



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 7UZJ / pdb_00007uzj
EMDB ID : EMD-26913
Title : Rat Kidney V1 complex with SidK and NCOA7B, State 1
Authors : Abbas, Y.M.; Rubinstein, J.L.
Deposited on : 2022-05-09
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

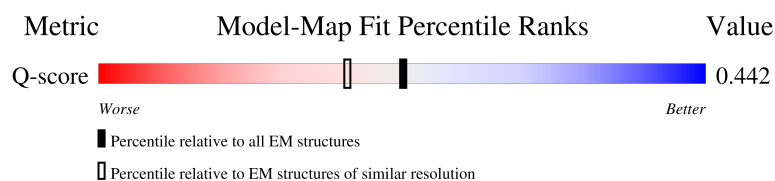
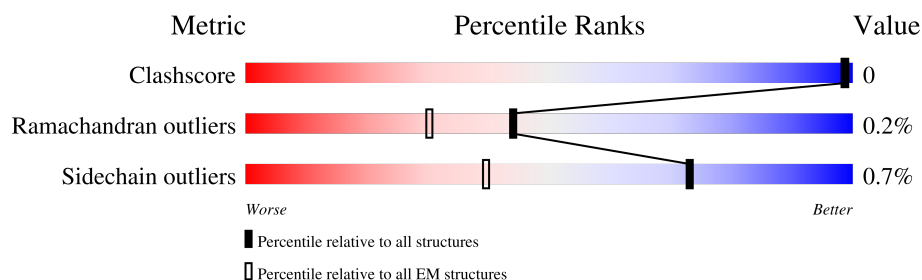
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



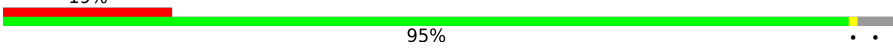
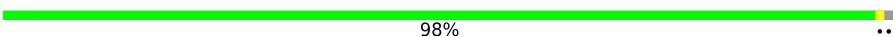
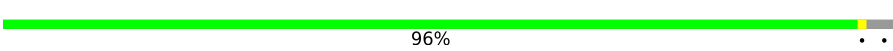
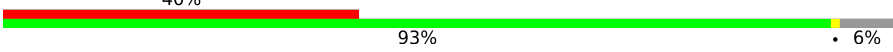
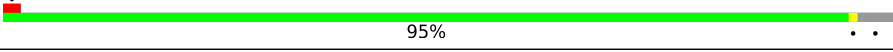
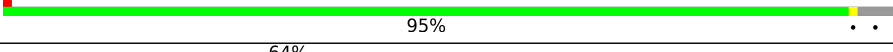
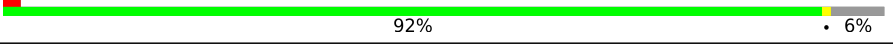
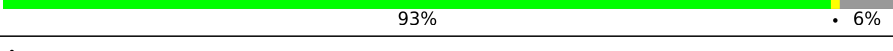
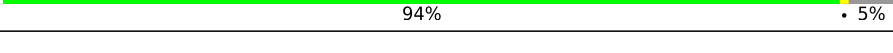
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	94% 5%
1	B	617	95% ..
1	C	617	96% ..
2	D	511	89% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	511	 89% • 9%
2	F	511	 88% • 11%
3	G	382	 92% • 6%
4	H	247	 26% 83% • 16%
5	I	226	 19% 95% • •
5	J	226	 98% • •
5	K	226	 96% • •
6	L	119	 60% 87% • • 8%
7	M	118	 40% 93% • 6%
7	N	118	 95% • •
7	O	118	 95% • •
8	P	483	 64% 88% • 11%
9	Q	280	 92% • 6%
9	R	280	 93% • 6%
9	S	280	 94% • 5%
10	T	221	 75% • 23%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 49624 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATPase H⁺-transporting V1 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	588	Total	C	N	O	S	0	0
			4568	2896	773	873	26		
1	B	601	Total	C	N	O	S	0	0
			4657	2952	787	891	27		
1	C	600	Total	C	N	O	S	0	0
			4648	2947	786	888	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	460	Total	C	N	O	S	0	0
			3603	2286	615	682	20		
2	E	464	Total	C	N	O	S	0	0
			3632	2301	619	692	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
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
4	H	207	Total	C	N	O	S	0	0
			1689	1072	308	304	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	218	Total	C	N	O	S	0	0
			1774	1118	314	332	10		
5	J	223	Total	C	N	O	S	0	0
			1808	1137	319	342	10		
5	K	218	Total	C	N	O	S	0	0
			1774	1118	314	332	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	111	Total	C	N	O	S	0	0
			914	560	172	179	3		
7	N	113	Total	C	N	O	S	0	0
			929	568	175	183	3		
7	O	113	Total	C	N	O	S	0	0
			929	568	175	183	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	430	Total	C	N	O	S	0	0
			3529	2239	608	656	26		

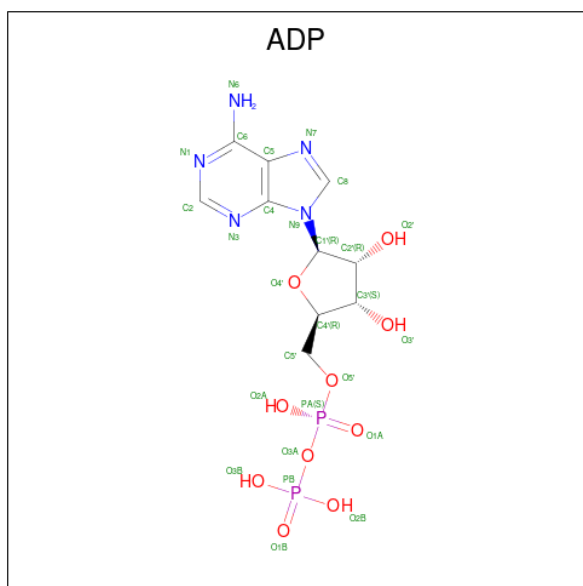
- Molecule 9 is a protein called Effector SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	262	Total	C	N	O	S	0	0
			2122	1348	356	408	10		
9	R	263	Total	C	N	O	S	0	0
			2126	1350	357	409	10		
9	S	266	Total	C	N	O	S	0	0
			2147	1363	361	412	11		

- Molecule 10 is a protein called Nuclear receptor coactivator 7B.

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

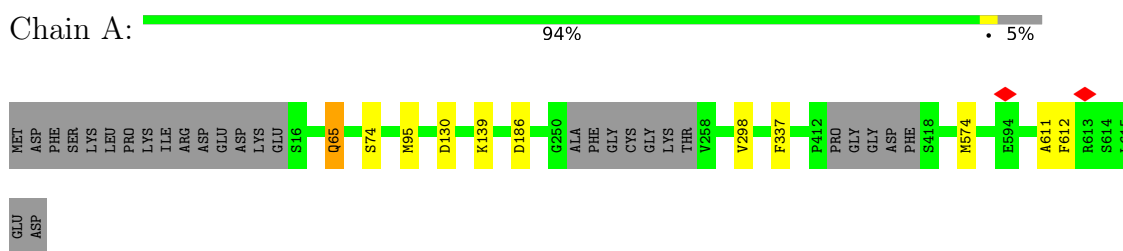
- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



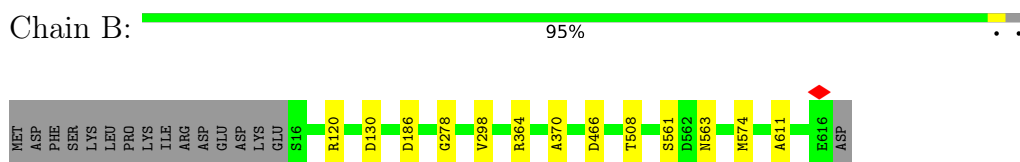
3 Residue-property plots [i](#)

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.

