Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 02:27 PM EST

PDB ID	:	7UZK
EMDB ID	:	EMD-26914
Title	:	Rat Kidney V1 complex lacking subunit H with SidK and NCOA7B, State 1
Authors	:	Abbas, Y.M.; Rubinstein, J.L.
Deposited on	:	2022-05-09
Resolution	:	3.00 Å(reported)

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

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

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

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

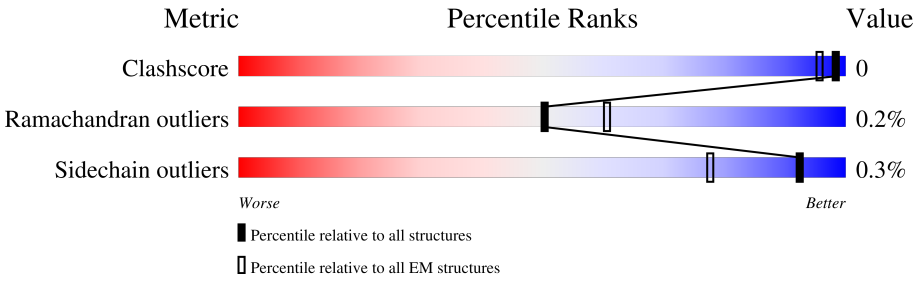
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=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	92% · 5%
1	B	617	93% · ·
1	C	617	94% · ·
2	D	511	87% · 10%
2	E	511	87% · 9%
2	F	511	85% · 11%
3	G	382	90% · 6%
4	H	247	79% · · 16%

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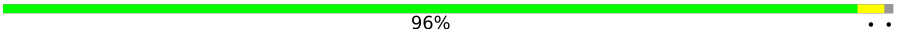
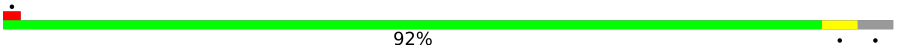
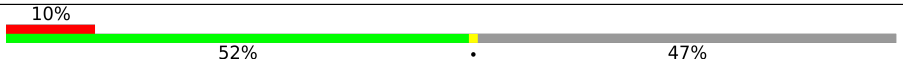
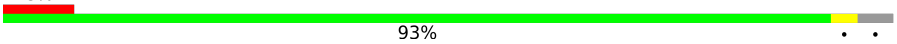
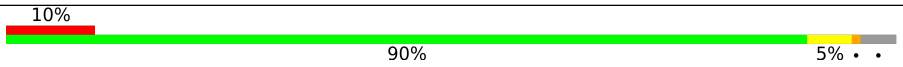
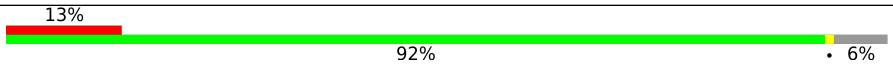
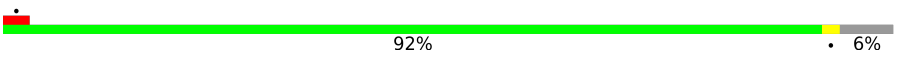
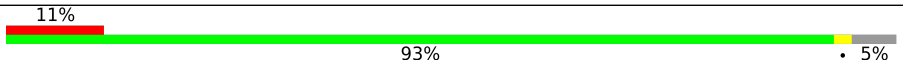
Mol	Chain	Length	Quality of chain
5	I	226	
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	Q	280	
8	R	280	
8	S	280	
9	T	221	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 45246 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	167	Total	C	N	O	S	0	0
			1341	847	241	246	7		
5	J	223	Total	C	N	O	S	0	0
			1807	1137	319	341	10		
5	K	218	Total	C	N	O	S	0	0
			1773	1118	314	331	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	62	Total	C	N	O	S	0	0
			501	311	86	101	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		

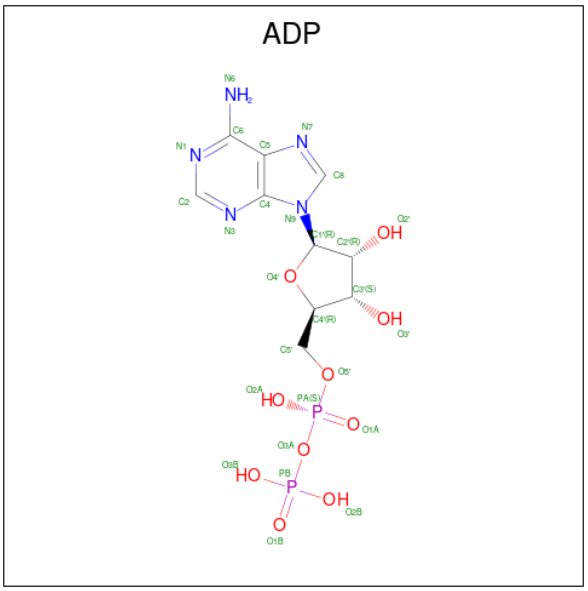
- Molecule 8 is a protein called Effector SidK.

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

- Molecule 9 is a protein called Nuclear receptor coactivator 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	170	Total	C	N	O	S	0	0
			1376	887	230	256	3		

- Molecule 10 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
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

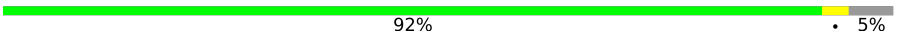
Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	

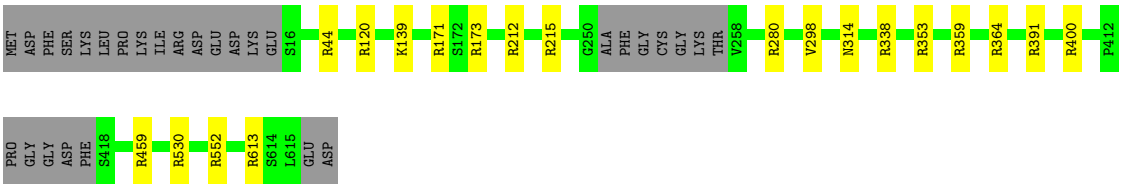
3 Residue-property plots (i)

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

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

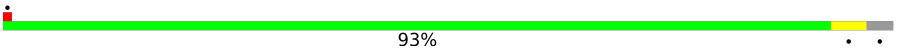
Chain A:

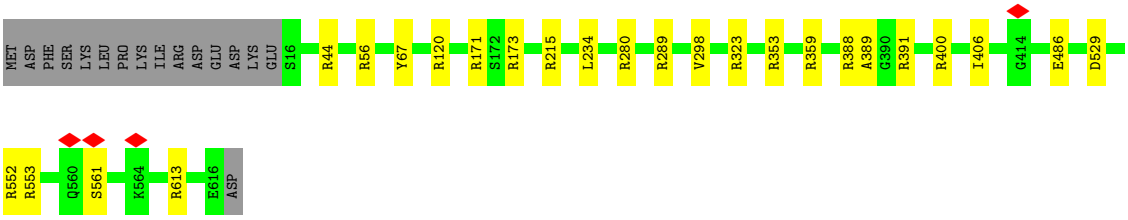




• Molecule 1: ATPase H+-transporting V1 subunit A

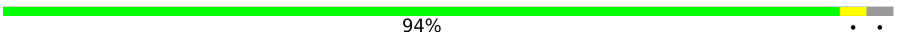
Chain B:





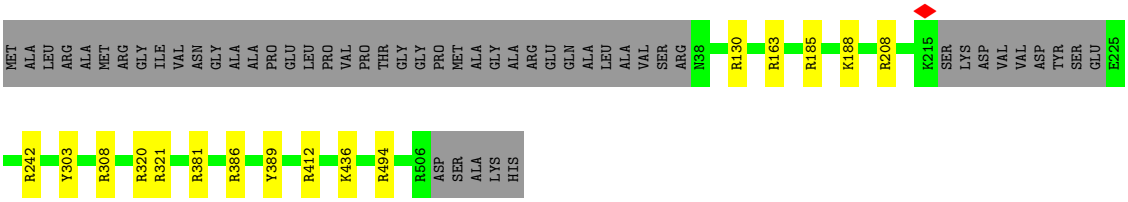
• Molecule 1: ATPase H+-transporting V1 subunit A

Chain C:

