



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:39 PM UTC

PDB ID : 7UWA / pdb_00007uwa
EMDB ID : EMD-26826
Title : Citrus V-ATPase State 1, H in contact with subunits AB
Authors : Abdelaziz, R.A.; Keon, K.A.; Schulze, W.X.; Schumacher, K.; Rubinstein, J.L.
Deposited on : 2022-05-03
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

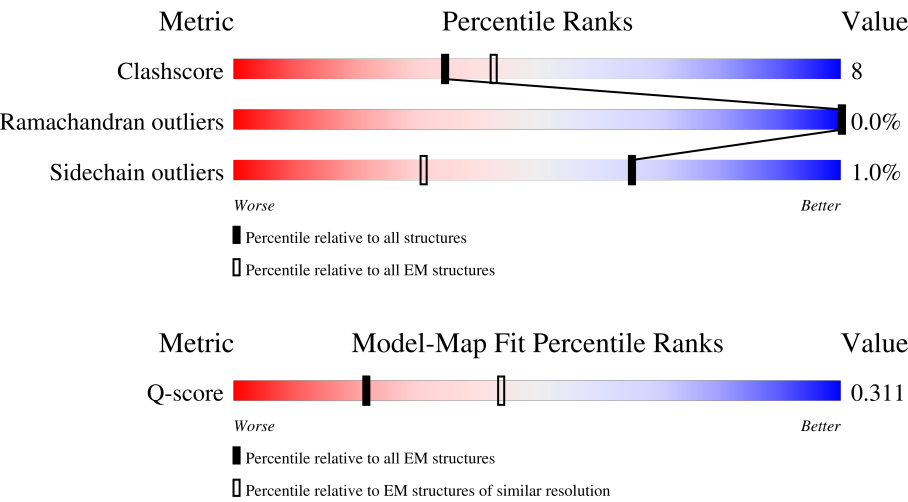
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	74%22%..
1	C	623	70%26%. .
1	E	623	9% 77%17%5%
2	B	488	7% 72%24%. .

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Mol	Chain	Length	Quality of chain
2	D	488	
2	F	488	
3	M	259	
4	N	130	
5	b	32	
6	c	182	
7	d	351	
8	g	164	
8	h	164	
8	i	164	
8	j	164	
8	k	164	
8	l	164	
8	m	164	
8	n	164	
8	o	164	
9	r	24	
10	G	230	
10	I	230	
10	K	230	
11	H	110	
11	J	110	
11	L	110	
12	O	375	
13	a	823	

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Mol	Chain	Length	Quality of chain
14	e	70	93% 6%
15	P	452	62% 90% 5% 5%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 46194 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	E	589	Total	C	N	O	S	0	0
			3935	2537	674	712	12		
1	A	603	Total	C	N	O	S	0	0
			4146	2671	714	746	15		
1	C	603	Total	C	N	O	S	0	0
			4252	2733	734	767	18		

- Molecule 2 is a protein called V-type proton ATPase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	460	Total	C	N	O	S	0	0
			3167	2058	544	557	8		
2	B	467	Total	C	N	O	S	0	0
			3213	2086	560	560	7		
2	D	463	Total	C	N	O	S	0	0
			3194	2069	547	569	9		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	213	Total	C	N	O	0	0
			1109	669	219	221		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	N	107	Total	C	N	O	0	0
			544	330	107	107		

- Molecule 5 is a protein called V-type proton ATPase subunit AP1 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	b	32	Total	C	N	O	0	0
			160	96	32	32		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	c	168	Total	C	N	O	0	0
			833	497	168	168		

- Molecule 7 is a protein called V-type proton ATPase subunit d2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	268	Total	C	N	O	0	0
			1344	806	268	270		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	153	Total	C	N	O	S	0	0
			764	456	153	154	1		
8	h	155	Total	C	N	O		0	0
			763	452	155	156			
8	i	156	Total	C	N	O		0	0
			780	463	156	161			
8	j	155	Total	C	N	O		0	0
			777	465	155	157			
8	k	155	Total	C	N	O	S	0	0
			769	458	155	155	1		
8	l	153	Total	C	N	O		0	0
			752	446	153	153			
8	m	155	Total	C	N	O		0	0
			769	458	155	156			
8	n	155	Total	C	N	O		0	0
			762	452	155	155			
8	o	152	Total	C	N	O		0	0
			737	433	152	152			

- Molecule 9 is a protein called V-type proton ATPase subunit AP2 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	r	24	Total	C	N	O	0	0
			120	72	24	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	204	Total	C	N	O	S	0	0
			1273	795	241	233	4		
10	I	207	Total	C	N	O	S	0	0
			1357	852	253	248	4		
10	K	217	Total	C	N	O	S	0	0
			1364	855	250	253	6		

- Molecule 11 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	97	Total	C	N	O	S	0	0
			555	343	110	101	1		
11	J	96	Total	C	N	O	S	0	0
			517	316	100	100	1		
11	L	101	Total	C	N	O	S	0	0
			582	357	112	112	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	311	Total	C	N	O	0	0
			1571	947	312	312		

- Molecule 13 is a protein called V-type proton ATPase subunit a3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	a	713	Total	C	N	O	0	0
			3590	2161	715	714		

- Molecule 14 is a protein called V-type proton ATPase subunit e1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	e	66	Total	C	N	O	0	0
			358	221	70	67		

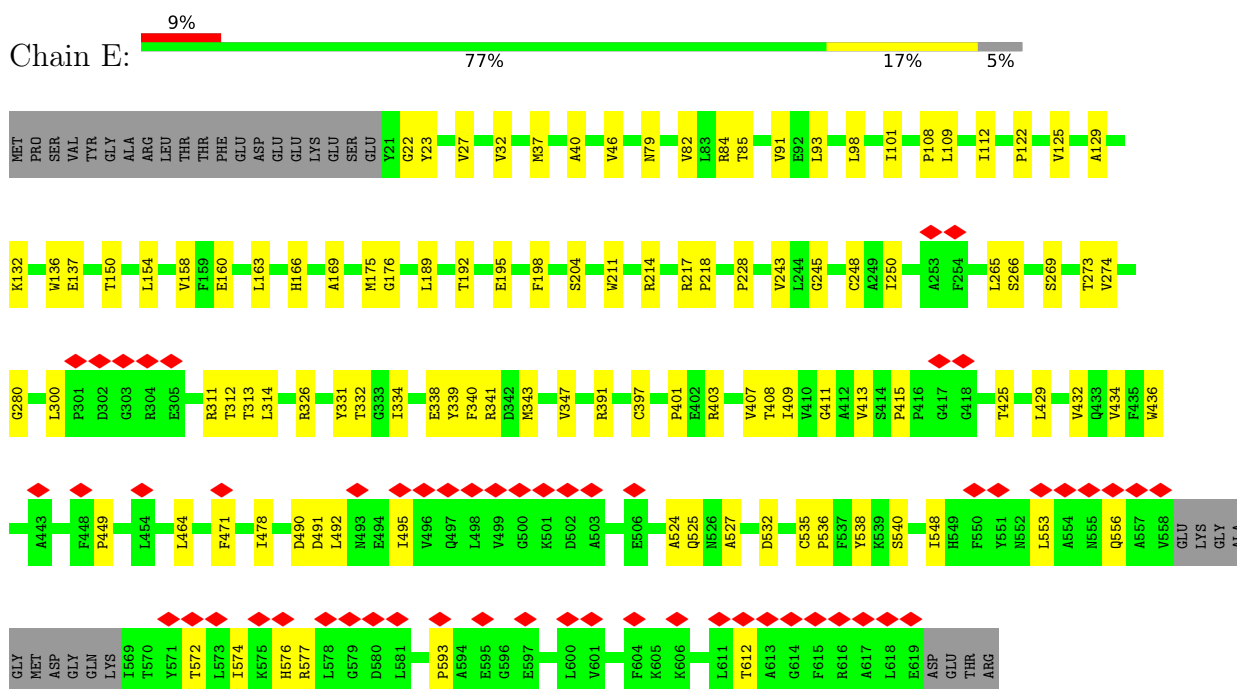
- Molecule 15 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	430	Total	C	N	O	0	0
			2137	1277	430	430		

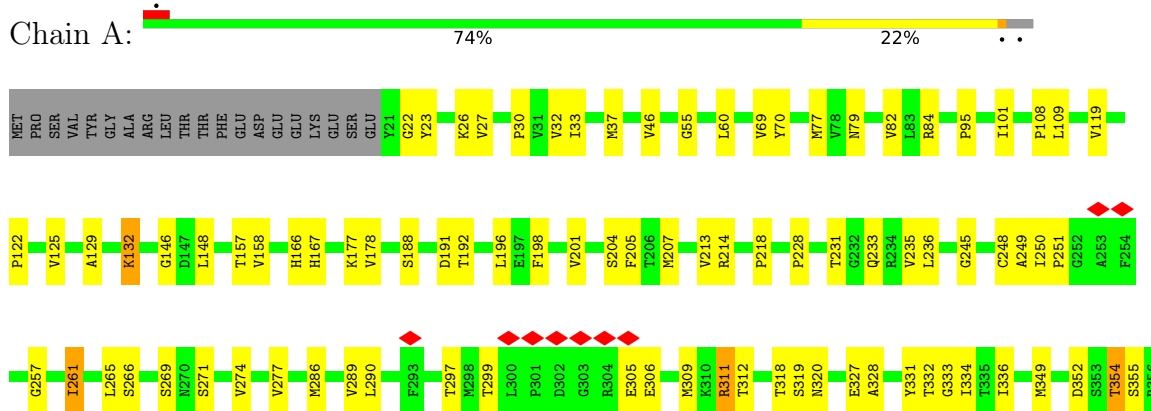
3 Residue-property plots

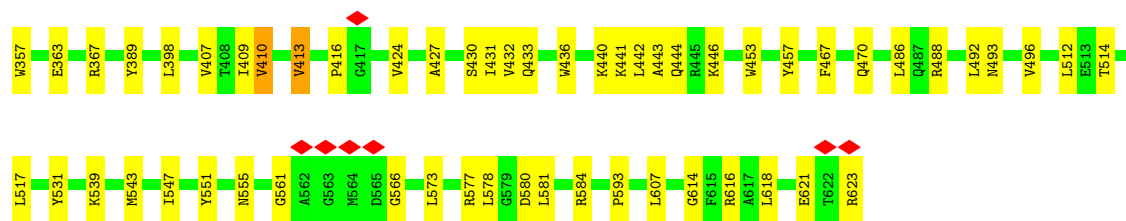
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





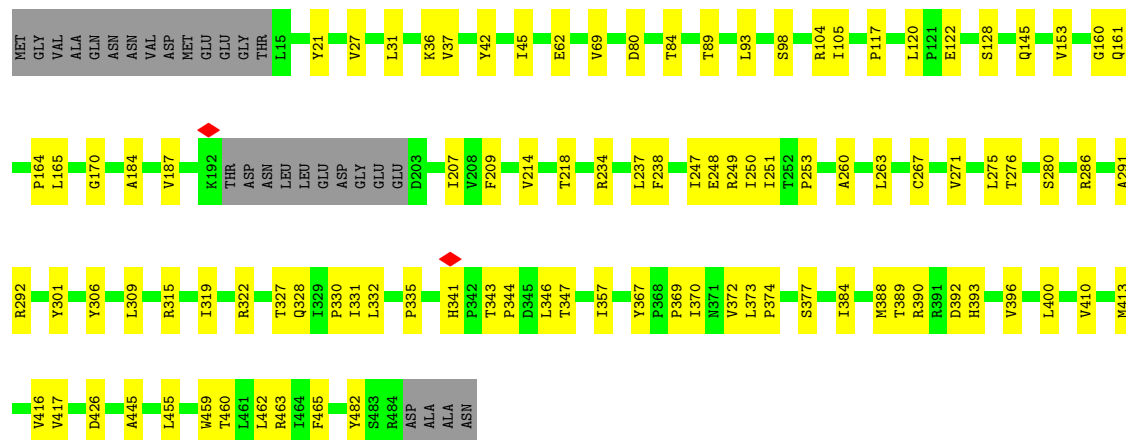
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain C: 70% 26% .

