



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 11:29 PM EST

PDB ID : 7U8P
EMDB ID : EMD-26386
Title : Structure of porcine kidney V-ATPase with SidK, Rotary State 1
Authors : Tan, Y.Z.; Keon, K.A.
Deposited on : 2022-03-09
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

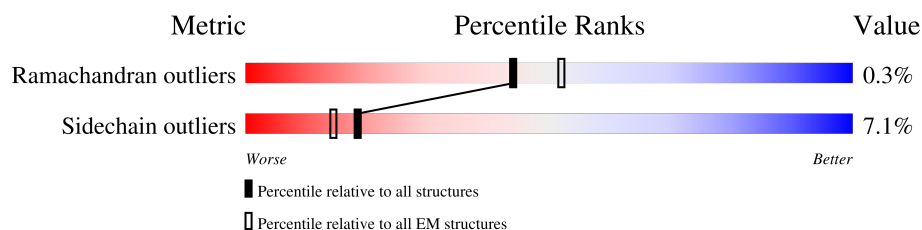
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.70 Å.

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




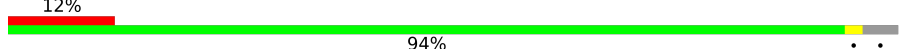
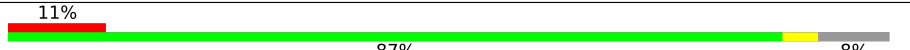
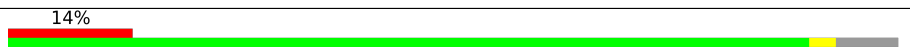

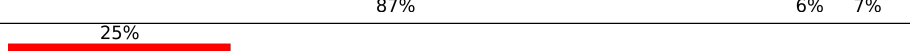
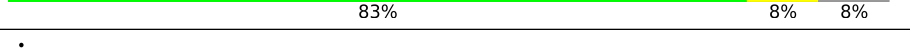




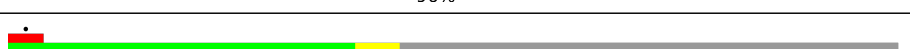
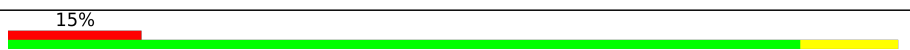


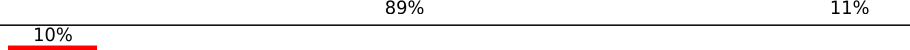
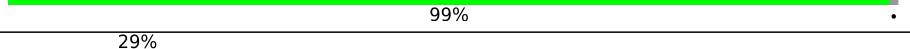

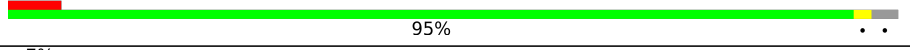
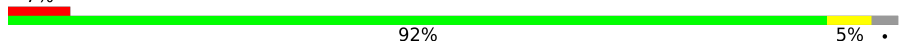
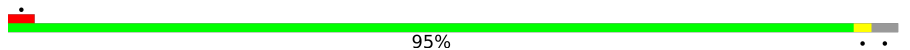
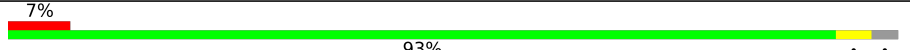

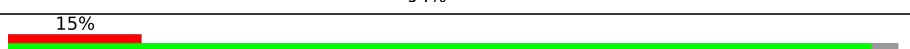
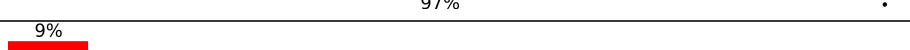
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	89% 6% 5%
1	B	617	92% 5% .
1	C	617	92% 5% .
2	D	515	83% 6% 11%
2	E	515	84% 5% 11%
2	F	515	80% 9% 11%
3	G	382	56% 87% 7% 6%
4	H	247	78% 8% 14%
5	I	226	90% 6% .

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Mol	Chain	Length	Quality of chain
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	Q	337	
8	R	337	
8	S	337	
9	T	483	
10	a	838	
11	b	205	
12	c	469	
13	d	351	
14	e	81	
15	f	98	
16	g	155	
16	h	155	
16	i	155	
16	j	155	
16	k	155	
16	l	155	
16	m	155	
16	n	155	
16	o	155	

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Mol	Chain	Length	Quality of chain
17	p	351	 <div>14% 85%</div>

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 69827 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 V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	587	Total	C	N	O	S	0	0
			4577	2904	776	873	24		
1	B	600	Total	C	N	O	S	0	0
			4661	2957	790	889	25		
1	C	600	Total	C	N	O	S	0	0
			4661	2957	790	889	25		

- Molecule 2 is a protein called Vacuolar proton pump subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	456	Total	C	N	O	S	0	0
			3572	2266	611	674	21		
2	E	458	Total	C	N	O	S	0	0
			3590	2278	615	676	21		
2	F	456	Total	C	N	O	S	0	0
			3572	2266	611	674	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	360	Total	C	N	O	S	0	0
			2935	1880	496	549	10		

- Molecule 4 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	213	Total	C	N	O	S	0	0
			1717	1089	309	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	217	Total	C	N	O	S	0	0
			1416	880	263	269	4		
5	J	218	Total	C	N	O	S	0	0
			1773	1118	317	329	9		
5	K	217	Total	C	N	O	S	0	0
			1766	1113	316	328	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total	C	N	O	S	0	0
			865	548	153	162	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	110	Total	C	N	O	S	0	0
			673	413	129	130	1		
7	N	110	Total	C	N	O	S	0	0
			906	556	172	175	3		
7	O	108	Total	C	N	O	S	0	0
			894	548	170	173	3		

- Molecule 8 is a protein called Bacterial effector protein SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	224	Total	C	N	O	S	0	0
			1824	1162	306	346	10		
8	R	206	Total	C	N	O	S	0	0
			1685	1073	285	319	8		
8	S	226	Total	C	N	O	S	0	0
			1836	1169	308	348	11		

- Molecule 9 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	427	Total	C	N	O	S	0	0
			3510	2230	606	651	23		

- Molecule 10 is a protein called V-type proton ATPase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	750	Total	C	N	O	S	0	0
			6099	3978	1017	1063	41		

- Molecule 11 is a protein called V-type proton ATPase 21 kDa proteolipid subunit isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	b	203	Total	C	N	O	S	0	0
			1498	993	237	258	10		

- Molecule 12 is a protein called ATPase H⁺ transporting accessory protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	206	Total	C	N	O	S	0	0
			1666	1087	270	302	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	350	Total	C	N	O	S	0	0
			2835	1829	462	530	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	80	Total	C	N	O	S	0	0
			652	451	98	98	5		

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	84	Total	C	N	O	S	0	0
			653	433	100	114	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	h	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	i	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		

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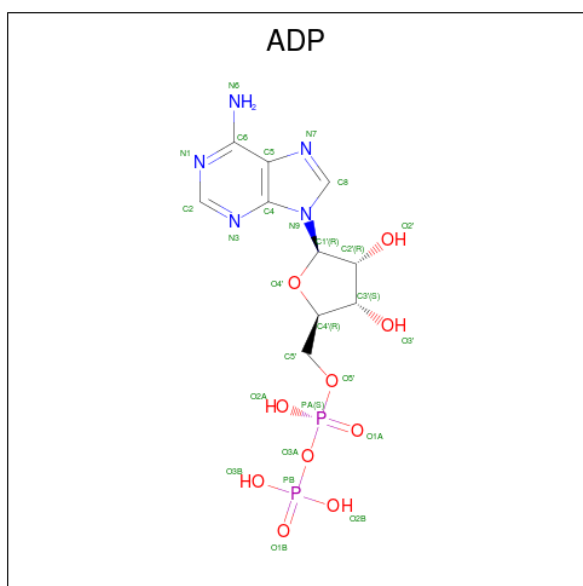
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Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	k	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	l	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	m	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	n	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	o	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		

- Molecule 17 is a protein called ATPase H(+)-transporting lysosomal accessory protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	p	53	Total	C	N	O	S	0	0
			442	297	65	76	4		

- 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).

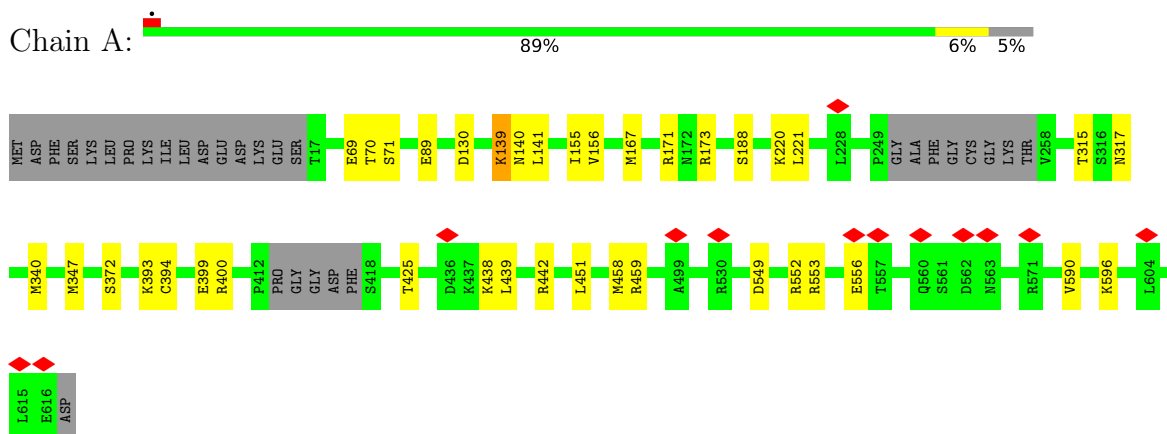


Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

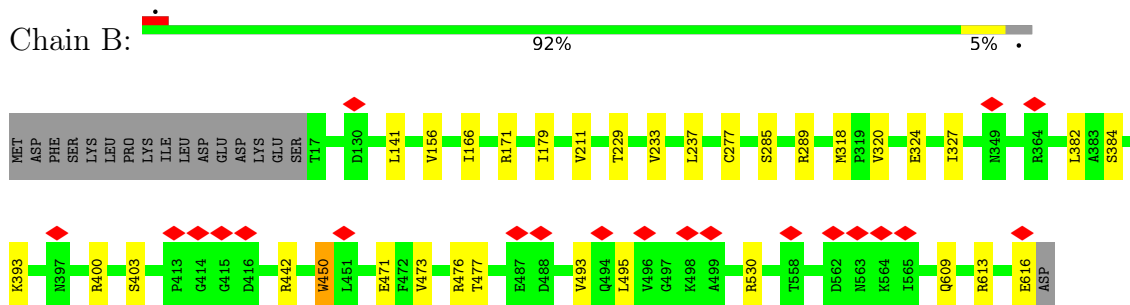
3 Residue-property plots

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

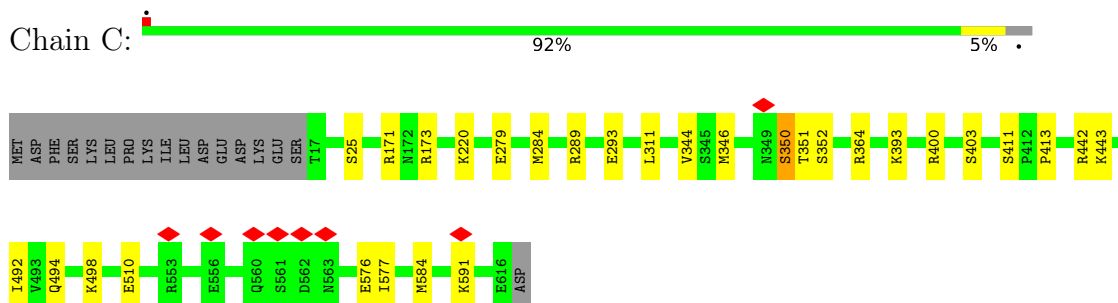
- Molecule 1: V-type proton ATPase catalytic subunit A