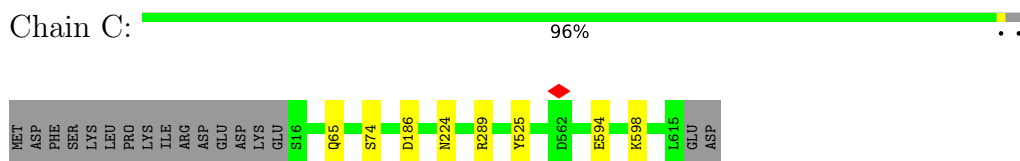
- Molecule 1: ATPase H⁺-transporting V1 subunit A



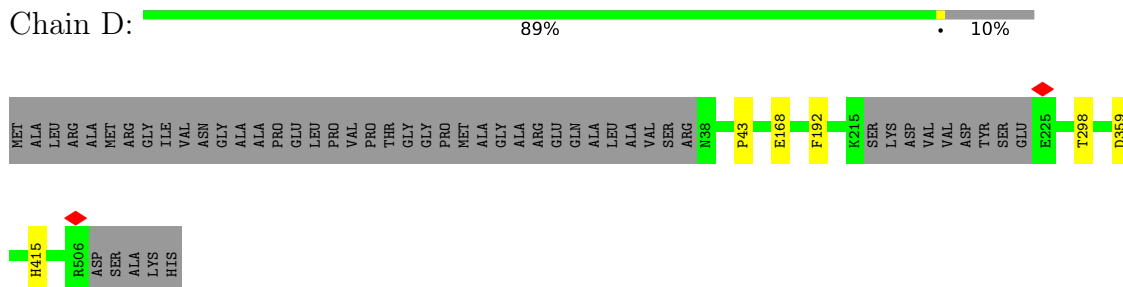
- Molecule 1: ATPase H⁺-transporting V1 subunit A



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

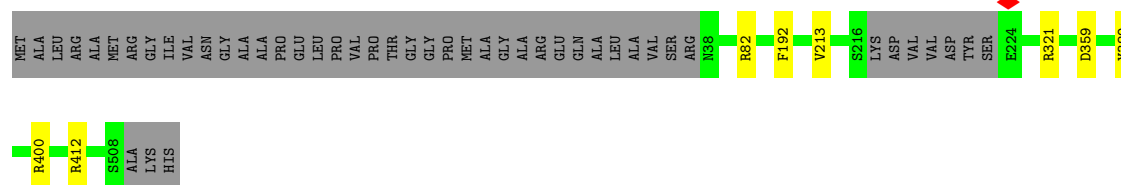


- Molecule 2: V-type proton ATPase subunit B, brain isoform



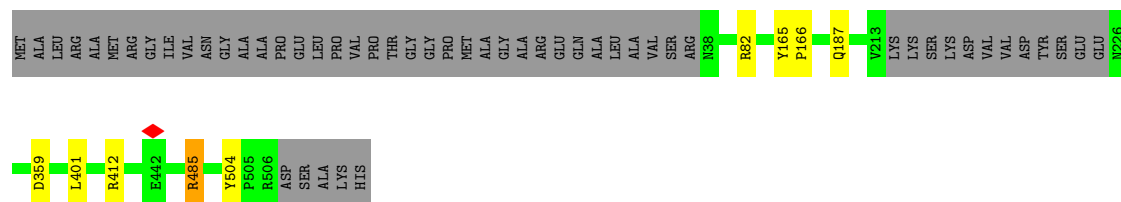
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain E:  89% 9%



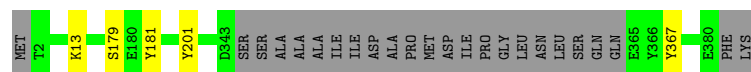
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain F:  88% 11%



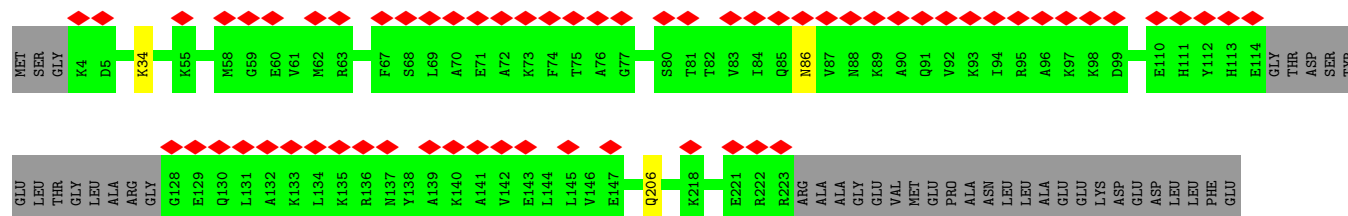
- Molecule 3: V-type proton ATPase subunit C 1

Chain G:  92% 6%

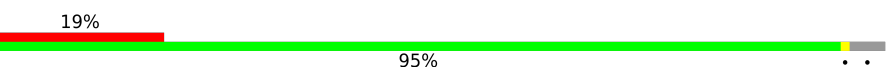


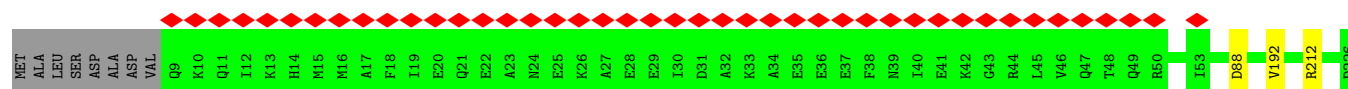
- Molecule 4: ATPase H⁺-transporting V1 subunit D

Chain H:  26% 83% 16%

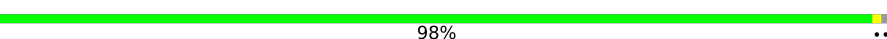


- Molecule 5: V-type proton ATPase subunit E 1

Chain I:  19% 95%



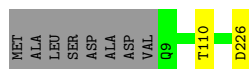
- Molecule 5: V-type proton ATPase subunit E 1

Chain J:  98%



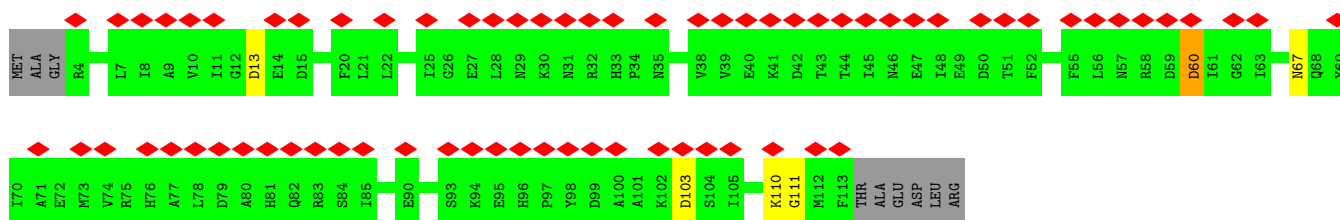
- Molecule 5: V-type proton ATPase subunit E 1

Chain K: 96%



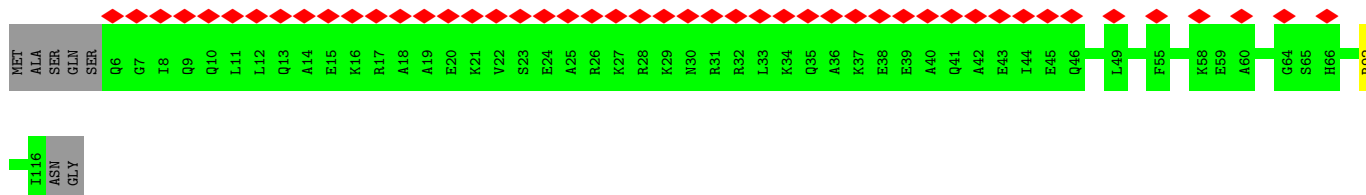
- Molecule 6: V-type proton ATPase subunit F

Chain L: 60%
87% 8%



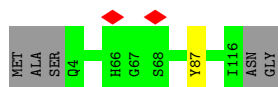
- Molecule 7: V-type proton ATPase subunit G

Chain M: 40%
93% 6%



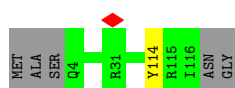
- Molecule 7: V-type proton ATPase subunit G