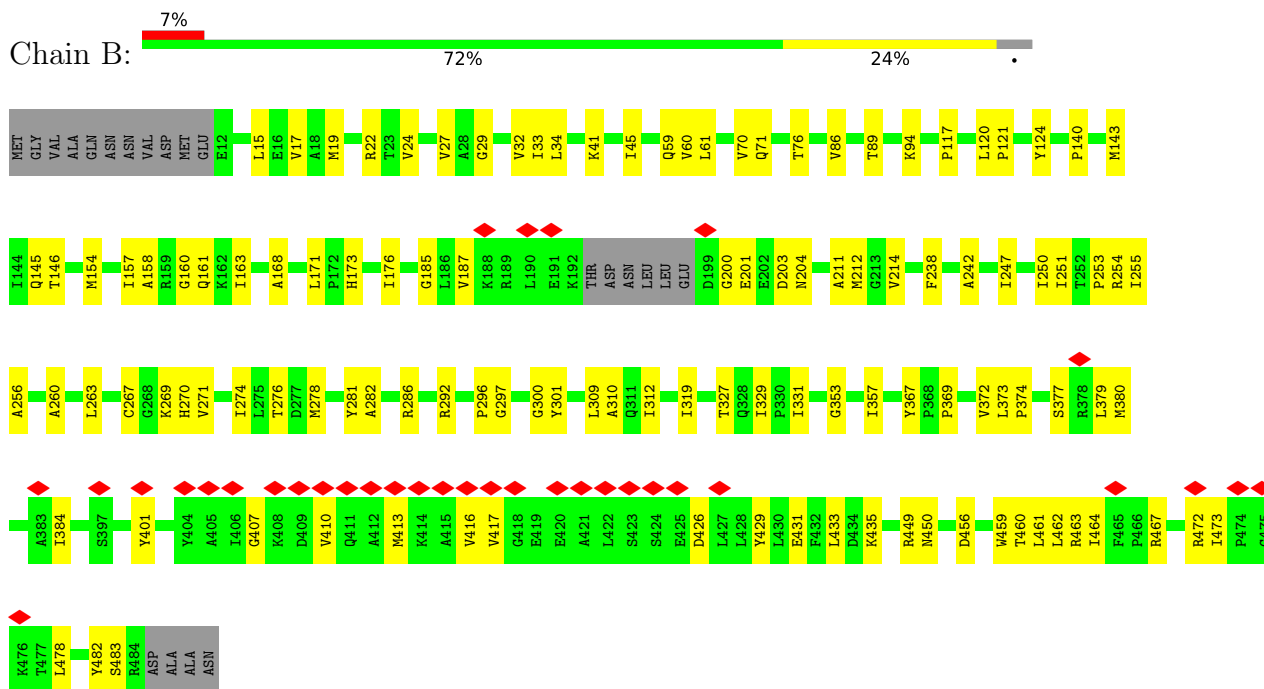


- Molecule 2: V-type proton ATPase subunit B2

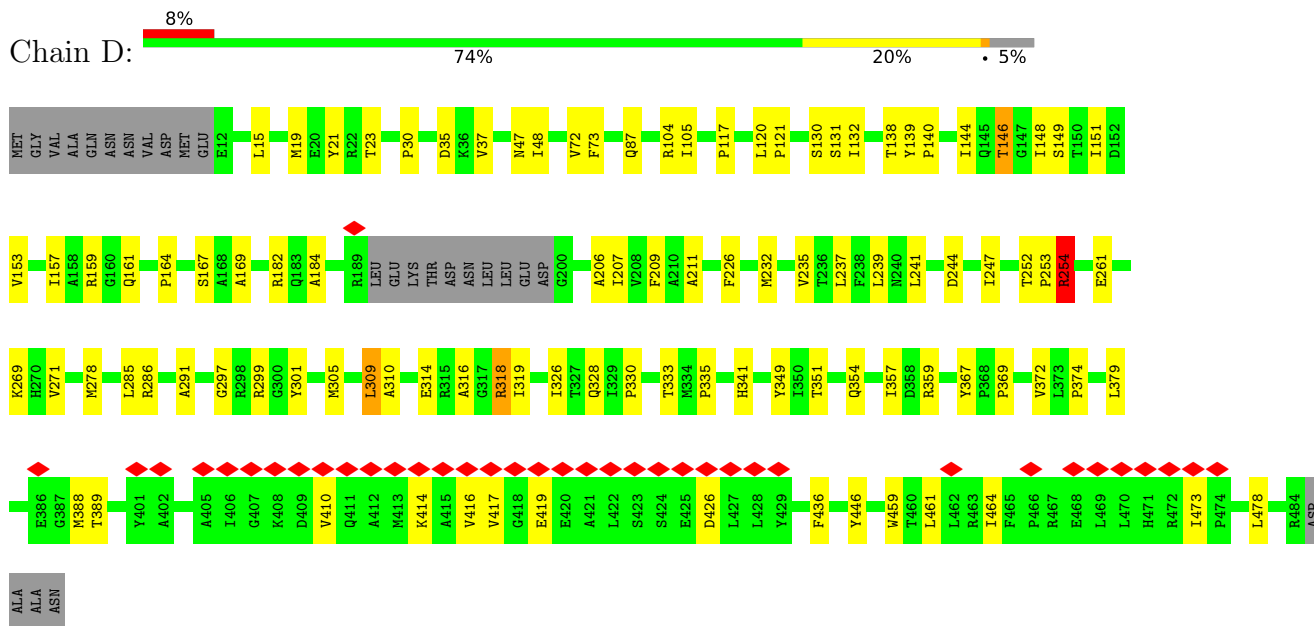
Chain F: 74% 20% 6%



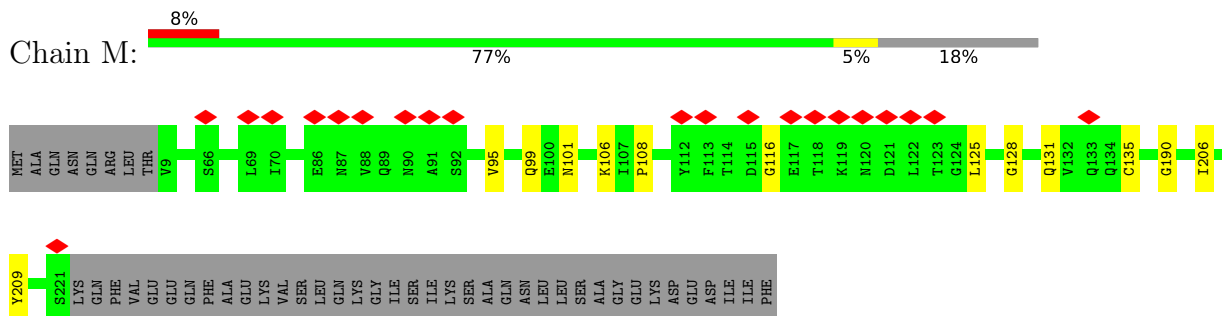
- Molecule 2: V-type proton ATPase subunit B2



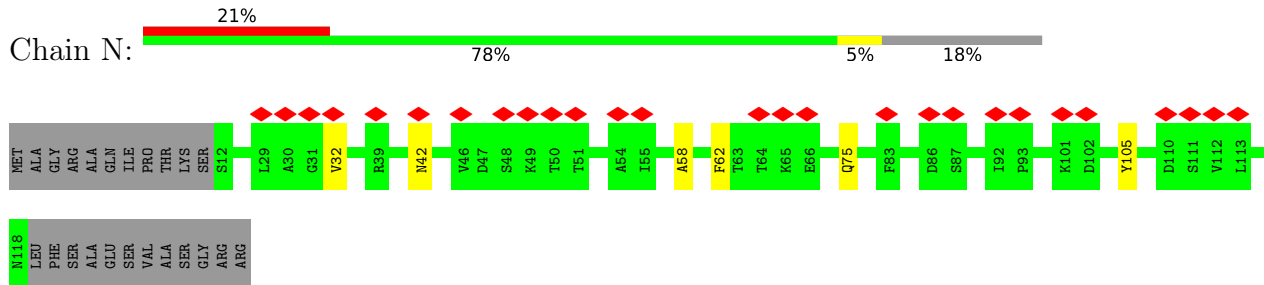
- Molecule 2: V-type proton ATPase subunit B2



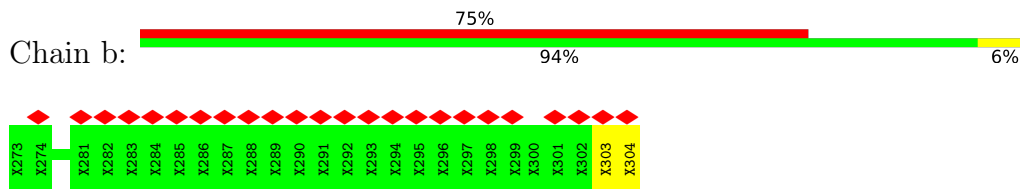
- Molecule 3: V-type proton ATPase subunit D



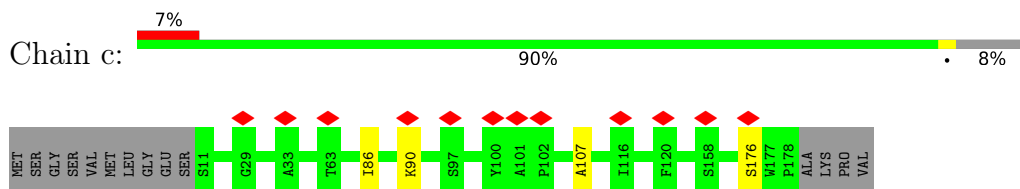
- Molecule 4: V-type proton ATPase subunit F



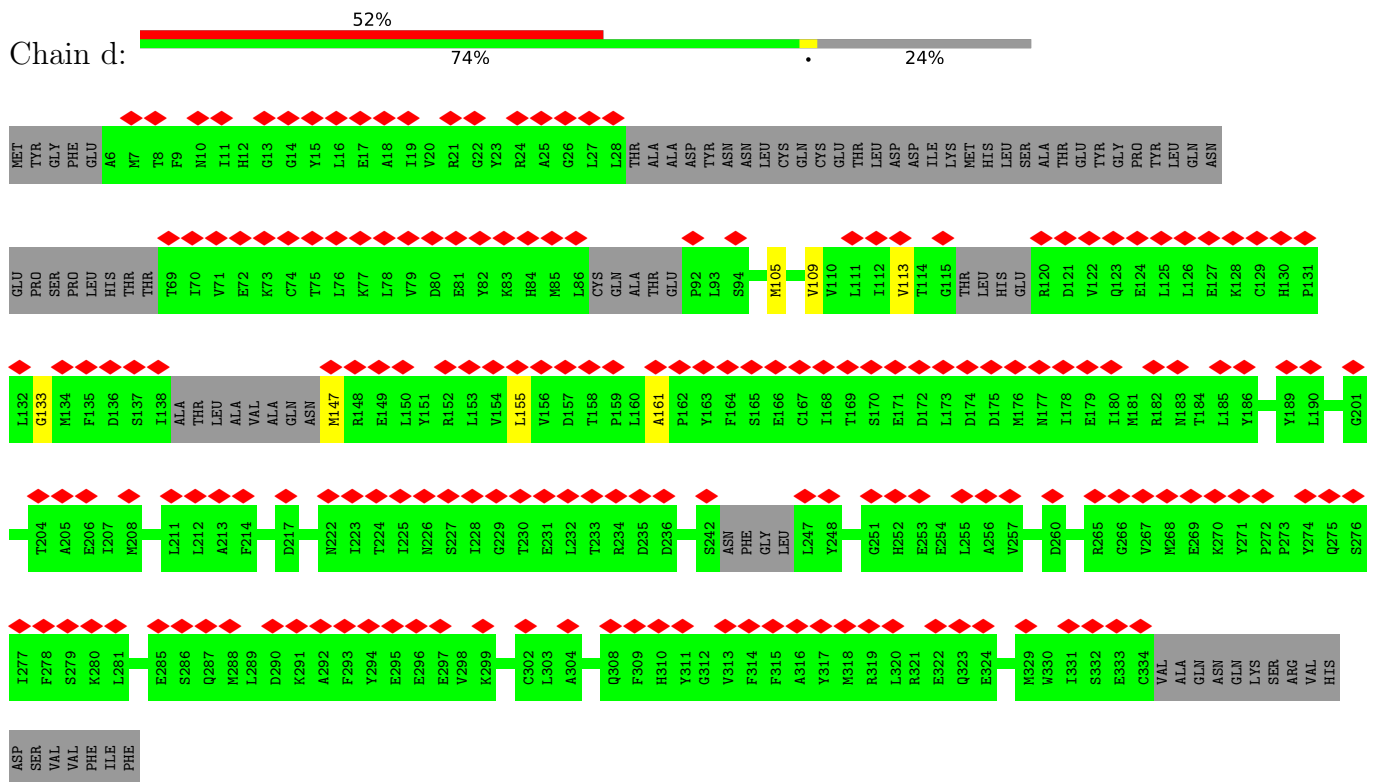
- Molecule 5: V-type proton ATPase subunit AP1 fragment



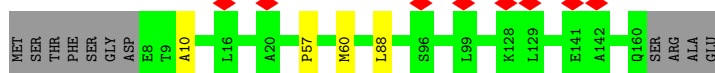
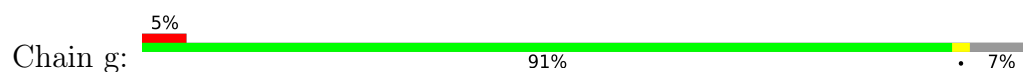
- Molecule 6: V-type proton ATPase subunit c"



- Molecule 7: V-type proton ATPase subunit d2



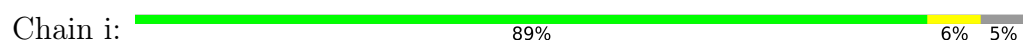
- Molecule 8: V-type proton ATPase subunit c



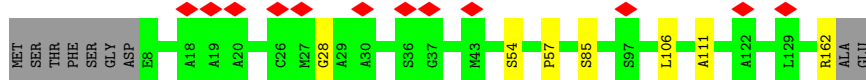
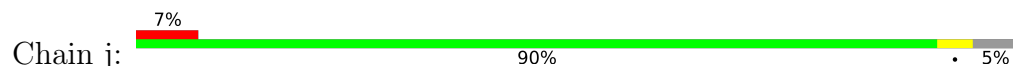
- Molecule 8: V-type proton ATPase subunit c



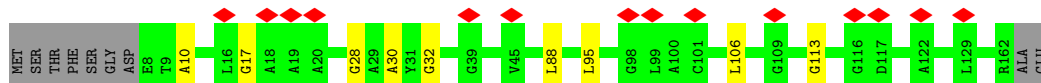
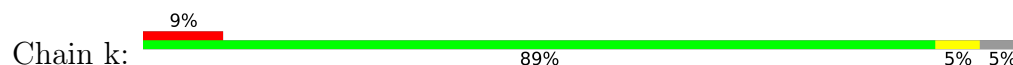
- Molecule 8: V-type proton ATPase subunit c



