
5	I	0.61	0/1825	0.94	10/2442 (0.4%)
5	J	0.62	0/1825	0.90	6/2442 (0.2%)
5	K	0.62	0/1825	0.92	9/2442 (0.4%)
6	L	0.64	0/889	0.99	5/1199 (0.4%)
7	M	0.66	0/928	1.00	10/1236 (0.8%)
7	N	0.65	0/943	0.95	9/1256 (0.7%)
7	O	0.67	0/943	0.97	6/1256 (0.5%)
8	P	0.67	0/3604	0.92	8/4854 (0.2%)
9	Q	0.61	0/2160	0.90	6/2910 (0.2%)
9	R	0.61	0/2164	0.87	6/2915 (0.2%)
9	S	0.62	0/2189	0.91	6/2947 (0.2%)
10	a	0.69	0/6322	0.93	17/8551 (0.2%)
11	b	0.62	0/1537	1.00	7/2088 (0.3%)
12	c	0.67	0/1707	0.98	4/2324 (0.2%)
13	d	0.65	0/2882	0.99	16/3903 (0.4%)
14	e	0.72	0/648	0.94	0/891
15	f	0.70	0/668	0.84	1/907 (0.1%)
16	g	0.60	0/1084	0.96	4/1466 (0.3%)
16	h	0.61	0/1084	0.92	3/1466 (0.2%)
16	i	0.58	0/1084	0.91	3/1466 (0.2%)
16	j	0.61	0/1084	0.92	3/1466 (0.2%)
16	k	0.60	0/1084	0.87	1/1466 (0.1%)
16	l	0.60	0/1084	0.87	1/1466 (0.1%)
16	m	0.62	0/1084	0.92	4/1466 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	n	0.62	0/1084	0.96	4/1466 (0.3%)
16	o	0.61	0/1084	0.93	2/1466 (0.1%)
17	p	0.73	0/436	1.04	0/598
All	All	0.64	0/73230	0.95	268/98915 (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	C	0	3
2	D	0	1
2	E	0	1
2	F	0	3
5	J	0	2
5	K	0	1
7	O	0	1
10	a	0	1
11	b	0	2
13	d	0	2
16	g	0	1
16	h	0	1
16	i	0	1
16	j	0	1
16	o	0	2
17	p	0	1
All	All	0	26

There are no bond length outliers.