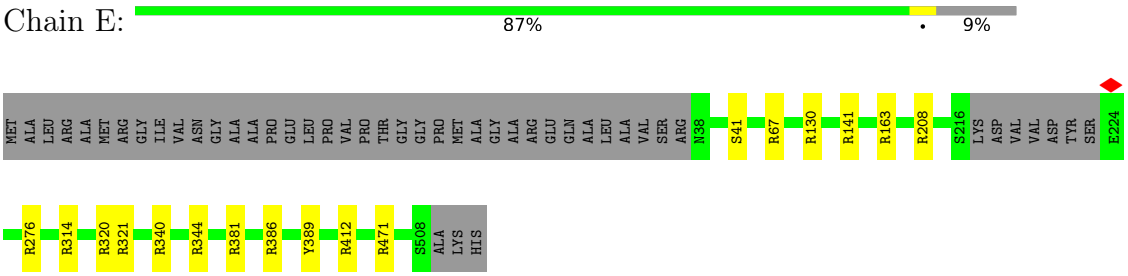


• Molecule 2: V-type proton ATPase subunit B, brain isoform

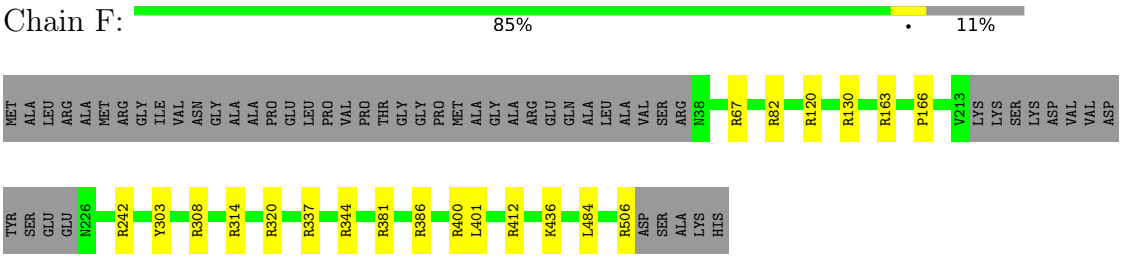
Chain D:



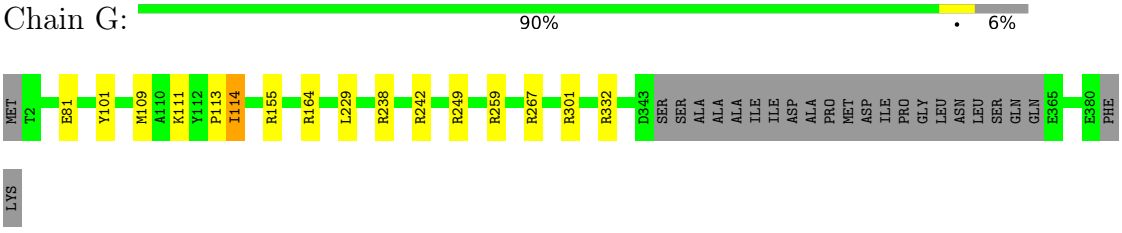
• Molecule 2: V-type proton ATPase subunit B, brain isoform



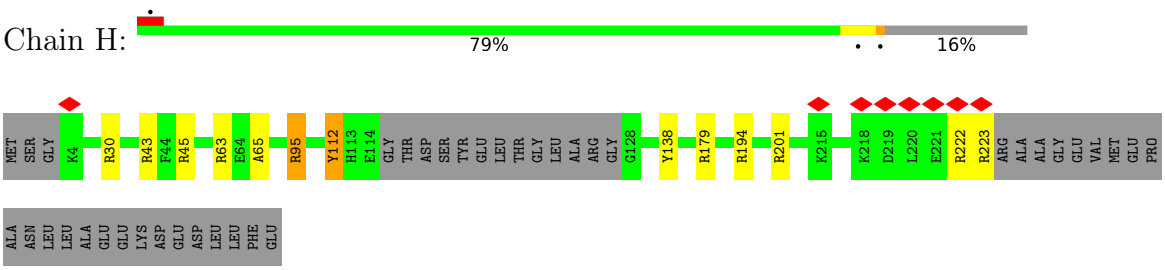
• Molecule 2: V-type proton ATPase subunit B, brain isoform



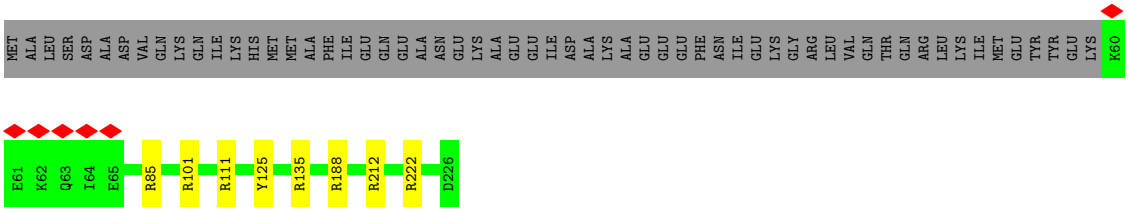
• Molecule 3: V-type proton ATPase subunit C 1



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

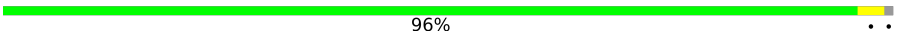


• Molecule 5: V-type proton ATPase subunit E 1



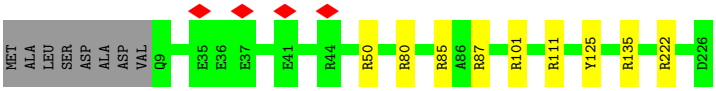
• Molecule 5: V-type proton ATPase subunit E 1

Chain J:



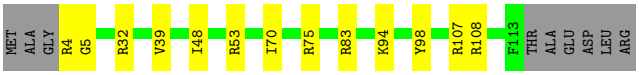
• Molecule 5: V-type proton ATPase subunit E 1

Chain K:



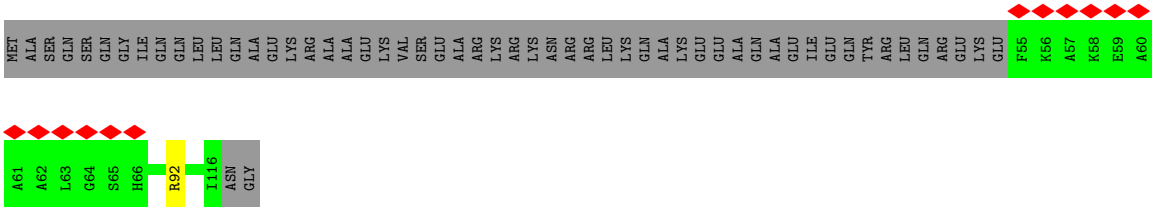
• Molecule 6: V-type proton ATPase subunit F

Chain L:



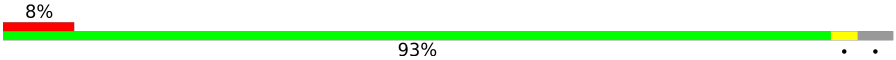
• Molecule 7: V-type proton ATPase subunit G

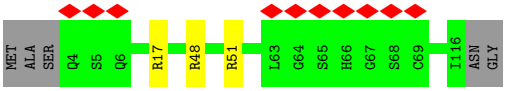
Chain M:



• Molecule 7: V-type proton ATPase subunit G

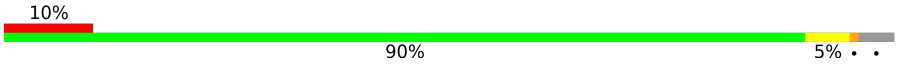
Chain N:

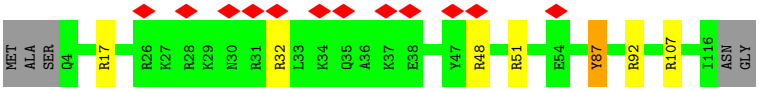




• Molecule 7: V-type proton ATPase subunit G

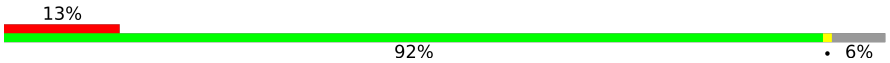
Chain O:

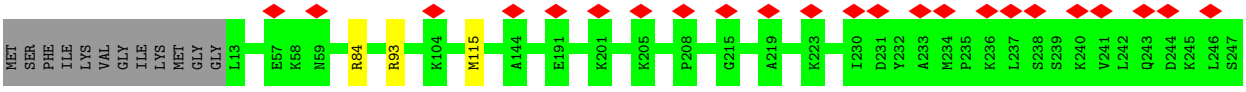


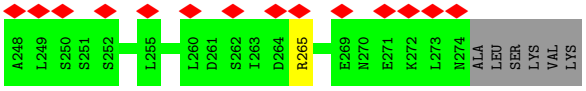


• Molecule 8: Effector SidK

Chain Q:

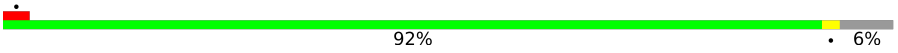


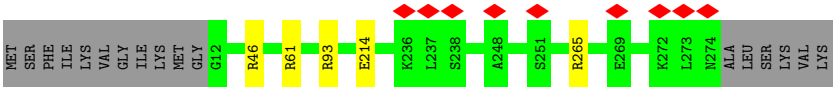




• Molecule 8: Effector SidK

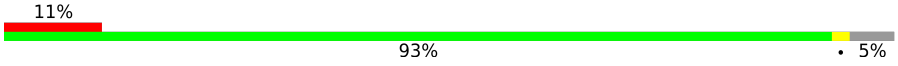
Chain R:

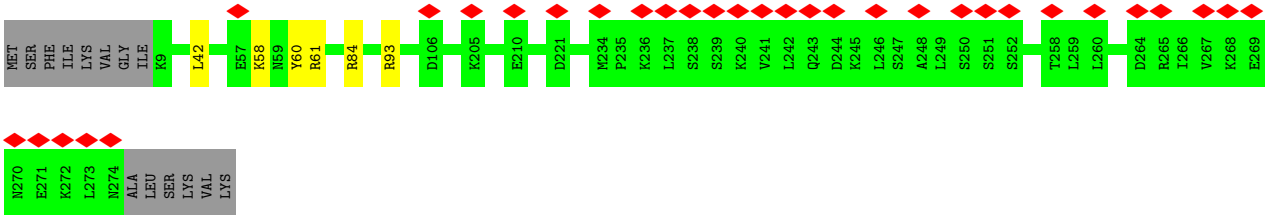




• Molecule 8: Effector SidK

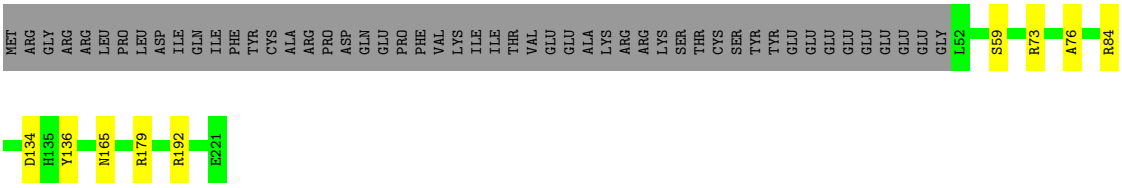
Chain S:





• Molecule 9: Nuclear receptor coactivator 7B

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175138	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 ($e^-/Å^2$)	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	94.198	Depositor
Minimum map value	-74.132	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.197	Depositor
Recommended contour level	3.0	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	0.63	0/4658	1.00	20/6304 (0.3%)
1	B	0.64	0/4752	1.00	18/6433 (0.3%)
1	C	0.64	0/4743	1.00	18/6421 (0.3%)
2	D	0.64	0/3674	0.98	11/4978 (0.2%)
2	E	0.63	0/3703	1.00	15/5017 (0.3%)
2	F	0.65	1/3647 (0.0%)	1.01	16/4944 (0.3%)
3	G	0.61	1/2973 (0.0%)	0.93	9/4016 (0.2%)
4	H	0.64	0/1705	1.03	10/2275 (0.4%)
5	I	0.61	0/1353	0.98	9/1815 (0.5%)
5	J	0.60	0/1824	0.91	5/2442 (0.2%)
5	K	0.61	0/1790	0.93	9/2395 (0.4%)
6	L	0.64	0/889	1.13	6/1199 (0.5%)
7	M	0.65	0/508	0.89	1/682 (0.1%)
7	N	0.64	0/937	0.93	3/1248 (0.2%)
7	O	0.65	0/937	0.96	8/1248 (0.6%)
8	Q	0.61	0/2156	0.88	3/2905 (0.1%)
8	R	0.60	0/2160	0.88	4/2910 (0.1%)
8	S	0.60	0/2181	0.87	3/2936 (0.1%)
9	T	0.65	1/1416 (0.1%)	0.96	4/1919 (0.2%)
All	All	0.63	3/46006 (0.0%)	0.97	172/62087 (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	B	0	1
2	D	0	3
2	E	0	1
2	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	76	ALA	C-N	6.00	1.47	1.34
2	F	484	LEU	C-N	-5.68	1.21	1.34
3	G	113	PRO	C-N	5.34	1.46	1.34