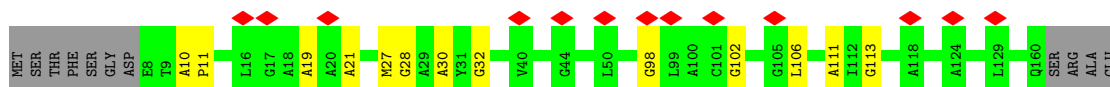
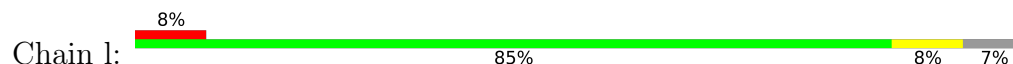
- Molecule 8: V-type proton ATPase subunit c



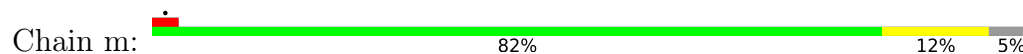
- Molecule 8: V-type proton ATPase subunit c



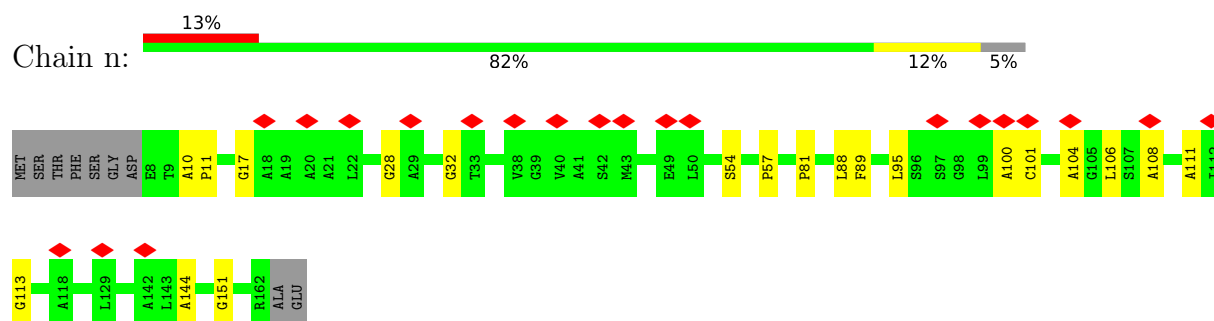
- Molecule 8: V-type proton ATPase subunit c



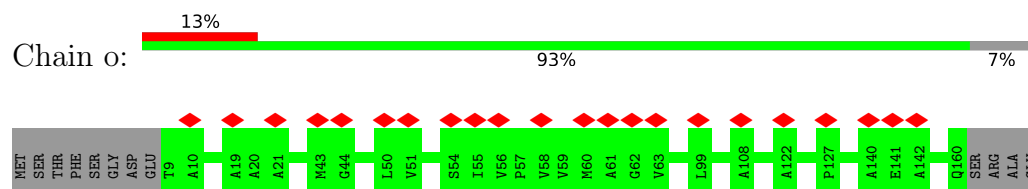
- Molecule 8: V-type proton ATPase subunit c



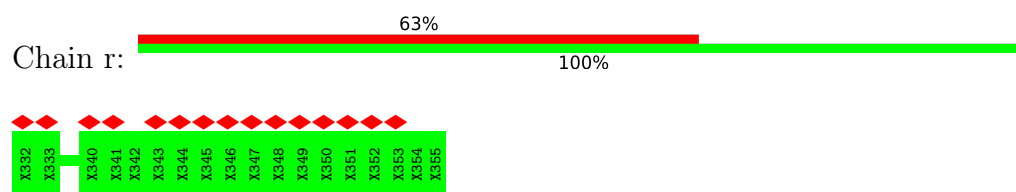
- Molecule 8: V-type proton ATPase subunit c



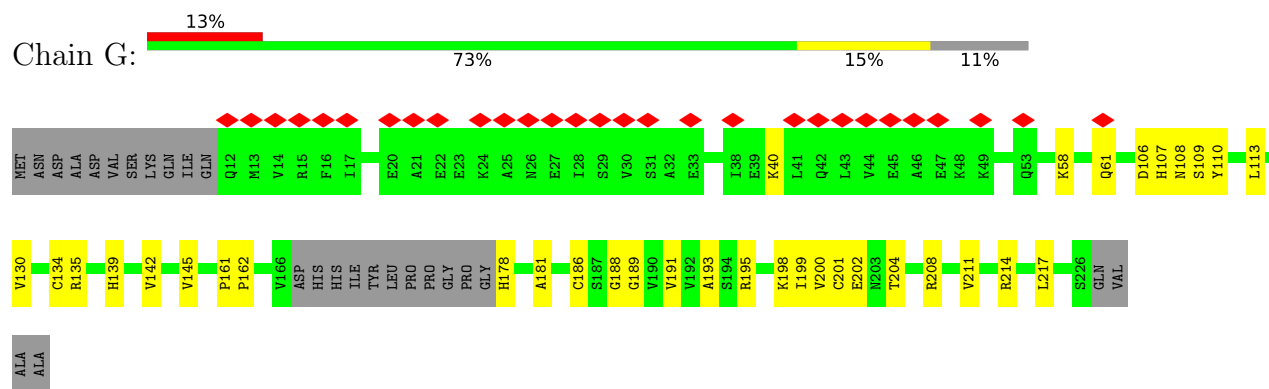
- Molecule 8: V-type proton ATPase subunit c



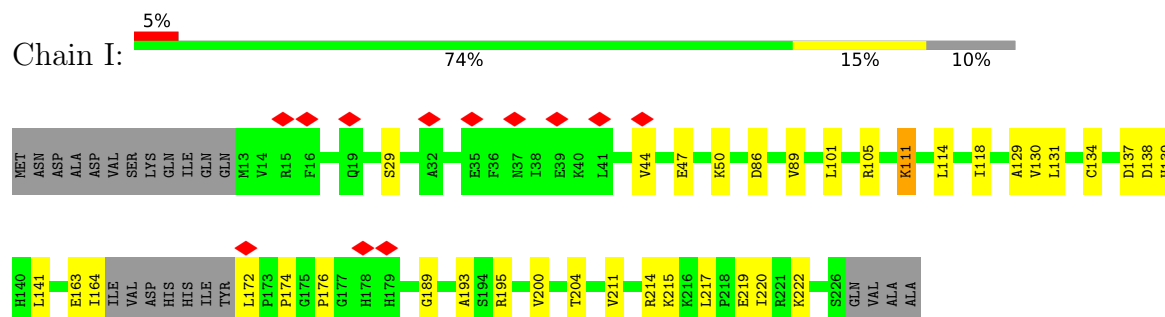
- Molecule 9: V-type proton ATPase subunit AP2 fragment



- Molecule 10: V-type proton ATPase subunit E

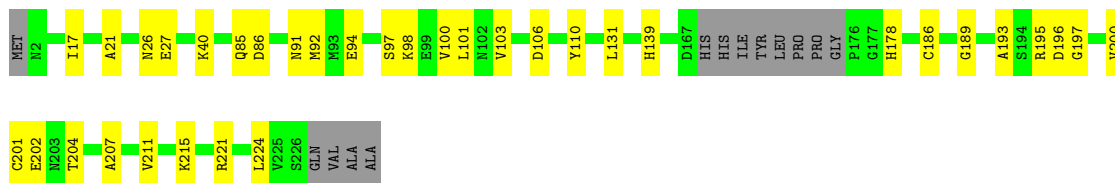


- Molecule 10: V-type proton ATPase subunit E



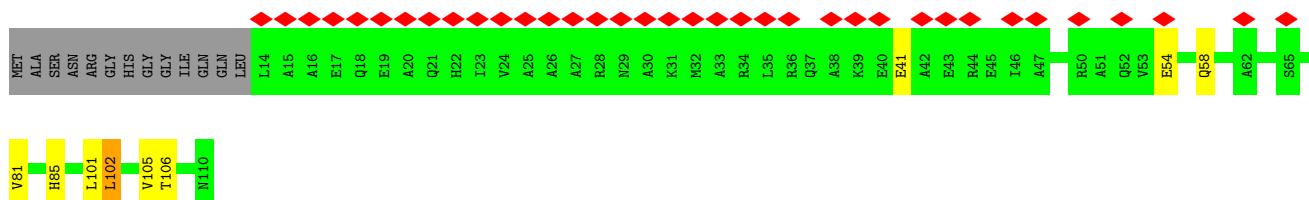
- Molecule 10: V-type proton ATPase subunit E

Chain K:



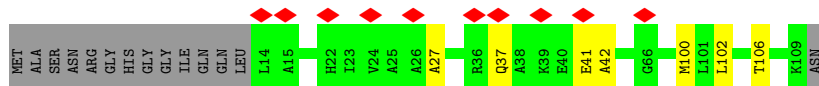
- Molecule 11: V-type proton ATPase subunit G

Chain H:



- Molecule 11: V-type proton ATPase subunit G

Chain J:



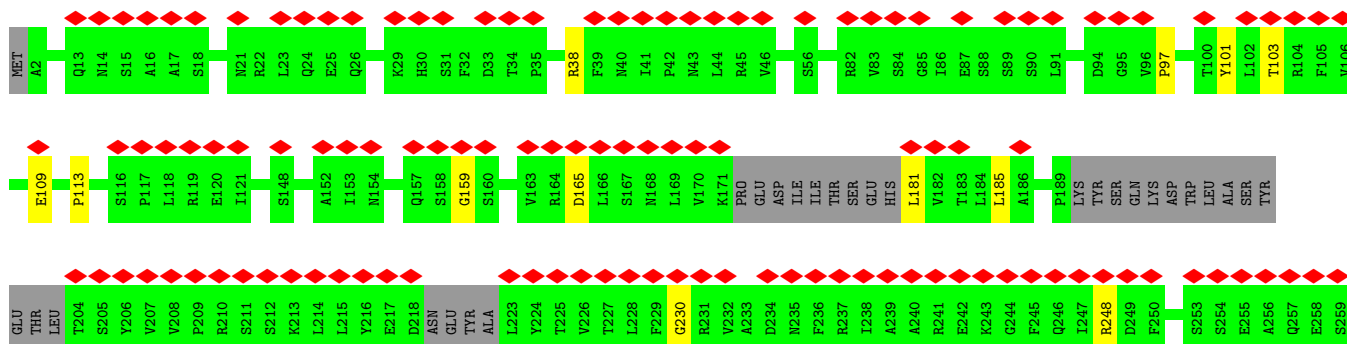
- Molecule 11: V-type proton ATPase subunit G

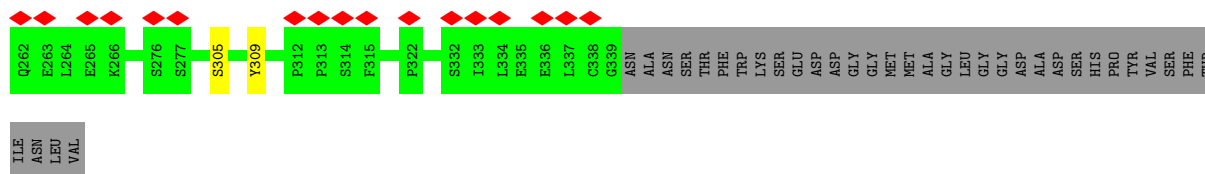
Chain L:



- Molecule 12: V-type proton ATPase subunit C

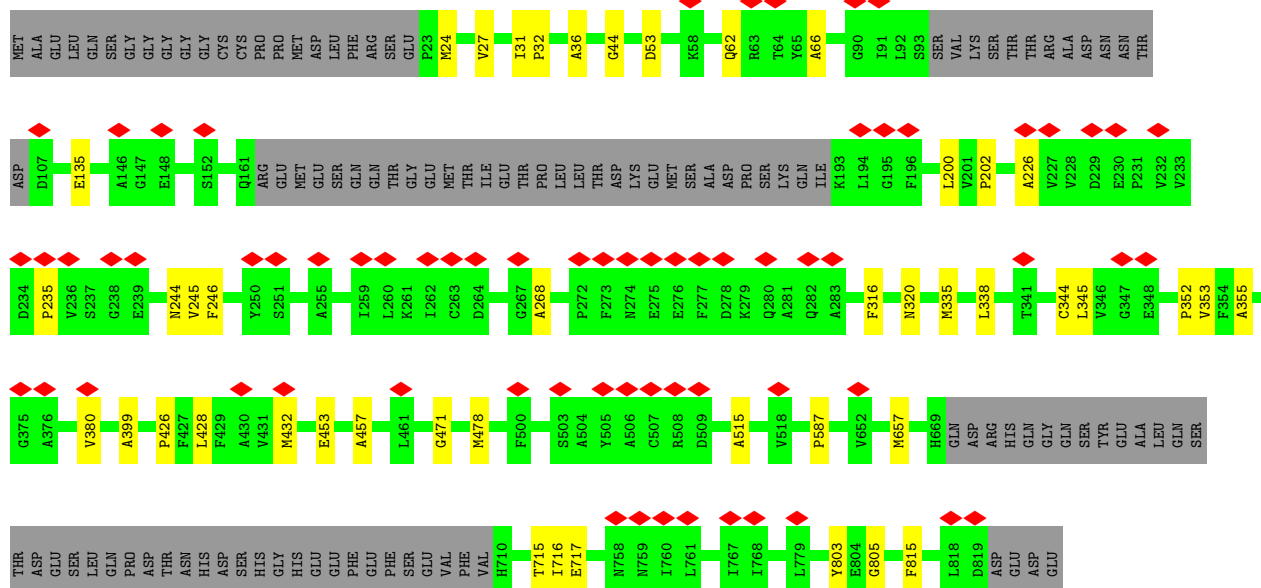
Chain O:





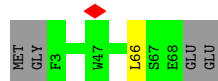
• Molecule 13: V-type proton ATPase subunit a3

Chain a:



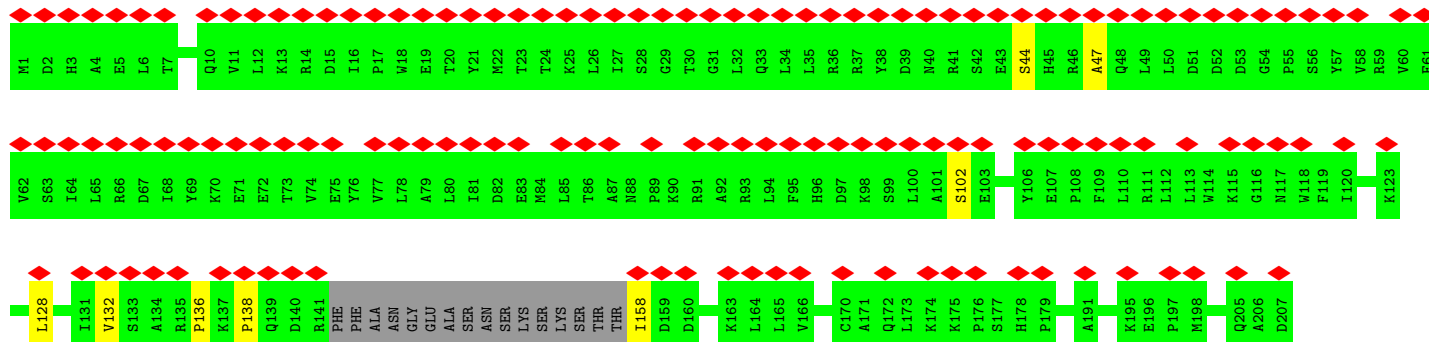
• Molecule 14: V-type proton ATPase subunit e1

Chain e:



• Molecule 15: V-type proton ATPase subunit H

Chain P:



G208	V209	K210	L211	L212	T213	P214	L215	I216	S217	P218	A219	S224	L228	A244	V245	K283	G284	N285	F286	I291	G294	L295	P296	Q297	V298	A304	S308	D309	E310	K324	D325	N326	I327	K328	R329	L330	S331	S332	F333	D334	K335	Y336	K337	Q338	E339	V340	L341	L342	G343	H344									
L345	D346	W347	S348	P349	M350	H351	K352	D353	P354	L355	F356	W357	R358	D359	N360	I361	T362	N363	F364	E365	E366	N367	D368	F369	Q370	I371	L372	R373	V374	L375	L376	T377	I378	L379	D380	T381	S382	S383	D384	P385	R386	A387	L388	A389	V390	A391	C392	F393	D394	L395	S396	Q397	F398	I399	Q400	Y401	H402	P403	A404
G405	R406	V407	I408	V409	T410	D411	L412	K413	A414	V418	M419	K420	L421	M422	N423	H424	E425	M426	T427	E428	V429	T430	K431	S432	A433	L434	L435	C436	I437	Q438	R439	L440	F441	L442	G443	A444	K445	Y446	ALA	SER	PHE	LEU	GLN	ALA															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31	Depositor
Minimum defocus (nm)	677.558	Depositor
Maximum defocus (nm)	3414.211	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.484	Depositor
Minimum map value	-0.391	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	485.1, 485.1, 485.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.617, 1.617, 1.617	Depositor

5 Model quality

5.1 Standard geometry

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	0.29	0/4244	0.52	4/5833 (0.1%)
1	C	0.17	0/4350	0.39	1/5958 (0.0%)
1	E	0.14	0/4023	0.34	0/5546
2	B	0.20	0/3277	0.40	0/4494
2	D	0.33	0/3257	0.56	3/4468 (0.1%)
2	F	0.20	0/3230	0.42	0/4434
3	M	0.15	0/1113	0.38	0/1548
4	N	0.18	0/548	0.57	1/767 (0.1%)
6	c	0.13	0/837	0.30	0/1164
7	d	0.13	0/1345	0.36	0/1870
8	g	0.14	0/769	0.30	0/1064
8	h	0.13	0/767	0.34	0/1062
8	i	0.13	0/785	0.35	0/1086
8	j	0.14	0/783	0.30	0/1084
8	k	0.14	0/774	0.29	0/1071
8	l	0.15	0/756	0.36	0/1047
8	m	0.16	0/774	0.33	0/1071
8	n	0.14	0/766	0.39	0/1061
8	o	0.14	0/736	0.30	0/1015
10	G	0.14	0/1283	0.37	0/1764
10	I	0.29	0/1374	0.52	0/1884
10	K	0.18	0/1377	0.39	0/1895
11	H	0.34	0/558	0.55	0/772
11	J	0.13	0/517	0.36	0/716
11	L	0.14	0/586	0.29	0/812
12	O	0.13	0/1578	0.33	0/2203
13	a	0.13	0/3613	0.36	0/5044
14	e	0.12	0/363	0.29	0/506
15	P	0.11	0/2135	0.34	0/2978
All	All	0.20	0/46518	0.41	9/64217 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	THR	CB-CA-C	9.88	119.61	109.83
2	D	253	PRO	N-CA-C	-7.89	106.48	114.68
1	A	261	ILE	N-CA-C	-7.02	103.46	110.62
1	A	355	SER	N-CA-C	-6.53	104.00	112.68
2	D	254	ARG	N-CA-C	-6.34	104.50	112.93
1	C	620	ASP	O-C-N	-6.03	115.27	122.15
2	D	309	LEU	N-CA-C	-5.96	105.09	112.90
1	A	352	ASP	N-CA-C	-5.91	106.71	112.97
4	N	42	ASN	CB-CA-C	-5.54	110.17	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	620	ASP	Mainchain

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	4146	0	3766	90	0
1	C	4252	0	3975	113	0
1	E	3935	0	3531	70	0
2	B	3213	0	3010	80	0
2	D	3194	0	2985	63	0
2	F	3167	0	2963	66	0
3	M	1109	0	597	9	0
4	N	544	0	279	2	0
5	b	160	0	35	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	c	833	0	446	2	0
7	d	1344	0	632	4	0
8	g	764	0	446	2	0
8	h	763	0	432	2	0
8	i	780	0	460	6	0
8	j	777	0	448	4	0
8	k	769	0	439	5	0
8	l	752	0	425	9	0
8	m	769	0	439	15	0
8	n	762	0	429	13	0
8	o	737	0	393	0	0
9	r	120	0	27	0	0
10	G	1273	0	1039	22	0
10	I	1357	0	1177	27	0
10	K	1364	0	1113	25	0
11	H	555	0	400	6	0
11	J	517	0	343	6	0
11	L	582	0	411	8	0
12	O	1571	0	752	7	0
13	a	3590	0	1768	25	0
14	e	358	0	170	1	0
15	P	2137	0	935	12	0
All	All	46194	0	34265	643	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 8.