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	93	ARG	NE-CZ-NH2	10.01	125.30	120.30
1	C	81	ARG	NE-CZ-NH2	9.79	125.20	120.30
1	B	308	ARG	NE-CZ-NH2	9.34	124.97	120.30
2	E	185	ARG	NE-CZ-NH2	8.98	124.79	120.30
2	E	321	ARG	NE-CZ-NH2	8.79	124.69	120.30
5	K	80	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	129	ARG	NE-CZ-NH2	8.26	124.43	120.30
9	R	93	ARG	NE-CZ-NH2	8.22	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	93	ARG	NE-CZ-NH2	8.20	124.40	120.30
6	L	107	ARG	NE-CZ-NH2	8.19	124.39	120.30
9	S	46	ARG	NE-CZ-NH2	8.16	124.38	120.30
2	E	141	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	B	120	ARG	NE-CZ-NH2	7.86	124.23	120.30
5	I	131	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	B	67	TYR	CB-CG-CD2	-7.81	116.31	121.00
13	d	182	ARG	NE-CZ-NH2	7.81	124.21	120.30
2	E	344	ARG	NE-CZ-NH2	7.74	124.17	120.30
10	a	447	ARG	NE-CZ-NH2	7.72	124.16	120.30
5	K	131	ARG	NE-CZ-NH2	7.71	124.16	120.30
7	M	48	ARG	NE-CZ-NH2	7.69	124.14	120.30
7	M	26	ARG	NE-CZ-NH2	7.66	124.13	120.30
7	O	32	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	F	400	ARG	NE-CZ-NH2	7.59	124.09	120.30
7	N	48	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	B	476	ARG	NE-CZ-NH2	7.52	124.06	120.30
7	O	115	ARG	NE-CZ-NH2	7.52	124.06	120.30
5	J	80	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	A	476	ARG	NE-CZ-NH2	7.47	124.04	120.30
9	S	31	ARG	NE-CZ-NH2	7.41	124.01	120.30
16	g	48	ARG	NE-CZ-NH2	7.41	124.00	120.30
2	F	208	ARG	NE-CZ-NH2	7.40	124.00	120.30
3	G	301	ARG	NE-CZ-NH2	7.38	123.99	120.30
3	G	155	ARG	NE-CZ-NH2	7.35	123.97	120.30
9	Q	31	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	B	44	ARG	NE-CZ-NH2	7.29	123.94	120.30
13	d	21	ARG	NE-CZ-NH1	-7.28	116.66	120.30
2	E	314	ARG	NE-CZ-NH2	7.28	123.94	120.30
2	F	386	ARG	NE-CZ-NH2	7.27	123.94	120.30
3	G	267	ARG	NE-CZ-NH2	7.26	123.93	120.30
7	M	32	ARG	NE-CZ-NH2	7.16	123.88	120.30
9	S	84	ARG	NE-CZ-NH2	7.07	123.83	120.30
16	n	48	ARG	NE-CZ-NH2	7.05	123.83	120.30
11	b	26	TYR	CB-CG-CD2	-7.05	116.77	121.00
13	d	120	ARG	NE-CZ-NH2	7.01	123.80	120.30
2	E	320	ARG	NE-CZ-NH2	7.01	123.80	120.30
16	l	88	ARG	NE-CZ-NH2	6.99	123.79	120.30
1	B	81	ARG	NE-CZ-NH2	6.97	123.78	120.30
5	J	101	ARG	NE-CZ-NH2	6.97	123.78	120.30
9	Q	84	ARG	NE-CZ-NH2	6.97	123.78	120.30
11	b	34	ARG	NE-CZ-NH2	6.96	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	38	ARG	NE-CZ-NH2	6.92	123.76	120.30
2	E	208	ARG	NE-CZ-NH2	6.91	123.76	120.30
2	F	276	ARG	NE-CZ-NH2	6.88	123.74	120.30
7	O	92	ARG	NE-CZ-NH2	6.87	123.73	120.30
16	h	119	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	C	459	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	B	212	ARG	NE-CZ-NH2	6.82	123.71	120.30
5	K	101	ARG	NE-CZ-NH2	6.82	123.71	120.30
4	H	30	ARG	NE-CZ-NH2	6.81	123.70	120.30
2	F	340	ARG	NE-CZ-NH2	6.80	123.70	120.30
16	m	88	ARG	NE-CZ-NH2	6.79	123.70	120.30
10	a	63	ARG	NE-CZ-NH2	6.78	123.69	120.30
5	I	101	ARG	NE-CZ-NH2	6.77	123.69	120.30
10	a	133	ARG	NE-CZ-NH2	6.76	123.68	120.30
13	d	293	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	B	323	ARG	NE-CZ-NH2	6.75	123.67	120.30
10	a	66	ARG	NE-CZ-NH2	6.71	123.66	120.30
11	b	135	TYR	CB-CG-CD1	-6.69	116.99	121.00
1	C	476	ARG	NE-CZ-NH2	6.66	123.63	120.30
10	a	387	ARG	NE-CZ-NH2	6.66	123.63	120.30
2	E	381	ARG	NE-CZ-NH2	6.65	123.62	120.30
2	F	381	ARG	NE-CZ-NH2	6.64	123.62	120.30
10	a	73	ARG	NE-CZ-NH2	6.63	123.61	120.30
9	S	61	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	B	280	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	323	ARG	NE-CZ-NH2	6.58	123.59	120.30
5	I	44	ARG	NE-CZ-NH2	6.57	123.58	120.30
13	d	7	LEU	CB-CA-C	6.57	122.67	110.20
1	B	308	ARG	CD-NE-CZ	6.56	132.79	123.60
2	D	208	ARG	NE-CZ-NH2	6.55	123.58	120.30
16	j	48	ARG	NE-CZ-NH2	6.53	123.56	120.30
16	o	48	ARG	NE-CZ-NH2	6.49	123.54	120.30
3	G	332	ARG	NE-CZ-NH2	6.47	123.54	120.30
2	F	337	ARG	NE-CZ-NH2	6.47	123.53	120.30
8	P	132	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	F	67	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	D	314	ARG	NE-CZ-NH2	6.41	123.50	120.30
7	M	51	ARG	NE-CZ-NH2	6.39	123.50	120.30
7	N	32	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	E	386	ARG	NE-CZ-NH2	6.36	123.48	120.30
5	J	188	ARG	NE-CZ-NH2	6.35	123.47	120.30
2	F	485	ARG	NE-CZ-NH2	6.34	123.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	377	ARG	NE-CZ-NH2	6.34	123.47	120.30
10	a	281	ARG	NE-CZ-NH2	6.32	123.46	120.30
13	d	218	ARG	NE-CZ-NH2	6.32	123.46	120.30
7	N	51	ARG	NE-CZ-NH2	6.32	123.46	120.30
8	P	143	ARG	NE-CZ-NH2	6.32	123.46	120.30
10	a	192	ARG	NE-CZ-NH2	6.30	123.45	120.30
16	m	48	ARG	NE-CZ-NH2	6.29	123.45	120.30
12	c	324	ARG	NE-CZ-NH2	6.27	123.44	120.30
7	M	17	ARG	NE-CZ-NH2	6.26	123.43	120.30
12	c	338	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	B	400	ARG	NE-CZ-NH2	6.19	123.40	120.30
8	P	210	ARG	NE-CZ-NH2	6.18	123.39	120.30
10	a	120	ARG	NE-CZ-NH2	6.17	123.38	120.30
12	c	448	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	B	289	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	359	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	A	280	ARG	NE-CZ-NH2	6.11	123.35	120.30
5	K	50	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	C	442	ARG	NE-CZ-NH2	6.10	123.35	120.30
10	a	241	ARG	NE-CZ-NH2	6.10	123.35	120.30
13	d	86	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	C	81	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
2	F	120	ARG	NE-CZ-NH2	6.06	123.33	120.30
7	N	17	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	364	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	C	289	ARG	NE-CZ-NH2	6.01	123.30	120.30
9	R	31	ARG	NE-CZ-NH2	6.00	123.30	120.30
13	d	327	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	A	601	TYR	CB-CG-CD2	-5.98	117.41	121.00
2	D	314	ARG	NE-CZ-NH1	-5.97	117.31	120.30
10	a	167	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	A	81	ARG	NE-CZ-NH2	5.97	123.28	120.30
2	E	67	ARG	NE-CZ-NH2	5.97	123.28	120.30
16	j	119	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	E	242	ARG	NE-CZ-NH2	5.95	123.28	120.30
2	D	485	ARG	NE-CZ-NH2	5.93	123.26	120.30
8	P	290	ARG	NE-CZ-NH2	5.93	123.27	120.30
3	G	309	ARG	NE-CZ-NH2	5.91	123.25	120.30
5	K	222	ARG	NE-CZ-NH2	5.91	123.25	120.30
10	a	56	ARG	NE-CZ-NH2	5.91	123.25	120.30
5	I	50	ARG	NE-CZ-NH2	5.90	123.25	120.30
6	L	79	ASP	CB-CG-OD1	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	320	ARG	NE-CZ-NH2	5.89	123.25	120.30
13	d	120	ARG	NE-CZ-NH1	-5.87	117.36	120.30
2	E	485	ARG	NE-CZ-NH2	5.86	123.23	120.30
2	F	185	ARG	NE-CZ-NH2	5.86	123.23	120.30
6	L	75	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	552	ARG	NE-CZ-NH2	5.85	123.23	120.30
5	K	188	ARG	NE-CZ-NH2	5.85	123.22	120.30
5	I	125	TYR	CB-CG-CD2	-5.85	117.49	121.00
10	a	768	ARG	NE-CZ-NH2	5.85	123.22	120.30
8	P	382	ARG	NE-CZ-NH2	5.84	123.22	120.30
16	h	48	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	C	215	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	C	552	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	F	321	ARG	NE-CZ-NH2	5.79	123.19	120.30
16	i	126	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	C	552	ARG	NE-CZ-NH1	-5.77	117.42	120.30
3	G	211	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	B	359	ARG	NE-CZ-NH2	5.76	123.18	120.30
5	J	135	ARG	NE-CZ-NH2	5.76	123.18	120.30
4	H	43	ARG	NE-CZ-NH2	5.75	123.17	120.30
7	O	32	ARG	NE-CZ-NH1	-5.72	117.44	120.30
13	d	21	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	459	ARG	NE-CZ-NH2	5.67	123.14	120.30
7	N	48	ARG	NE-CZ-NH1	-5.67	117.46	120.30
6	L	53	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	C	120	ARG	NE-CZ-NH2	5.66	123.13	120.30
16	k	126	ARG	NE-CZ-NH2	5.66	123.13	120.30
15	f	88	ARG	NE-CZ-NH2	5.63	123.12	120.30
16	i	144	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	B	552	ARG	NE-CZ-NH2	5.63	123.11	120.30
16	h	144	TYR	CB-CG-CD2	-5.63	117.62	121.00
2	E	314	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	B	442	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	C	391	ARG	NE-CZ-NH2	5.60	123.10	120.30
11	b	103	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	B	391	ARG	NE-CZ-NH2	5.59	123.09	120.30
16	g	126	ARG	NE-CZ-NH2	5.56	123.08	120.30
2	F	308	ARG	NE-CZ-NH2	5.55	123.08	120.30
16	j	126	ARG	NE-CZ-NH2	5.54	123.07	120.30
16	n	88	ARG	NE-CZ-NH2	5.54	123.07	120.30
9	Q	153	ARG	NE-CZ-NH2	5.52	123.06	120.30
2	D	44	ARG	NE-CZ-NH2	5.51	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	129	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	C	104	ARG	NE-CZ-NH2	5.47	123.04	120.30
2	D	506	ARG	NE-CZ-NH2	5.47	123.03	120.30
9	S	83	ARG	NE-CZ-NH2	5.47	123.03	120.30
3	G	249	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	E	208	ARG	NE-CZ-NH1	-5.45	117.57	120.30
5	I	137	ARG	NE-CZ-NH2	5.45	123.03	120.30
9	R	265	ARG	NE-CZ-NH2	5.45	123.02	120.30
5	I	212	ARG	NE-CZ-NH2	5.45	123.02	120.30
2	F	344	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	571	ARG	NE-CZ-NH2	5.44	123.02	120.30
4	H	167	ARG	NE-CZ-NH2	5.44	123.02	120.30
9	Q	83	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	F	120	ARG	NE-CZ-NH1	-5.43	117.59	120.30
10	a	338	ARG	NE-CZ-NH2	5.43	123.01	120.30