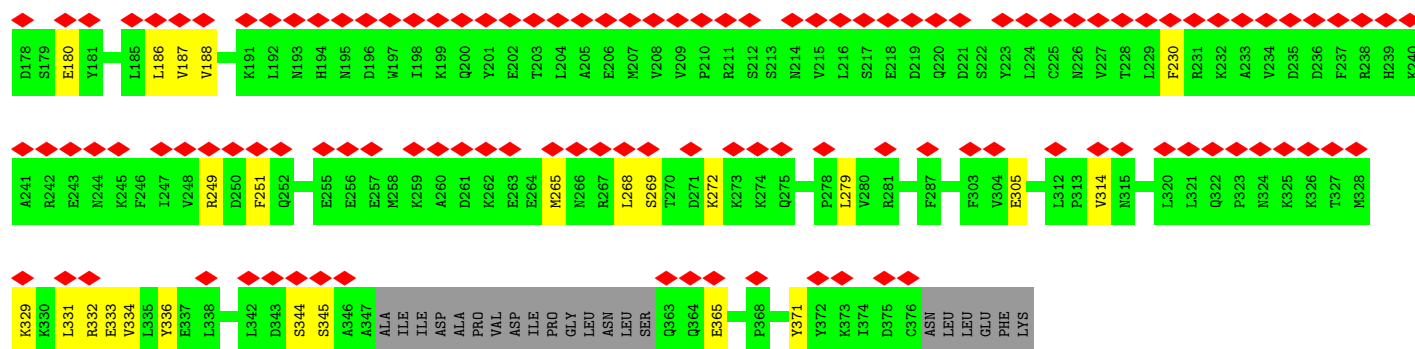


- Molecule 1: V-type proton ATPase catalytic subunit A

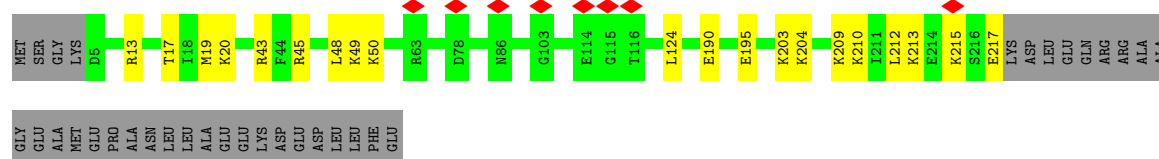
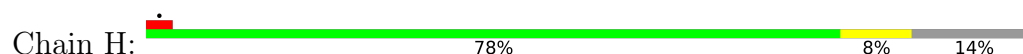


- Molecule 1: V-type proton ATPase catalytic subunit A

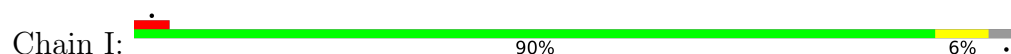




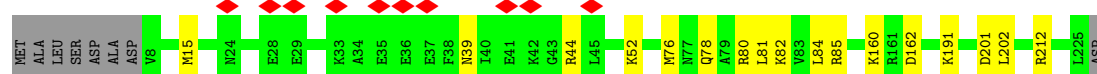
• Molecule 4: V-type proton ATPase subunit D



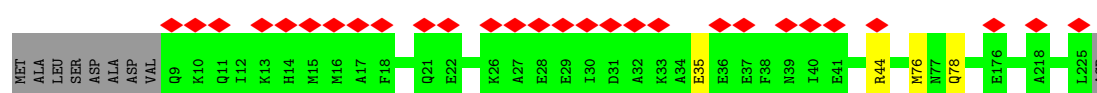
• Molecule 5: V-type proton ATPase subunit E 1



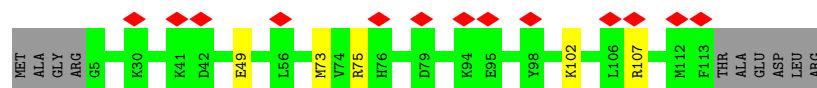
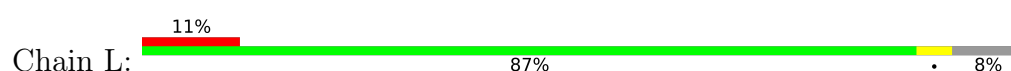
• Molecule 5: V-type proton ATPase subunit E 1



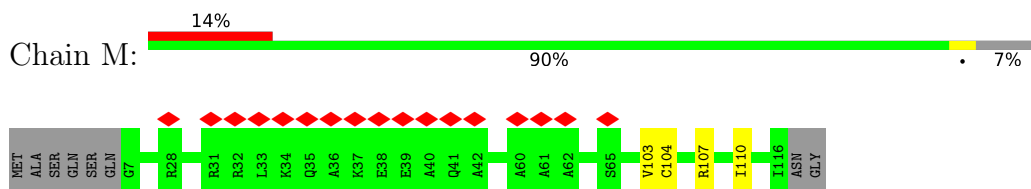
• Molecule 5: V-type proton ATPase subunit E 1



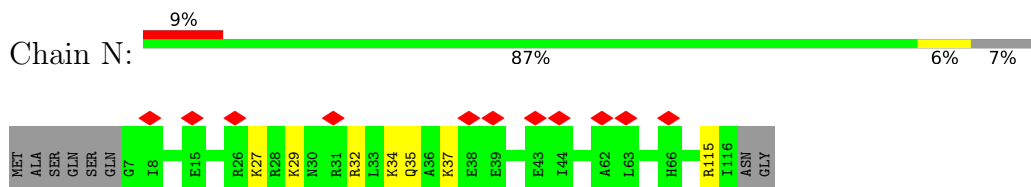
• Molecule 6: V-type proton ATPase subunit F



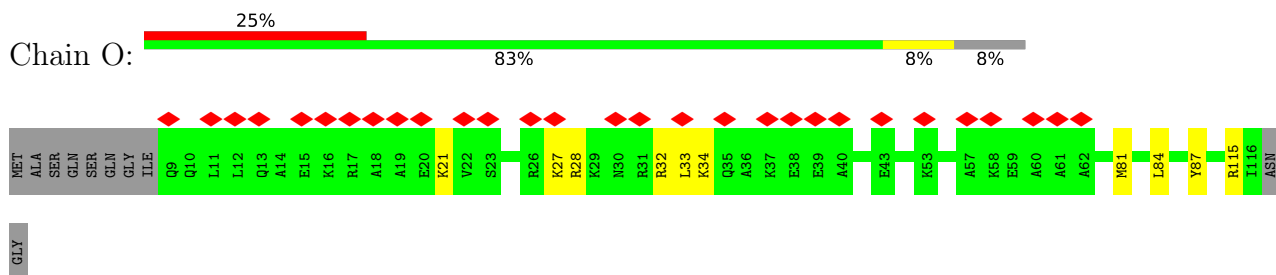
- Molecule 7: V-type proton ATPase subunit G



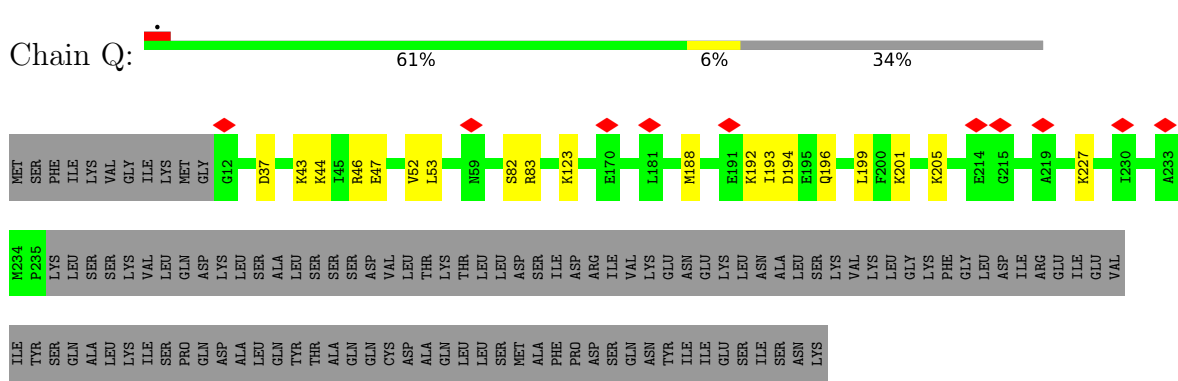
- Molecule 7: V-type proton ATPase subunit G



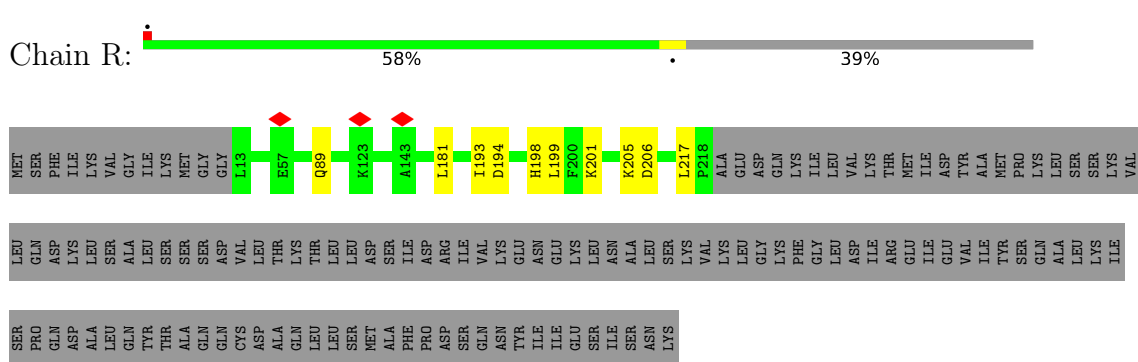
- Molecule 7: V-type proton ATPase subunit G



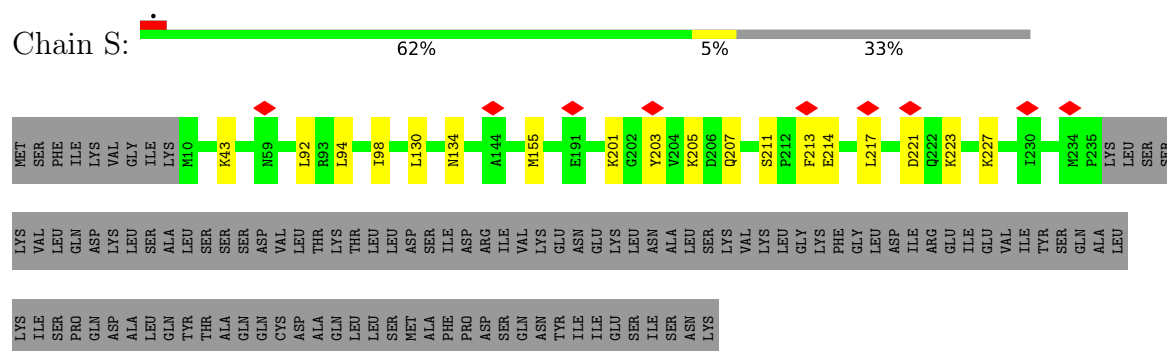
- Molecule 8: Bacterial effector protein SidK