All (643) 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)
15:P:365:GLU:HA	15:P:369:PHE:HA	1.58	0.86
1:A:492:LEU:HD11	1:A:512:LEU:HD11	1.58	0.84
1:A:277:VAL:HG21	1:A:349:MET:HE2	1.65	0.79
10:G:214:ARG:HA	10:G:217:LEU:HD12	1.65	0.79
1:C:26:LYS:HB3	1:C:33:ILE:HB	1.64	0.78
1:E:228:PRO:HA	1:E:243:VAL:HA	1.67	0.76
10:G:211:VAL:HA	10:G:214:ARG:HH12	1.49	0.76
2:B:61:LEU:HD13	2:B:292:ARG:HD2	1.70	0.73
2:F:160:GLY:H	2:F:327:THR:HG22	1.54	0.73
2:F:328:GLN:HG3	2:F:330:PRO:HD3	1.71	0.72
1:C:320:ASN:ND2	2:D:314:GLU:O	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:108:ASN:OD1	10:G:109:SER:N	2.23	0.72
10:G:189:GLY:HA3	10:G:204:THR:HA	1.70	0.71
10:I:219:GLU:HA	10:I:222:LYS:HG2	1.71	0.71
1:C:132:LYS:O	1:C:190:LYS:NZ	2.21	0.71
1:A:251:PRO:HA	1:A:413:VAL:HG12	1.73	0.71
15:P:291:ILE:O	15:P:295:LEU:N	2.22	0.70
4:N:75:GLN:HA	4:N:105:TYR:HA	1.73	0.70
2:B:168:ALA:H	2:B:171:LEU:HD12	1.57	0.70
10:K:211:VAL:HG22	10:K:215:LYS:HZ2	1.55	0.70
1:C:239:LEU:O	1:C:483:ARG:NH2	2.25	0.69
1:C:320:ASN:HB3	2:D:131:SER:HB2	1.73	0.69
2:D:148:ILE:HG22	2:D:151:ILE:HG22	1.72	0.69
1:A:213:VAL:HG13	1:A:214:ARG:HD2	1.75	0.69
1:C:163:LEU:HD12	1:C:306:GLU:HG2	1.74	0.69
2:D:140:PRO:HA	2:D:318:ARG:HD3	1.74	0.69
1:C:334:ILE:HA	1:C:349:MET:HE1	1.75	0.69
8:n:17:GLY:HA3	8:n:95:LEU:HA	1.76	0.68
1:A:440:LYS:O	1:A:443:ALA:N	2.25	0.68
6:c:86:ILE:O	6:c:90:LYS:N	2.26	0.68
8:n:28:GLY:HA3	8:n:106:LEU:HA	1.76	0.68
10:I:130:VAL:H	10:I:164:ILE:HD13	1.59	0.68
8:k:28:GLY:HA3	8:k:106:LEU:HA	1.75	0.67
12:O:38:ARG:HA	12:O:103:THR:HA	1.75	0.67
1:E:122:PRO:HG2	1:E:125:VAL:HB	1.77	0.67
2:B:143:MET:HA	2:B:158:ALA:HA	1.77	0.67
1:C:572:THR:O	1:C:576:HIS:ND1	2.27	0.66
1:A:573:LEU:O	1:A:577:ARG:N	2.29	0.66
10:I:211:VAL:HG12	10:I:215:LYS:NZ	2.11	0.66
1:C:543:MET:HE2	1:C:588:GLN:HG3	1.78	0.66
8:m:17:GLY:HA3	8:m:95:LEU:HA	1.77	0.65
10:K:189:GLY:HA3	10:K:204:THR:HA	1.78	0.65
1:C:47:ARG:HB2	1:C:83:LEU:HB2	1.78	0.65
12:O:159:GLY:HA2	12:O:165:ASP:HA	1.78	0.65
1:C:581:LEU:HD13	1:C:611:LEU:HA	1.79	0.65
1:A:299:THR:HB	1:A:305:GLU:HG2	1.80	0.64
1:A:108:PRO:HD3	1:A:129:ALA:HA	1.80	0.64
15:P:294:GLY:O	15:P:298:VAL:N	2.30	0.64
2:F:105:ILE:HG22	2:F:237:LEU:HB3	1.79	0.64
2:F:31:LEU:HD21	2:F:291:ALA:HB1	1.79	0.63
1:E:23:TYR:HB2	1:E:79:ASN:HA	1.81	0.63
1:E:136:TRP:CD1	1:E:160:GLU:HA	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:163:GLU:O	10:I:172:LEU:N	2.31	0.63
1:C:535:CYS:SG	1:C:540:SER:OG	2.56	0.63
8:m:19:ALA:HA	8:n:100:ALA:HB2	1.81	0.63
10:K:40:LYS:HG2	11:L:39:LYS:HA	1.79	0.63
1:E:154:LEU:HD23	1:E:169:ALA:HB2	1.81	0.63
2:F:276:THR:HA	2:F:331:ILE:HB	1.80	0.62
2:B:27:VAL:HG13	2:B:32:VAL:HG12	1.81	0.62
1:C:241:PRO:HG3	1:C:479:ARG:HH12	1.64	0.62
1:C:543:MET:HG3	1:C:588:GLN:NE2	2.14	0.62
1:E:217:ARG:HD3	1:E:218:PRO:HD2	1.82	0.62
2:D:367:TYR:O	2:D:369:PRO:HD3	2.00	0.62
2:F:286:ARG:HE	2:F:301:TYR:HA	1.63	0.62
2:B:463:ARG:NH1	2:B:483:SER:O	2.33	0.62
12:O:97:PRO:O	12:O:101:TYR:N	2.33	0.62
13:a:44:GLY:O	13:a:815:PHE:N	2.33	0.61
1:C:252:GLY:HA3	1:C:258:LYS:HE3	1.82	0.61
2:F:459:TRP:O	2:F:463:ARG:HD2	2.00	0.61
2:D:182:ARG:HH12	2:D:446:TYR:HE2	1.49	0.61
8:n:10:ALA:HB2	8:n:88:LEU:HA	1.82	0.61
13:a:338:LEU:HA	13:a:345:LEU:HA	1.82	0.61
1:C:167:HIS:HB2	1:C:343:MET:HG3	1.83	0.61
4:N:58:ALA:O	4:N:62:PHE:N	2.30	0.61
1:E:574:ILE:HA	1:E:577:ARG:HG2	1.81	0.61
1:A:37:MET:HE2	1:A:37:MET:HA	1.83	0.60
1:A:218:PRO:HB2	1:A:398:LEU:HD11	1.83	0.60
1:A:319:SER:HB3	2:B:310:ALA:HB1	1.82	0.60
5:b:303:UNK:O	5:b:304:UNK:CB	2.49	0.60
2:D:226:PHE:HB3	2:D:232:MET:HE2	1.82	0.60
1:E:22:GLY:O	1:E:82:VAL:N	2.33	0.60
1:E:413:VAL:HG12	1:E:415:PRO:HD3	1.81	0.60
1:E:250:ILE:HD11	1:E:436:TRP:HE3	1.67	0.60
2:F:332:LEU:HD11	2:F:343:THR:HG22	1.84	0.60
1:C:72:GLU:O	1:C:123:ARG:NH1	2.34	0.60
1:C:101:ILE:HG12	1:C:314:LEU:HD12	1.83	0.60
2:D:169:ALA:O	2:D:359:ARG:NH2	2.34	0.60
1:C:222:LYS:HG2	1:C:395:VAL:HG12	1.84	0.60
1:E:154:LEU:HD12	1:E:401:PRO:HD2	1.82	0.60
2:B:276:THR:HA	2:B:331:ILE:HG12	1.83	0.60
2:D:105:ILE:HG23	2:D:237:LEU:HB2	1.82	0.59
7:d:113:VAL:O	7:d:147:MET:N	2.35	0.59
1:A:318:THR:OG1	1:A:320:ASN:OD1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:HD13	1:C:170:LEU:HD22	1.83	0.59
13:a:53:ASP:HA	13:a:335:MET:HA	1.84	0.59
2:F:306:TYR:HB2	2:F:346:LEU:HD11	1.84	0.59
2:D:414:LYS:HE3	2:D:419:GLU:HA	1.84	0.59
13:a:202:PRO:HA	13:a:244:ASN:H	1.67	0.59
1:C:267:LYS:HE2	1:C:293:PHE:HE1	1.67	0.59
2:D:207:ILE:HB	2:D:235:VAL:HG22	1.84	0.59
1:E:46:VAL:HG23	1:E:84:ARG:HA	1.85	0.59
1:E:245:GLY:H	1:E:408:THR:HB	1.69	0.58
10:G:193:ALA:HA	10:G:200:VAL:HA	1.84	0.58
1:C:300:LEU:HD21	1:C:304:ARG:HG2	1.84	0.58
10:I:211:VAL:HG12	10:I:215:LYS:HZ1	1.66	0.58
1:E:228:PRO:HB3	1:E:464:LEU:HD11	1.85	0.58
1:A:257:GLY:HA2	1:A:261:ILE:HB	1.85	0.58
1:C:266:SER:O	1:C:311:ARG:NH2	2.36	0.58
1:C:135:LEU:HB3	1:C:186:GLN:HB3	1.86	0.58
1:E:415:PRO:HB3	1:E:425:THR:HG21	1.85	0.58
1:C:398:LEU:O	1:C:403:ARG:NH2	2.32	0.58
1:A:551:TYR:O	1:A:555:ASN:ND2	2.38	0.57
2:B:161:GLN:HE22	2:B:379:LEU:HB2	1.68	0.57
2:D:146:THR:HG21	2:D:151:ILE:HD13	1.85	0.57
7:d:109:VAL:O	7:d:113:VAL:N	2.27	0.57
10:K:186:CYS:HG	10:K:204:THR:HG1	1.47	0.57
1:E:176:GLY:HA2	1:E:198:PHE:HB2	1.84	0.57
2:F:306:TYR:HA	2:F:346:LEU:HD21	1.87	0.57
2:B:431:GLU:O	2:B:435:LYS:HG3	2.05	0.57
10:K:106:ASP:O	10:K:110:TYR:HB2	2.05	0.57
2:D:73:PHE:HA	2:D:247:ILE:HG21	1.87	0.57
2:D:167:SER:HB2	2:D:357:ILE:HD12	1.87	0.57
1:A:23:TYR:HB2	1:A:79:ASN:HA	1.87	0.56
2:D:461:LEU:HD13	2:D:464:ILE:HD12	1.87	0.56
10:G:106:ASP:OD2	10:G:107:HIS:N	2.37	0.56
1:E:397:CYS:SG	1:E:403:ARG:HD3	2.44	0.56
8:k:17:GLY:HA3	8:k:95:LEU:HA	1.87	0.56
10:I:139:HIS:CE1	10:I:176:PRO:HD2	2.40	0.56
2:B:140:PRO:HG2	2:B:379:LEU:HD13	1.87	0.56
2:D:459:TRP:HE1	2:D:478:LEU:HB2	1.70	0.56
8:m:28:GLY:HA3	8:m:106:LEU:HA	1.88	0.56
15:P:138:PRO:O	15:P:158:ILE:N	2.38	0.56
1:C:49:GLY:HA2	1:C:80:ASP:HB3	1.88	0.56
1:A:309:MET:HA	1:A:312:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TYR:HA	1:A:334:ILE:HG22	1.88	0.56
1:C:22:GLY:O	1:C:82:VAL:N	2.36	0.56
3:M:125:LEU:H	3:M:128:GLY:HA3	1.71	0.56
10:G:134:CYS:O	10:G:178:HIS:NE2	2.37	0.56
10:G:142:VAL:HA	10:G:145:VAL:HG12	1.88	0.56
1:A:251:PRO:HB2	1:A:416:PRO:HD3	1.87	0.56
8:j:28:GLY:HA3	8:j:106:LEU:HA	1.87	0.56
2:B:203:ASP:HA	2:B:270:HIS:HD2	1.70	0.56
1:E:273:THR:HG23	1:E:347:VAL:HG23	1.89	0.55
1:E:478:ILE:HG12	1:E:548:ILE:HG21	1.88	0.55
1:A:266:SER:HA	1:A:274:VAL:HG21	1.89	0.55
2:B:467:ARG:HH21	2:B:482:TYR:HB3	1.72	0.55
1:A:265:LEU:HA	1:A:269:SER:HB3	1.89	0.55
1:C:577:ARG:HG3	1:C:618:LEU:HD13	1.89	0.55
2:B:171:LEU:HD13	2:B:357:ILE:HG22	1.89	0.55
2:D:104:ARG:NH2	2:D:117:PRO:O	2.35	0.55
2:F:460:THR:HA	2:F:463:ARG:HD3	1.89	0.55
2:B:59:GLN:HB3	2:B:71:GLN:HE21	1.71	0.55
3:M:99:GLN:HA	3:M:108:PRO:HA	1.89	0.55
1:A:561:GLY:HA2	1:A:566:GLY:HA3	1.89	0.54
2:B:373:LEU:HB3	2:B:374:PRO:HD3	1.89	0.54
13:a:200:LEU:HA	13:a:246:PHE:H	1.72	0.54
13:a:399:ALA:HB2	13:a:471:GLY:HA2	1.89	0.54
1:E:341:ARG:HD3	1:E:407:VAL:HG23	1.89	0.54
1:A:517:LEU:HD23	1:A:547:ILE:HG23	1.89	0.54
2:B:163:ILE:HD13	2:B:353:GLY:HA3	1.88	0.54
1:E:338:GLU:HA	1:E:341:ARG:HG2	1.88	0.54
1:C:331:TYR:HA	1:C:334:ILE:HG22	1.90	0.54
1:C:119:VAL:HG21	2:D:319:ILE:HG12	1.89	0.54
1:C:289:VAL:HG13	1:C:293:PHE:CE2	2.43	0.54
11:L:102:LEU:HA	11:L:105:VAL:HG22	1.90	0.54
1:E:27:VAL:HG13	1:E:32:VAL:HG22	1.90	0.54
1:E:553:LEU:HA	1:E:556:GLN:HE22	1.72	0.54
2:B:145:GLN:HB2	2:B:187:VAL:HB	1.90	0.54
2:B:410:VAL:HG11	2:B:426:ASP:HA	1.89	0.54
1:C:341:ARG:HD2	1:C:395:VAL:HG22	1.88	0.54
13:a:24:MET:HA	13:a:353:VAL:H	1.72	0.54
1:C:539:LYS:HB2	1:C:604:PHE:HE2	1.71	0.54
13:a:587:PRO:HB2	13:a:657:MET:HA	1.90	0.54
10:G:191:VAL:HG12	10:G:202:GLU:HG2	1.90	0.53
2:B:154:MET:HE3	2:B:372:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ALA:HA	1:C:394:LYS:HE2	1.89	0.53
1:C:550:PHE:HB2	1:C:611:LEU:HD21	1.89	0.53
12:O:185:LEU:O	12:O:248:ARG:N	2.34	0.53
1:A:578:LEU:HD12	1:A:581:LEU:HD12	1.90	0.53
8:m:10:ALA:HB2	8:m:88:LEU:HA	1.89	0.53
2:B:296:PRO:HB2	2:B:300:GLY:HA2	1.91	0.53
1:C:28:SER:OG	1:C:367:ARG:NH2	2.41	0.53
2:F:332:LEU:HD13	2:F:347:THR:HG21	1.90	0.53
1:C:279:CYS:HB2	1:C:326:ARG:HG3	1.90	0.53
1:C:353:SER:H	1:C:412:ALA:HB3	1.74	0.53
10:K:131:LEU:HD23	10:K:195:ARG:HA	1.90	0.53
2:F:31:LEU:HD12	2:F:69:VAL:HG22	1.91	0.53
2:F:249:ARG:HD2	2:F:280:SER:HB3	1.91	0.53
2:F:413:MET:O	2:F:417:VAL:HG22	2.08	0.53
1:C:37:MET:HE3	1:C:37:MET:HA	1.91	0.53
2:D:211:ALA:HB3	2:D:239:LEU:HA	1.91	0.53
2:D:354:GLN:NE2	2:D:374:PRO:O	2.42	0.53
2:B:253:PRO:HB2	2:B:312:ILE:HD11	1.91	0.52
2:D:241:LEU:N	2:D:244:ASP:OD2	2.42	0.52
1:E:195:GLU:HA	1:E:204:SER:HA	1.91	0.52
2:F:145:GLN:HG3	2:F:187:VAL:HG22	1.90	0.52
10:G:106:ASP:OD1	10:G:109:SER:OG	2.27	0.52
1:C:341:ARG:HG3	1:C:406:SER:N	2.24	0.52
2:D:21:TYR:CE2	2:D:37:VAL:HA	2.44	0.52
10:I:189:GLY:HA3	10:I:204:THR:HA	1.90	0.52
12:O:181:LEU:HA	12:O:230:GLY:HA3	1.92	0.52
13:a:27:VAL:HA	13:a:380:VAL:HA	1.90	0.52
2:F:390:ARG:HH22	2:F:455:LEU:HB3	1.75	0.52
8:k:32:GLY:HA2	8:k:113:GLY:HA3	1.91	0.52
1:C:214:ARG:O	1:C:391:ARG:NH2	2.43	0.52
2:B:297:GLY:N	2:B:301:TYR:O	2.37	0.52
10:G:181:ALA:HB3	10:G:186:CYS:HB2	1.92	0.52
2:D:299:ARG:HH21	3:M:190:GLY:HA3	1.73	0.52
10:I:86:ASP:HA	10:I:89:VAL:HG22	1.91	0.52
1:A:196:LEU:HD12	1:A:205:PHE:HE2	1.75	0.52
2:B:254:ARG:NH2	2:B:281:TYR:OH	2.43	0.51
1:E:132:LYS:HA	1:E:189:LEU:HB2	1.92	0.51
2:F:36:LYS:HE3	2:F:36:LYS:HA	1.91	0.51
2:B:19:MET:HE3	2:B:19:MET:HA	1.91	0.51
1:C:134:THR:OG1	1:C:136:TRP:NE1	2.43	0.51
1:E:40:ALA:HA	1:E:84:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:LEU:HD12	2:B:464:ILE:HD12	1.92	0.51
1:A:22:GLY:O	1:A:82:VAL:N	2.35	0.51
1:A:132:LYS:O	1:A:188:SER:HB2	2.10	0.51
2:B:416:VAL:HG13	2:B:417:VAL:HG13	1.92	0.51
2:F:165:LEU:HD23	2:F:331:ILE:HD12	1.92	0.51
1:A:27:VAL:HG13	1:A:32:VAL:HG22	1.93	0.51
1:A:427:ALA:O	1:A:430:SER:OG	2.23	0.51
1:C:578:LEU:HD11	1:C:581:LEU:HD12	1.92	0.51