10	a	6	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	400	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	553	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	104	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	A	530	ARG	NE-CZ-NH2	5.40	123.00	120.30
10	a	429	ARG	NE-CZ-NH2	5.39	123.00	120.30
5	I	135	ARG	NE-CZ-NH2	5.39	123.00	120.30
8	P	117	ARG	NE-CZ-NH2	5.39	123.00	120.30
16	g	68	TYR	CB-CG-CD2	-5.39	117.77	121.00
2	E	400	ARG	NE-CZ-NH2	5.39	123.00	120.30
16	n	119	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	120	ARG	NE-CZ-NH2	5.38	122.99	120.30
4	H	168	ARG	NE-CZ-NH2	5.37	122.99	120.30
7	M	48	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	B	129	ARG	NE-CZ-NH2	5.36	122.98	120.30
7	N	107	ARG	NE-CZ-NH2	5.36	122.98	120.30
7	O	51	ARG	NE-CZ-NH2	5.36	122.98	120.30
13	d	197	CYS	CA-CB-SG	-5.35	104.36	114.00
9	R	46	ARG	NE-CZ-NH2	5.35	122.97	120.30
16	i	68	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	D	67	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	381	ARG	NE-CZ-NH2	5.31	122.96	120.30
8	P	423	ARG	NE-CZ-NH2	5.31	122.95	120.30
16	n	119	ARG	NE-CZ-NH2	5.31	122.95	120.30
13	d	7	LEU	N-CA-CB	-5.30	99.79	110.40
2	E	506	ARG	NE-CZ-NH2	5.30	122.95	120.30
9	Q	61	ARG	NE-CZ-NH2	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH2	5.29	122.95	120.30
5	K	212	ARG	NE-CZ-NH2	5.27	122.94	120.30
7	M	92	ARG	NE-CZ-NH2	5.27	122.94	120.30
5	K	222	ARG	NE-CZ-NH1	-5.26	117.67	120.30
7	M	92	ARG	NE-CZ-NH1	-5.26	117.67	120.30
6	L	75	ARG	NE-CZ-NH1	-5.26	117.67	120.30
7	N	28	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	E	120	ARG	NE-CZ-NH2	5.25	122.93	120.30
7	M	115	ARG	NE-CZ-NH2	5.24	122.92	120.30
5	J	50	ARG	NE-CZ-NH2	5.23	122.92	120.30
5	I	111	ARG	NE-CZ-NH1	-5.23	117.69	120.30
9	R	61	ARG	NE-CZ-NH2	5.23	122.91	120.30
7	N	26	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	F	163	ARG	NE-CZ-NH2	5.21	122.91	120.30
7	O	87	TYR	CB-CG-CD2	-5.21	117.87	121.00
5	J	125	TYR	CB-CG-CD2	-5.21	117.88	121.00
3	G	164	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	C	44	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	338	ARG	NE-CZ-NH2	5.18	122.89	120.30
16	m	126	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	104	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	C	171	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	F	242	ARG	NE-CZ-NH2	5.18	122.89	120.30
16	o	144	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	B	552	ARG	NE-CZ-NH1	-5.17	117.71	120.30
7	M	107	ARG	NE-CZ-NH2	5.17	122.89	120.30
11	b	34	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	C	571	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	E	271	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	571	ARG	NE-CZ-NH2	5.14	122.87	120.30
13	d	237	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	C	338	ARG	NE-CZ-NH2	5.13	122.86	120.30
16	m	119	ARG	NE-CZ-NH2	5.12	122.86	120.30
16	g	48	ARG	NE-CZ-NH1	-5.12	117.74	120.30
13	d	341	ARG	NE-CZ-NH2	5.11	122.86	120.30
2	D	412	ARG	NE-CZ-NH2	5.11	122.85	120.30
4	H	63	ARG	NE-CZ-NH2	5.09	122.84	120.30
4	H	112	TYR	CB-CG-CD2	-5.08	117.95	121.00
13	d	339	ARG	NE-CZ-NH2	5.07	122.83	120.30
5	I	188	ARG	NE-CZ-NH2	5.07	122.83	120.30
11	b	18	CYS	CA-CB-SG	-5.05	104.91	114.00
1	C	613	ARG	NE-CZ-NH2	5.04	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	c	338	ARG	NE-CZ-NH1	-5.04	117.78	120.30
7	N	92	ARG	NE-CZ-NH2	5.04	122.82	120.30
9	R	84	ARG	NE-CZ-NH2	5.03	122.81	120.30
5	K	87	ARG	NE-CZ-NH2	5.01	122.81	120.30
13	d	194	TYR	CB-CG-CD1	-5.01	117.99	121.00
2	D	242	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	A	232	ARG	NE-CZ-NH2	5.01	122.80	120.30
3	G	242	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	364	ARG	Sidechain
1	A	67	TYR	Sidechain
1	C	280	ARG	Sidechain
1	C	364	ARG	Sidechain
1	C	377	TYR	Sidechain
2	D	389	TYR	Sidechain
2	E	389	TYR	Sidechain
2	F	185	ARG	Sidechain
2	F	389	TYR	Sidechain
2	F	82	ARG	Sidechain
5	J	137	ARG	Sidechain
5	J	57	TYR	Sidechain
5	K	137	ARG	Sidechain
7	O	92	ARG	Sidechain
10	a	816	TYR	Sidechain
11	b	26	TYR	Sidechain
11	b	8	TYR	Sidechain
13	d	164	PHE	Sidechain
13	d	21	ARG	Sidechain
16	g	32	TYR	Sidechain
16	h	144	TYR	Sidechain
16	i	10	TYR	Sidechain
16	j	32	TYR	Sidechain
16	o	10	TYR	Sidechain
16	o	119	ARG	Sidechain
17	p	303	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4632	0	4628	3	0
1	B	4651	0	4644	6	0
1	C	4666	0	4655	2	0
2	D	3604	0	3608	2	0
2	E	3603	0	3608	1	0
2	F	3576	0	3576	6	0
3	G	2919	0	2961	3	0
4	H	1760	0	1869	0	0
5	I	1808	0	1880	1	0
5	J	1808	0	1880	1	0
5	K	1808	0	1880	0	0
6	L	875	0	883	0	0
7	M	920	0	918	0	0
7	N	935	0	931	0	0
7	O	935	0	931	0	0
8	P	3537	0	3510	1	0
9	Q	2126	0	2165	1	0
9	R	2130	0	2168	0	0
9	S	2155	0	2201	0	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	C	27	0	12	0	0
All	All	71930	0	72924	22	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 (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD21	1:A:448:VAL:HG21	1.82	0.61
1:C:387:GLU:HG3	2:D:264:ALA:HB3	1.88	0.54
1:B:104:ARG:HB3	1:B:109:ILE:HD11	1.92	0.52
1:B:387:GLU:HG3	2:F:264:ALA:HB3	1.91	0.52
3:G:379:LEU:H	3:G:379:LEU:HD23	1.75	0.51
3:G:186:LEU:HD13	3:G:251:PHE:H	1.76	0.51
1:B:275:VAL:HG11	1:B:330:GLY:HA3	1.94	0.49
1:A:67:TYR:CE1	1:A:321:ALA:HB1	2.49	0.48
2:D:406:ILE:HD12	2:D:415:HIS:CE1	2.50	0.46
8:P:90:VAL:HA	8:P:93:ILE:HG22	1.99	0.44
2:F:166:PRO:HG2	2:F:401:LEU:HD13	2.01	0.43
2:E:274:THR:HB	2:E:275:PRO:HD3	2.00	0.43
3:G:185:LEU:C	3:G:186:LEU:HD12	2.39	0.42
5:I:123:GLY:HA3	5:I:183:ILE:HD13	2.02	0.42
5:J:88:ASP:HA	5:J:91:ILE:HG22	2.00	0.42
1:B:387:GLU:CG	2:F:264:ALA:HB3	2.50	0.42
1:B:383:ALA:HB1	2:F:264:ALA:HB1	2.02	0.41
1:B:153:TYR:CZ	1:B:166:ILE:HG22	2.56	0.41
1:C:353:ARG:HD2	2:F:328:TYR:CZ	2.56	0.41
9:Q:94:LEU:HD23	9:Q:94:LEU:C	2.40	0.41
2:F:415:HIS:CD2	2:F:477:LEU:HD21	2.56	0.41
1:A:234:LEU:HD22	1:A:433:TRP:CD1	2.57	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	593/617 (96%)	564 (95%)	28 (5%)	1 (0%)	47	79
1	B	598/617 (97%)	575 (96%)	22 (4%)	1 (0%)	47	79
1	C	600/617 (97%)	578 (96%)	21 (4%)	1 (0%)	47	79
2	D	456/511 (89%)	436 (96%)	20 (4%)	0	100	100
2	E	456/511 (89%)	430 (94%)	26 (6%)	0	100	100
2	F	453/511 (89%)	433 (96%)	20 (4%)	0	100	100
3	G	354/382 (93%)	348 (98%)	6 (2%)	0	100	100
4	H	216/247 (87%)	212 (98%)	4 (2%)	0	100	100
5	I	221/226 (98%)	218 (99%)	3 (1%)	0	100	100
5	J	221/226 (98%)	217 (98%)	4 (2%)	0	100	100
5	K	221/226 (98%)	216 (98%)	5 (2%)	0	100	100
6	L	108/119 (91%)	104 (96%)	4 (4%)	0	100	100
7	M	110/118 (93%)	109 (99%)	1 (1%)	0	100	100
7	N	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	O	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
8	P	427/483 (88%)	422 (99%)	5 (1%)	0	100	100
9	Q	261/280 (93%)	256 (98%)	5 (2%)	0	100	100
9	R	262/280 (94%)	258 (98%)	4 (2%)	0	100	100
9	S	265/280 (95%)	257 (97%)	8 (3%)	0	100	100
10	a	751/838 (90%)	728 (97%)	23 (3%)	0	100	100
11	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
12	c	202/463 (44%)	189 (94%)	13 (6%)	0	100	100
13	d	346/351 (99%)	338 (98%)	7 (2%)	1 (0%)	41	74
14	e	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
15	f	82/98 (84%)	81 (99%)	1 (1%)	0	100	100
16	g	148/155 (96%)	148 (100%)	0	0	100	100
16	h	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	i	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	22	60
16	j	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	k	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	m	148/155 (96%)	145 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	n	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	o	148/155 (96%)	148 (100%)	0	0	100	100
17	p	49/350 (14%)	44 (90%)	5 (10%)	0	100	100
All	All	9084/10268 (88%)	8822 (97%)	257 (3%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	i	10	TYR
1	B	389	ALA
1	C	139	LYS
13	d	339	ARG
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	506/524 (97%)	502 (99%)	4 (1%)	81	89
1	B	507/524 (97%)	504 (99%)	3 (1%)	86	92
1	C	509/524 (97%)	503 (99%)	6 (1%)	71	84
2	D	394/431 (91%)	392 (100%)	2 (0%)	88	94
2	E	394/431 (91%)	393 (100%)	1 (0%)	92	96
2	F	391/431 (91%)	381 (97%)	10 (3%)	46	69
3	G	325/344 (94%)	324 (100%)	1 (0%)	92	96
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%)	195 (100%)	1 (0%)	88	94
5	K	196/198 (99%)	196 (100%)	0	100	100
6	L	94/100 (94%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	P	389/428 (91%)	387 (100%)	2 (0%)	88	94
9	Q	241/255 (94%)	241 (100%)	0	100	100
9	R	241/255 (94%)	240 (100%)	1 (0%)	91	95
9	S	244/255 (96%)	244 (100%)	0	100	100
10	a	674/743 (91%)	674 (100%)	0	100	100
11	b	156/158 (99%)	152 (97%)	4 (3%)	46	69
12	c	182/395 (46%)	180 (99%)	2 (1%)	73	85
13	d	303/306 (99%)	298 (98%)	5 (2%)	60	78
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%)	108 (99%)	1 (1%)	78	88
16	h	109/113 (96%)	108 (99%)	1 (1%)	78	88
16	i	109/113 (96%)	109 (100%)	0	100	100
16	j	109/113 (96%)	108 (99%)	1 (1%)	78	88
16	k	109/113 (96%)	109 (100%)	0	100	100
16	l	109/113 (96%)	108 (99%)	1 (1%)	78	88
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%)	109 (100%)	0	100	100
17	p	46/313 (15%)	46 (100%)	0	100	100
All	All	7784/8694 (90%)	7738 (99%)	46 (1%)	86	92