Chain N: 95%



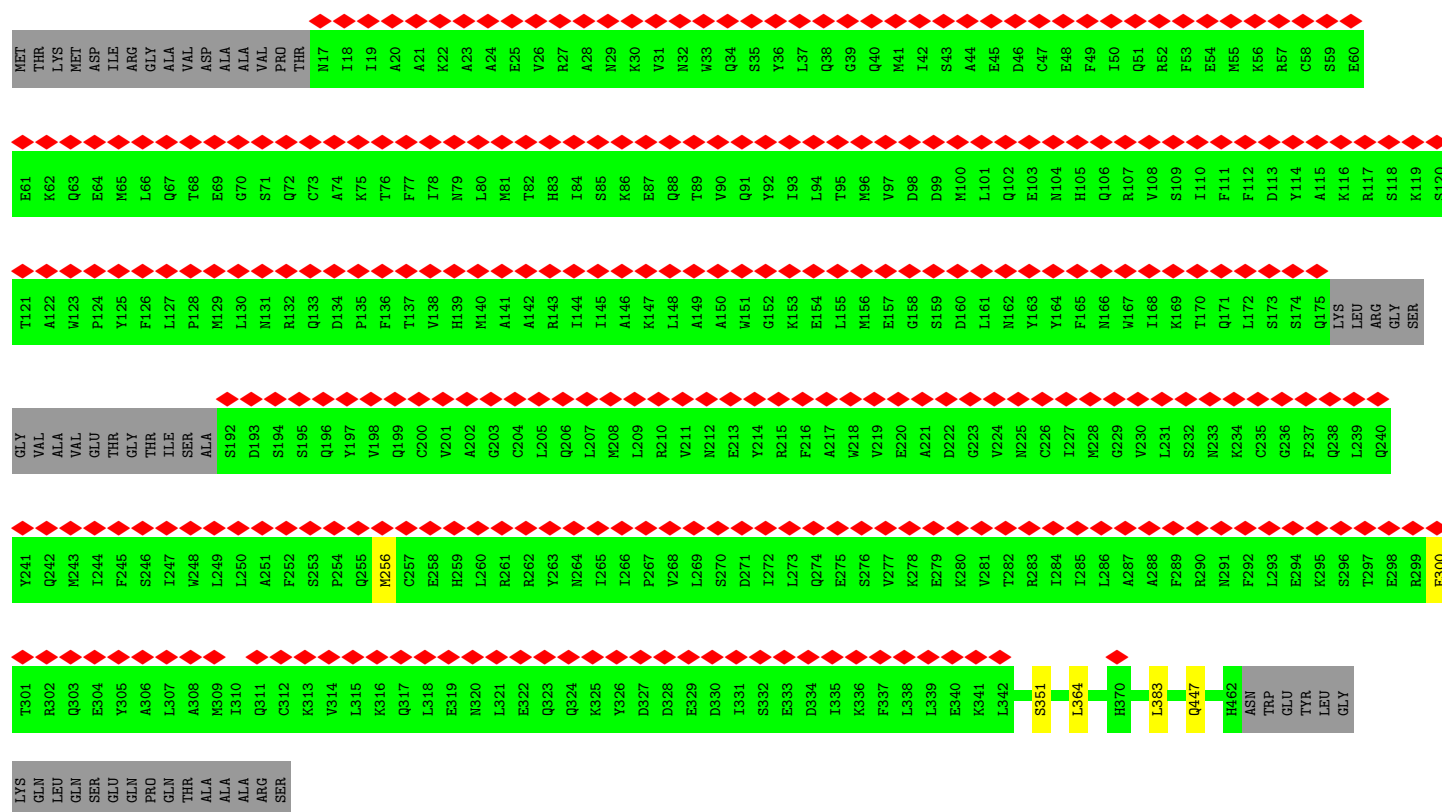
- Molecule 7: V-type proton ATPase subunit G

Chain O: 95%

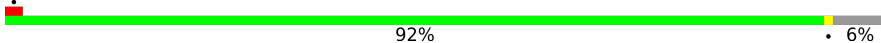


- Molecule 8: V-type proton ATPase subunit H

Chain P: 



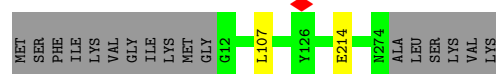
• Molecule 9: Effector SidK

Chain Q: 

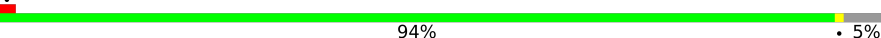


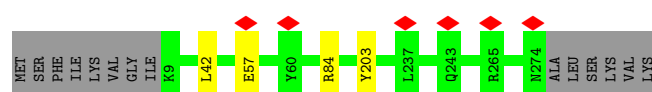
• Molecule 9: Effector SidK

Chain R: 



• Molecule 9: Effector SidK

Chain S: 



• Molecule 10: Nuclear receptor coactivator 7B



MET	ARG	GLY	ARG	ARG	LEU	PRO	LEU	ASP	ILE	GLN	ILE	PHE	TYR	CYS	ALA	ARG	PRO	ASP	GLN	GLU	PRO	PHE	VAL	LYS	ILE	ILE	THR	VAL	GLU	GLU	ALA	LYS	ARG	ARG	LYS	SER	THR	CYS	SER	TYR	TYR	GLU	GLU	GLU	GLU	GLU	GLU	GLY	L152	H58	S59	R77	S148
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	------

L182	E221
------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46258	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 ($e^-/\text{\AA}^2$)	40.826	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	86.955	Depositor
Minimum map value	-52.139	Depositor
Average map value	0.006	Depositor
Map value standard deviation	1.169	Depositor
Recommended contour level	3	Depositor
Map size (Å)	370.99997, 370.99997, 370.99997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.73	0/4658	1.23	1/6304 (0.0%)
1	B	0.73	0/4752	1.23	2/6433 (0.0%)
1	C	0.74	0/4743	1.24	2/6421 (0.0%)
2	D	0.74	0/3674	1.23	4/4978 (0.1%)
2	E	0.73	0/3703	1.25	2/5017 (0.0%)
2	F	0.73	0/3647	1.23	2/4944 (0.0%)
3	G	0.69	0/2973	1.19	0/4016
4	H	0.74	0/1705	1.22	1/2275 (0.0%)
5	I	0.70	0/1791	1.22	0/2395
5	J	0.68	0/1825	1.19	0/2442
5	K	0.68	0/1791	1.19	1/2395 (0.0%)
6	L	0.88	0/889	1.41	4/1199 (0.3%)
7	M	0.75	0/922	1.26	0/1228
7	N	0.73	0/937	1.24	0/1248
7	O	0.72	0/937	1.25	0/1248
8	P	0.76	0/3596	1.30	0/4843
9	Q	0.71	0/2156	1.24	0/2905
9	R	0.69	0/2160	1.22	0/2910
9	S	0.71	0/2181	1.24	2/2936 (0.1%)
10	T	0.76	0/1417	1.26	1/1919 (0.1%)
All	All	0.73	0/50457	1.24	22/68056 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
2	E	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	3
3	G	0	3
7	M	0	1
7	O	0	1
9	S	0	2
All	All	0	16

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	60	ASP	CA-CB-CG	7.42	120.02	112.60
6	L	67	ASN	CA-CB-CG	6.58	119.18	112.60
1	B	466	ASP	CA-CB-CG	6.50	119.10	112.60
1	C	186	ASP	CA-CB-CG	6.22	118.82	112.60
2	E	359	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	186	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	186	ASP	CA-CB-CG	5.72	118.32	112.60
2	D	359	ASP	CA-CB-CG	5.58	118.17	112.60
2	D	415	HIS	CA-CB-CG	5.56	119.36	113.80
6	L	103	ASP	CA-C-N	5.53	128.45	120.38
6	L	103	ASP	C-N-CA	5.53	128.45	120.38
2	F	359	ASP	CA-CB-CG	5.46	118.06	112.60
4	H	206	GLN	OE1-CD-NE2	-5.19	117.41	122.60
2	D	298	THR	N-CA-C	5.18	119.61	113.28
5	K	226	ASP	CA-CB-CG	5.17	117.77	112.60
2	E	192	PHE	CA-CB-CG	5.16	118.95	113.80
2	F	187	GLN	OE1-CD-NE2	-5.10	117.50	122.60
9	S	57	GLU	CA-C-N	5.10	129.49	120.87
9	S	57	GLU	C-N-CA	5.10	129.49	120.87
10	T	58	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	C	65	GLN	OE1-CD-NE2	-5.06	117.54	122.60
2	D	192	PHE	CA-CB-CG	5.03	118.83	113.80