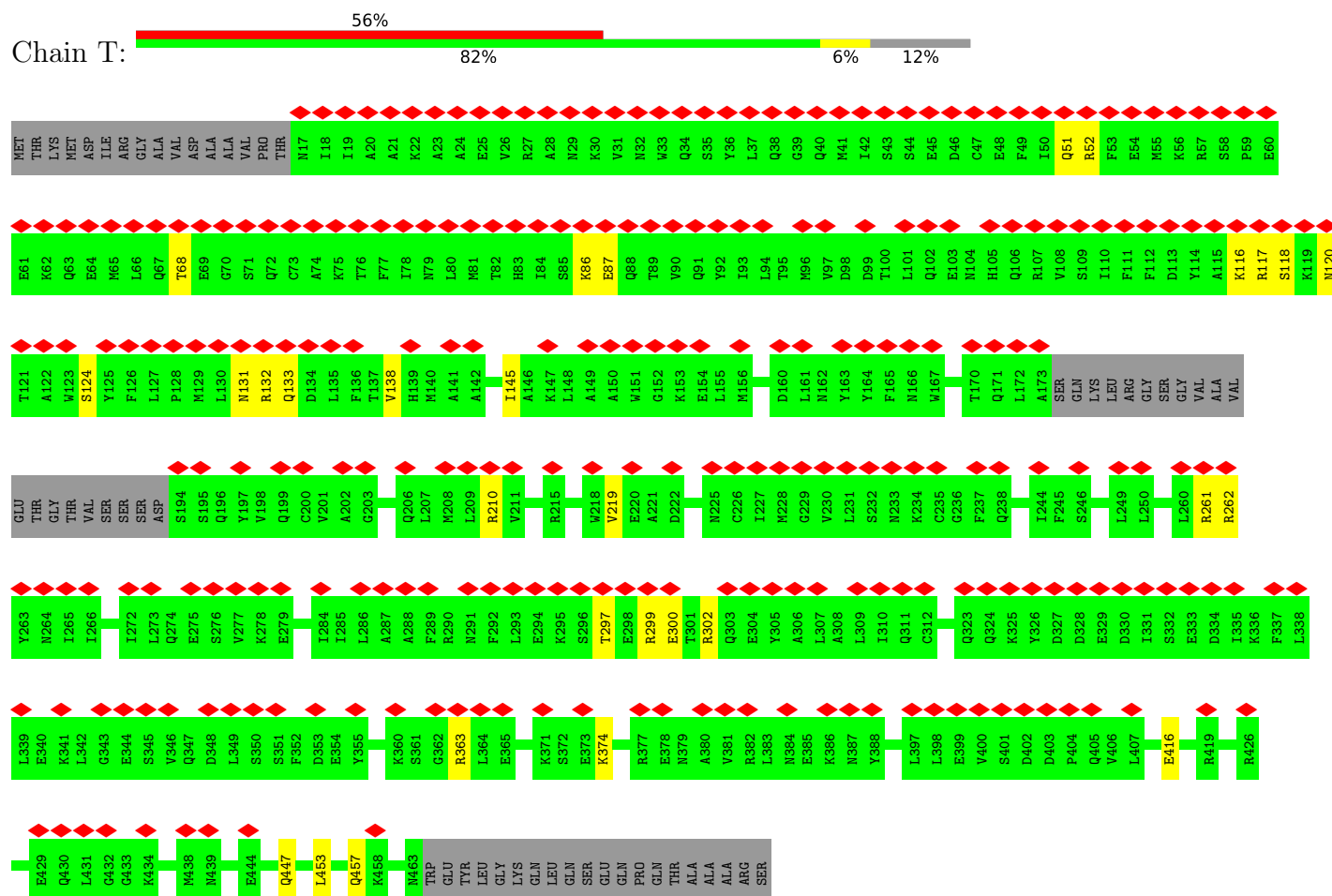
- Molecule 8: Bacterial effector protein SidK



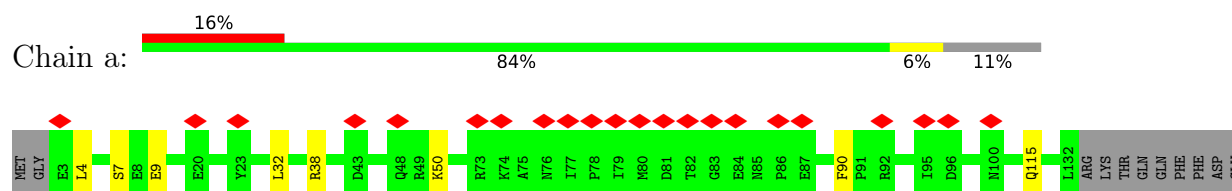
- Molecule 8: Bacterial effector protein SidK

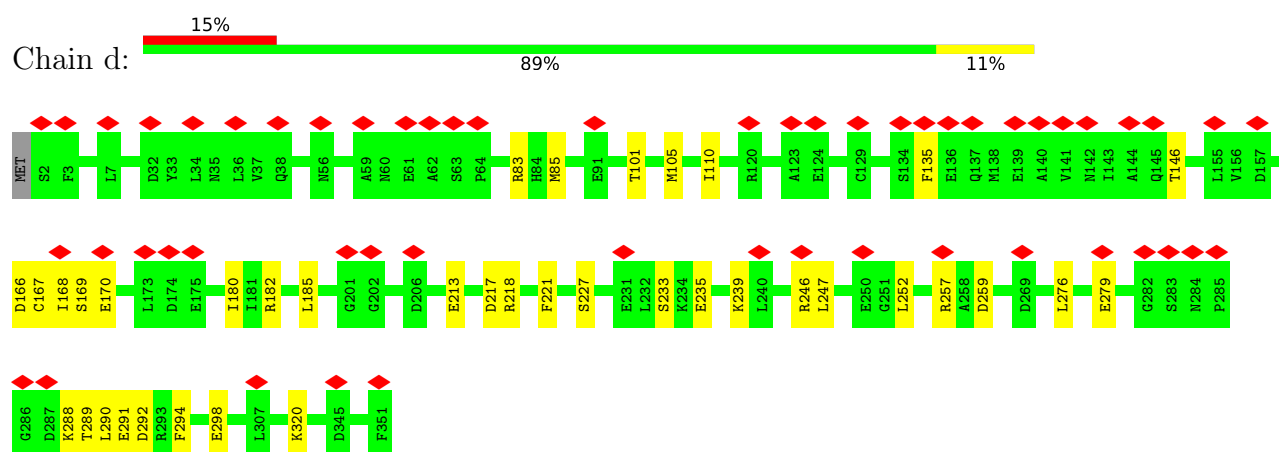


- Molecule 9: V-type proton ATPase subunit H

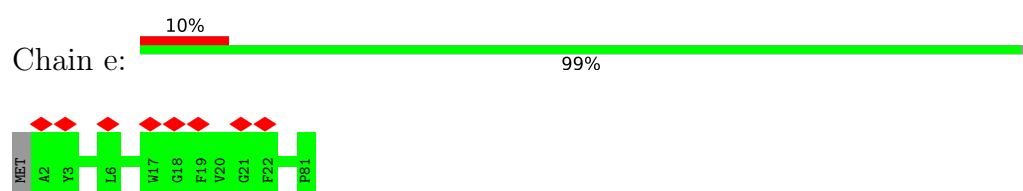


- Molecule 10: V-type proton ATPase subunit a

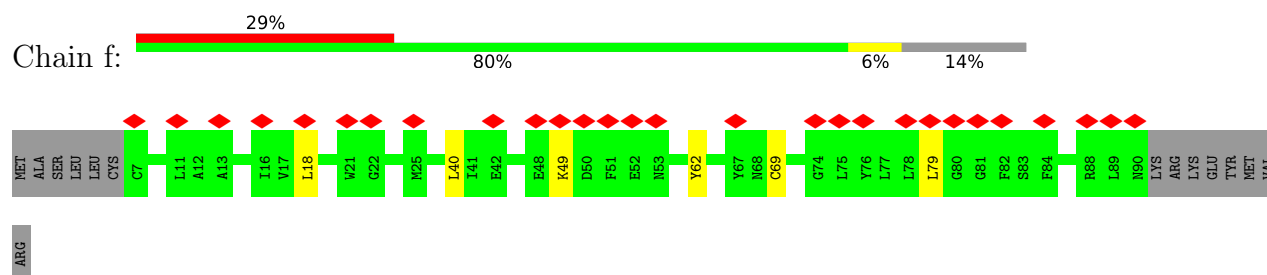




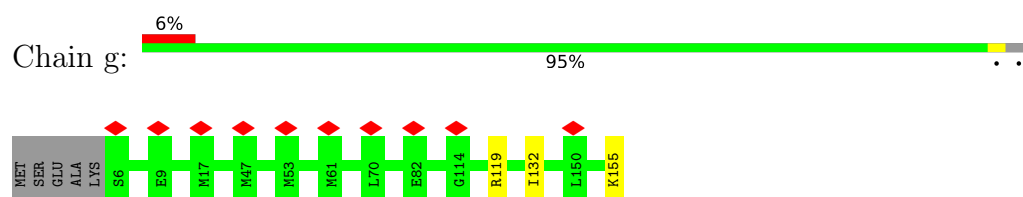
- Molecule 14: V-type proton ATPase subunit



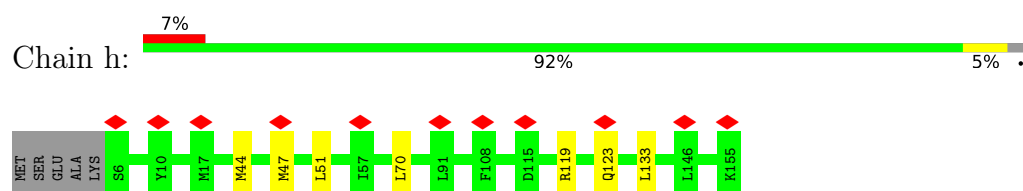
- Molecule 15: Ribonuclease kappa



- Molecule 16: V-type proton ATPase proteolipid subunit

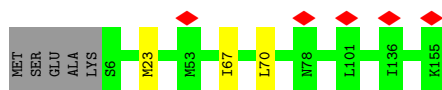


- Molecule 16: V-type proton ATPase proteolipid subunit

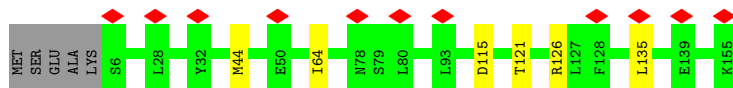
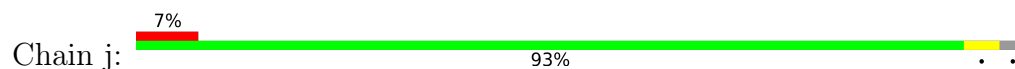


- Molecule 16: V-type proton ATPase proteolipid subunit

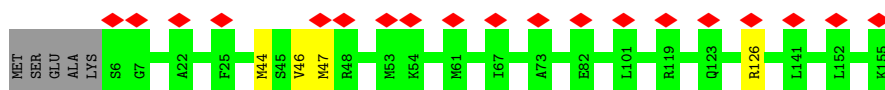




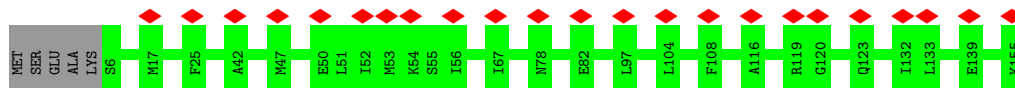
- Molecule 16: V-type proton ATPase proteolipid subunit



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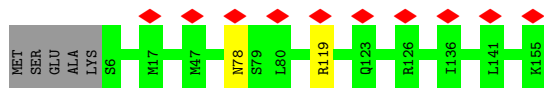
- Molecule 16: V-type proton ATPase proteolipid subunit