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	308	ARG
1	A	400	ARG
1	A	430	GLN
1	B	173	ARG
1	B	220	LYS

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Mol	Chain	Res	Type
1	B	311	LEU
1	C	228	LEU
1	C	286	GLU
1	C	289	ARG
1	C	443	LYS
1	C	510	GLU
1	C	568	SER
2	D	356	MET
2	D	472	THR
2	E	359	ASP
2	F	106	ASP
2	F	167	GLU
2	F	185	ARG
2	F	226	ASN
2	F	227	PHE
2	F	293	VAL
2	F	347	SER
2	F	400	ARG
2	F	402	MET
2	F	419	SER
3	G	229	LEU
5	J	208	MET
8	P	169	LYS
8	P	460	MET
9	R	270	ASN
11	b	34	ARG
11	b	35	PHE
11	b	67	TRP
11	b	70	TYR
12	c	398	PHE
12	c	403	GLU
13	d	7	LEU
13	d	24	LYS
13	d	45	LEU
13	d	57	PHE
13	d	311	HIS
16	g	139	GLU
16	h	12	SER
16	j	10	TYR
16	l	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	415	HIS
12	c	364	HIS
12	c	391	HIS
13	d	84	HIS
13	d	340	HIS
16	g	123	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	C	801	-	24,29,29	1.14	2 (8%)	29,45,45	1.31	3 (10%)

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	C	801	-	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	801	ADP	C5-C4	-2.27	1.34	1.40
18	C	801	ADP	O4'-C1'	2.25	1.44	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	801	ADP	C4-C5-N7	4.39	113.98	109.40
18	C	801	ADP	N6-C6-N1	-2.29	113.82	118.57
18	C	801	ADP	C2-N1-C6	-2.19	115.01	118.75

There are no chirality outliers.

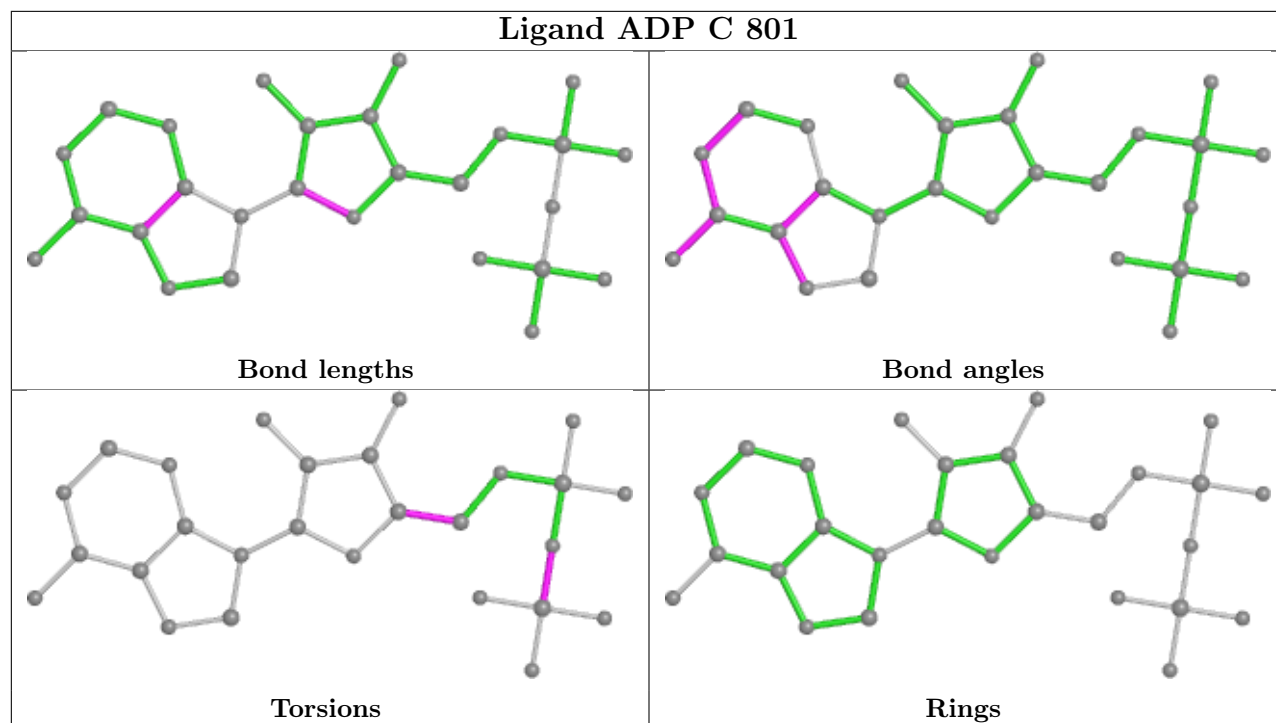
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	801	ADP	O4'-C4'-C5'-O5'
18	C	801	ADP	PA-O3A-PB-O1B
18	C	801	ADP	C3'-C4'-C5'-O5'
18	C	801	ADP	PA-O3A-PB-O2B
18	C	801	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 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.