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Q	93	ARG	NE-CZ-NH1	9.59	125.09	120.30
8	R	93	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	400	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	391	ARG	NE-CZ-NH1	8.89	124.75	120.30
2	F	308	ARG	NE-CZ-NH1	8.67	124.63	120.30
5	I	212	ARG	NE-CZ-NH1	8.65	124.62	120.30
2	F	320	ARG	NE-CZ-NH1	8.41	124.50	120.30
2	F	400	ARG	NE-CZ-NH1	8.24	124.42	120.30
2	F	130	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	613	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	B	215	ARG	NE-CZ-NH1	8.00	124.30	120.30
8	S	93	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	B	391	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	400	ARG	NE-CZ-NH1	7.88	124.24	120.30
4	H	63	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	E	130	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	C	212	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	44	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	E	67	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	552	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	D	320	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	C	280	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	364	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	D	130	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	215	ARG	NE-CZ-NH1	7.15	123.88	120.30
6	L	107	ARG	NE-CZ-NH1	7.13	123.87	120.30
3	G	155	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	323	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	44	ARG	NE-CZ-NH1	7.07	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	215	ARG	NE-CZ-NH1	7.03	123.81	120.30
3	G	267	ARG	NE-CZ-NH1	7.00	123.80	120.30
7	O	32	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	613	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	388	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	212	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	C	571	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	F	381	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	D	185	ARG	NE-CZ-NH1	6.78	123.69	120.30
7	O	17	ARG	NE-CZ-NH1	6.78	123.69	120.30
7	N	17	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	104	ARG	NE-CZ-NH1	6.66	123.63	120.30
4	H	95	ARG	NE-CZ-NH1	6.66	123.63	120.30
4	H	43	ARG	NE-CZ-NH1	6.62	123.61	120.30
5	J	135	ARG	NE-CZ-NH1	6.62	123.61	120.30
8	R	46	ARG	NE-CZ-NH1	6.60	123.60	120.30
5	J	111	ARG	NE-CZ-NH1	6.59	123.59	120.30
4	H	194	ARG	NE-CZ-NH1	6.58	123.59	120.30
3	G	301	ARG	NE-CZ-NH1	6.57	123.58	120.30
2	E	412	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	171	ARG	NE-CZ-NH1	6.48	123.54	120.30
8	Q	84	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	553	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	171	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	F	67	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	364	ARG	NE-CZ-NH1	6.39	123.49	120.30
5	K	80	ARG	NE-CZ-NH1	6.37	123.48	120.30
3	G	249	ARG	NE-CZ-NH1	6.36	123.48	120.30
7	N	51	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	G	164	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	613	ARG	NE-CZ-NH1	6.31	123.45	120.30
3	G	242	ARG	NE-CZ-NH1	6.31	123.45	120.30
2	D	381	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	E	163	ARG	NE-CZ-NH1	6.29	123.44	120.30
8	S	61	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	359	ARG	NE-CZ-NH1	6.28	123.44	120.30
9	T	84	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	F	242	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	F	506	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	44	ARG	NE-CZ-NH1	6.23	123.41	120.30
5	K	111	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	E	208	ARG	NE-CZ-NH1	6.21	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	84	ARG	NE-CZ-NH1	6.20	123.40	120.30
5	K	85	ARG	NE-CZ-NH1	6.19	123.40	120.30
2	D	242	ARG	NE-CZ-NH1	6.15	123.38	120.30
5	K	50	ARG	NE-CZ-NH1	6.11	123.35	120.30
5	K	101	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	552	ARG	NE-CZ-NH1	6.10	123.35	120.30
8	R	265	ARG	NE-CZ-NH1	6.08	123.34	120.30
4	H	223	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	173	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	E	381	ARG	NE-CZ-NH1	6.07	123.33	120.30
7	M	92	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	E	320	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	F	314	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	D	208	ARG	NE-CZ-NH1	5.99	123.29	120.30
9	T	192	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	81	ARG	NE-CZ-NH1	5.97	123.28	120.30
5	K	135	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	C	171	ARG	NE-CZ-NH1	5.93	123.26	120.30
2	D	412	ARG	NE-CZ-NH1	5.91	123.25	120.30
3	G	259	ARG	NE-CZ-NH1	5.89	123.25	120.30
4	H	30	ARG	NE-CZ-NH1	5.87	123.24	120.30
6	L	108	ARG	NE-CZ-NH1	5.87	123.23	120.30
5	I	125	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	C	353	ARG	NE-CZ-NH1	5.87	123.23	120.30
3	G	238	ARG	NE-CZ-NH1	5.82	123.21	120.30
4	H	201	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	C	359	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	D	386	ARG	NE-CZ-NH1	5.76	123.18	120.30
9	T	179	ARG	NE-CZ-NH1	5.74	123.17	120.30
5	K	125	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	215	ARG	NE-CZ-NH2	-5.73	117.44	120.30
6	L	75	ARG	NE-CZ-NH1	5.72	123.16	120.30
5	J	199	ARG	NE-CZ-NH1	5.71	123.16	120.30
8	Q	265	ARG	NE-CZ-NH1	5.70	123.15	120.30
4	H	222	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	280	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	F	344	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	F	412	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	G	332	ARG	NE-CZ-NH2	5.66	123.13	120.30
2	D	321	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	E	314	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	400	ARG	NE-CZ-NH1	5.63	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	215	ARG	NE-CZ-NH2	-5.60	117.50	120.30
7	O	17	ARG	NE-CZ-NH2	-5.59	117.51	120.30
5	I	101	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	67	TYR	CB-CG-CD2	-5.58	117.65	121.00
2	D	308	ARG	NE-CZ-NH1	5.58	123.09	120.30
7	N	48	ARG	NE-CZ-NH1	5.58	123.09	120.30
6	L	53	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	F	163	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	F	386	ARG	NE-CZ-NH1	5.54	123.07	120.30
5	K	87	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	E	340	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	D	163	ARG	NE-CZ-NH1	5.47	123.04	120.30
4	H	179	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	F	484	LEU	O-C-N	-5.44	113.99	122.70
1	A	120	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	173	ARG	NE-CZ-NH2	5.44	123.02	120.30
6	L	83	ARG	NE-CZ-NH1	5.42	123.01	120.30
5	I	222	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	F	337	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	359	ARG	NE-CZ-NH1	5.37	122.99	120.30
2	E	344	ARG	NE-CZ-NH1	5.36	122.98	120.30
6	L	32	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	E	276	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	391	ARG	NE-CZ-NH1	5.33	122.97	120.30
8	R	61	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	338	ARG	NE-CZ-NH1	5.31	122.95	120.30
7	O	107	ARG	NE-CZ-NH1	5.26	122.93	120.30
5	I	188	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	530	ARG	NE-CZ-NH1	5.26	122.93	120.30
5	I	85	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	364	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	353	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	E	386	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	459	ARG	NE-CZ-NH1	5.21	122.91	120.30
4	H	45	ARG	NE-CZ-NH1	5.20	122.90	120.30
7	O	51	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	338	ARG	NE-CZ-NH1	5.19	122.89	120.30
5	I	222	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	289	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	289	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	E	471	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	552	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	308	ARG	NE-CZ-NH1	5.14	122.87	120.30
7	O	87	TYR	CB-CG-CD2	-5.09	117.94	121.00
5	J	125	TYR	CB-CG-CD2	-5.08	117.95	121.00
5	K	222	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	E	141	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	E	321	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	442	ARG	NE-CZ-NH1	5.04	122.82	120.30
7	O	48	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	280	ARG	NE-CZ-NH1	5.04	122.82	120.30
5	I	135	ARG	NE-CZ-NH1	5.04	122.82	120.30
9	T	73	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	F	120	ARG	NE-CZ-NH1	5.03	122.81	120.30
5	I	111	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	353	ARG	NE-CZ-NH1	5.02	122.81	120.30
5	J	222	ARG	NE-CZ-NH1	5.02	122.81	120.30
7	O	92	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ARG	Sidechain
2	D	303	TYR	Sidechain
2	D	389	TYR	Sidechain
2	D	494	ARG	Sidechain
2	E	389	TYR	Sidechain
2	F	303	TYR	Sidechain
2	F	82	ARG	Sidechain
3	G	101	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	4568	0	4570	0	0
1	B	4657	0	4649	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4648	0	4643	1	0
2	D	3603	0	3608	0	0
2	E	3632	0	3628	0	0
2	F	3576	0	3575	1	0
3	G	2919	0	2961	1	0
4	H	1689	0	1807	4	0
5	I	1341	0	1423	0	0
5	J	1807	0	1880	1	0
5	K	1773	0	1853	0	0
6	L	875	0	883	3	0
7	M	501	0	480	0	0
7	N	929	0	926	0	0
7	O	929	0	926	0	0
8	Q	2122	0	2162	1	0
8	R	2126	0	2165	0	0
8	S	2147	0	2190	2	0
9	T	1376	0	1315	1	0
10	C	27	0	12	0	0
11	C	1	0	0	0	0
All	All	45246	0	45656	14	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 (14) 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	1.43	0.99
4:H:95:ARG:HG3	4:H:112:TYR:CE2	2.20	0.75
4:H:112:TYR:OH	6:L:5:GLY:HA3	2.09	0.53
4:H:112:TYR:OH	6:L:4:ARG:O	2.27	0.51
3:G:109:MET:SD	3:G:114:ILE:HG12	2.52	0.49
2:F:166:PRO:HG2	2:F:401:LEU:HD13	1.95	0.49
5:J:136:CYS:CB	5:J:144:VAL:HG21	2.45	0.47
8:Q:115:MET:N	8:Q:115:MET:HE2	2.30	0.46
4:H:65:ALA:HB1	4:H:138:TYR:CZ	2.50	0.46
9:T:136:TYR:CE2	9:T:165:ASN:HB2	2.54	0.42
8:S:58:LYS:HD3	8:S:60:TYR:HE2	1.84	0.42
6:L:39:VAL:HG21	6:L:70:ILE:HD12	2.03	0.41
8:S:58:LYS:HD3	8:S:60:TYR:CE2	2.55	0.41
1:B:389:ALA:HB2	1:B:406:ILE:HG12	2.01	0.41

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%)	570 (98%)	11 (2%)	1 (0%)	47 82
1	B	599/617 (97%)	581 (97%)	15 (2%)	3 (0%)	29 68
1	C	598/617 (97%)	577 (96%)	20 (3%)	1 (0%)	47 82
2	D	456/511 (89%)	444 (97%)	12 (3%)	0	100 100
2	E	460/511 (90%)	446 (97%)	13 (3%)	1 (0%)	47 82
2	F	453/511 (89%)	439 (97%)	14 (3%)	0	100 100
3	G	354/382 (93%)	342 (97%)	11 (3%)	1 (0%)	41 76
4	H	203/247 (82%)	198 (98%)	5 (2%)	0	100 100
5	I	165/226 (73%)	165 (100%)	0	0	100 100
5	J	221/226 (98%)	221 (100%)	0	0	100 100
5	K	216/226 (96%)	215 (100%)	1 (0%)	0	100 100
6	L	108/119 (91%)	91 (84%)	16 (15%)	1 (1%)	17 55
7	M	60/118 (51%)	59 (98%)	1 (2%)	0	100 100
7	N	111/118 (94%)	110 (99%)	1 (1%)	0	100 100
7	O	111/118 (94%)	109 (98%)	2 (2%)	0	100 100
8	Q	260/280 (93%)	254 (98%)	6 (2%)	0	100 100
8	R	261/280 (93%)	256 (98%)	4 (2%)	1 (0%)	34 72
8	S	264/280 (94%)	255 (97%)	9 (3%)	0	100 100
9	T	168/221 (76%)	160 (95%)	8 (5%)	0	100 100
All	All	5650/6225 (91%)	5492 (97%)	149 (3%)	9 (0%)	50 82

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	VAL
6	L	94	LYS
1	A	139	LYS
1	B	561	SER
2	E	41	SER
1	B	234	LEU
3	G	81	GLU
8	R	214	GLU
1	C	298	VAL