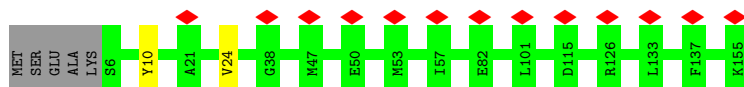
- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 17: ATPase H(+)-transporting lysosomal accessory protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24327	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	100.00	Depositor
Maximum defocus (nm)	3911.445	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.443	Depositor
Minimum map value	-0.604	Depositor
Average map value	0.168	Depositor
Map value standard deviation	0.283	Depositor
Recommended contour level	0.75	Depositor
Map size (\AA)	184.88861, 215.4487, 307.129	wwPDB
Map dimensions	121, 141, 201	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.528005, 1.528005, 1.528005	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

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	0.53	0/4668	0.78	0/6324
1	B	0.47	0/4757	0.69	0/6446
1	C	0.50	0/4757	0.72	0/6446
2	D	0.52	0/3644	0.72	0/4939
2	E	0.54	0/3662	0.77	0/4961
2	F	0.55	0/3644	0.78	0/4939
3	G	0.54	0/2989	0.80	0/4038
4	H	0.51	0/1735	0.81	0/2321
5	I	0.45	0/1427	0.65	0/1948
5	J	0.47	0/1790	0.72	0/2396
5	K	0.42	0/1783	0.69	0/2386
6	L	0.54	0/879	0.88	0/1186
7	M	0.34	0/678	0.53	0/933
7	N	0.38	0/914	0.67	0/1218
7	O	0.40	0/902	0.65	0/1202
8	Q	0.44	0/1858	0.68	0/2505
8	R	0.53	0/1717	0.78	0/2315
8	S	0.47	0/1870	0.68	0/2520
9	T	0.46	0/3576	0.71	0/4818
10	a	0.50	0/6252	0.73	0/8459
11	b	0.42	0/1532	0.69	0/2083
12	c	0.57	0/1721	0.80	0/2345
13	d	0.49	0/2901	0.70	0/3930
14	e	0.45	0/679	0.69	0/934
15	f	0.52	0/669	0.75	0/907
16	g	0.47	0/1073	0.73	0/1453
16	h	0.53	0/1073	0.73	0/1453
16	i	0.49	0/1073	0.79	0/1453
16	j	0.52	0/1073	0.82	0/1453
16	k	0.41	0/1073	0.67	0/1453
16	l	0.32	0/1073	0.54	0/1453
16	m	0.48	0/1073	0.72	0/1453

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	n	0.51	0/1073	0.80	0/1453
16	o	0.40	0/1073	0.64	0/1453
17	p	0.47	0/456	0.78	0/625
All	All	0.49	0/71117	0.73	0/96201

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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	581/617 (94%)	545 (94%)	35 (6%)	1 (0%)	47	78
1	B	598/617 (97%)	562 (94%)	34 (6%)	2 (0%)	41	74
1	C	598/617 (97%)	577 (96%)	18 (3%)	3 (0%)	29	66
2	D	452/515 (88%)	419 (93%)	33 (7%)	0	100	100
2	E	454/515 (88%)	426 (94%)	25 (6%)	3 (1%)	22	59
2	F	452/515 (88%)	430 (95%)	21 (5%)	1 (0%)	47	78
3	G	356/382 (93%)	337 (95%)	16 (4%)	3 (1%)	19	56
4	H	211/247 (85%)	203 (96%)	8 (4%)	0	100	100
5	I	215/226 (95%)	209 (97%)	6 (3%)	0	100	100
5	J	216/226 (96%)	211 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	215/226 (95%)	209 (97%)	6 (3%)	0	100	100
6	L	107/119 (90%)	97 (91%)	10 (9%)	0	100	100
7	M	108/118 (92%)	108 (100%)	0	0	100	100
7	N	108/118 (92%)	107 (99%)	1 (1%)	0	100	100
7	O	106/118 (90%)	106 (100%)	0	0	100	100
8	Q	222/337 (66%)	215 (97%)	7 (3%)	0	100	100
8	R	204/337 (60%)	196 (96%)	8 (4%)	0	100	100
8	S	224/337 (66%)	215 (96%)	8 (4%)	1 (0%)	34	69
9	T	423/483 (88%)	399 (94%)	22 (5%)	2 (0%)	29	66
10	a	744/838 (89%)	706 (95%)	34 (5%)	4 (0%)	29	66
11	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
12	c	204/469 (44%)	181 (89%)	23 (11%)	0	100	100
13	d	348/351 (99%)	334 (96%)	14 (4%)	0	100	100
14	e	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
15	f	82/98 (84%)	79 (96%)	3 (4%)	0	100	100
16	g	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	22	59
16	h	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	i	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
16	j	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
16	k	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
16	l	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
16	m	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	n	148/155 (96%)	138 (93%)	10 (7%)	0	100	100
16	o	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	22	59
17	p	51/351 (14%)	48 (94%)	2 (4%)	1 (2%)	7	39
All	All	8890/10458 (85%)	8472 (95%)	395 (4%)	23 (0%)	44	74

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	a	90	PHE
1	C	498	LYS
2	E	372	TYR

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Mol	Chain	Res	Type
2	F	341	SER
3	G	251	PHE
16	o	10	TYR
1	A	139	LYS
2	E	293	ASP
9	T	120	ASN
10	a	4	LEU
10	a	583	LEU
1	B	171	ARG
1	C	413	PRO
3	G	344	SER
8	S	98	ILE
10	a	432	SER
1	B	450	TRP
1	C	350	SER
2	E	208	LYS
9	T	124	SER
17	p	298	TYR
16	g	132	ILE
3	G	314	VAL

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	501/525 (95%)	463 (92%)	38 (8%)	13	43
1	B	508/525 (97%)	476 (94%)	32 (6%)	18	49
1	C	508/525 (97%)	480 (94%)	28 (6%)	21	53
2	D	390/438 (89%)	359 (92%)	31 (8%)	12	42
2	E	392/438 (90%)	371 (95%)	21 (5%)	22	54
2	F	390/438 (89%)	347 (89%)	43 (11%)	6	29
3	G	325/344 (94%)	302 (93%)	23 (7%)	14	45
4	H	184/211 (87%)	164 (89%)	20 (11%)	6	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	96/197 (49%)	82 (85%)	14 (15%)	3	18
5	J	191/197 (97%)	174 (91%)	17 (9%)	9	37
5	K	190/197 (96%)	186 (98%)	4 (2%)	53	74
6	L	93/100 (93%)	88 (95%)	5 (5%)	22	54
7	M	33/101 (33%)	29 (88%)	4 (12%)	5	24
7	N	95/101 (94%)	88 (93%)	7 (7%)	13	44
7	O	94/101 (93%)	84 (89%)	10 (11%)	6	30
8	Q	203/305 (67%)	184 (91%)	19 (9%)	8	35
8	R	188/305 (62%)	178 (95%)	10 (5%)	22	54
8	S	204/305 (67%)	187 (92%)	17 (8%)	11	40
9	T	385/429 (90%)	358 (93%)	27 (7%)	15	45
10	a	668/743 (90%)	622 (93%)	46 (7%)	15	46
11	b	156/158 (99%)	149 (96%)	7 (4%)	27	57
12	c	179/387 (46%)	156 (87%)	23 (13%)	4	23
13	d	305/306 (100%)	267 (88%)	38 (12%)	4	23
14	e	71/72 (99%)	71 (100%)	0	100	100
15	f	70/83 (84%)	64 (91%)	6 (9%)	10	39
16	g	105/109 (96%)	103 (98%)	2 (2%)	57	76
16	h	105/109 (96%)	98 (93%)	7 (7%)	16	47
16	i	105/109 (96%)	102 (97%)	3 (3%)	42	66
16	j	105/109 (96%)	99 (94%)	6 (6%)	20	52
16	k	105/109 (96%)	101 (96%)	4 (4%)	33	61
16	l	105/109 (96%)	105 (100%)	0	100	100
16	m	105/109 (96%)	95 (90%)	10 (10%)	8	34
16	n	105/109 (96%)	103 (98%)	2 (2%)	57	76
16	o	105/109 (96%)	104 (99%)	1 (1%)	76	86
17	p	48/311 (15%)	45 (94%)	3 (6%)	18	49
All	All	7412/8823 (84%)	6884 (93%)	528 (7%)	18	45

All (528) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLU

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Mol	Chain	Res	Type
1	A	70	THR
1	A	71	SER
1	A	89	GLU
1	A	130	ASP
1	A	139	LYS
1	A	140	ASN
1	A	141	LEU
1	A	155	ILE
1	A	156	VAL
1	A	167	MET
1	A	171	ARG
1	A	173	ARG
1	A	188	SER
1	A	220	LYS
1	A	221	LEU
1	A	315	THR
1	A	317	ASN
1	A	340	MET
1	A	347	MET
1	A	372	SER
1	A	393	LYS
1	A	394	CYS
1	A	399	GLU
1	A	400	ARG
1	A	425	THR
1	A	438	LYS
1	A	439	LEU
1	A	442	ARG
1	A	451	LEU
1	A	458	MET
1	A	459	ARG
1	A	549	ASP
1	A	552	ARG
1	A	553	ARG
1	A	556	GLU
1	A	590	VAL
1	A	596	LYS
1	B	141	LEU
1	B	156	VAL
1	B	166	ILE
1	B	179	ILE
1	B	211	VAL

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Mol	Chain	Res	Type
1	B	229	THR
1	B	233	VAL
1	B	237	LEU
1	B	277	CYS
1	B	285	SER
1	B	289	ARG
1	B	318	MET
1	B	320	VAL
1	B	324	GLU
1	B	327	ILE
1	B	382	LEU
1	B	384	SER
1	B	393	LYS
1	B	400	ARG
1	B	403	SER
1	B	442	ARG
1	B	450	TRP
1	B	471	GLU
1	B	473	VAL
1	B	476	ARG
1	B	477	THR
1	B	493	VAL
1	B	495	LEU
1	B	530	ARG
1	B	609	GLN
1	B	613	ARG
1	B	616	GLU
1	C	25	SER
1	C	171	ARG
1	C	173	ARG
1	C	220	LYS
1	C	279	GLU
1	C	284	MET
1	C	289	ARG
1	C	293	GLU
1	C	311	LEU
1	C	344	VAL
1	C	346	MET
1	C	350	SER
1	C	351	THR
1	C	352	SER
1	C	364	ARG

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Mol	Chain	Res	Type
1	C	393	LYS
1	C	400	ARG
1	C	403	SER
1	C	411	SER
1	C	442	ARG
1	C	443	LYS
1	C	492	ILE
1	C	494	GLN
1	C	510	GLU
1	C	576	GLU
1	C	577	ILE
1	C	584	MET
1	C	591	LYS
2	D	33	TYR
2	D	82	GLU
2	D	105	THR
2	D	112	ILE
2	D	147	ILE
2	D	166	THR
2	D	168	ILE
2	D	175	ASN
2	D	270	ARG
2	D	315	ARG
2	D	321	MET
2	D	327	THR
2	D	353	ASP
2	D	380	ARG
2	D	381	GLN
2	D	404	MET
2	D	405	THR
2	D	406	ARG
2	D	407	LYS
2	D	411	ASP
2	D	447	GLU
2	D	458	ASN
2	D	463	GLU
2	D	464	LYS
2	D	465	ARG
2	D	466	SER
2	D	469	GLU
2	D	473	LEU
2	D	487	LYS