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ARG	Sidechain
1	C	525	TYR	Sidechain
2	E	389	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	400	ARG	Sidechain
2	E	412	ARG	Sidechain
2	E	82	ARG	Sidechain
2	F	165	TYR	Sidechain
2	F	412	ARG	Sidechain
2	F	82	ARG	Sidechain
3	G	181	TYR	Sidechain
3	G	201	TYR	Sidechain
3	G	367	TYR	Sidechain
7	M	92	ARG	Sidechain
7	O	114	TYR	Sidechain
9	S	203	TYR	Sidechain
9	S	84	ARG	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	4568	0	4570	4	0
1	B	4657	0	4649	1	0
1	C	4648	0	4643	1	0
2	D	3603	0	3608	1	0
2	E	3632	0	3628	0	0
2	F	3576	0	3576	2	0
3	G	2919	0	2961	0	0
4	H	1689	0	1807	0	0
5	I	1774	0	1853	1	0
5	J	1808	0	1880	0	0
5	K	1774	0	1853	0	0
6	L	875	0	883	0	0
7	M	914	0	913	0	0
7	N	929	0	926	0	0
7	O	929	0	926	0	0
8	P	3529	0	3504	0	0
9	Q	2122	0	2162	0	0
9	R	2126	0	2165	0	0
9	S	2147	0	2190	0	0
10	T	1377	0	1315	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	27	0	12	0	0
12	C	1	0	0	0	0
All	All	49624	0	50024	9	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 (9) 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:C:594:GLU:HG2	1:C:598:LYS:HE2	1.73	0.69
1:A:574:MET:HE3	1:A:611:ALA:HB3	1.92	0.51
2:F:166:PRO:HG2	2:F:401:LEU:HD13	1.92	0.51
1:B:574:MET:HE3	1:B:611:ALA:HB3	1.97	0.47
1:A:574:MET:HE1	1:A:612:PHE:CE1	2.52	0.45
2:F:485:ARG:HD2	2:F:504:TYR:O	2.17	0.45
1:A:65:GLN:O	1:A:65:GLN:HG2	2.19	0.42
1:A:95:MET:HE2	1:A:337:PHE:CE2	2.54	0.41
2:D:43:PRO:HB2	5:I:192:VAL:CG2	2.52	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	582/617 (94%)	563 (97%)	17 (3%)	2 (0%)	36	65
1	B	599/617 (97%)	578 (96%)	17 (3%)	4 (1%)	18	49
1	C	598/617 (97%)	571 (96%)	27 (4%)	0	100	100
2	D	456/511 (89%)	443 (97%)	13 (3%)	0	100	100
2	E	460/511 (90%)	437 (95%)	23 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	453/511 (89%)	438 (97%)	15 (3%)	0	100	100
3	G	354/382 (93%)	338 (96%)	16 (4%)	0	100	100
4	H	203/247 (82%)	198 (98%)	5 (2%)	0	100	100
5	I	216/226 (96%)	215 (100%)	1 (0%)	0	100	100
5	J	221/226 (98%)	219 (99%)	2 (1%)	0	100	100
5	K	216/226 (96%)	211 (98%)	5 (2%)	0	100	100
6	L	108/119 (91%)	98 (91%)	8 (7%)	2 (2%)	6	28
7	M	109/118 (92%)	105 (96%)	4 (4%)	0	100	100
7	N	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
7	O	111/118 (94%)	108 (97%)	3 (3%)	0	100	100
8	P	426/483 (88%)	420 (99%)	5 (1%)	1 (0%)	43	71
9	Q	260/280 (93%)	250 (96%)	8 (3%)	2 (1%)	16	45
9	R	261/280 (93%)	253 (97%)	7 (3%)	1 (0%)	30	60
9	S	264/280 (94%)	257 (97%)	7 (3%)	0	100	100
10	T	168/221 (76%)	158 (94%)	8 (5%)	2 (1%)	10	37
All	All	6176/6708 (92%)	5970 (97%)	192 (3%)	14 (0%)	44	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	110	LYS
9	R	214	GLU
1	A	298	VAL
8	P	351	SER
1	A	139	LYS
1	B	561	SER
1	B	278	GLY
1	B	370	ALA
9	Q	61	ARG
10	T	59	SER
9	Q	62	PHE
1	B	298	VAL
6	L	111	GLY
10	T	148	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	500/524 (95%)	497 (99%)	3 (1%)	78	81
1	B	508/524 (97%)	504 (99%)	4 (1%)	73	79
1	C	507/524 (97%)	504 (99%)	3 (1%)	78	81
2	D	394/431 (91%)	393 (100%)	1 (0%)	86	86
2	E	398/431 (92%)	396 (100%)	2 (0%)	81	83
2	F	391/431 (91%)	390 (100%)	1 (0%)	86	86
3	G	325/344 (94%)	323 (99%)	2 (1%)	78	81
4	H	182/212 (86%)	180 (99%)	2 (1%)	65	76
5	I	192/198 (97%)	190 (99%)	2 (1%)	68	76
5	J	196/198 (99%)	194 (99%)	2 (1%)	68	76
5	K	192/198 (97%)	191 (100%)	1 (0%)	81	83
6	L	94/100 (94%)	92 (98%)	2 (2%)	47	67
7	M	96/101 (95%)	96 (100%)	0	100	100
7	N	98/101 (97%)	97 (99%)	1 (1%)	68	76
7	O	98/101 (97%)	98 (100%)	0	100	100
8	P	388/428 (91%)	383 (99%)	5 (1%)	61	74
9	Q	241/255 (94%)	239 (99%)	2 (1%)	73	79
9	R	241/255 (94%)	240 (100%)	1 (0%)	84	84
9	S	243/255 (95%)	242 (100%)	1 (0%)	84	84
10	T	148/195 (76%)	146 (99%)	2 (1%)	59	73
All	All	5432/5806 (94%)	5395 (99%)	37 (1%)	73	80

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	74	SER
1	A	130	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	130	ASP
1	B	364	ARG
1	B	508	THR
1	B	563	ASN
1	C	74	SER
1	C	224	ASN
1	C	289	ARG
2	D	168	GLU
2	E	213	VAL
2	E	321	ARG
2	F	485	ARG
3	G	13	LYS
3	G	179	SER
4	H	34	LYS
4	H	86	ASN
5	I	88	ASP
5	I	212	ARG
5	J	80	ARG
5	J	116	LEU
5	K	110	THR
6	L	13	ASP
6	L	60	ASP
7	N	87	TYR
8	P	256	MET
8	P	300	GLU
8	P	364	LEU
8	P	383	LEU
8	P	447	GLN
9	Q	42	LEU
9	Q	274	ASN
9	R	107	LEU
9	S	42	LEU
10	T	77	ARG
10	T	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	B	65	GLN
1	B	164	HIS
1	B	184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	231	GLN
1	B	521	GLN
1	C	140	ASN
1	C	184	ASN
2	D	181	ASN
2	D	384	HIS
2	D	420	ASN
2	D	461	ASN
2	E	73	HIS
2	E	156	GLN
2	E	181	ASN
2	E	205	GLN
2	E	209	GLN
2	E	358	ASN
2	F	181	ASN
2	F	205	GLN
2	F	209	GLN
2	F	251	ASN
2	F	384	HIS
2	F	433	GLN
3	G	120	ASN
3	G	193	ASN
3	G	226	ASN
4	H	111	HIS
4	H	113	HIS
5	I	9	GLN
5	I	122	GLN
5	J	11	GLN
5	J	77	ASN
5	J	149	GLN
5	K	66	GLN
6	L	31	ASN
6	L	35	ASN
6	L	96	HIS
7	M	6	GLN
7	M	10	GLN
7	M	13	GLN
7	N	10	GLN
7	O	9	GLN
7	O	10	GLN
8	P	17	ASN
8	P	175	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	P	196	GLN
8	P	199	GLN
8	P	233	ASN
8	P	238	GLN
8	P	242	GLN
8	P	435	GLN
8	P	439	ASN
9	Q	207	GLN
9	Q	243	GLN
9	S	162	GLN
9	S	196	GLN
9	S	222	GLN
10	T	213	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	ADP	C	701	12	28,29,29	1.20	2 (7%)	43,45,45	1.20	5 (11%)