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	500/524 (95%)	498 (100%)	2 (0%)	91 97
1	B	508/524 (97%)	506 (100%)	2 (0%)	91 97
1	C	507/524 (97%)	507 (100%)	0	100 100
2	D	394/431 (91%)	392 (100%)	2 (0%)	88 96
2	E	398/431 (92%)	398 (100%)	0	100 100
2	F	391/431 (91%)	390 (100%)	1 (0%)	92 97
3	G	325/344 (94%)	322 (99%)	3 (1%)	78 92
4	H	182/212 (86%)	181 (100%)	1 (0%)	88 96
5	I	147/198 (74%)	147 (100%)	0	100 100
5	J	196/198 (99%)	196 (100%)	0	100 100
5	K	192/198 (97%)	192 (100%)	0	100 100
6	L	94/100 (94%)	92 (98%)	2 (2%)	53 82
7	M	55/101 (54%)	55 (100%)	0	100 100
7	N	98/101 (97%)	98 (100%)	0	100 100
7	O	98/101 (97%)	97 (99%)	1 (1%)	76 91
8	Q	241/255 (94%)	241 (100%)	0	100 100
8	R	241/255 (94%)	241 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	S	243/255 (95%)	242 (100%)	1 (0%)	91 97
9	T	148/195 (76%)	146 (99%)	2 (1%)	67 88
All	All	4958/5378 (92%)	4941 (100%)	17 (0%)	92 97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	VAL
1	A	314	ASN
1	B	486	GLU
1	B	529	ASP
2	D	188	LYS
2	D	436	LYS
2	F	436	LYS
3	G	111	LYS
3	G	114	ILE
3	G	229	LEU
4	H	112	TYR
6	L	48	ILE
6	L	98	TYR
7	O	87	TYR
8	S	42	LEU
9	T	59	SER
9	T	134	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	38	ASN
9	T	56	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)

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	$\#\|Z\| > 2$
10	ADP	C	701	11	24,29,29	1.24	4 (16%)	29,45,45	1.43	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
10	ADP	C	701	11	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	701	ADP	O4'-C1'	3.20	1.45	1.41
10	C	701	ADP	C5-C4	-2.16	1.35	1.40
10	C	701	ADP	PB-O3B	-2.03	1.47	1.54
10	C	701	ADP	PB-O2B	-2.00	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	701	ADP	C4-C5-N7	4.24	113.82	109.40
10	C	701	ADP	O2B-PB-O3A	3.36	115.92	104.64
10	C	701	ADP	PA-O3A-PB	-2.44	124.45	132.83
10	C	701	ADP	N6-C6-N1	-2.24	113.92	118.57
10	C	701	ADP	C2-N1-C6	-2.01	115.32	118.75

There are no chirality outliers.

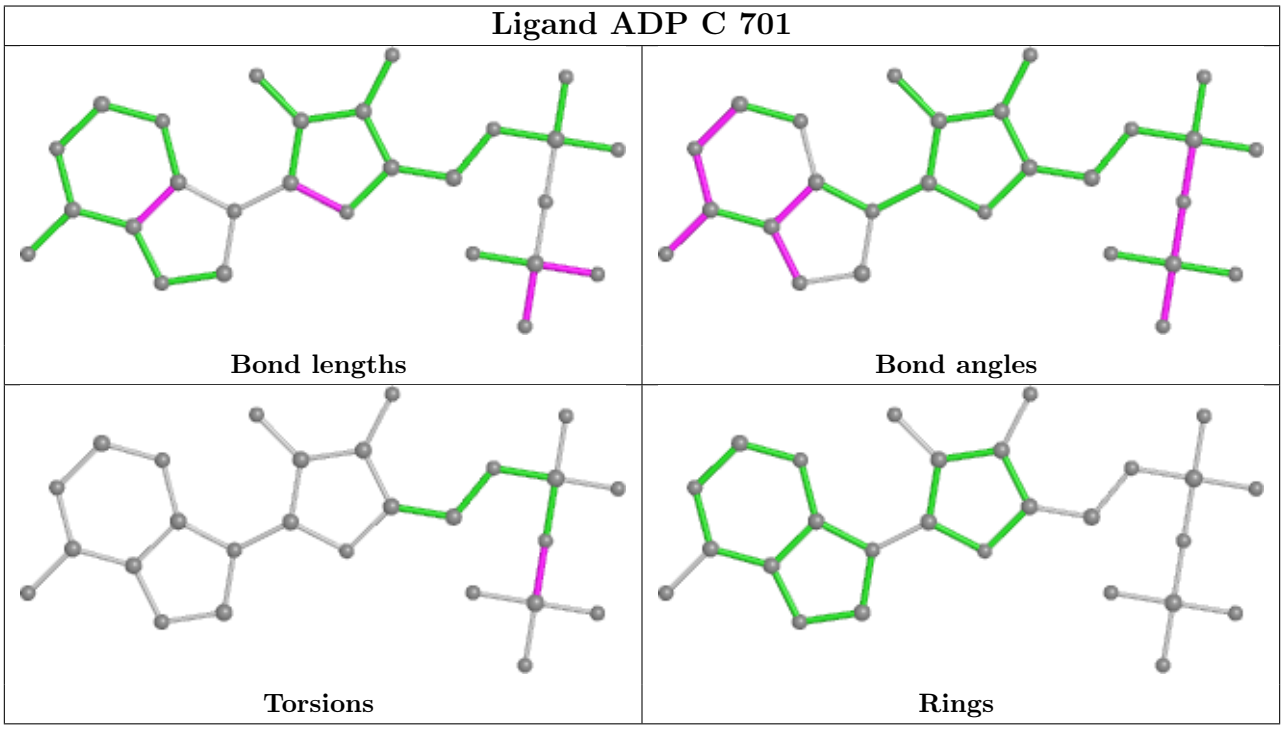
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	701	ADP	PA-O3A-PB-O2B
10	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

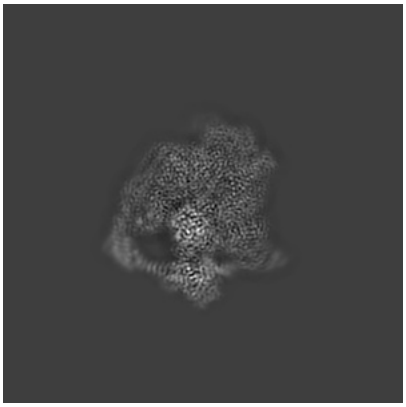
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26914. These allow visual inspection of the internal detail of the map and identification of artifacts.

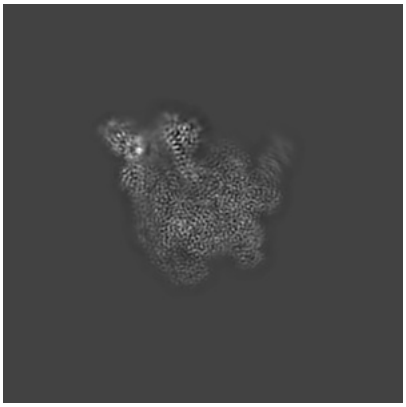
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

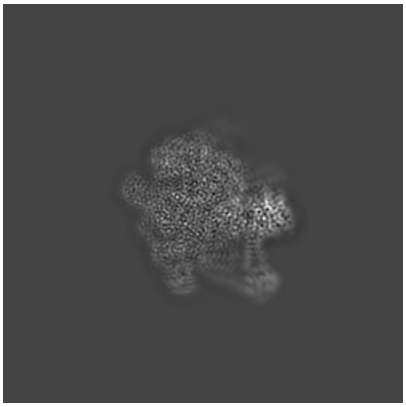
6.1.1 Primary map



X



Y

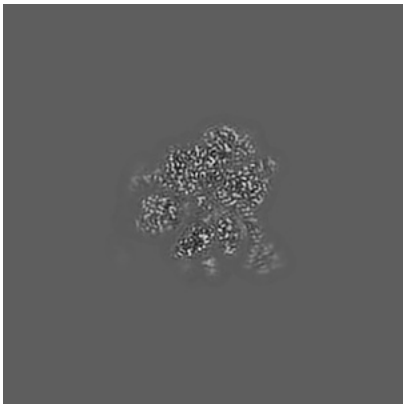


Z

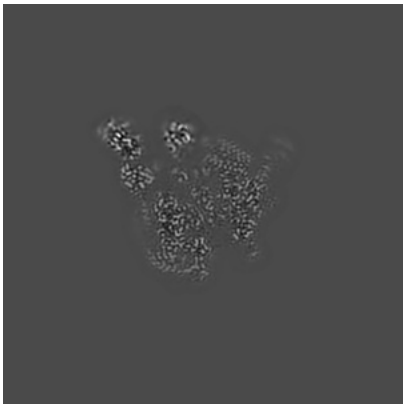
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 175