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Mol	Chain	Res	Type
2	D	489	ILE
2	D	493	MET
2	E	39	VAL
2	E	40	THR
2	E	120	ASP
2	E	121	MET
2	E	124	ARG
2	E	131	LYS
2	E	139	VAL
2	E	159	TYR
2	E	248	MET
2	E	252	CYS
2	E	257	LEU
2	E	271	LEU
2	E	299	GLU
2	E	323	THR
2	E	366	ILE
2	E	405	THR
2	E	407	LYS
2	E	411	ASP
2	E	453	GLU
2	E	497	PHE
2	E	500	ARG
2	F	72	ASN
2	F	77	SER
2	F	96	THR
2	F	97	SER
2	F	99	ILE
2	F	120	ASP
2	F	121	MET
2	F	122	LEU
2	F	124	ARG
2	F	138	VAL
2	F	139	VAL
2	F	158	ILE
2	F	161	GLU
2	F	237	PHE
2	F	240	SER
2	F	257	LEU
2	F	262	THR
2	F	263	ILE
2	F	266	ILE

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Mol	Chain	Res	Type
2	F	267	ILE
2	F	268	THR
2	F	271	LEU
2	F	274	THR
2	F	299	GLU
2	F	302	ARG
2	F	310	GLU
2	F	311	VAL
2	F	321	MET
2	F	328	ILE
2	F	334	ARG
2	F	362	LEU
2	F	371	ILE
2	F	375	ARG
2	F	377	LEU
2	F	388	VAL
2	F	389	LEU
2	F	392	LEU
2	F	394	ARG
2	F	411	ASP
2	F	459	GLN
2	F	483	LYS
2	F	487	LYS
2	F	489	ILE
3	G	155	ARG
3	G	162	LEU
3	G	180	GLU
3	G	186	LEU
3	G	187	VAL
3	G	188	VAL
3	G	230	PHE
3	G	249	ARG
3	G	265	MET
3	G	268	LEU
3	G	269	SER
3	G	272	LYS
3	G	279	LEU
3	G	305	GLU
3	G	329	LYS
3	G	331	LEU
3	G	332	ARG
3	G	333	GLU

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Mol	Chain	Res	Type
3	G	334	VAL
3	G	336	TYR
3	G	345	SER
3	G	365	GLU
3	G	371	TYR
4	H	13	ARG
4	H	17	THR
4	H	19	MET
4	H	20	LYS
4	H	43	ARG
4	H	45	ARG
4	H	48	LEU
4	H	49	LYS
4	H	50	LYS
4	H	124	LEU
4	H	190	GLU
4	H	195	GLU
4	H	203	LYS
4	H	204	LYS
4	H	209	LYS
4	H	210	LYS
4	H	212	LEU
4	H	213	LYS
4	H	215	LYS
4	H	217	GLU
5	I	126	GLN
5	I	127	LEU
5	I	132	MET
5	I	156	LYS
5	I	159	THR
5	I	164	ASP
5	I	177	ILE
5	I	181	VAL
5	I	188	ARG
5	I	193	SER
5	I	195	THR
5	I	197	GLU
5	I	199	ARG
5	I	200	LEU
5	J	15	MET
5	J	39	ASN
5	J	44	ARG

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Mol	Chain	Res	Type
5	J	52	LYS
5	J	76	MET
5	J	78	GLN
5	J	80	ARG
5	J	81	LEU
5	J	82	LYS
5	J	84	LEU
5	J	85	ARG
5	J	160	LYS
5	J	162	ASP
5	J	191	LYS
5	J	201	ASP
5	J	202	LEU
5	J	212	ARG
5	K	35	GLU
5	K	44	ARG
5	K	76	MET
5	K	78	GLN
6	L	49	GLU
6	L	73	MET
6	L	75	ARG
6	L	102	LYS
6	L	107	ARG
7	M	103	VAL
7	M	104	CYS
7	M	107	ARG
7	M	110	ILE
7	N	27	LYS
7	N	29	LYS
7	N	32	ARG
7	N	34	LYS
7	N	35	GLN
7	N	37	LYS
7	N	115	ARG
7	O	21	LYS
7	O	27	LYS
7	O	28	ARG
7	O	32	ARG
7	O	33	LEU
7	O	34	LYS
7	O	81	MET
7	O	84	LEU

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Mol	Chain	Res	Type
7	O	87	TYR
7	O	115	ARG
8	Q	37	ASP
8	Q	43	LYS
8	Q	44	LYS
8	Q	46	ARG
8	Q	47	GLU
8	Q	52	VAL
8	Q	53	LEU
8	Q	82	SER
8	Q	83	ARG
8	Q	123	LYS
8	Q	188	MET
8	Q	192	LYS
8	Q	193	ILE
8	Q	194	ASP
8	Q	196	GLN
8	Q	199	LEU
8	Q	201	LYS
8	Q	205	LYS
8	Q	227	LYS
8	R	89	GLN
8	R	181	LEU
8	R	193	ILE
8	R	194	ASP
8	R	198	HIS
8	R	199	LEU
8	R	201	LYS
8	R	205	LYS
8	R	206	ASP
8	R	217	LEU
8	S	43	LYS
8	S	92	LEU
8	S	94	LEU
8	S	130	LEU
8	S	134	ASN
8	S	155	MET
8	S	201	LYS
8	S	203	TYR
8	S	205	LYS
8	S	207	GLN
8	S	211	SER

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Mol	Chain	Res	Type
8	S	213	PHE
8	S	214	GLU
8	S	217	LEU
8	S	221	ASP
8	S	223	LYS
8	S	227	LYS
9	T	51	GLN
9	T	52	ARG
9	T	68	THR
9	T	86	LYS
9	T	87	GLU
9	T	116	LYS
9	T	117	ARG
9	T	118	SER
9	T	131	ASN
9	T	132	ARG
9	T	133	GLN
9	T	138	VAL
9	T	145	ILE
9	T	210	ARG
9	T	219	VAL
9	T	261	ARG
9	T	262	ARG
9	T	297	THR
9	T	299	ARG
9	T	300	GLU
9	T	302	ARG
9	T	363	ARG
9	T	374	LYS
9	T	416	GLU
9	T	447	GLN
9	T	453	LEU
9	T	457	GLN
10	a	7	SER
10	a	9	GLU
10	a	32	LEU
10	a	38	ARG
10	a	50	LYS
10	a	115	GLN
10	a	185	ARG
10	a	186	MET
10	a	195	VAL

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Mol	Chain	Res	Type
10	a	274	GLN
10	a	277	ASP
10	a	281	ARG
10	a	284	GLN
10	a	310	CYS
10	a	322	GLU
10	a	323	VAL
10	a	385	THR
10	a	388	GLU
10	a	394	TYR
10	a	439	MET
10	a	445	SER
10	a	528	ASN
10	a	530	LEU
10	a	532	PHE
10	a	534	ASN
10	a	538	MET
10	a	550	MET
10	a	554	SER
10	a	587	LEU
10	a	646	LEU
10	a	653	LEU
10	a	654	ILE
10	a	659	LEU
10	a	660	ARG
10	a	721	GLN
10	a	738	SER
10	a	740	LEU
10	a	742	LEU
10	a	745	LEU
10	a	776	LEU
10	a	805	ARG
10	a	812	GLN
10	a	829	GLU
10	a	830	HIS
10	a	831	ILE
10	a	832	ARG
11	b	37	VAL
11	b	41	LEU
11	b	43	GLU
11	b	112	SER
11	b	114	MET

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Mol	Chain	Res	Type
11	b	184	SER
11	b	200	ARG
12	c	274	SER
12	c	282	GLU
12	c	284	LEU
12	c	289	PHE
12	c	303	ASP
12	c	305	VAL
12	c	313	ASP
12	c	323	LYS
12	c	325	ILE
12	c	326	LEU
12	c	332	GLN
12	c	333	VAL
12	c	334	SER
12	c	336	ARG
12	c	337	HIS
12	c	338	TRP
12	c	339	PHE
12	c	343	ARG
12	c	344	LEU
12	c	394	LEU
12	c	395	THR
12	c	410	ARG
12	c	452	MET
13	d	83	ARG
13	d	85	MET
13	d	101	THR
13	d	105	MET
13	d	110	ILE
13	d	135	PHE
13	d	146	THR
13	d	166	ASP
13	d	167	CYS
13	d	168	ILE
13	d	169	SER
13	d	170	GLU
13	d	180	ILE
13	d	182	ARG
13	d	185	LEU
13	d	213	GLU
13	d	217	ASP

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Mol	Chain	Res	Type
13	d	218	ARG
13	d	221	PHE
13	d	227	SER
13	d	233	SER
13	d	235	GLU
13	d	239	LYS
13	d	246	ARG
13	d	247	LEU
13	d	252	LEU
13	d	257	ARG
13	d	259	ASP
13	d	276	LEU
13	d	279	GLU
13	d	288	LYS
13	d	289	THR
13	d	290	LEU
13	d	291	GLU
13	d	292	ASP
13	d	294	PHE
13	d	298	GLU
13	d	320	LYS
15	f	18	LEU
15	f	40	LEU
15	f	49	LYS
15	f	62	TYR
15	f	69	CYS
15	f	79	LEU
16	g	119	ARG
16	g	155	LYS
16	h	44	MET
16	h	47	MET
16	h	51	LEU
16	h	70	LEU
16	h	119	ARG
16	h	123	GLN
16	h	133	LEU
16	i	23	MET
16	i	67	ILE
16	i	70	LEU
16	j	44	MET
16	j	64	ILE
16	j	115	ASP

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Mol	Chain	Res	Type
16	j	121	THR
16	j	126	ARG
16	j	135	LEU
16	k	44	MET
16	k	46	VAL
16	k	47	MET
16	k	126	ARG
16	m	16	VAL
16	m	32	TYR
16	m	56	ILE
16	m	61	MET
16	m	64	ILE
16	m	136	ILE
16	m	139	GLU
16	m	140	VAL
16	m	141	LEU
16	m	143	LEU
16	n	78	ASN
16	n	119	ARG
16	o	24	VAL
17	p	296	LEU
17	p	332	MET
17	p	343	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	172	ASN
1	A	317	ASN
1	B	157	ASN
2	E	256	ASN
2	F	256	ASN
2	F	259	ASN
5	I	122	GLN
5	J	47	GLN
5	J	126	GLN
5	J	149	GLN
5	J	205	GLN
7	O	30	ASN
8	Q	127	HIS
8	R	184	HIS

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Mol	Chain	Res	Type
8	S	165	GLN
8	S	177	GLN
9	T	457	GLN
10	a	534	ASN
10	a	626	ASN
11	b	90	ASN
11	b	168	GLN
12	c	332	GLN
12	c	337	HIS
12	c	405	ASN
16	h	123	GLN
16	i	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	ADP	C	701	-	24,29,29	0.71	0	29,45,45	0.78	1 (3%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	701	ADP	C5-C6-N6	2.12	123.58	120.35

There are no chirality outliers.