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
11	ADP	C	701	12	-	2/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	701	ADP	PA-O3A	-3.32	1.55	1.59
11	C	701	ADP	C5-C4	-2.16	1.35	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	701	ADP	C5-C4-N3	-2.84	122.80	126.72
11	C	701	ADP	C4-C5-N7	2.81	113.80	110.58
11	C	701	ADP	C2-N1-C6	-2.32	114.92	118.73
11	C	701	ADP	O2B-PB-O3A	2.23	112.13	104.64
11	C	701	ADP	C5-C6-N1	2.14	122.93	117.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

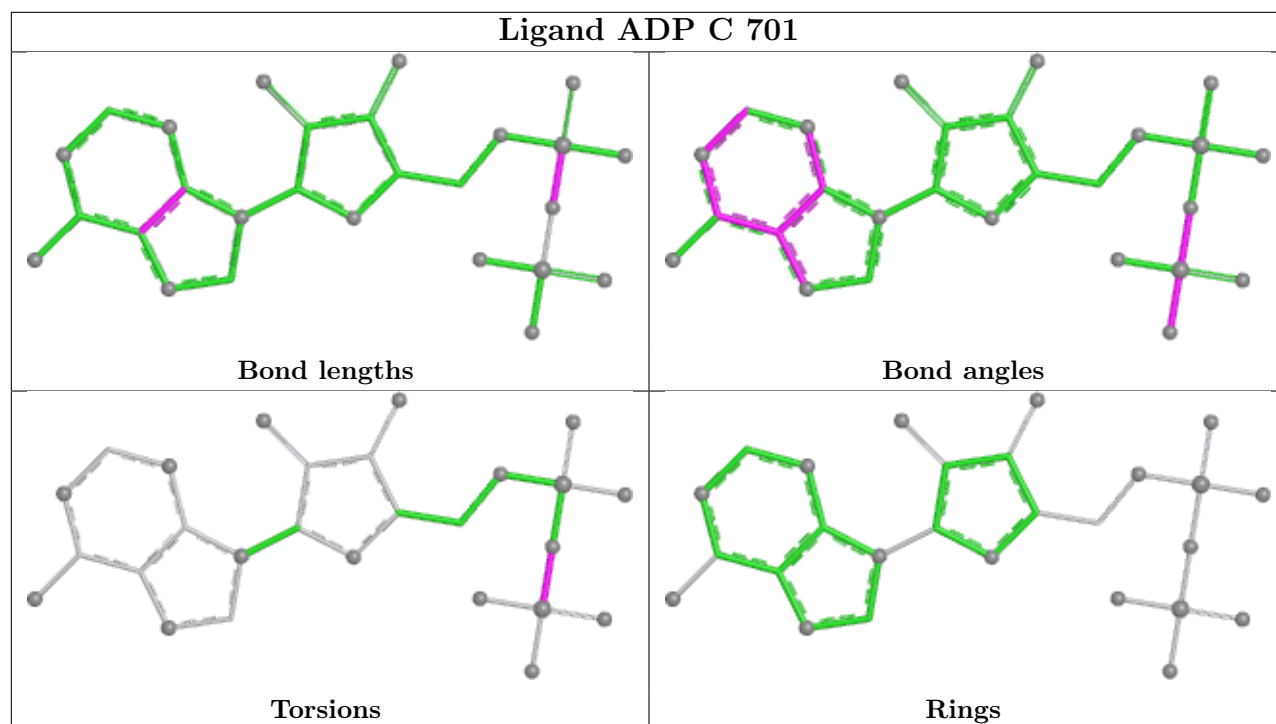
Mol	Chain	Res	Type	Atoms
11	C	701	ADP	PA-O3A-PB-O2B
11	C	701	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

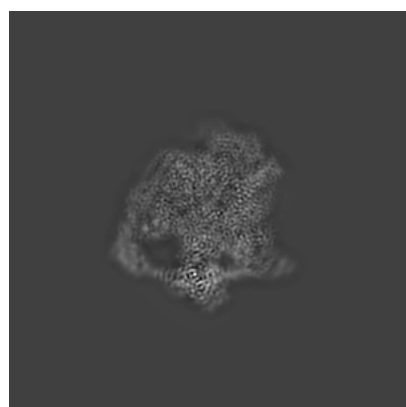
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26913. These allow visual inspection of the internal detail of the map and identification of artifacts.

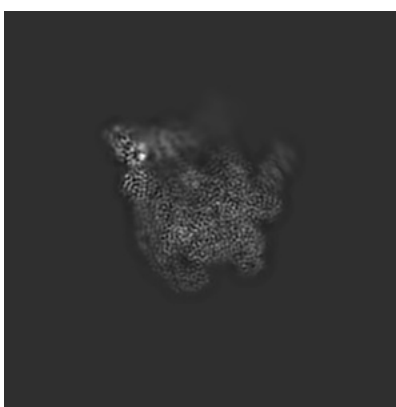
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

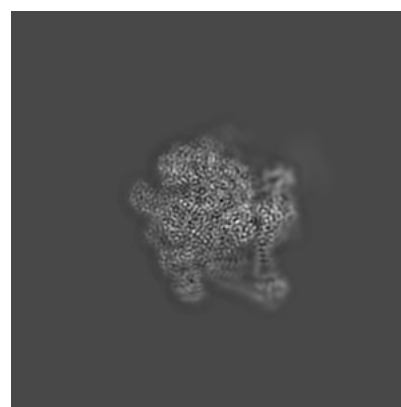
6.1.1 Primary map



X



Y

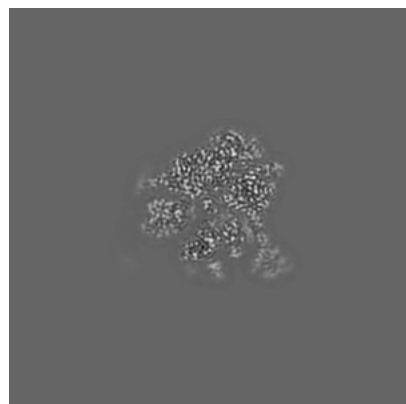


Z

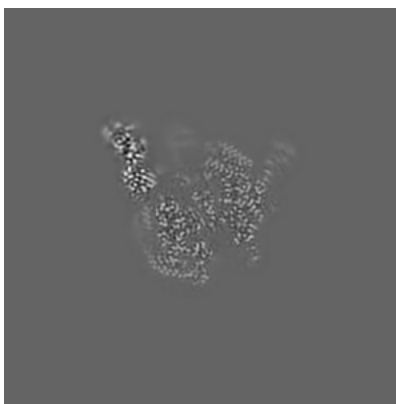
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