Y Index: 175

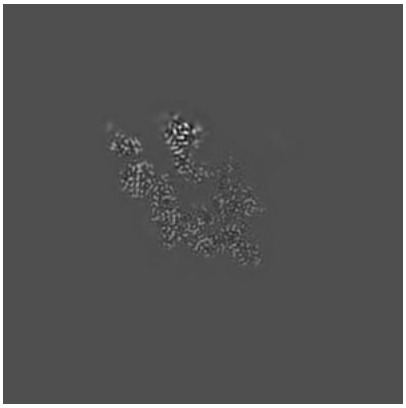
Z Index: 175

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

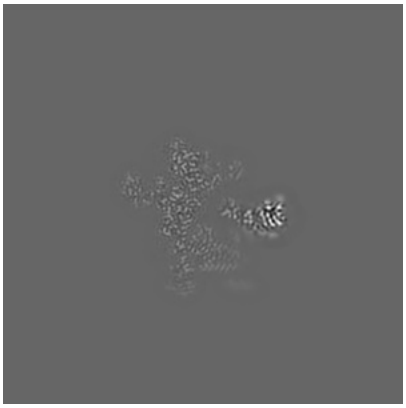
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 157



Y Index: 162

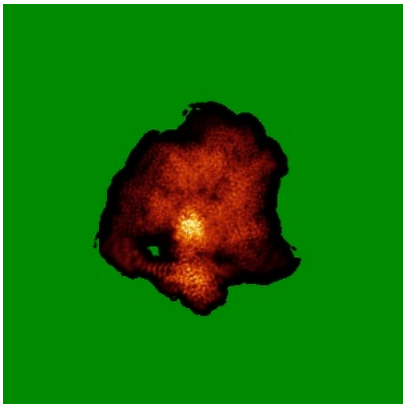


Z Index: 158

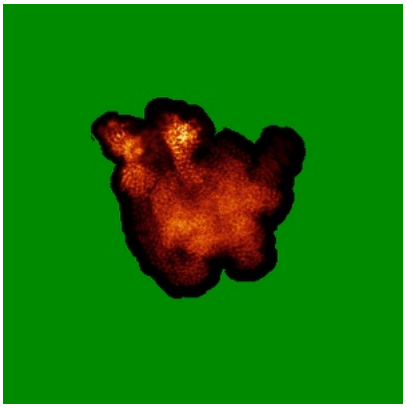
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

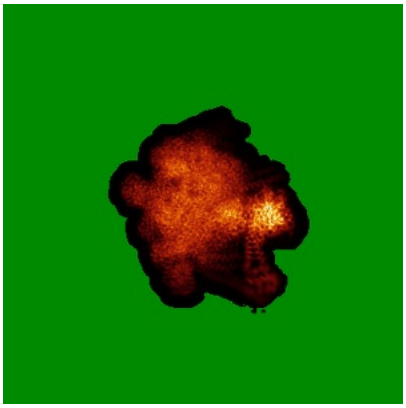
6.4.1 Primary map



X



Y

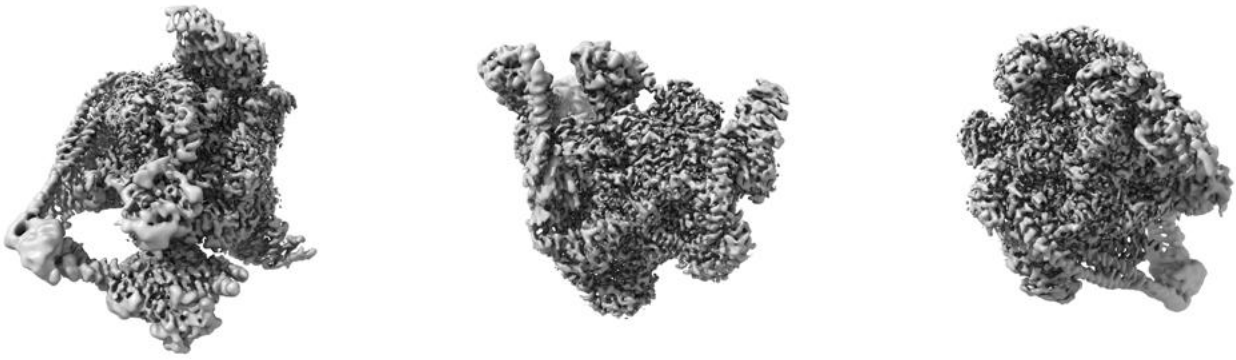


Z

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.

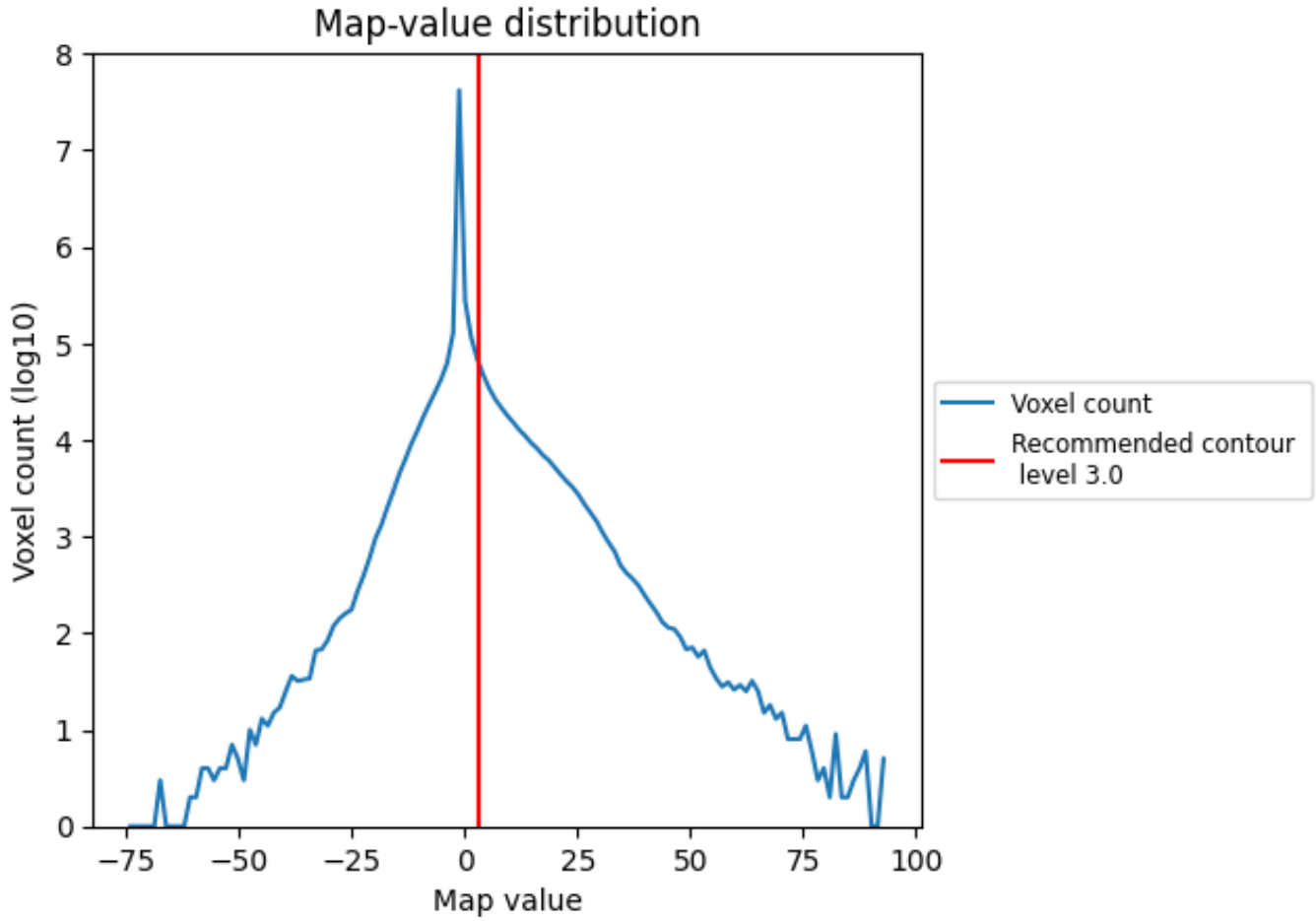
6.6 Mask visualisation (i)