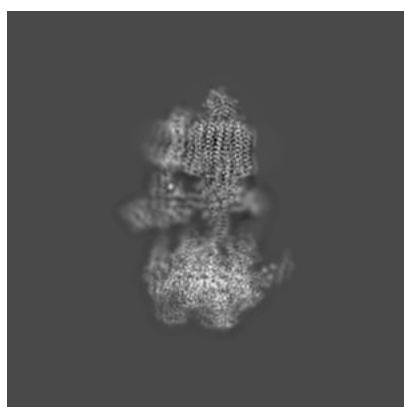
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26909. These allow visual inspection of the internal detail of the map and identification of artifacts.

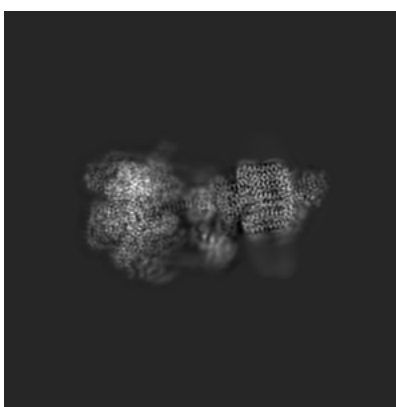
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

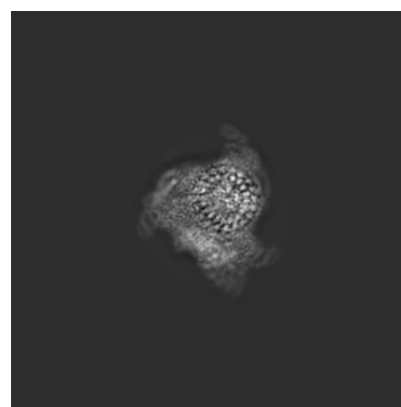
6.1.1 Primary map



X



Y



Z

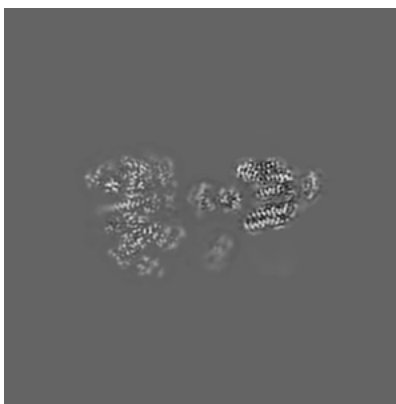
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 170



Y Index: 170

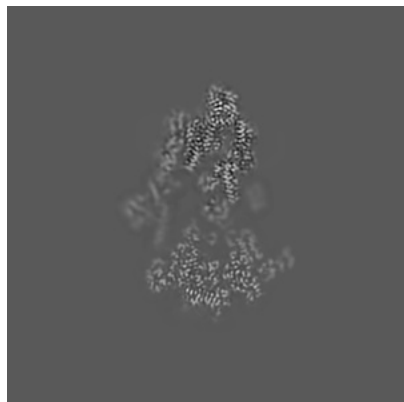


Z Index: 170

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

6.3 Largest variance slices [\(i\)](#)

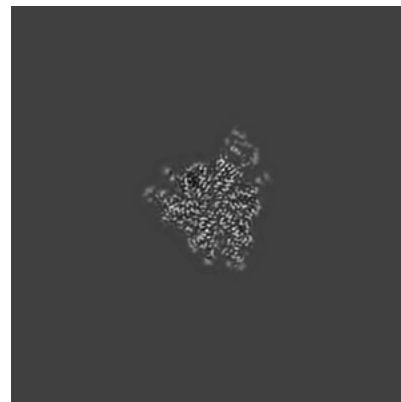
6.3.1 Primary map



X Index: 184



Y Index: 179

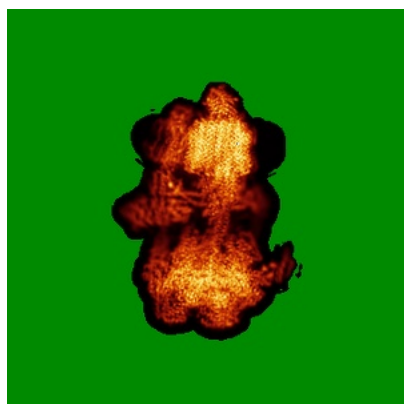


Z Index: 110

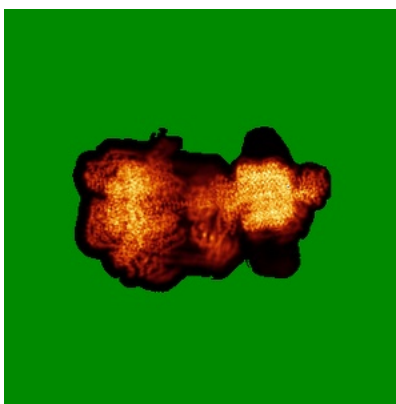
The images above show the largest variance slices of the map in three orthogonal directions.