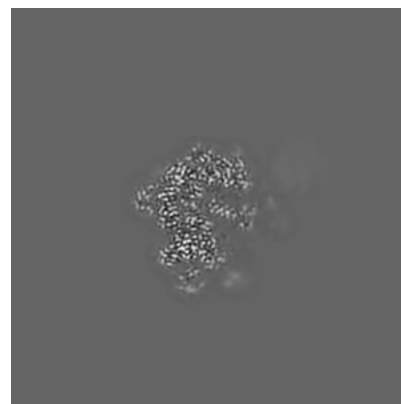
6.2.1 Primary map



X Index: 175



Y Index: 175

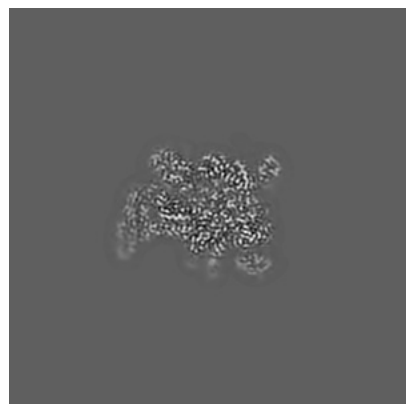


Z Index: 175

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

6.3 Largest variance slices [i](#)

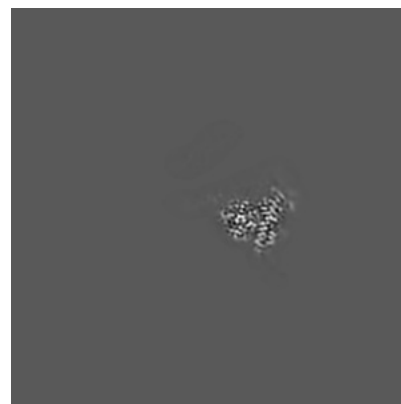
6.3.1 Primary map



X Index: 157



Y Index: 162

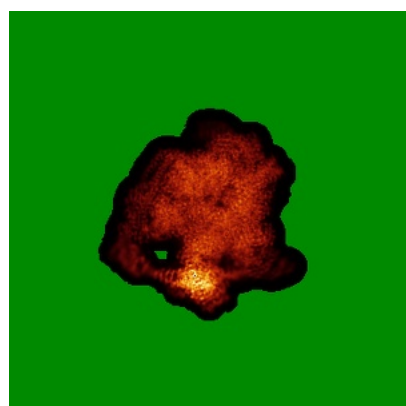


Z Index: 111

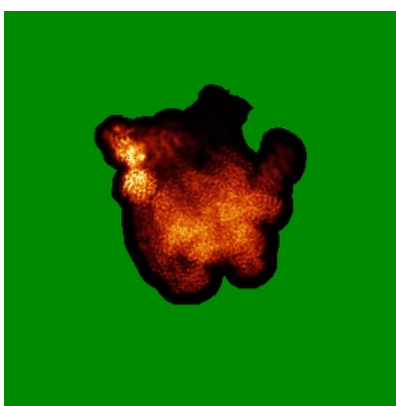
The images above show the largest variance slices of the map in three orthogonal directions.

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

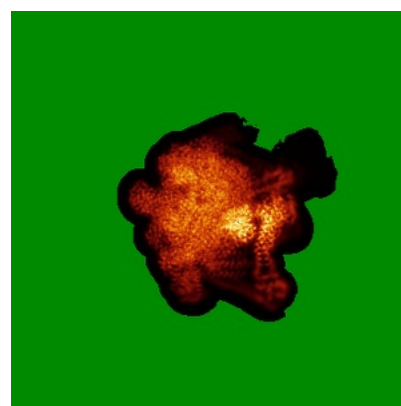
6.4.1 Primary map



X



Y

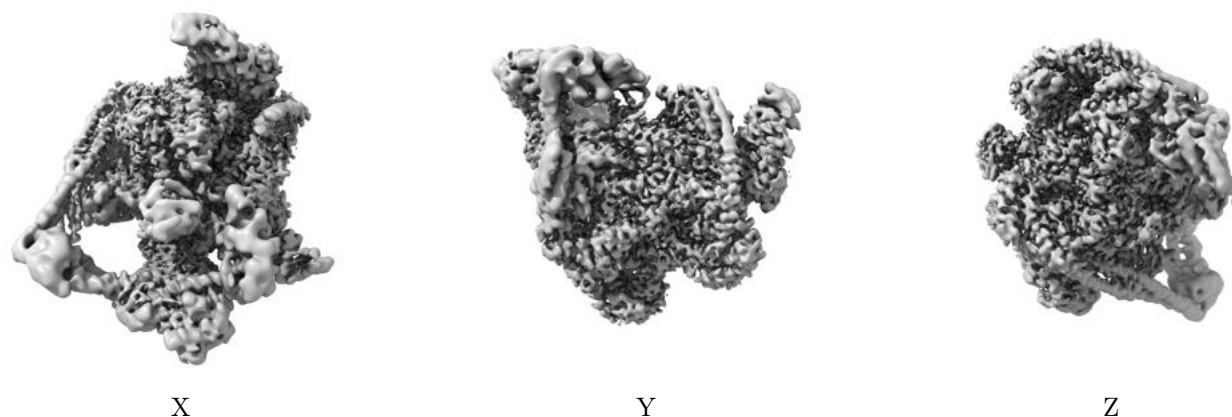


Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

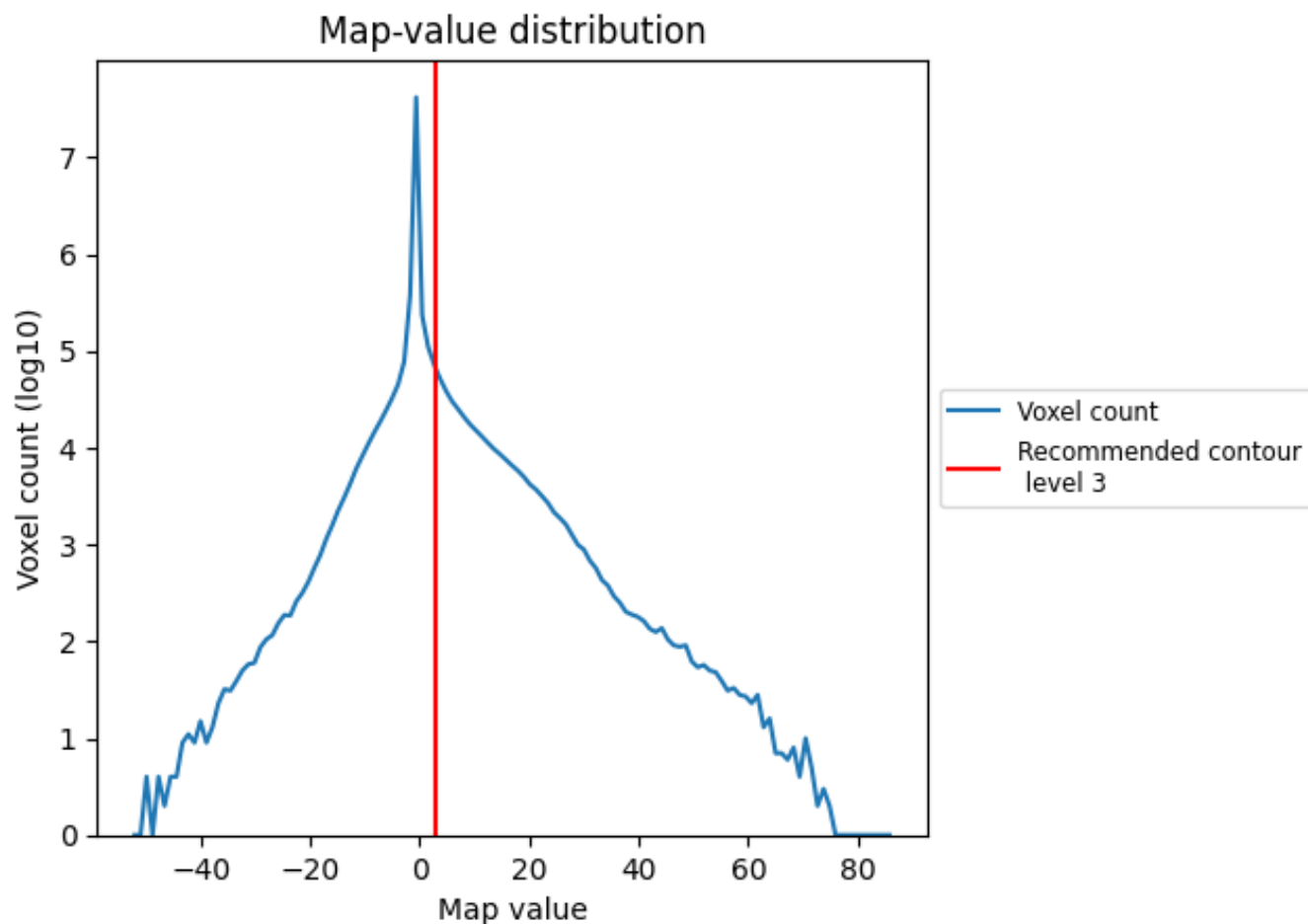
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