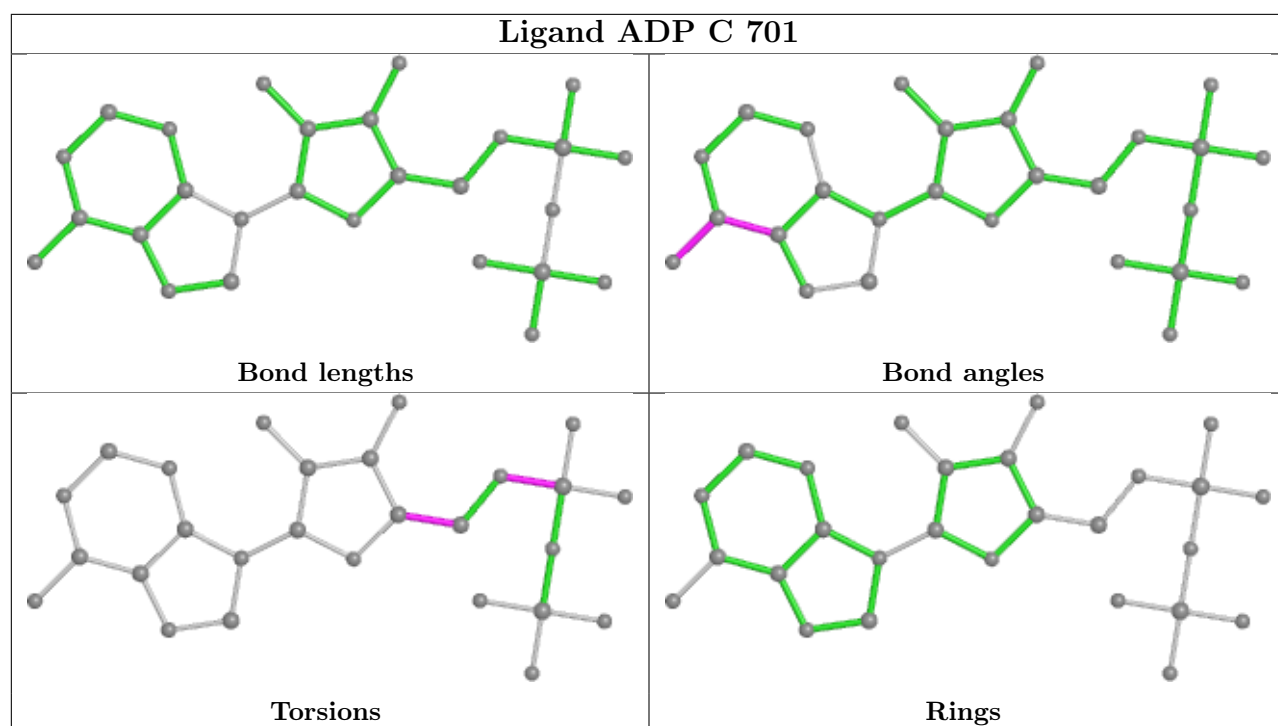
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	701	ADP	C5'-O5'-PA-O3A
18	C	701	ADP	O4'-C4'-C5'-O5'
18	C	701	ADP	C3'-C4'-C5'-O5'
18	C	701	ADP	C5'-O5'-PA-O1A
18	C	701	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

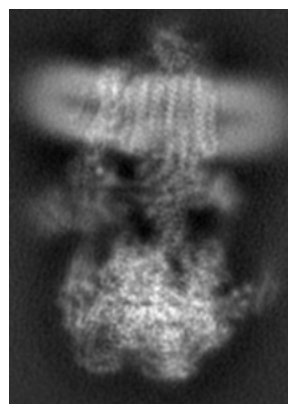
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26386. These allow visual inspection of the internal detail of the map and identification of artifacts.

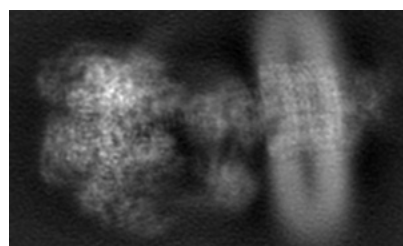
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

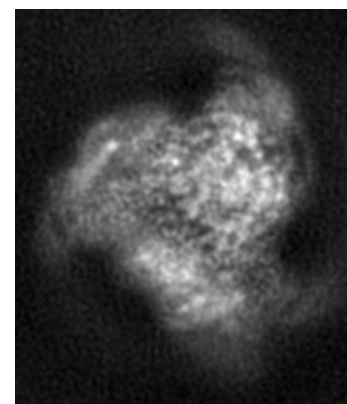
6.1.1 Primary map



X



Y

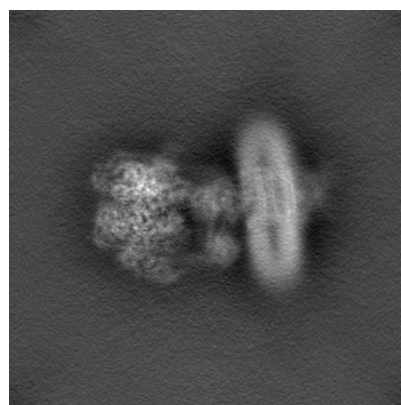


Z

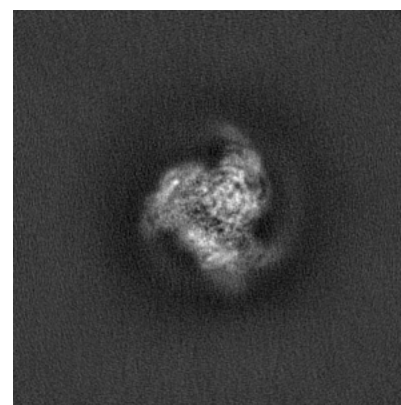
6.1.2 Raw map



X



Y



Z

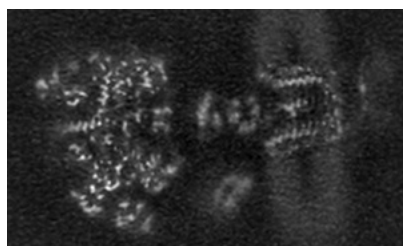
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

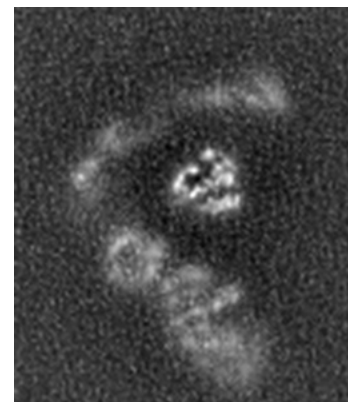
6.2.1 Primary map



X Index: 60

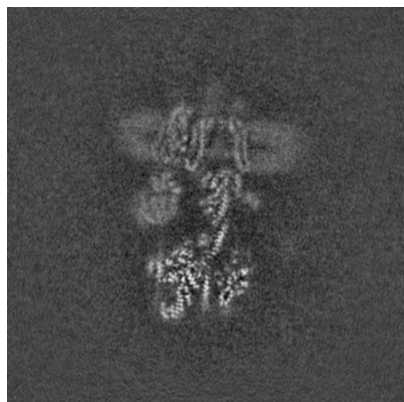


Y Index: 70

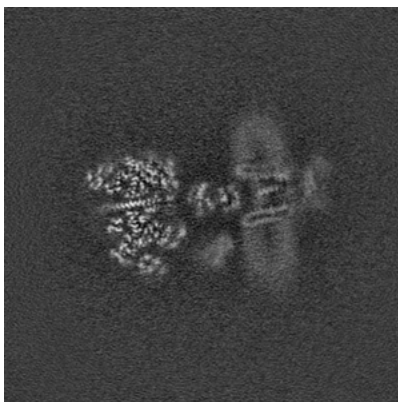


Z Index: 100

6.2.2 Raw map



X Index: 150



Y Index: 150

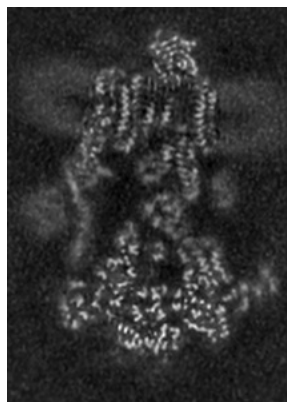


Z Index: 150

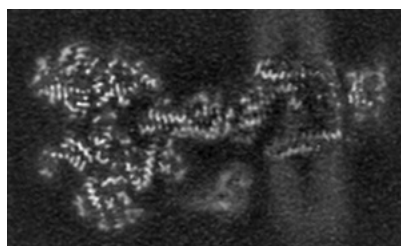
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

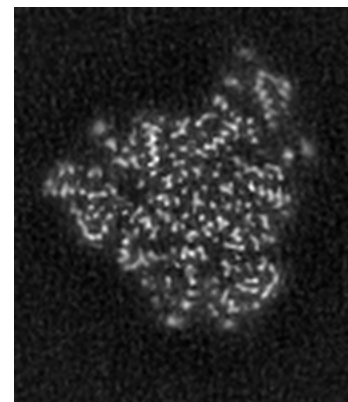
6.3.1 Primary map



X Index: 73

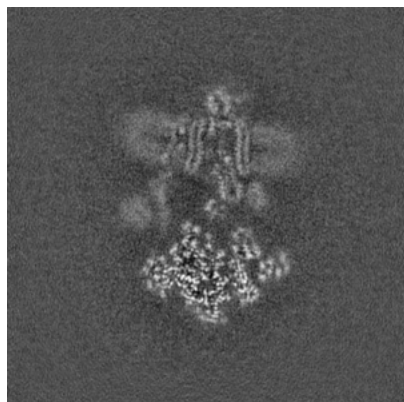


Y Index: 78

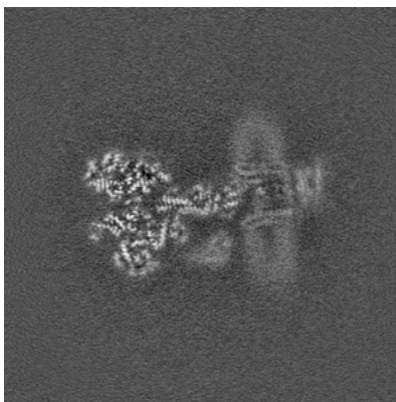


Z Index: 47

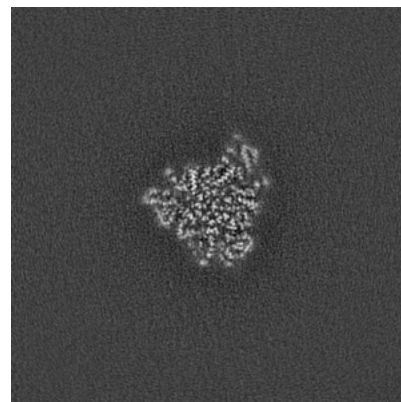
6.3.2 Raw map



X Index: 166



Y Index: 156

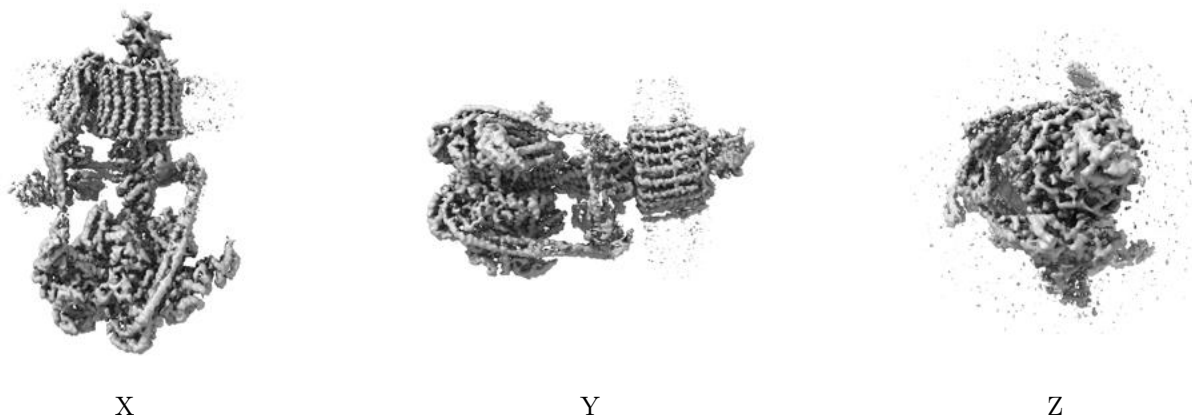


Z Index: 95

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

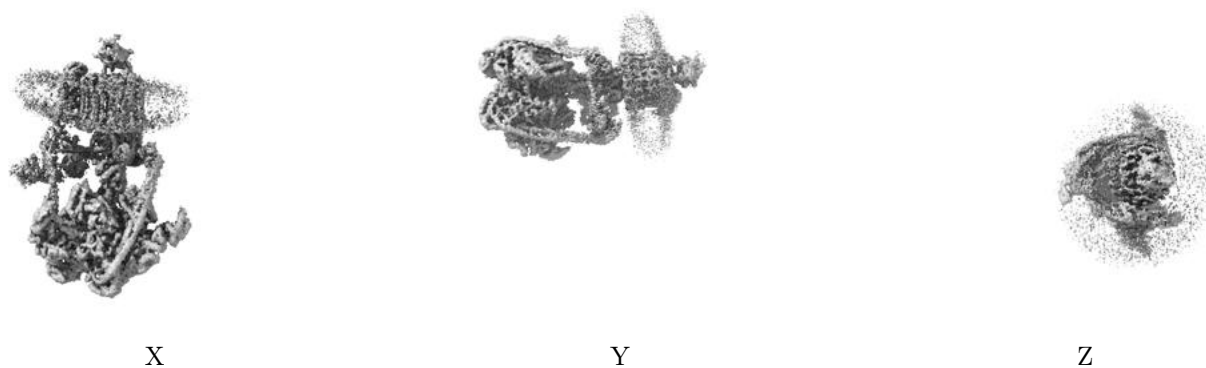
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