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

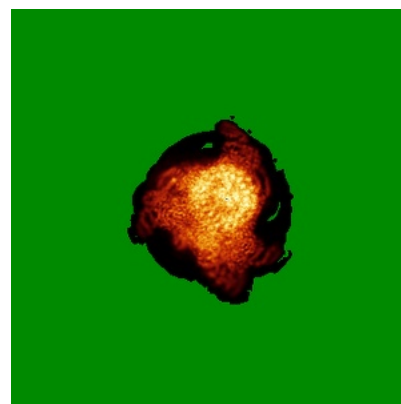
6.4.1 Primary map



X



Y

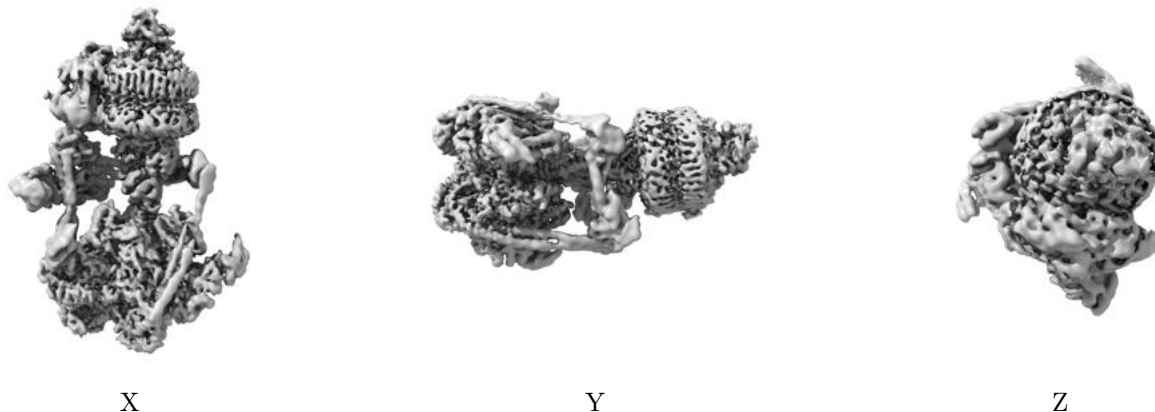


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

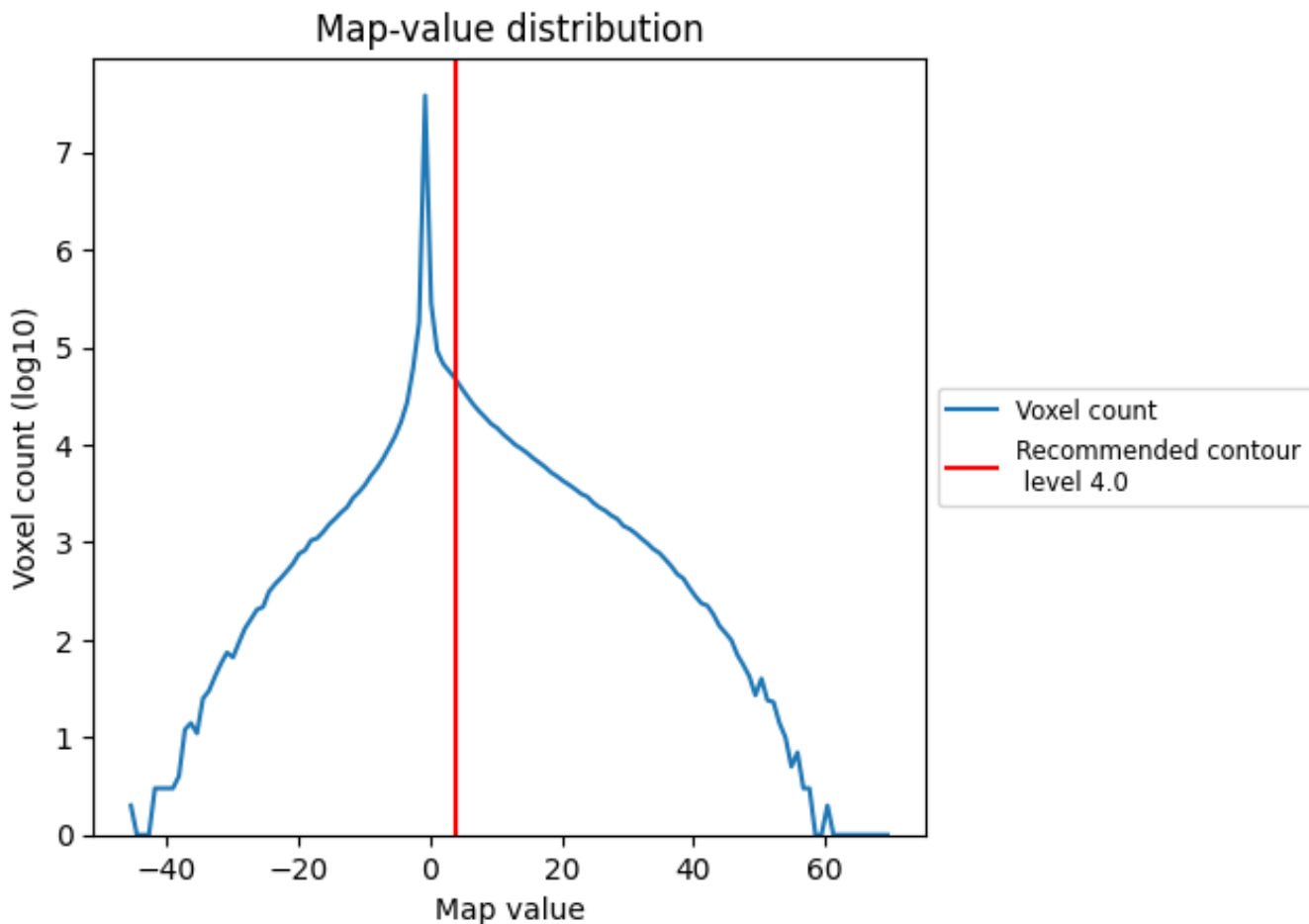
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

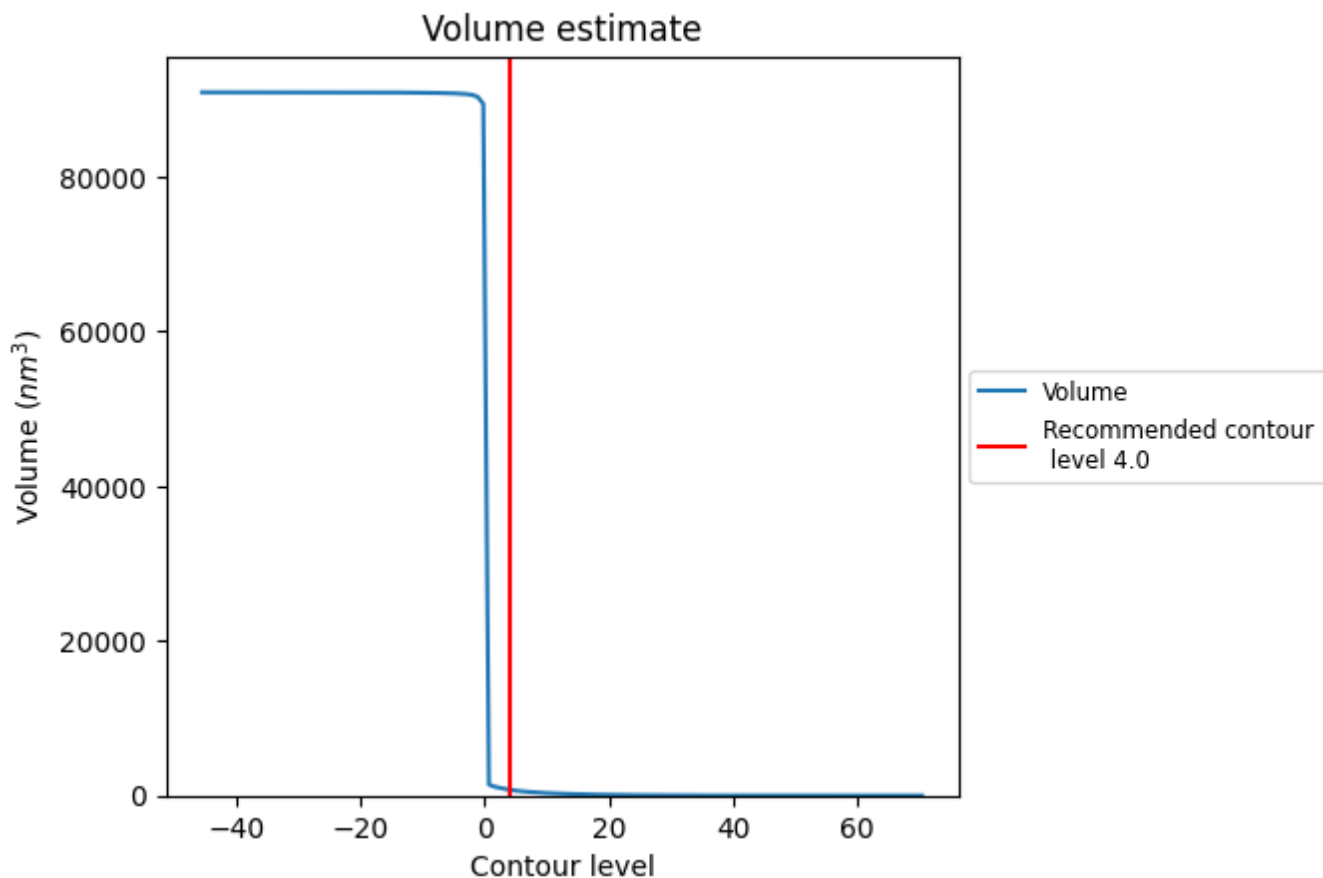
This section contains the results of statistical analysis of the map.