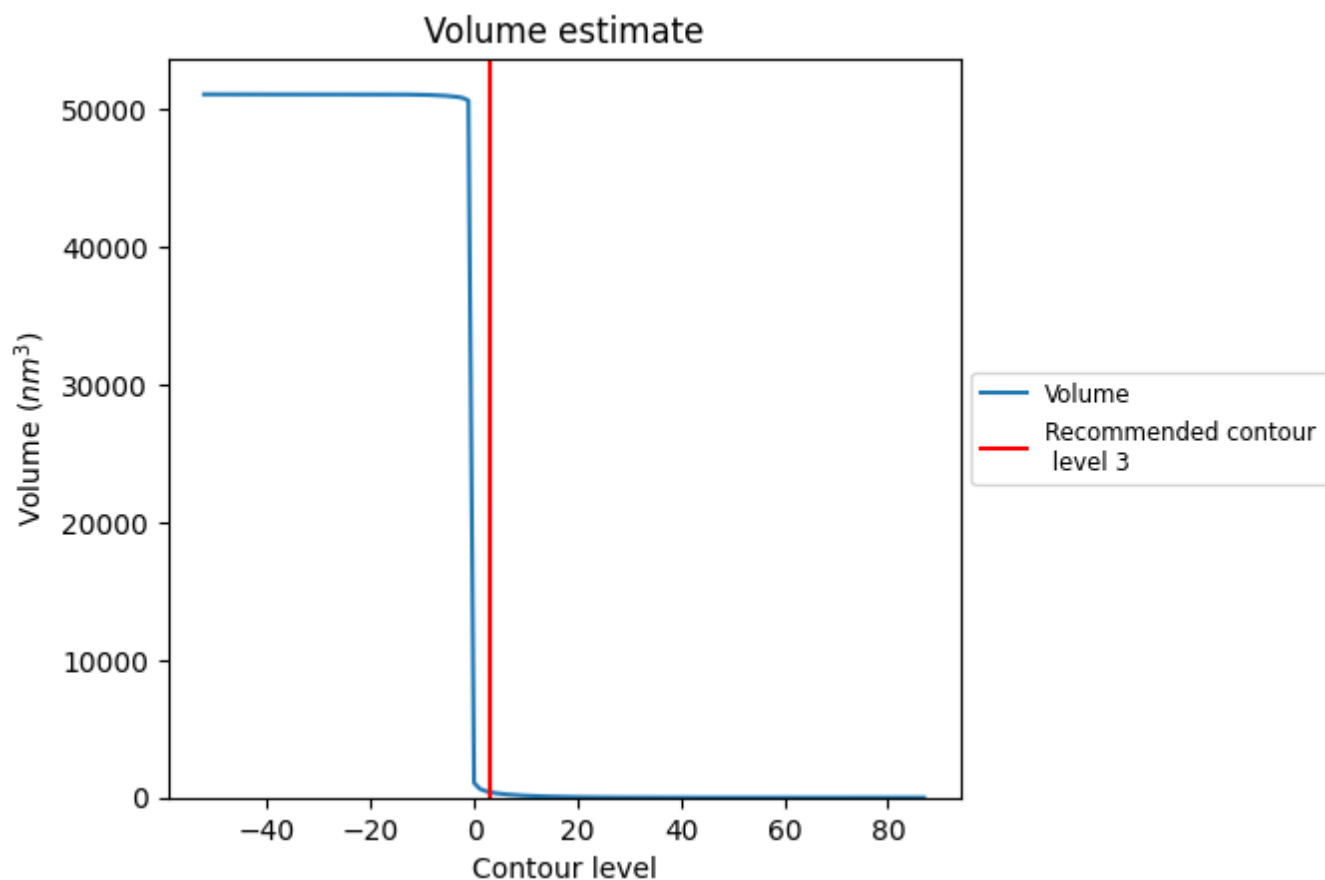
This section contains the results of statistical analysis of the map.

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.

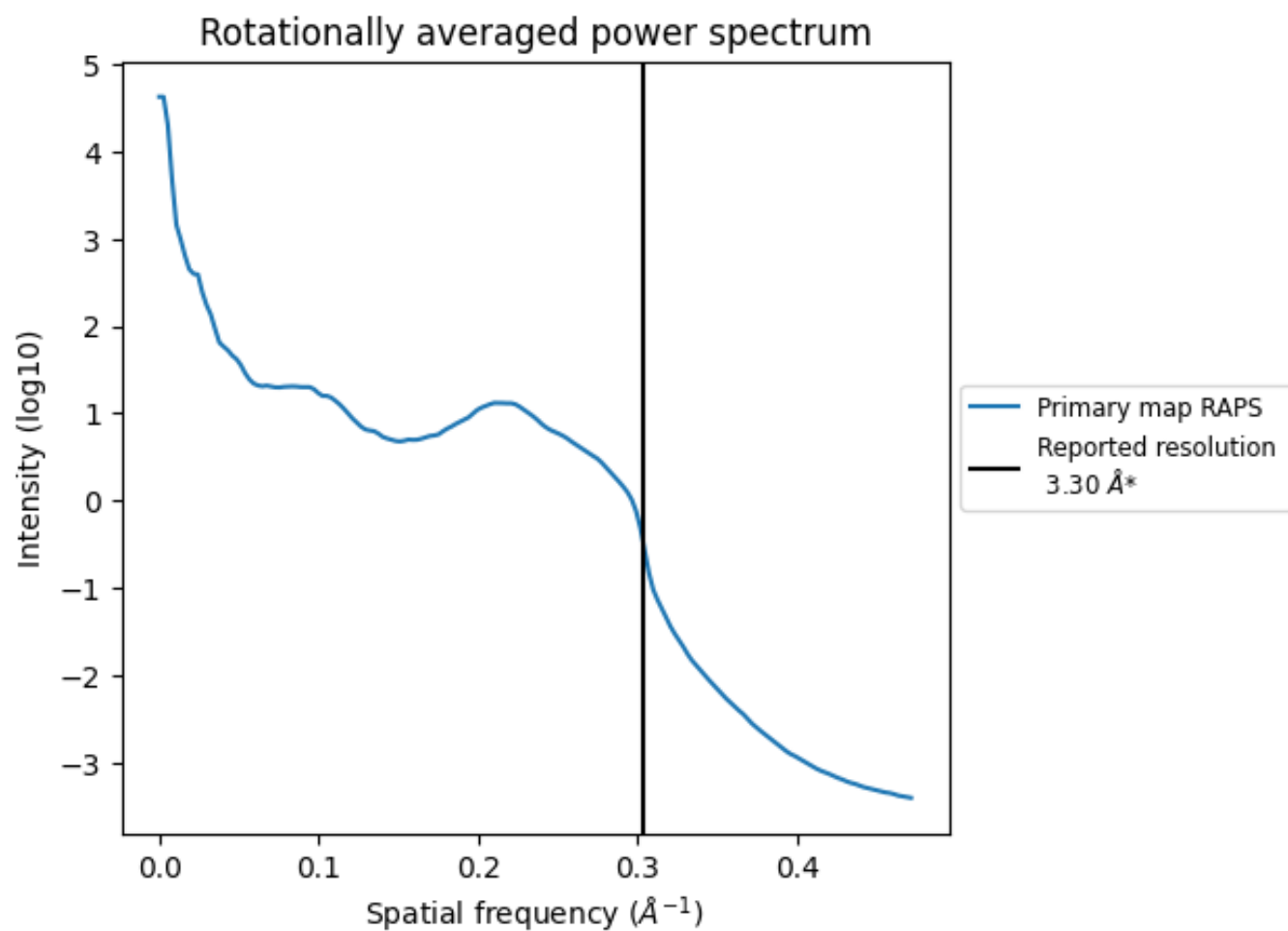
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 405 nm³; this corresponds to an approximate mass of 366 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