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

7 Map analysis

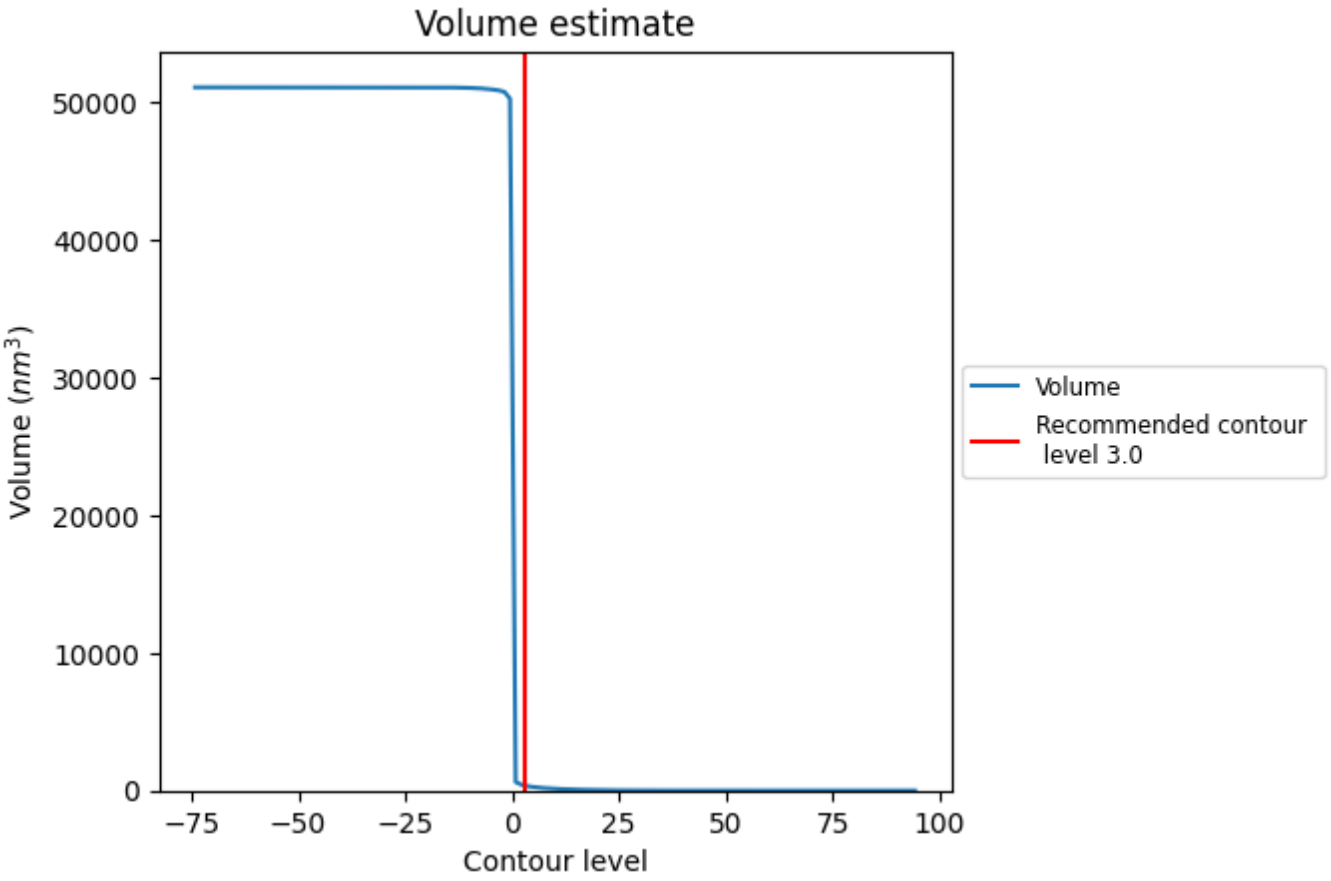
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

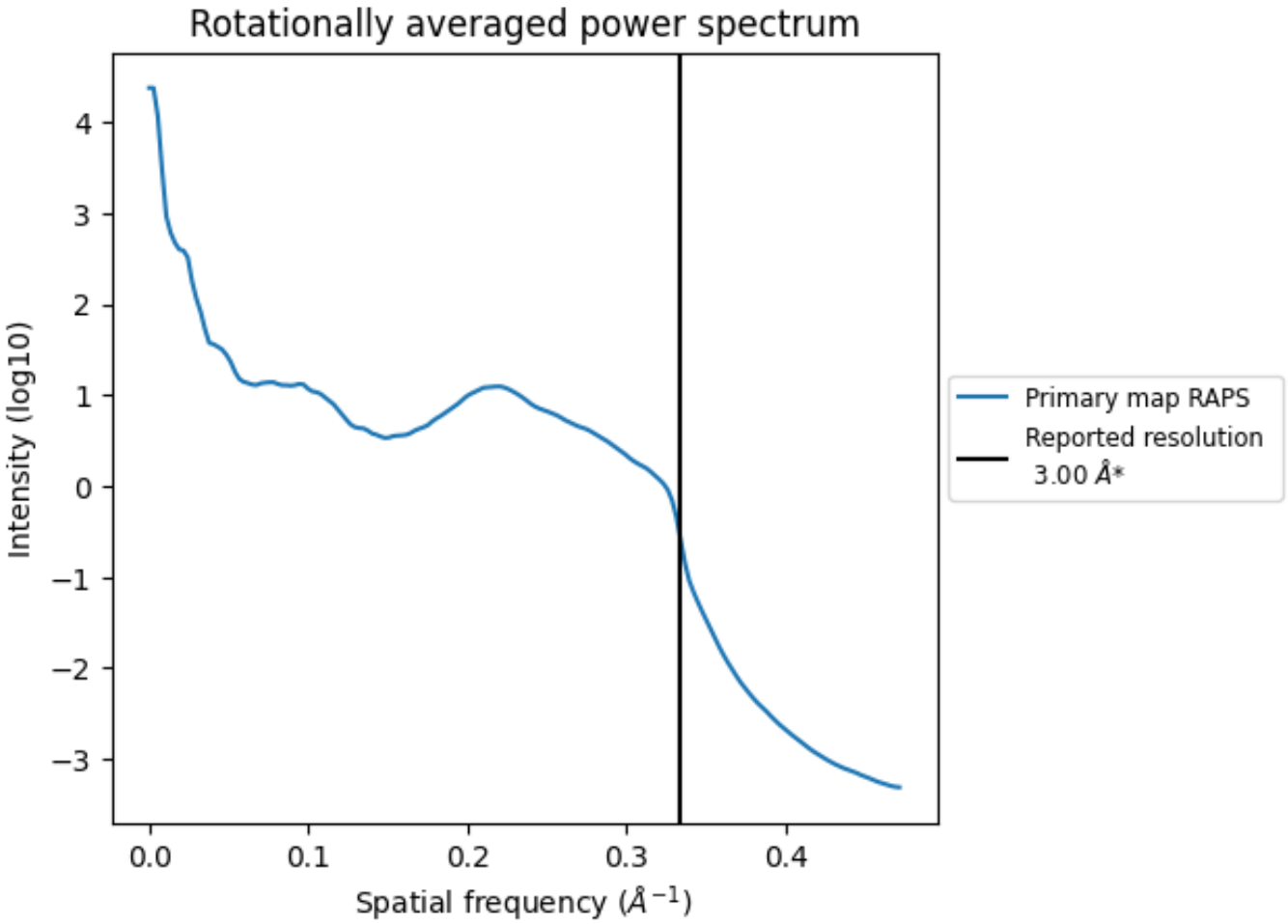
7.2 Volume estimate (i)



The volume at the recommended contour level is 366 nm^3; this corresponds to an approximate mass of 331 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 0.333 $Å^{-1}$

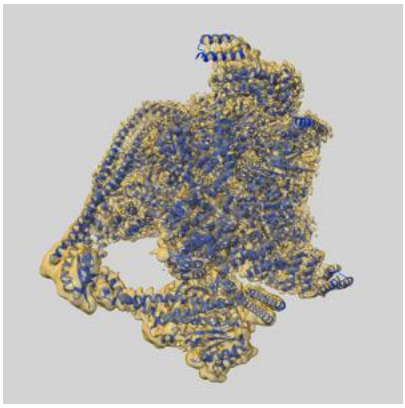
8 Fourier-Shell correlation (i)

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

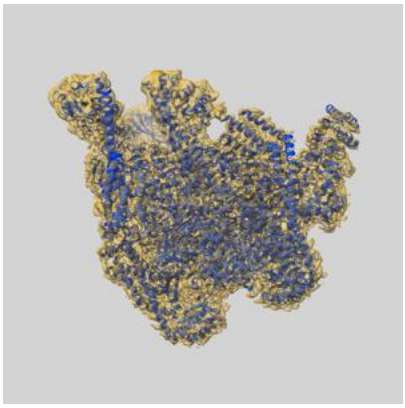
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26914 and PDB model 7UZK. Per-residue inclusion information can be found in section 3 on page 7.