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.

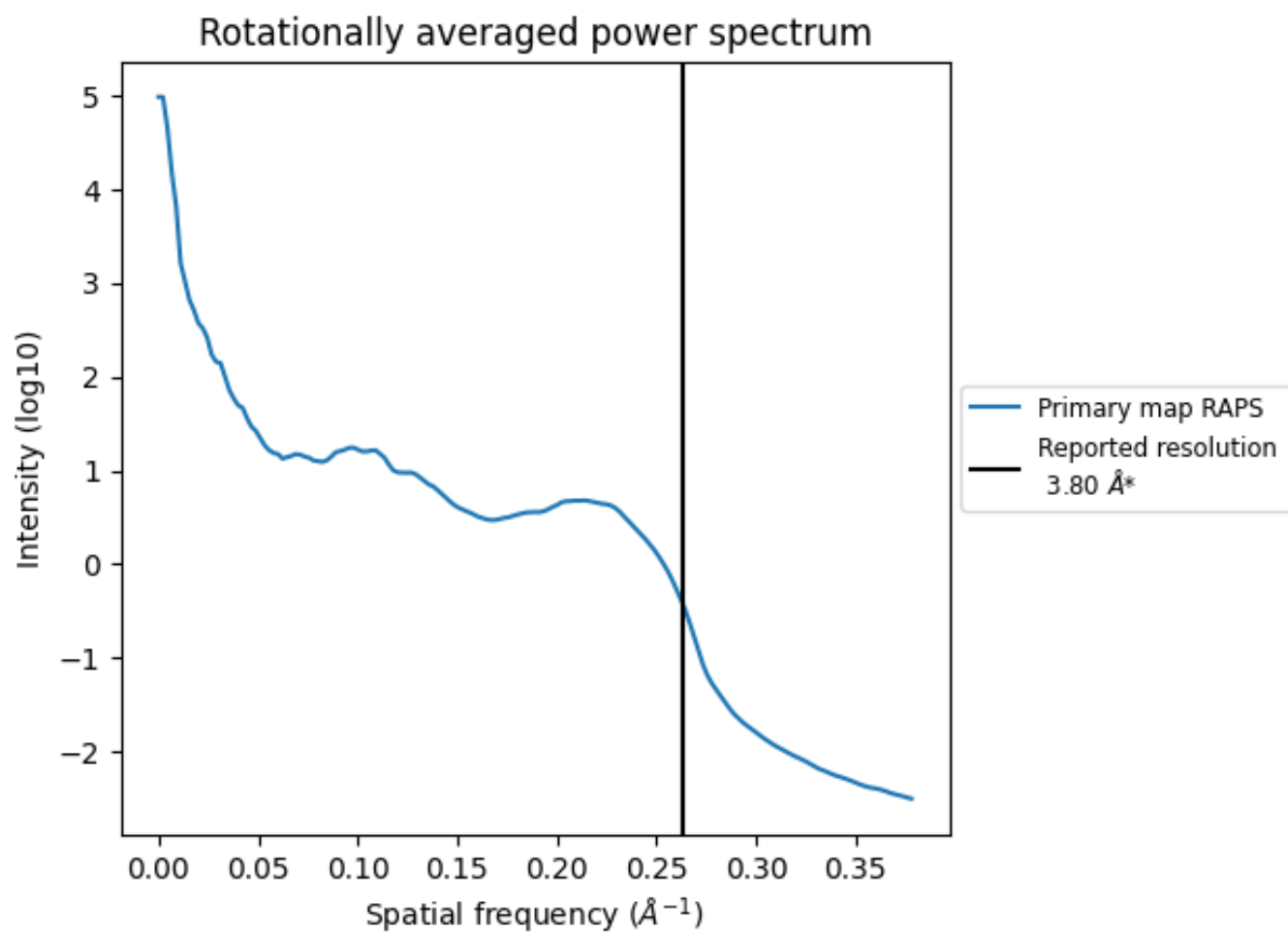
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 758 nm^3 ; this corresponds to an approximate mass of 685 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 0.263 Å⁻¹

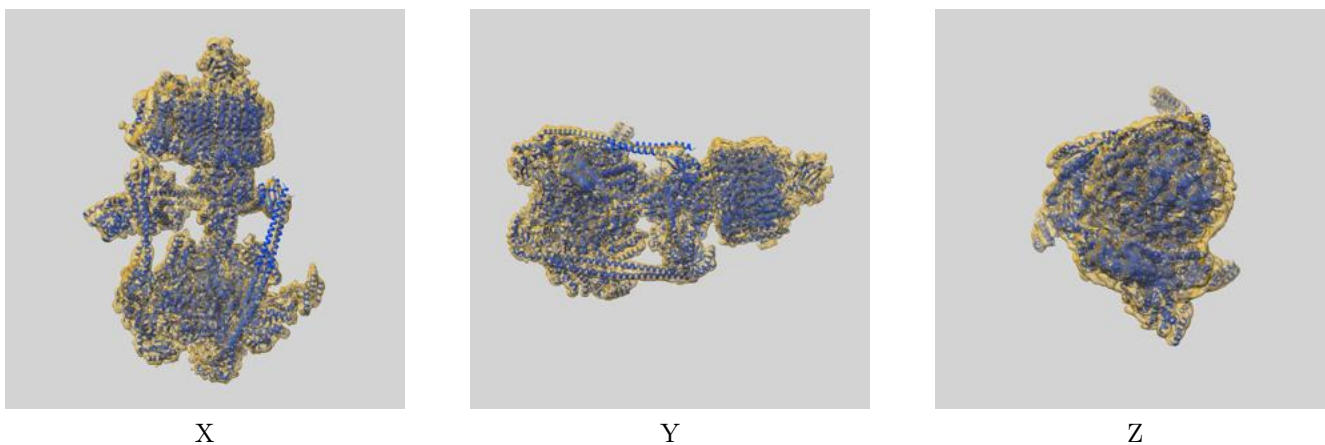
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

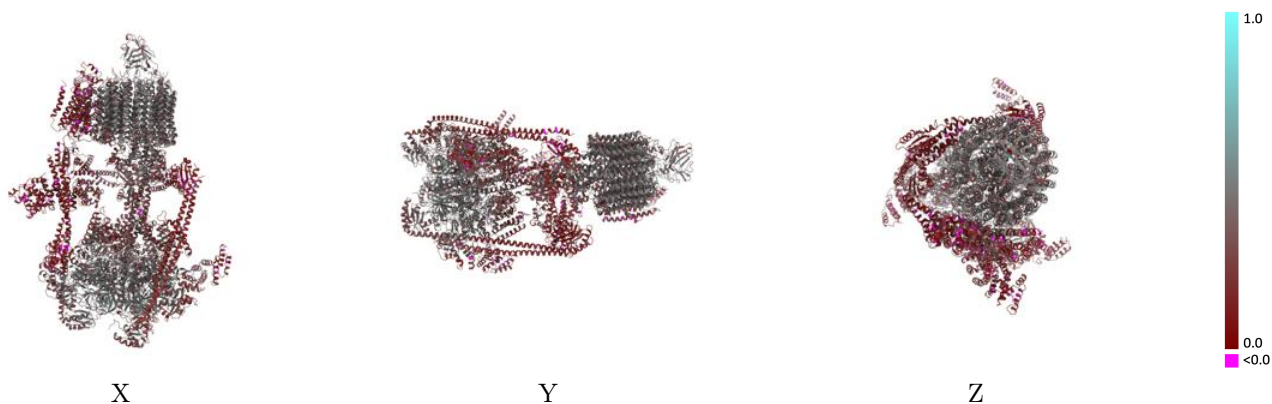
This section contains information regarding the fit between EMDB map EMD-26909 and PDB model 7UZF. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