1:E:409:ILE:HG22	1:E:411:GLY:H	1.76	0.51
2:B:120:LEU:O	10:K:221:ARG:NH1	2.43	0.51
1:C:57:ILE:HD13	1:C:67:ILE:HG13	1.93	0.51
1:A:621:GLU:HG3	1:A:623:ARG:H	1.76	0.51
2:B:276:THR:HG23	2:B:331:ILE:HD11	1.93	0.51
1:C:213:VAL:HG12	1:C:331:TYR:HB3	1.92	0.51
3:M:206:ILE:HA	3:M:209:TYR:CE1	2.46	0.51
11:L:49:HIS:O	11:L:52:GLN:HG3	2.11	0.51
1:A:26:LYS:HB3	1:A:33:ILE:HB	1.92	0.50
2:D:23:THR:OG1	2:D:35:ASP:O	2.27	0.50
10:I:211:VAL:HA	10:I:214:ARG:HG2	1.94	0.50
2:D:301:TYR:CD1	2:D:305:MET:HE1	2.46	0.50
8:l:19:ALA:HB1	8:m:100:ALA:HB2	1.93	0.50
10:I:44:VAL:HG11	11:J:42:ALA:C	2.36	0.50
1:C:282:ARG:NH2	2:D:349:TYR:O	2.43	0.50
13:a:32:PRO:HA	13:a:344:CYS:HA	1.92	0.50
1:C:496:VAL:O	1:C:500:GLY:N	2.44	0.50
1:E:331:TYR:HA	1:E:334:ILE:HG22	1.94	0.50
2:B:200:GLY:O	2:B:204:ASN:N	2.45	0.50
2:B:211:ALA:HA	2:B:276:THR:HB	1.94	0.50
1:C:121:ILE:HG12	2:D:131:SER:O	2.11	0.50
1:C:429:LEU:HA	1:C:432:VAL:HG12	1.94	0.50
1:E:490:ASP:OD1	1:E:491:ASP:N	2.45	0.50
1:A:235:VAL:HG13	1:A:236:LEU:HD12	1.92	0.50
1:C:282:ARG:HB2	1:C:285:GLU:HG3	1.94	0.50
2:B:160:GLY:N	2:B:327:THR:OG1	2.36	0.50
2:B:286:ARG:HH11	1:C:373:ALA:HB1	1.77	0.50
13:a:515:ALA:HB3	14:e:66:LEU:H	1.77	0.50
1:E:553:LEU:HD13	1:E:612:THR:HA	1.93	0.49
1:C:257:GLY:O	1:C:260:VAL:HG12	2.12	0.49
11:H:81:VAL:O	11:H:85:HIS:ND1	2.45	0.49
10:I:29:SER:HB2	11:J:27:ALA:HB1	1.94	0.49
13:a:62:GLN:C	13:a:66:ALA:HB3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:THR:HA	1:E:175:MET:HA	1.94	0.49
10:K:131:LEU:N	10:K:193:ALA:O	2.34	0.49
10:K:224:LEU:HD21	11:L:86:LEU:HD11	1.93	0.49
1:C:23:TYR:HB2	1:C:79:ASN:HA	1.93	0.49
8:k:10:ALA:HB2	8:k:88:LEU:HA	1.93	0.49
10:K:85:GLN:HG2	11:L:86:LEU:HD21	1.94	0.49
2:F:416:VAL:HG23	2:F:417:VAL:HG13	1.93	0.49
15:P:369:PHE:O	15:P:373:ARG:N	2.37	0.49
1:E:535:CYS:SG	1:E:540:SER:OG	2.54	0.49
1:A:539:LYS:HG2	1:A:543:MET:HE2	1.94	0.49
8:i:10:ALA:N	8:i:11:PRO:HD2	2.28	0.49
8:m:21:ALA:HA	8:m:102:GLY:HA3	1.95	0.49
2:F:27:VAL:O	1:A:60:LEU:N	2.44	0.49
1:C:581:LEU:HD22	1:C:584:ARG:NH1	2.28	0.49
2:D:48:ILE:HD13	2:D:72:VAL:HG12	1.94	0.49
2:D:416:VAL:HG23	2:D:417:VAL:HG23	1.94	0.49
1:A:277:VAL:HG11	1:A:333:GLY:HA3	1.94	0.49
1:A:441:LYS:HA	1:A:444:GLN:NE2	2.28	0.49
15:P:44:SER:HA	15:P:47:ALA:HB3	1.95	0.49
2:B:145:GLN:N	2:B:185:GLY:O	2.44	0.48
1:C:577:ARG:CZ	1:C:618:LEU:HB3	2.43	0.48
10:I:101:LEU:O	10:I:105:ARG:HG2	2.13	0.48
1:A:442:LEU:HD11	1:A:453:TRP:HZ3	1.78	0.48
1:C:300:LEU:HD23	1:C:300:LEU:H	1.77	0.48
1:C:605:LYS:O	1:C:609:GLU:HG2	2.13	0.48
2:D:164:PRO:HG3	2:D:351:THR:HG21	1.94	0.48
1:E:91:VAL:HG21	1:E:332:THR:HG23	1.95	0.48
2:F:373:LEU:HB3	2:F:374:PRO:HD3	1.95	0.48
1:A:77:MET:HE3	2:B:41:LYS:HD3	1.93	0.48
1:E:211:TRP:CZ2	1:E:218:PRO:HD3	2.48	0.48
1:C:278:GLY:H	1:C:316:ALA:HB2	1.79	0.48
13:a:202:PRO:HG3	13:a:268:ALA:HB2	1.94	0.48
1:E:265:LEU:HG	1:E:269:SER:HB3	1.95	0.48
10:K:26:ASN:OD1	10:K:27:GLU:N	2.46	0.48
2:B:247:ILE:O	2:B:250:ILE:HG22	2.13	0.48
1:C:298:MET:SD	1:C:311:ARG:NH1	2.86	0.48
12:O:109:GLU:O	12:O:113:PRO:HD2	2.14	0.48
1:A:213:VAL:HG22	1:A:331:TYR:HB3	1.95	0.48
2:B:286:ARG:HD3	2:B:301:TYR:HA	1.96	0.48
10:I:164:ILE:HA	10:I:172:LEU:N	2.28	0.48
1:C:603:LYS:O	1:C:606:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:385:PRO:O	15:P:389:ALA:N	2.45	0.48
1:A:119:VAL:HG21	2:B:319:ILE:HD11	1.95	0.48
1:A:119:VAL:HG11	2:B:319:ILE:HD11	1.94	0.48
1:A:188:SER:N	1:A:191:ASP:OD2	2.38	0.48
6:c:107:ALA:HB2	6:c:176:SER:H	1.79	0.48
10:G:58:LYS:HA	10:G:61:GLN:HE21	1.79	0.48
2:F:184:ALA:O	2:F:234:ARG:NH1	2.46	0.48
13:a:715:THR:C	13:a:717:GLU:H	2.22	0.48
15:P:128:LEU:O	15:P:132:VAL:N	2.47	0.48
13:a:352:PRO:HB2	13:a:355:ALA:HB3	1.96	0.47
2:F:45:ILE:O	2:F:89:THR:OG1	2.29	0.47
1:C:70:TYR:HD1	1:C:325:ALA:HA	1.78	0.47
2:D:144:ILE:HB	2:D:157:ILE:HG23	1.95	0.47
10:K:193:ALA:HB2	10:K:200:VAL:HG23	1.95	0.47
1:A:233:GLN:HB2	1:A:236:LEU:HB2	1.96	0.47
2:B:282:ALA:HB1	2:B:301:TYR:HE2	1.79	0.47
1:A:192:THR:OG1	1:A:204:SER:OG	2.32	0.47
2:B:456:ASP:O	2:B:460:THR:HG23	2.14	0.47
3:M:101:ASN:HA	3:M:106:LYS:HA	1.97	0.47
8:m:54:SER:O	8:m:57:PRO:HD2	2.15	0.47
10:K:139:HIS:HB2	10:K:178:HIS:CE1	2.50	0.47
2:D:120:LEU:HD12	2:D:121:PRO:HD2	1.96	0.47
1:E:101:ILE:HG23	1:E:109:LEU:HB2	1.97	0.47
1:E:136:TRP:HD1	1:E:160:GLU:HA	1.79	0.47
2:F:42:TYR:HH	2:F:292:ARG:HH22	1.55	0.47
2:F:465:PHE:O	2:F:482:TYR:OH	2.32	0.47
1:C:166:HIS:CD2	1:C:343:MET:HE1	2.50	0.47
1:C:245:GLY:H	1:C:408:THR:HG1	1.57	0.47
8:n:11:PRO:HB3	8:n:81:PRO:HG3	1.97	0.47
8:n:32:GLY:CA	8:n:113:GLY:HA3	2.44	0.47
11:J:37:GLN:O	11:J:41:GLU:OE1	2.33	0.47
13:a:428:LEU:O	13:a:432:MET:N	2.48	0.47
1:C:315:VAL:HG12	1:C:315:VAL:O	2.15	0.47
8:k:30:ALA:HB1	8:l:111:ALA:HB2	1.96	0.47
10:G:139:HIS:HA	10:G:142:VAL:HG12	1.96	0.47
10:K:40:LYS:HG3	11:L:42:ALA:HB3	1.97	0.47
2:F:275:LEU:O	2:F:331:ILE:N	2.33	0.47
2:F:370:ILE:HD12	2:F:370:ILE:H	1.79	0.47
2:F:413:MET:HA	2:F:416:VAL:HG22	1.96	0.47
1:A:228:PRO:HG3	1:A:467:PHE:CE2	2.50	0.47
13:a:426:PRO:HB3	13:a:478:MET:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:PRO:HB3	10:I:86:ASP:OD2	2.15	0.46
1:C:33:ILE:HD13	1:C:66:THR:HA	1.97	0.46
1:C:584:ARG:HH22	1:C:607:LEU:HA	1.80	0.46
8:g:10:ALA:HB2	8:g:88:LEU:HA	1.96	0.46
1:A:248:CYS:HB2	1:A:410:VAL:HA	1.96	0.46
1:A:55:GLY:HA2	1:A:70:TYR:HD1	1.80	0.46
2:B:449:ARG:HH11	2:B:450:ASN:H	1.61	0.46
1:C:414:SER:HB2	2:D:349:TYR:CE1	2.50	0.46
2:D:473:ILE:HD13	2:D:478:LEU:HD23	1.96	0.46
8:n:101:CYS:CB	8:n:151:GLY:HA3	2.45	0.46
1:E:340:PHE:O	1:E:343:MET:HG3	2.14	0.46
1:A:249:ALA:HB2	1:A:432:VAL:HG11	1.97	0.46
1:E:553:LEU:HA	1:E:556:GLN:NE2	2.30	0.46
2:F:388:MET:O	2:F:389:THR:OG1	2.23	0.46
1:A:198:PHE:O	1:A:201:VAL:HG22	2.15	0.46
1:A:349:MET:HB3	1:A:409:ILE:HD13	1.98	0.46
2:D:30:PRO:HG2	2:D:291:ALA:HB1	1.98	0.46
8:m:11:PRO:HG2	8:n:89:PHE:CB	2.46	0.46
10:G:134:CYS:SG	10:G:135:ARG:N	2.89	0.46
1:A:46:VAL:HG12	1:A:84:ARG:HA	1.96	0.46
1:A:122:PRO:HG2	1:A:125:VAL:HB	1.98	0.46
2:B:367:TYR:O	2:B:369:PRO:HD3	2.16	0.46
1:C:59:ARG:O	1:C:66:THR:N	2.38	0.46
1:C:276:TYR:CE1	1:C:286:MET:HE1	2.50	0.46
1:C:306:GLU:OE2	1:C:310:LYS:HD2	2.16	0.46
10:I:29:SER:OG	11:J:27:ALA:O	2.30	0.46
10:K:91:ASN:HA	10:K:94:GLU:HG2	1.97	0.46
1:E:214:ARG:O	1:E:391:ARG:NH1	2.49	0.46
1:E:274:VAL:HG13	1:E:312:THR:HG23	1.96	0.46
2:F:184:ALA:HB3	2:F:207:ILE:HD11	1.97	0.46
1:C:578:LEU:HG	1:C:581:LEU:HB2	1.96	0.46
2:D:299:ARG:NH2	3:M:190:GLY:HA3	2.31	0.46
2:D:410:VAL:HG11	2:D:426:ASP:O	2.16	0.46
2:B:212:MET:HE1	2:B:278:MET:HE1	1.98	0.46
2:B:94:LYS:HB3	2:B:124:TYR:HB3	1.98	0.46
1:E:266:SER:O	1:E:311:ARG:NH2	2.32	0.46
1:C:341:ARG:HB2	1:C:407:VAL:HG23	1.97	0.46
2:D:209:PHE:HB3	2:D:237:LEU:HD23	1.97	0.46
10:I:47:GLU:HA	10:I:50:LYS:HG2	1.98	0.46
1:E:536:PRO:HD3	1:E:593:PRO:HG3	1.98	0.45
1:C:158:VAL:HG13	1:C:166:HIS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:57:PRO:HA	8:g:60:MET:HG2	1.97	0.45
13:a:316:PHE:O	13:a:320:ASN:N	2.49	0.45
1:E:158:VAL:HG13	1:E:166:HIS:HB3	1.98	0.45
2:F:209:PHE:O	2:F:238:PHE:N	2.45	0.45
2:B:260:ALA:HB1	2:B:271:VAL:HG11	1.98	0.45
2:B:478:LEU:O	2:B:482:TYR:N	2.50	0.45
7:d:155:LEU:HA	7:d:161:ALA:HB3	1.97	0.45
8:l:28:GLY:HA3	8:l:106:LEU:HA	1.98	0.45
10:K:98:LYS:HA	10:K:101:LEU:HD12	1.98	0.45
15:P:224:SER:O	15:P:228:LEU:N	2.45	0.45
13:a:31:ILE:O	13:a:345:LEU:N	2.49	0.45
1:A:101:ILE:HG12	1:A:290:LEU:HD22	1.98	0.45
2:B:15:LEU:HD23	2:B:15:LEU:H	1.81	0.45
2:B:263:LEU:O	2:B:267:CYS:HB3	2.16	0.45
1:C:189:LEU:HA	1:C:207:MET:HE2	1.98	0.45
11:H:102:LEU:HD23	11:H:102:LEU:HA	1.75	0.45
1:E:37:MET:HG3	1:E:84:ARG:HD2	1.97	0.45
1:E:280:GLY:HA2	1:E:326:ARG:HD2	1.98	0.45
1:C:513:GLU:C	1:C:515:ALA:H	2.25	0.45
13:a:135:GLU:HA	13:a:235:PRO:HA	1.99	0.45
1:A:274:VAL:O	1:A:312:THR:HA	2.17	0.45
2:B:357:ILE:HG23	2:B:369:PRO:HB2	1.98	0.45
1:C:385:LEU:HD23	1:C:431:ILE:HD11	1.98	0.45
2:D:144:ILE:HD11	2:D:159:ARG:HA	1.99	0.45
2:D:149:SER:O	2:D:153:VAL:HG23	2.16	0.45
2:D:328:GLN:HG3	2:D:330:PRO:HD3	1.98	0.45
2:D:335:PRO:HG2	2:D:341:HIS:CD2	2.52	0.45
13:a:803:TYR:O	13:a:805:GLY:N	2.50	0.45
1:E:91:VAL:HG12	1:E:93:LEU:HD22	1.99	0.45
1:E:101:ILE:HD12	1:E:314:LEU:O	2.17	0.45
1:E:527:ALA:N	1:E:532:ASP:OD1	2.49	0.45
2:D:388:MET:HG2	2:D:389:THR:HG23	1.98	0.45
7:d:105:MET:HA	7:d:133:GLY:O	2.17	0.45
8:n:54:SER:O	8:n:57:PRO:HD2	2.17	0.45
1:E:192:THR:OG1	1:E:204:SER:OG	2.34	0.45
1:A:354:THR:HA	1:A:357:TRP:HB3	1.99	0.45
2:B:120:LEU:HD12	2:B:121:PRO:HD2	1.99	0.45
1:C:581:LEU:HD22	1:C:584:ARG:HH11	1.82	0.45
1:E:250:ILE:O	1:E:413:VAL:N	2.50	0.45
1:A:250:ILE:HG22	1:A:436:TRP:HB2	1.99	0.45
2:D:47:ASN:OD1	2:D:87:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:m:26:CYS:CB	8:n:104:ALA:HA	2.47	0.45
1:A:297:THR:OG1	1:A:306:GLU:O	2.32	0.44
1:E:93:LEU:HD12	1:E:339:TYR:CD2	2.51	0.44
1:E:429:LEU:HA	1:E:432:VAL:HG12	1.99	0.44
1:A:363:GLU:O	1:A:367:ARG:HG2	2.17	0.44
2:B:459:TRP:HZ3	2:B:478:LEU:HD23	1.81	0.44
1:A:101:ILE:HG22	1:A:109:LEU:HD12	1.99	0.44
2:D:167:SER:O	2:D:333:THR:HA	2.17	0.44
1:E:492:LEU:HA	1:E:495:ILE:HB	1.98	0.44
2:F:27:VAL:HB	1:A:60:LEU:HB2	1.99	0.44
1:A:580:ASP:OD1	1:A:581:LEU:N	2.48	0.44
8:l:32:GLY:HA2	8:l:113:GLY:HA3	2.00	0.44
10:I:134:CYS:SG	10:I:176:PRO:HG3	2.58	0.44
10:K:17:ILE:O	10:K:21:ALA:HB3	2.18	0.44
2:F:98:SER:HB2	2:F:122:GLU:H	1.82	0.44
2:F:260:ALA:HB1	2:F:271:VAL:HG11	1.99	0.44
2:D:252:THR:C	2:D:254:ARG:H	2.24	0.44
10:G:40:LYS:HA	11:H:41:GLU:CB	2.48	0.44
2:F:104:ARG:NH2	2:F:117:PRO:O	2.50	0.44
1:A:311:ARG:HE	1:A:311:ARG:HB2	1.40	0.44
1:A:618:LEU:HA	1:A:621:GLU:HG2	1.99	0.44
1:A:26:LYS:HD2	1:A:33:ILE:HD12	1.99	0.44
3:M:206:ILE:HA	3:M:209:TYR:CD1	2.52	0.44
10:K:196:ASP:OD2	10:K:197:GLY:N	2.51	0.44
1:E:248:CYS:HA	1:E:434:VAL:O	2.17	0.44
1:E:471:PHE:HZ	1:E:538:TYR:HA	1.83	0.44
10:I:111:LYS:HZ2	10:I:141:LEU:HD22	1.83	0.44
1:E:37:MET:HB3	1:E:40:ALA:HB2	2.00	0.44
2:F:384:ILE:HG23	2:F:393:HIS:HB3	2.00	0.44
2:D:309:LEU:HD23	2:D:309:LEU:HA	1.74	0.44
10:G:113:LEU:HD11	11:H:106:THR:HA	2.00	0.44