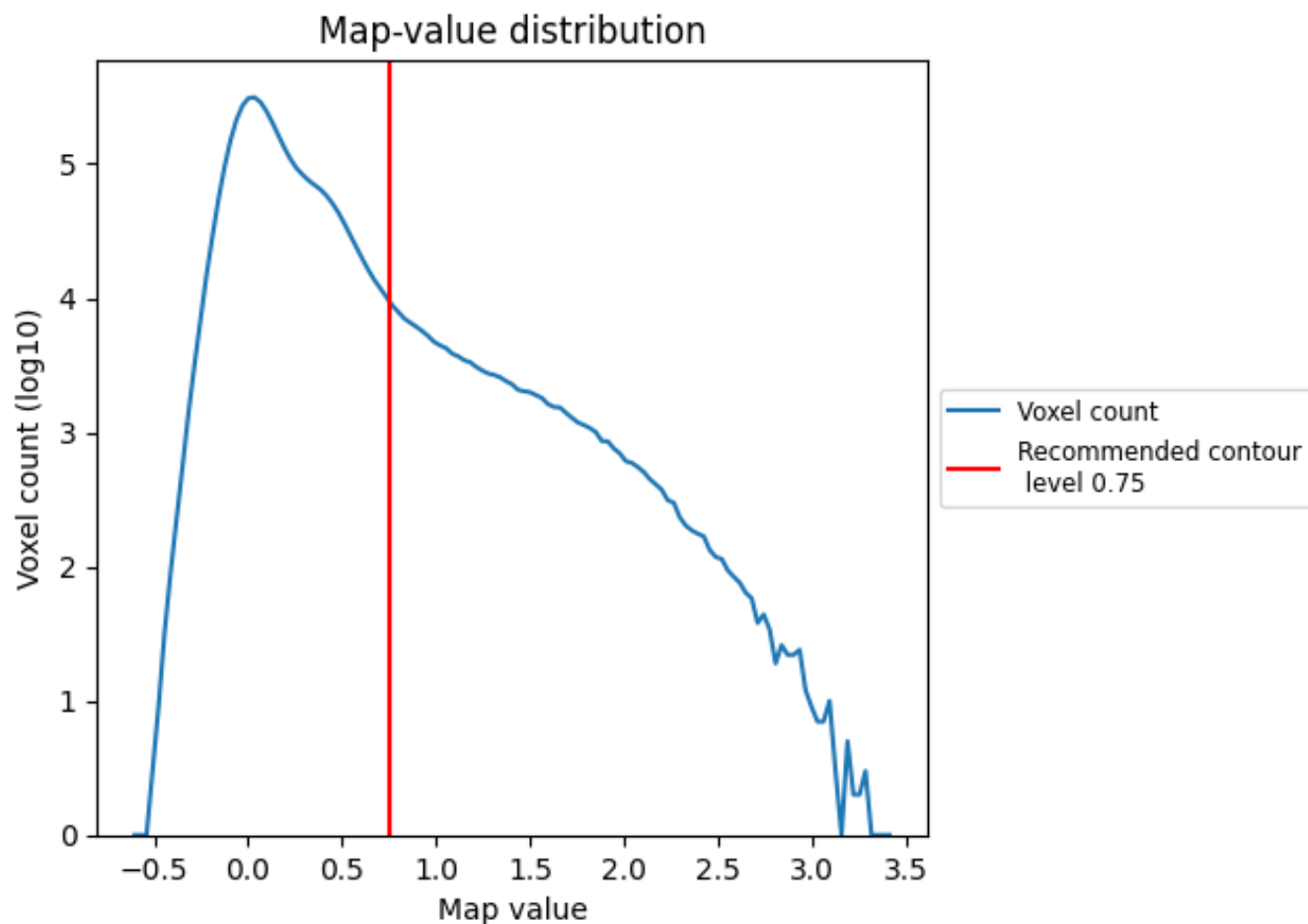
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

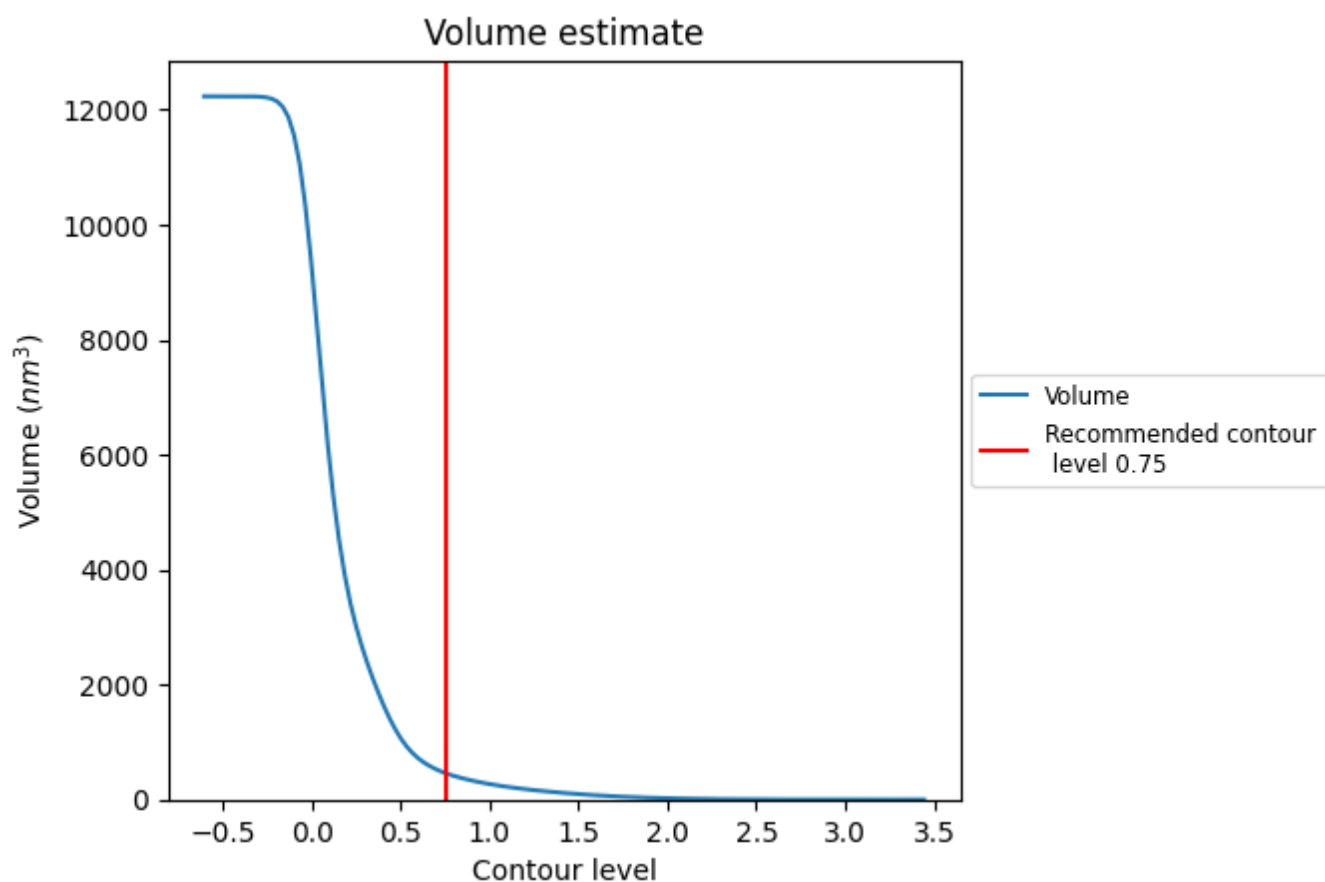
This section contains the results of statistical analysis of the map.

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 463 nm³; this corresponds to an approximate mass of 418 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.

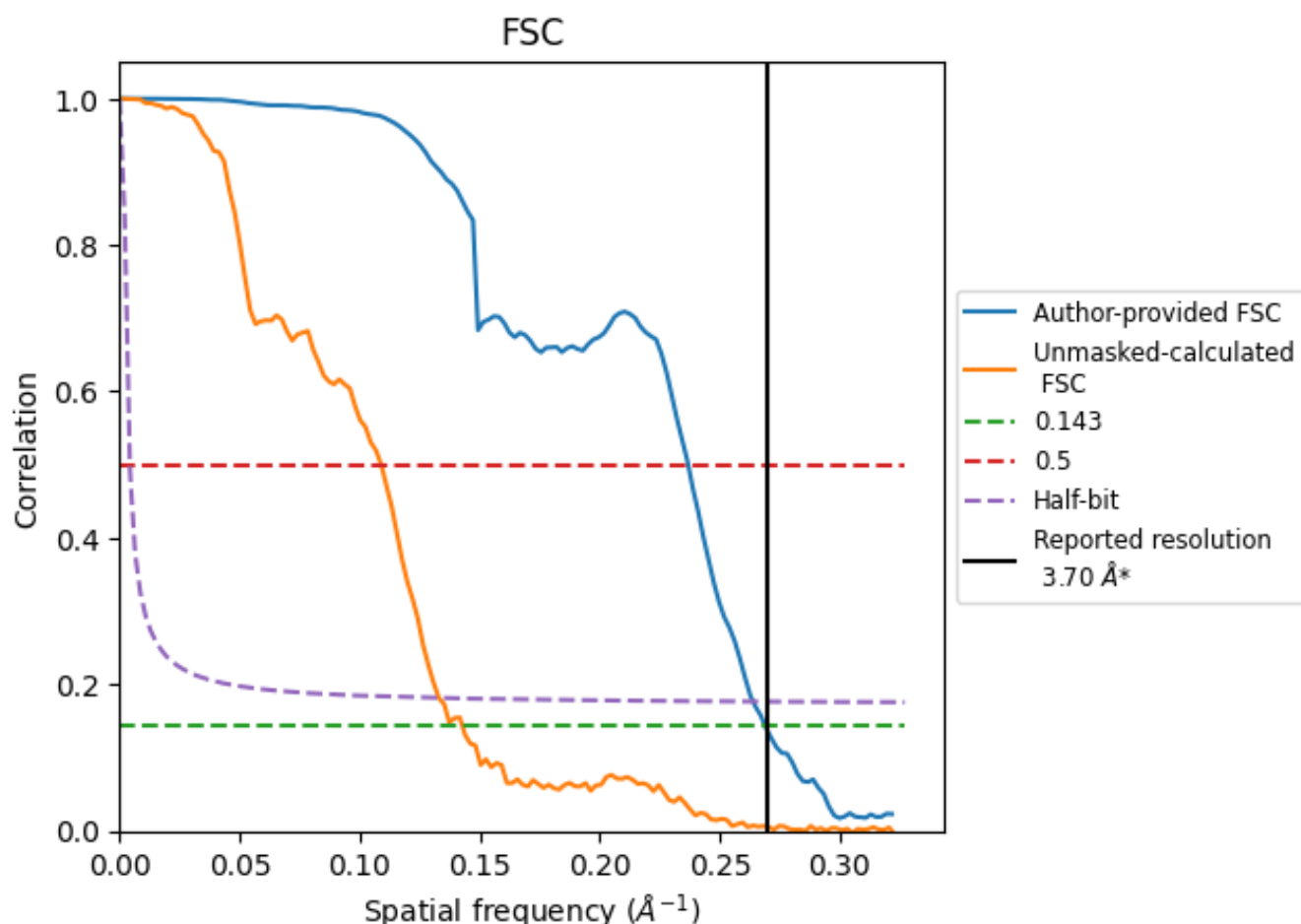
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