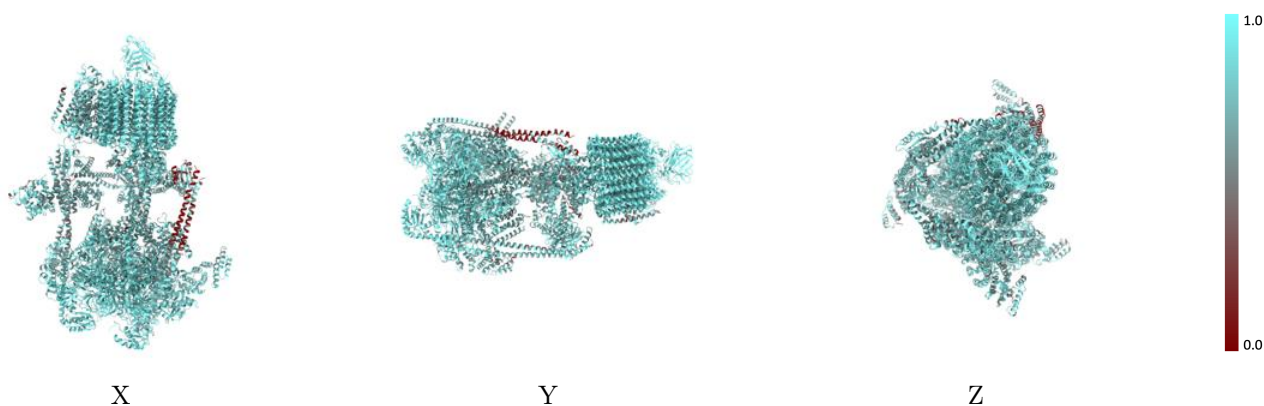
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



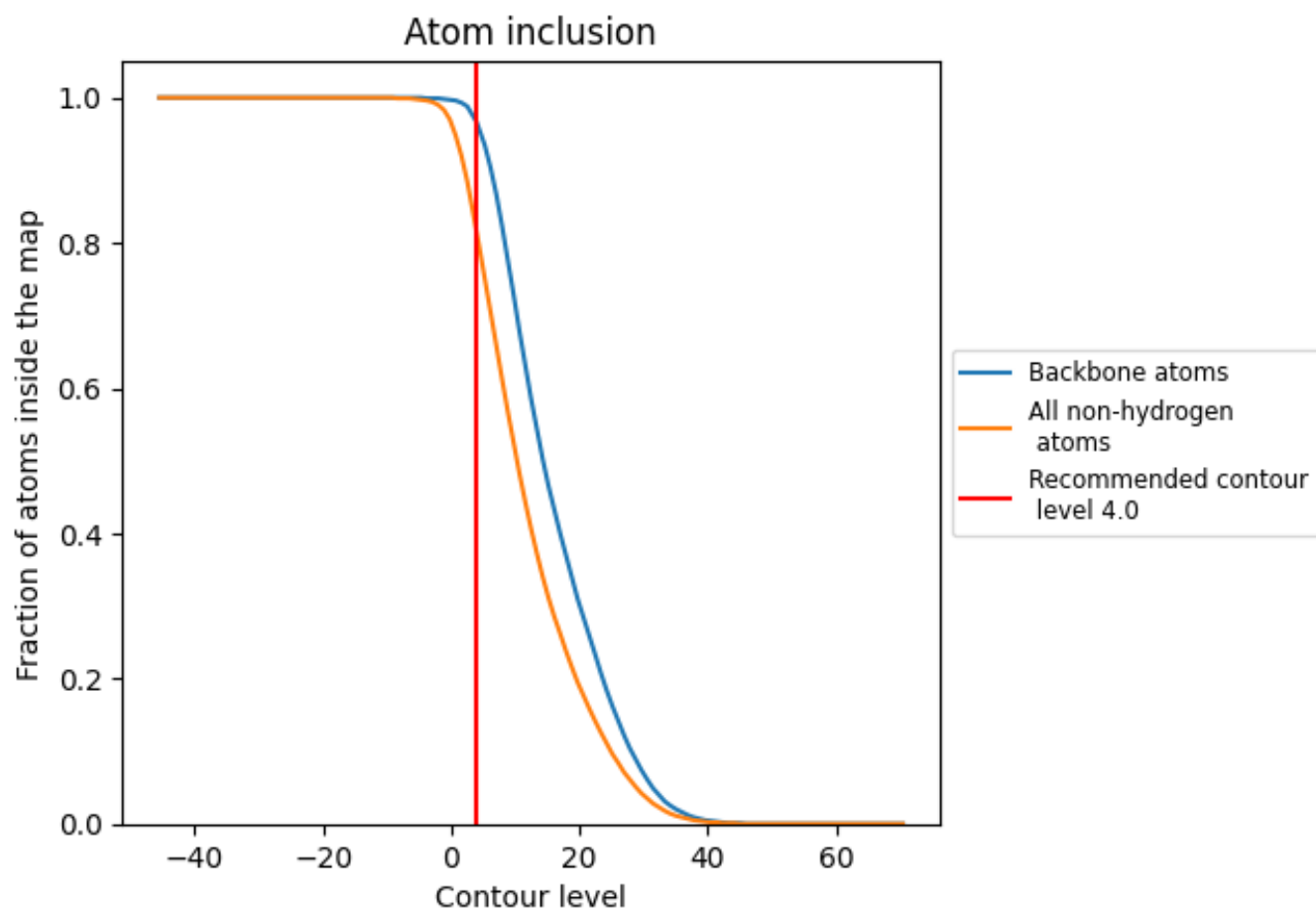
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).









































































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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8150	 0.3320
A	 0.8450	 0.3890
B	 0.8420	 0.3830
C	 0.8620	 0.4050
D	 0.8690	 0.4160
E	 0.8880	 0.4360
F	 0.8560	 0.4060
G	 0.6710	 0.1440
H	 0.7980	 0.3450
I	 0.7970	 0.2990
J	 0.8010	 0.2910
K	 0.6660	 0.2770
L	 0.7570	 0.2920
M	 0.7310	 0.2310
N	 0.7710	 0.2470
O	 0.5830	 0.2160
P	 0.7820	 0.1670
Q	 0.7490	 0.2400
R	 0.7920	 0.2690
S	 0.7550	 0.2510
a	 0.7610	 0.1960
b	 0.8880	 0.4350
c	 0.9010	 0.4180
d	 0.8470	 0.3890
e	 0.7550	 0.1860
f	 0.7320	 0.1450
g	 0.8830	 0.4290
h	 0.8850	 0.4310
i	 0.8730	 0.4240
j	 0.8700	 0.4150
k	 0.8660	 0.4160
l	 0.8730	 0.4260
m	 0.8810	 0.4300
n	 0.8780	 0.4420
o	 0.8810	 0.4370
p	 0.8670	 0.3960