2:F:80:ASP:O	2:F:84:THR:OG1	2.25	0.43
2:D:297:GLY:N	2:D:301:TYR:O	2.40	0.43
8:h:28:GLY:HA3	8:h:106:LEU:HA	2.00	0.43
10:I:193:ALA:HA	10:I:200:VAL:HA	1.99	0.43
2:B:146:THR:HG21	2:B:157:ILE:HD12	1.98	0.43
1:C:327:GLU:HG3	1:C:357:TRP:HE1	1.83	0.43
8:m:32:GLY:HA2	8:m:113:GLY:CA	2.48	0.43
10:G:110:TYR:OH	10:G:188:GLY:HA3	2.18	0.43
2:F:170:GLY:HA2	1:A:457:TYR:CE2	2.54	0.43
1:A:531:TYR:HA	1:A:593:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:THR:O	2:B:463:ARG:HG2	2.18	0.43
2:D:286:ARG:HD3	2:D:301:TYR:CD1	2.53	0.43
8:j:54:SER:O	8:j:57:PRO:HD2	2.18	0.43
8:m:34:ALA:HB2	8:n:111:ALA:HA	2.00	0.43
10:I:220:ILE:HD11	11:J:100:MET:SD	2.58	0.43
1:A:580:ASP:HB2	15:P:423:ASN:C	2.43	0.43
1:C:108:PRO:HB2	1:C:111:THR:OG1	2.18	0.43
1:C:585:LEU:O	1:C:588:GLN:HG2	2.18	0.43
2:D:148:ILE:CG2	2:D:151:ILE:HG22	2.42	0.43
1:E:46:VAL:HA	1:E:85:THR:HG23	2.01	0.43
1:E:98:LEU:HA	1:E:313:THR:OG1	2.19	0.43
1:E:137:GLU:OE2	1:E:137:GLU:N	2.50	0.43
1:A:148:LEU:HA	1:A:177:LYS:HD3	2.00	0.43
1:A:245:GLY:HA2	1:A:407:VAL:O	2.18	0.43
2:B:161:GLN:NE2	2:B:377:SER:OG	2.51	0.43
2:B:309:LEU:O	2:B:312:ILE:HG22	2.17	0.43
1:C:245:GLY:HA2	1:C:407:VAL:O	2.19	0.43
15:P:418:VAL:HA	15:P:433:ALA:HB1	2.00	0.43
1:A:488:ARG:HH12	1:A:492:LEU:HB3	1.82	0.43
1:C:97:ILE:HG23	1:C:130:LEU:HD11	2.01	0.43
8:i:21:ALA:HB2	8:i:98:GLY:HA2	2.01	0.43
1:E:108:PRO:HD3	1:E:129:ALA:HA	2.01	0.43
1:C:243:VAL:HG12	1:C:460:TYR:CE2	2.53	0.43
8:n:108:ALA:HB3	8:n:144:ALA:HB2	2.00	0.43
2:F:62:GLU:O	2:F:69:VAL:HG12	2.18	0.43
1:A:614:GLY:C	1:A:616:ARG:H	2.27	0.43
2:D:372:VAL:HG11	2:D:436:PHE:HZ	1.83	0.43
8:l:30:ALA:HB3	8:m:107:SER:OG	2.19	0.43
15:P:102:SER:HA	15:P:136:PRO:HA	2.00	0.43
2:F:128:SER:HA	2:F:315:ARG:HH12	1.84	0.43
2:F:161:GLN:NE2	2:F:377:SER:OG	2.43	0.43
2:D:316:ALA:HA	2:D:326:ILE:HB	2.01	0.43
1:E:572:THR:CG2	1:E:576:HIS:CE1	3.02	0.42
1:C:535:CYS:HA	1:C:539:LYS:HE3	2.01	0.42
2:D:15:LEU:HD11	10:G:208:ARG:CZ	2.49	0.42
1:E:449:PRO:HG3	1:E:524:ALA:HA	2.01	0.42
2:F:21:TYR:CE1	2:F:37:VAL:HA	2.54	0.42
2:F:250:ILE:O	2:F:253:PRO:HD2	2.19	0.42
1:A:389:TYR:HB2	1:A:431:ILE:HD12	2.01	0.42
2:B:154:MET:HB2	2:B:401:TYR:OH	2.19	0.42
1:C:478:ILE:HD13	1:C:545:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ALA:O	2:D:271:VAL:HG13	2.19	0.42
2:F:392:ASP:O	2:F:396:VAL:HG13	2.19	0.42
2:B:201:GLU:O	2:B:269:LYS:NZ	2.41	0.42
1:E:112:ILE:HG12	1:E:125:VAL:HG21	2.02	0.42
2:B:173:HIS:HA	2:B:176:ILE:HG12	2.00	0.42
8:l:27:MET:HA	8:m:107:SER:OG	2.19	0.42
2:F:164:PRO:HB3	2:F:330:PRO:HG2	2.01	0.42
1:A:446:LYS:O	2:B:472:ARG:NH1	2.52	0.42
1:A:584:ARG:NH2	1:A:607:LEU:HA	2.33	0.42
2:B:462:LEU:HD13	2:B:473:ILE:HD11	2.01	0.42
8:m:90:ASP:O	8:m:158:ALA:HB1	2.19	0.42
12:O:305:SER:O	12:O:309:TYR:N	2.53	0.42
13:a:31:ILE:N	13:a:345:LEU:O	2.51	0.42
13:a:226:ALA:HB3	13:a:245:VAL:H	1.85	0.42
2:F:247:ILE:O	2:F:251:ILE:HG23	2.19	0.42
2:F:319:ILE:HG22	2:F:322:ARG:H	1.83	0.42
2:B:60:VAL:HG22	2:B:70:VAL:HG22	2.02	0.42
2:D:161:GLN:CD	2:D:379:LEU:HB2	2.44	0.42
2:D:286:ARG:HB2	2:D:301:TYR:CD1	2.54	0.42
8:j:85:SER:N	8:j:162:ARG:O	2.53	0.42
10:I:131:LEU:HG	10:I:174:PRO:HG2	2.02	0.42
2:F:357:ILE:HD11	2:F:369:PRO:HG2	2.00	0.42
10:K:204:THR:HG23	10:K:207:ALA:H	1.84	0.42
1:E:27:VAL:HG22	1:E:32:VAL:HG13	2.02	0.42
2:F:153:VAL:HA	2:F:393:HIS:NE2	2.35	0.42
1:A:30:PRO:O	1:A:69:VAL:HG23	2.20	0.42
2:B:274:ILE:HD13	2:B:329:ILE:HB	2.01	0.42
2:B:309:LEU:HA	2:B:312:ILE:HG22	2.02	0.42
2:D:459:TRP:NE1	2:D:478:LEU:HB2	2.33	0.42
10:K:92:MET:HE1	11:L:94:GLN:HB2	2.02	0.42
10:K:97:SER:O	10:K:100:VAL:HG22	2.20	0.42
13:a:453:GLU:O	13:a:457:ALA:N	2.47	0.42
2:F:367:TYR:O	2:F:369:PRO:HD3	2.19	0.42
2:F:410:VAL:HG11	2:F:426:ASP:O	2.19	0.42
2:B:117:PRO:HB2	10:K:86:ASP:OD2	2.20	0.42
1:C:29:GLY:HA3	1:C:367:ARG:HH12	1.84	0.42
1:C:371:MET:HE3	1:C:371:MET:HB2	1.86	0.42
11:J:102:LEU:O	11:J:106:THR:HG23	2.19	0.42
1:A:286:MET:HA	1:A:289:VAL:HG22	2.01	0.42
2:B:17:VAL:HG11	10:K:202:GLU:O	2.20	0.42
2:B:429:TYR:O	2:B:433:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:54:GLU:HA	11:H:58:GLN:OE1	2.20	0.42
13:a:32:PRO:O	13:a:36:ALA:N	2.53	0.42
1:A:95:PRO:HD2	1:A:207:MET:HB3	2.01	0.41
1:A:158:VAL:O	1:A:166:HIS:N	2.52	0.41
2:B:242:ALA:HB1	1:C:386:ALA:HB1	2.02	0.41
1:C:467:PHE:O	1:C:470:GLN:HG3	2.20	0.41
1:C:522:TYR:HD1	1:C:543:MET:SD	2.42	0.41
8:i:17:GLY:HA3	8:i:95:LEU:HA	2.02	0.41
10:G:130:VAL:C	10:G:195:ARG:HH21	2.27	0.41
2:F:218:THR:HG23	1:A:433:GLN:HE22	1.85	0.41
1:A:328:ALA:O	1:A:332:THR:HG23	2.20	0.41
2:D:261:GLU:HA	2:D:326:ILE:HD11	2.02	0.41
2:B:19:MET:HE1	10:K:201:CYS:SG	2.60	0.41
2:B:45:ILE:O	2:B:89:THR:OG1	2.30	0.41
2:B:211:ALA:HB1	2:B:214:VAL:HG11	2.01	0.41
1:C:292:ASP:OD1	1:C:293:PHE:N	2.53	0.41
1:C:583:TYR:HA	1:C:586:VAL:HG12	2.02	0.41
8:h:30:ALA:HB1	8:i:111:ALA:HB2	2.02	0.41
8:m:10:ALA:HB3	8:m:11:PRO:HD3	2.02	0.41
10:G:161:PRO:HA	10:G:162:PRO:HD3	1.87	0.41
1:E:245:GLY:HA2	1:E:407:VAL:O	2.20	0.41
1:A:332:THR:O	1:A:336:ILE:HG12	2.19	0.41
1:A:467:PHE:O	1:A:470:GLN:HG3	2.20	0.41
2:B:238:PHE:HE2	2:B:256:ALA:HA	1.85	0.41
8:l:21:ALA:HA	8:l:102:GLY:HA3	2.02	0.41
2:B:380:MET:O	2:B:384:ILE:HG12	2.21	0.41
2:B:461:LEU:HA	2:B:464:ILE:HD12	2.02	0.41
1:C:511:THR:HA	1:C:551:TYR:HE1	1.85	0.41
10:K:103:VAL:HG21	11:L:102:LEU:HD12	2.03	0.41
1:E:40:ALA:HA	1:E:84:ARG:NH2	2.36	0.41
2:F:249:ARG:HH11	2:F:280:SER:HB3	1.85	0.41
2:F:396:VAL:O	2:F:400:LEU:HD23	2.21	0.41
1:A:453:TRP:CD1	1:A:486:LEU:HD13	2.56	0.41
2:B:157:ILE:HG12	2:B:163:ILE:HG13	2.03	0.41
1:C:375:SER:OG	1:C:423:PRO:HG2	2.21	0.41
1:C:616:ARG:O	1:C:620:ASP:N	2.43	0.41
10:I:217:LEU:HD12	10:I:217:LEU:HA	1.91	0.41
2:F:120:LEU:HD12	2:F:120:LEU:HA	1.93	0.41
2:F:263:LEU:O	2:F:267:CYS:HB2	2.21	0.41
2:F:367:TYR:CE2	2:F:445:ALA:HA	2.56	0.41
1:A:327:GLU:HA	1:A:357:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:NH1	1:A:492:LEU:HB3	2.36	0.41
1:A:514:THR:HG21	1:A:551:TYR:HB2	2.03	0.41
1:C:137:GLU:O	1:C:158:VAL:HG23	2.21	0.41
1:C:319:SER:HB3	2:D:310:ALA:HB1	2.03	0.41
1:C:437:GLY:HA3	1:C:455:ILE:HG13	2.03	0.41
1:C:452:ASN:OD1	1:C:455:ILE:HG12	2.21	0.41
2:D:269:LYS:HE3	2:D:269:LYS:HB3	1.89	0.41
10:I:129:ALA:HB1	10:I:195:ARG:HD3	2.03	0.41
1:E:572:THR:CG2	1:E:576:HIS:HE1	2.34	0.41
2:F:248:GLU:HA	2:F:251:ILE:HG12	2.02	0.41
1:A:157:THR:HA	1:A:167:HIS:HA	2.03	0.41
1:C:284:ASN:HD22	1:C:284:ASN:HA	1.71	0.41
1:C:300:LEU:HB2	1:C:301:PRO:HD2	2.01	0.41
1:C:317:ASN:HB2	1:C:321:MET:HG3	2.03	0.41
2:D:19:MET:HE1	10:G:201:CYS:HB2	2.03	0.41
2:D:184:ALA:HB3	2:D:207:ILE:HD11	2.03	0.41
8:i:34:ALA:HB2	8:j:111:ALA:HA	2.03	0.41
10:G:198:LYS:HB2	10:G:199:ILE:HD12	2.03	0.41
10:I:138:ASP:O	10:I:141:LEU:HG	2.20	0.41
10:I:139:HIS:ND1	10:I:176:PRO:HD2	2.36	0.41
2:F:335:PRO:HG2	2:F:341:HIS:CE1	2.55	0.41
2:B:34:LEU:HD13	2:B:86:VAL:HG11	2.03	0.41
2:B:251:ILE:HG22	2:B:255:ILE:HG12	2.03	0.41
2:B:413:MET:O	2:B:417:VAL:HG22	2.21	0.41
1:C:349:MET:HG2	1:C:350:MET:N	2.36	0.41
8:l:21:ALA:HB2	8:l:98:GLY:O	2.21	0.41
2:F:343:THR:HB	2:F:344:PRO:HD3	2.02	0.40
1:A:493:ASN:HA	1:A:496:VAL:HG12	2.03	0.40
1:C:27:VAL:HG22	1:C:32:VAL:HG13	2.03	0.40
1:C:282:ARG:HH21	2:D:349:TYR:C	2.29	0.40
1:C:394:LYS:HG3	1:C:406:SER:HB2	2.03	0.40
1:E:163:LEU:HD11	1:E:300:LEU:HD21	2.02	0.40
1:C:137:GLU:O	1:C:137:GLU:HG2	2.21	0.40
1:C:332:THR:HA	1:C:335:THR:HG22	2.03	0.40
3:M:95:VAL:HA	3:M:116:GLY:HA3	2.03	0.40
3:M:131:GLN:O	3:M:135:CYS:N	2.53	0.40
8:l:10:ALA:N	8:l:11:PRO:HD2	2.36	0.40
8:n:32:GLY:HA2	8:n:113:GLY:HA3	2.03	0.40
10:I:137:ASP:N	10:I:137:ASP:OD1	2.50	0.40
1:E:449:PRO:HD3	1:E:525:GLN:O	2.21	0.40
2:F:309:LEU:HD12	2:F:346:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:N	1:A:178:VAL:O	2.32	0.40
2:B:278:MET:N	2:B:278:MET:HE2	2.36	0.40
2:F:45:ILE:HD13	2:F:93:LEU:HD13	2.03	0.40
2:F:214:VAL:HB	2:F:218:THR:OG1	2.22	0.40
1:A:132:LYS:H	1:A:132:LYS:HG3	1.51	0.40
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.87	0.40
2:B:407:GLY:HA2	2:B:429:TYR:HB3	2.03	0.40
1:C:175:MET:O	1:C:198:PHE:HB2	2.21	0.40
1:C:263:GLN:HB3	1:C:267:LYS:HE3	2.03	0.40
11:H:101:LEU:O	11:H:105:VAL:HG23	2.21	0.40
10:I:211:VAL:HG12	10:I:215:LYS:HZ2	1.85	0.40
2:F:462:LEU:HD23	2:F:462:LEU:HA	1.88	0.40
2:B:29:GLY:O	2:B:76:THR:OG1	2.32	0.40
1:C:228:PRO:HG3	1:C:467:PHE:CE2	2.56	0.40
1:C:288:GLU:HA	1:C:291:MET:HG3	2.04	0.40
1:C:548:ILE:HD12	1:C:548:ILE:HA	1.88	0.40
8:i:45:VAL:O	8:i:48:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	601/623 (96%)	577 (96%)	24 (4%)	0	100	100
1	C	601/623 (96%)	571 (95%)	29 (5%)	1 (0%)	43	77
1	E	585/623 (94%)	567 (97%)	18 (3%)	0	100	100
2	B	463/488 (95%)	442 (96%)	21 (4%)	0	100	100
2	D	459/488 (94%)	432 (94%)	27 (6%)	0	100	100
2	F	456/488 (93%)	437 (96%)	19 (4%)	0	100	100
3	M	211/259 (82%)	195 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	105/130 (81%)	87 (83%)	17 (16%)	1 (1%)	12	47
6	c	166/182 (91%)	160 (96%)	6 (4%)	0	100	100
7	d	256/351 (73%)	246 (96%)	10 (4%)	0	100	100
8	g	151/164 (92%)	149 (99%)	2 (1%)	0	100	100
8	h	153/164 (93%)	149 (97%)	4 (3%)	0	100	100
8	i	154/164 (94%)	149 (97%)	5 (3%)	0	100	100
8	j	153/164 (93%)	151 (99%)	2 (1%)	0	100	100
8	k	153/164 (93%)	152 (99%)	1 (1%)	0	100	100
8	l	151/164 (92%)	148 (98%)	3 (2%)	0	100	100
8	m	153/164 (93%)	150 (98%)	3 (2%)	0	100	100
8	n	153/164 (93%)	153 (100%)	0	0	100	100
8	o	150/164 (92%)	147 (98%)	3 (2%)	0	100	100
10	G	200/230 (87%)	195 (98%)	5 (2%)	0	100	100
10	I	203/230 (88%)	200 (98%)	3 (2%)	0	100	100
10	K	213/230 (93%)	203 (95%)	10 (5%)	0	100	100
11	H	95/110 (86%)	93 (98%)	2 (2%)	0	100	100
11	J	94/110 (86%)	94 (100%)	0	0	100	100
11	L	99/110 (90%)	99 (100%)	0	0	100	100
12	O	303/375 (81%)	287 (95%)	16 (5%)	0	100	100
13	a	705/823 (86%)	677 (96%)	27 (4%)	1 (0%)	48	83
14	e	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
15	P	426/452 (94%)	406 (95%)	20 (5%)	0	100	100
All	All	7676/8471 (91%)	7379 (96%)	294 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	448	PHE
4	N	32	VAL
13	a	716	ILE