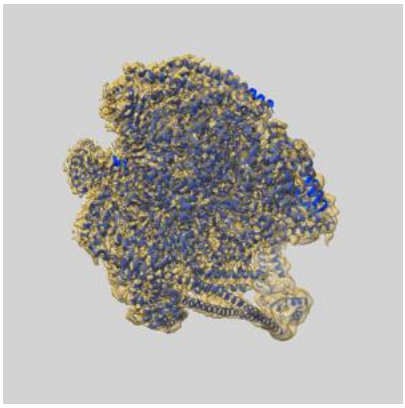
9.1 Map-model overlay



X



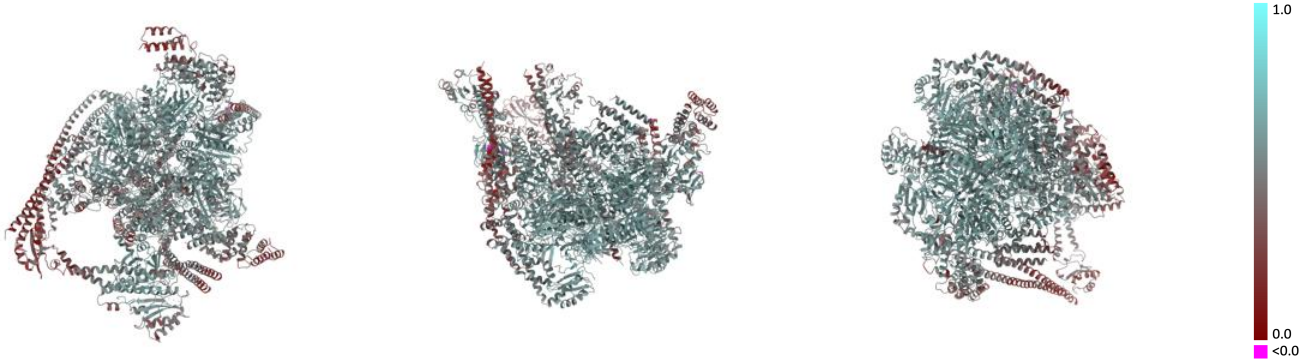
Y



Z

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.

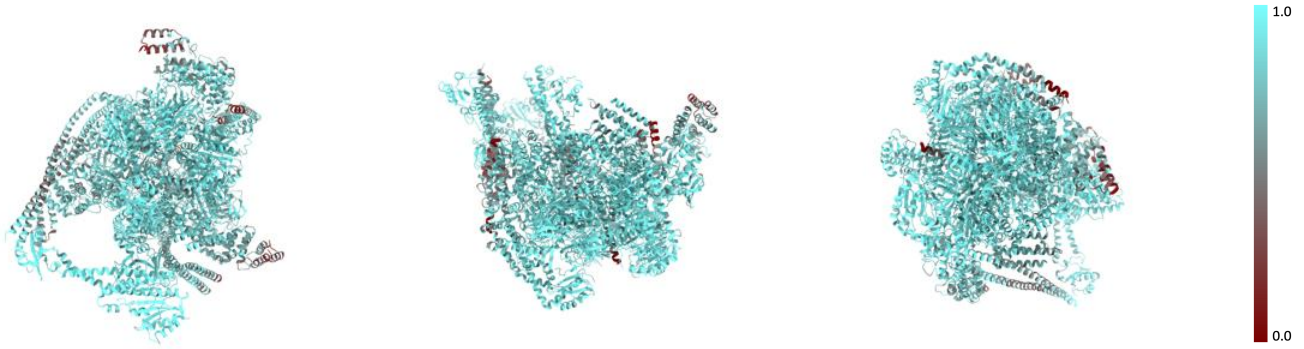
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

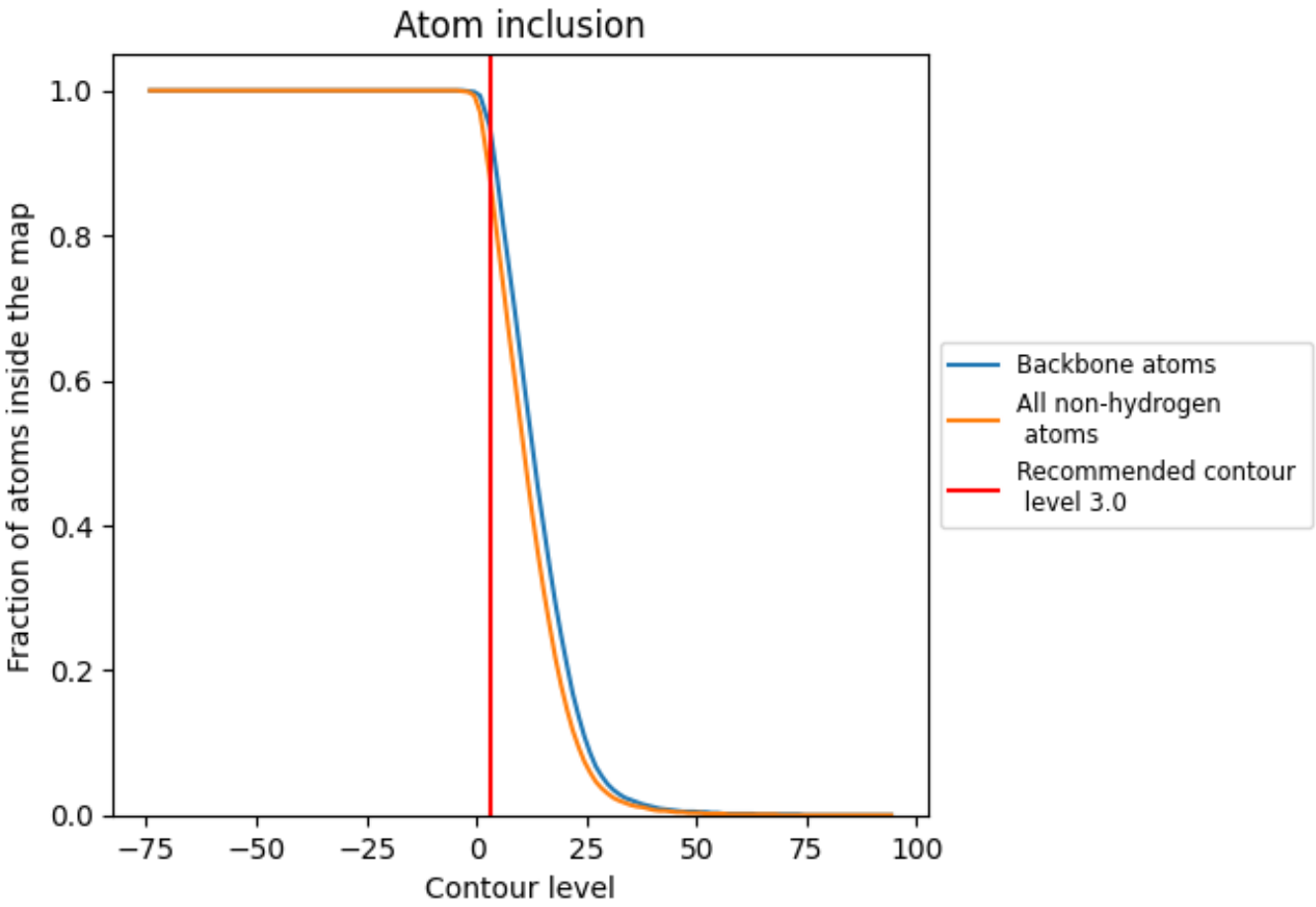
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.8830	0.5310
A	0.9200	0.5780
B	0.9020	0.5620
C	0.9270	0.5890
D	0.9380	0.5960
E	0.9560	0.6080
F	0.9480	0.6020
G	0.9390	0.4350
H	0.8700	0.4860
I	0.8530	0.5360
J	0.8660	0.5050
K	0.8410	0.4730
L	0.9490	0.4600
M	0.6730	0.4570
N	0.7430	0.4100
O	0.7130	0.3720
Q	0.7000	0.4180
R	0.8080	0.4610
S	0.7140	0.4330
T	0.9670	0.5920