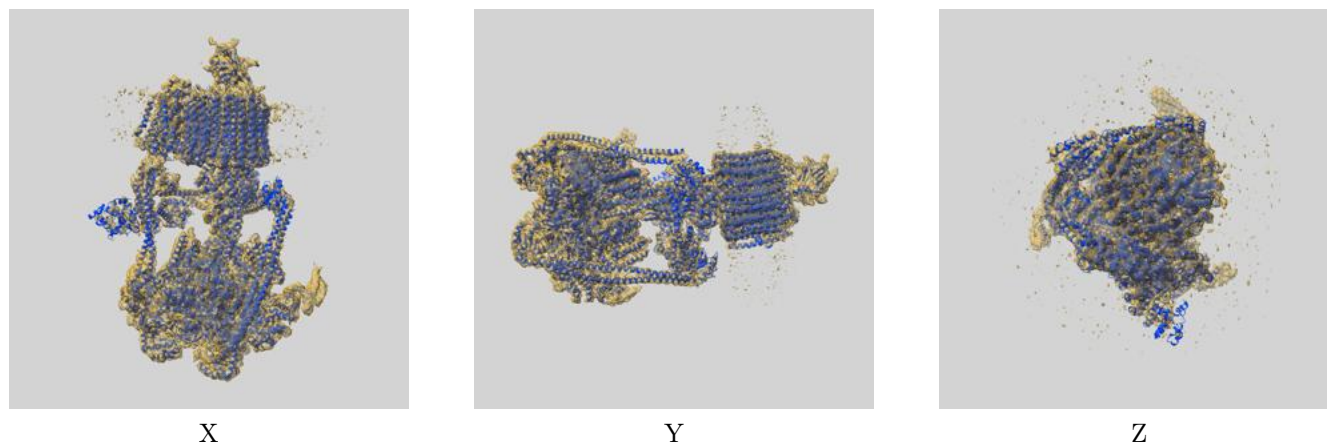
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.22	3.79
Unmasked-calculated*	7.00	9.17	7.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

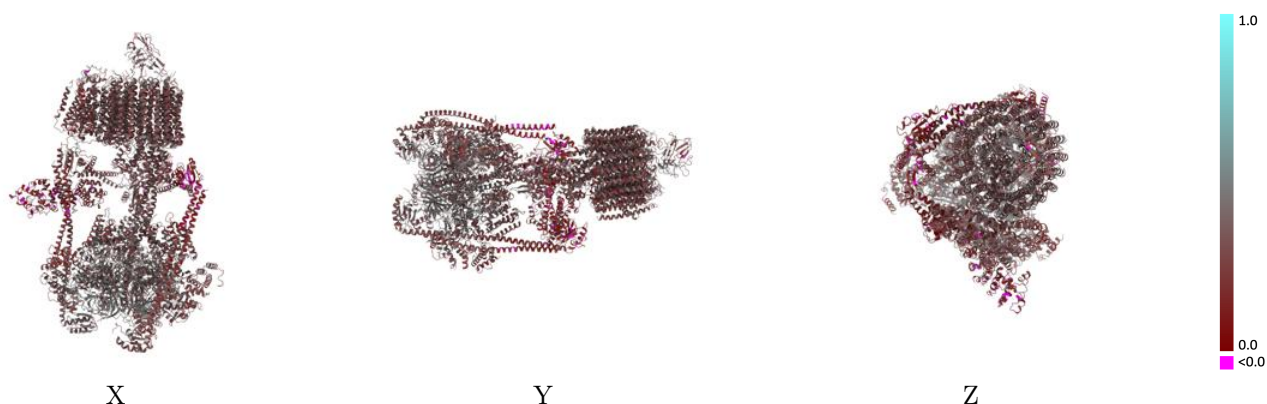
This section contains information regarding the fit between EMDB map EMD-26386 and PDB model 7U8P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



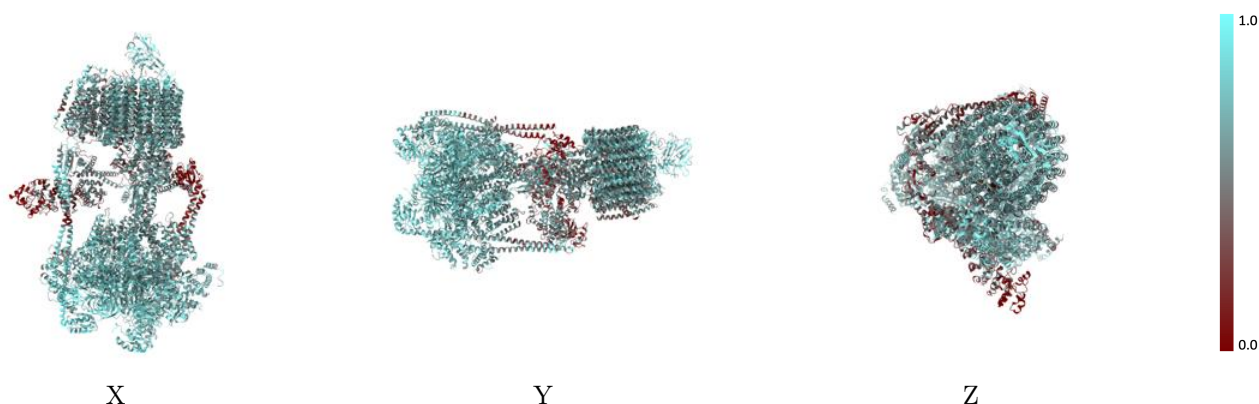
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



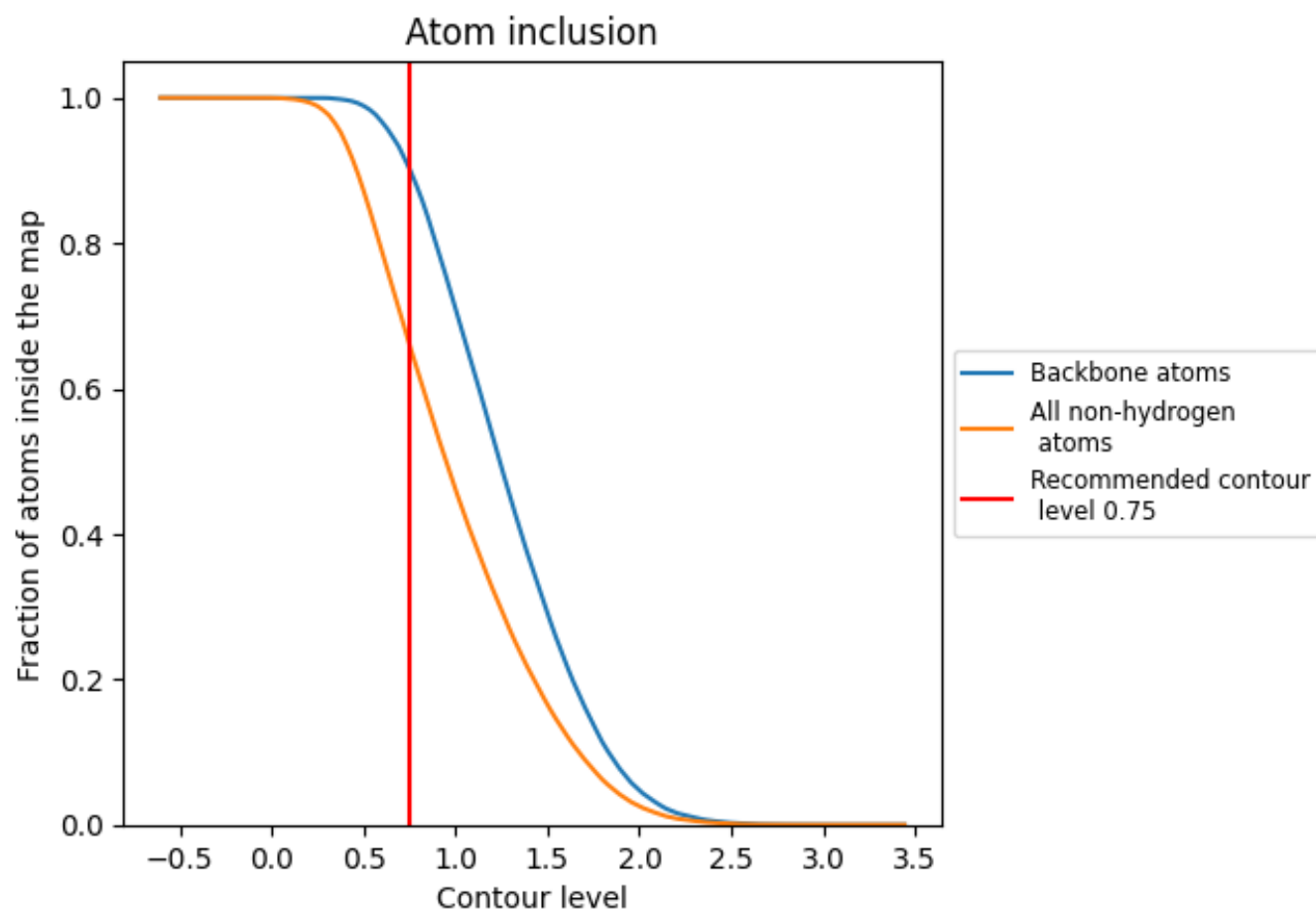
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6602	 0.3340
A	 0.7603	 0.3950
B	 0.7485	 0.3800
C	 0.7820	 0.3980
D	 0.7921	 0.4110
E	 0.7988	 0.4150
F	 0.7809	 0.4040
G	 0.3101	 0.1650
H	 0.7002	 0.3600
I	 0.8095	 0.3470
J	 0.7241	 0.3200
K	 0.6443	 0.3020
L	 0.6408	 0.3400
M	 0.7481	 0.3000
N	 0.6527	 0.2740
O	 0.5742	 0.2610
Q	 0.7145	 0.3110
R	 0.7221	 0.3170
S	 0.6877	 0.3100
T	 0.3034	 0.1780
a	 0.5598	 0.2840
b	 0.6655	 0.3380
c	 0.7245	 0.3530
d	 0.5883	 0.3320
e	 0.6334	 0.3410
f	 0.4969	 0.2690
g	 0.6571	 0.3510
h	 0.6208	 0.3280
i	 0.6590	 0.3390
j	 0.6399	 0.3400
k	 0.5931	 0.3340
l	 0.5931	 0.3190
m	 0.6141	 0.3260
n	 0.6457	 0.3260
o	 0.6590	 0.3300
p	 0.5870	 0.3650