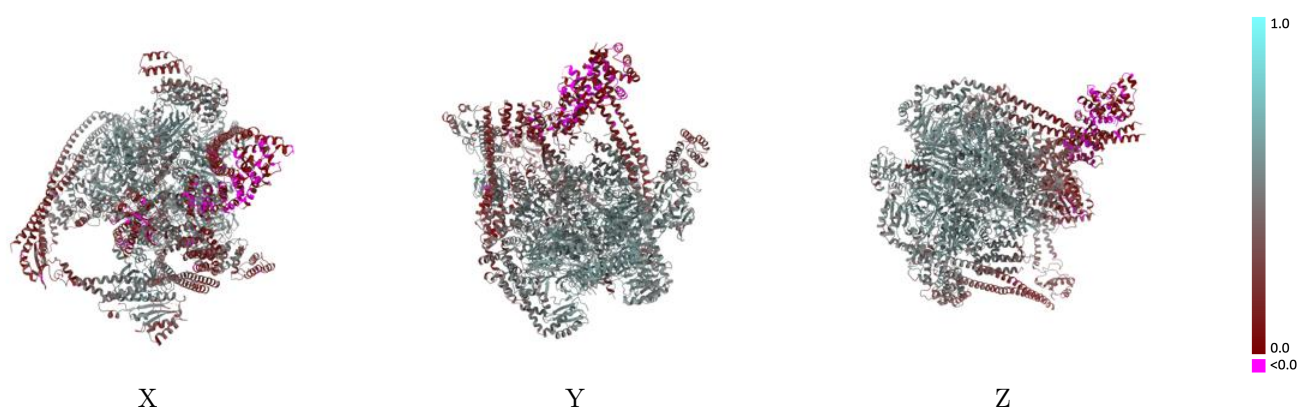
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-26913 and PDB model 7UZJ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

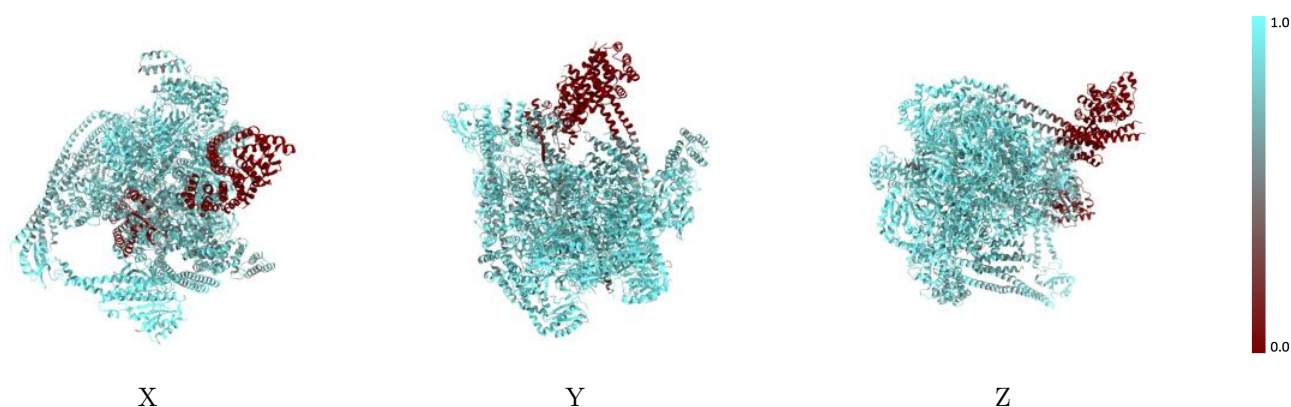
This section was not generated.

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



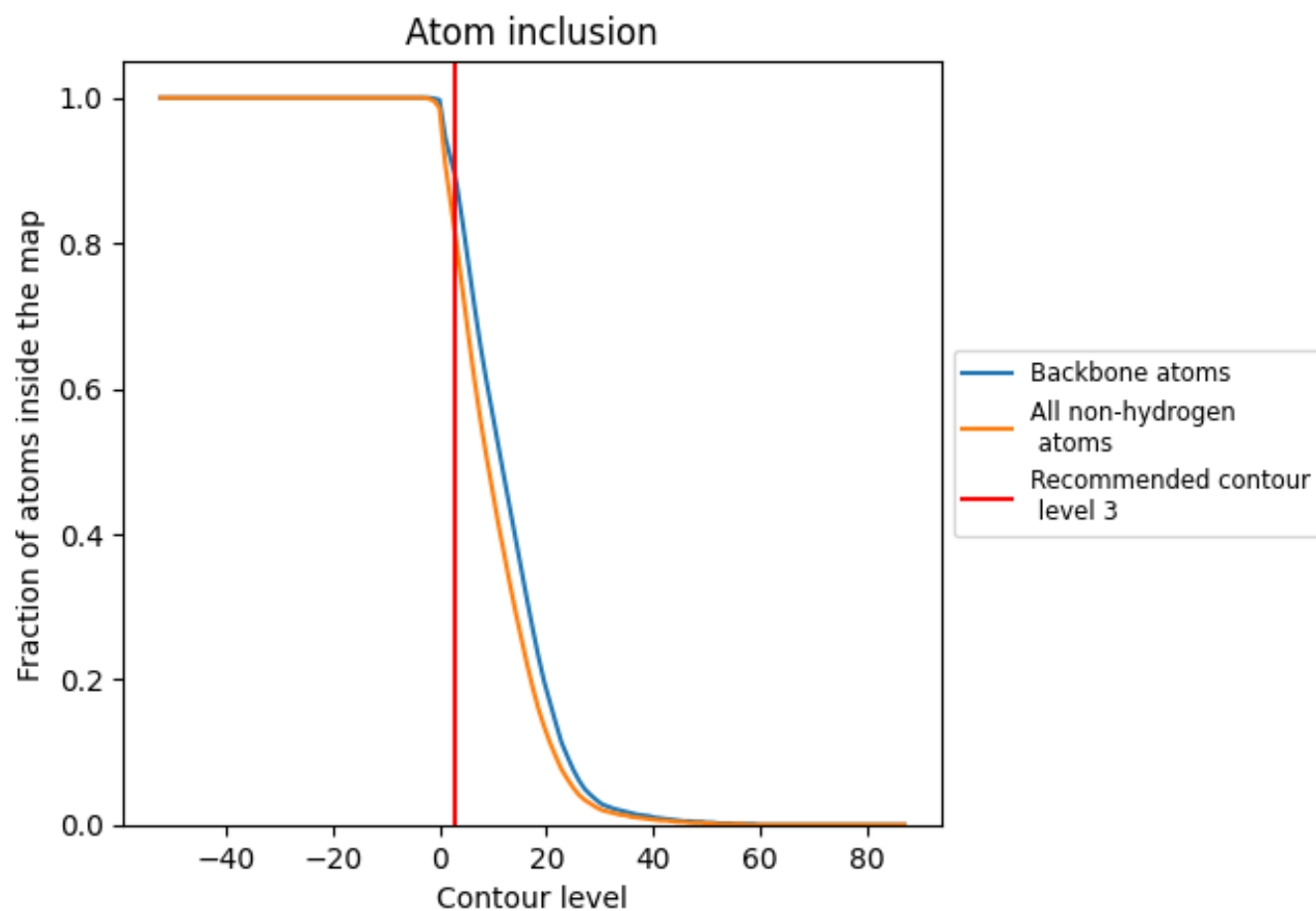
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.4420
A	 0.8920	 0.5090
B	 0.8970	 0.5190
C	 0.9150	 0.5410
D	 0.9330	 0.5540
E	 0.9390	 0.5590
F	 0.9380	 0.5610
G	 0.9250	 0.3730
H	 0.5850	 0.3490
I	 0.7030	 0.4030
J	 0.8760	 0.4540
K	 0.8450	 0.4210
L	 0.2990	 0.1560
M	 0.4940	 0.3030
N	 0.8120	 0.3540
O	 0.7870	 0.3330
P	 0.2160	 0.0900
Q	 0.7930	 0.3840
R	 0.8260	 0.4100
S	 0.8020	 0.4000
T	 0.9700	 0.5460