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	357/517 (69%)	350 (98%)	7 (2%)	48	66
1	C	387/517 (75%)	386 (100%)	1 (0%)	86	84
1	E	328/517 (63%)	328 (100%)	0	100	100
2	B	275/413 (67%)	272 (99%)	3 (1%)	65	74
2	D	279/413 (68%)	270 (97%)	9 (3%)	34	56
2	F	275/413 (67%)	274 (100%)	1 (0%)	84	82
3	M	17/225 (8%)	17 (100%)	0	100	100
4	N	6/111 (5%)	6 (100%)	0	100	100
6	c	5/139 (4%)	5 (100%)	0	100	100
7	d	9/312 (3%)	9 (100%)	0	100	100
8	g	8/115 (7%)	8 (100%)	0	100	100
8	h	6/115 (5%)	6 (100%)	0	100	100
8	i	11/115 (10%)	11 (100%)	0	100	100
8	j	8/115 (7%)	8 (100%)	0	100	100
8	k	7/115 (6%)	7 (100%)	0	100	100
8	l	5/115 (4%)	5 (100%)	0	100	100
8	m	7/115 (6%)	7 (100%)	0	100	100
8	n	5/115 (4%)	5 (100%)	0	100	100
10	G	87/206 (42%)	87 (100%)	0	100	100
10	I	108/206 (52%)	105 (97%)	3 (3%)	38	59
10	K	96/206 (47%)	96 (100%)	0	100	100
11	H	21/87 (24%)	20 (95%)	1 (5%)	23	45
11	J	14/87 (16%)	14 (100%)	0	100	100
11	L	25/87 (29%)	25 (100%)	0	100	100
12	O	13/336 (4%)	13 (100%)	0	100	100
13	a	27/715 (4%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	e	4/63 (6%)	4 (100%)	0	100	100
All	All	2390/6490 (37%)	2365 (99%)	25 (1%)	65	76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	372	VAL
1	A	132	LYS
1	A	231	THR
1	A	271	SER
1	A	311	ARG
1	A	410	VAL
1	A	413	VAL
1	A	424	VAL
2	B	22	ARG
2	B	24	VAL
2	B	33	ILE
1	C	284	ASN
2	D	130	SER
2	D	132	ILE
2	D	138	THR
2	D	139	TYR
2	D	146	THR
2	D	254	ARG
2	D	278	MET
2	D	285	LEU
2	D	318	ARG
11	H	102	LEU
10	I	111	LYS
10	I	114	LEU
10	I	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	79	ASN
1	E	167	HIS
1	E	270	ASN
2	F	145	GLN
2	F	220	GLN
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	487	GLN
2	B	71	GLN
2	B	161	GLN
1	C	86	HIS
1	C	284	ASN
1	C	433	GLN
1	C	555	ASN
2	D	328	GLN
10	G	61	GLN
10	G	203	ASN
10	I	179	HIS
10	K	37	ASN
10	K	83	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

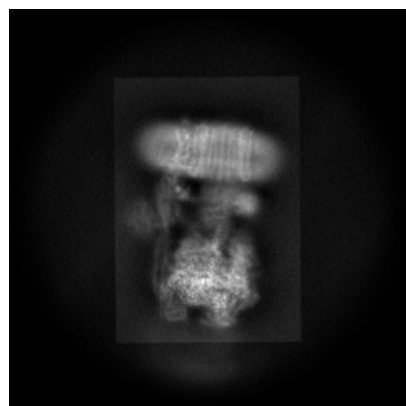
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26826. These allow visual inspection of the internal detail of the map and identification of artifacts.

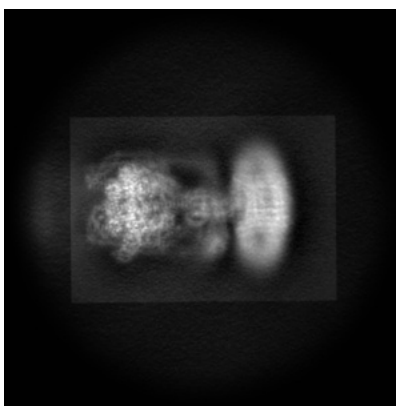
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

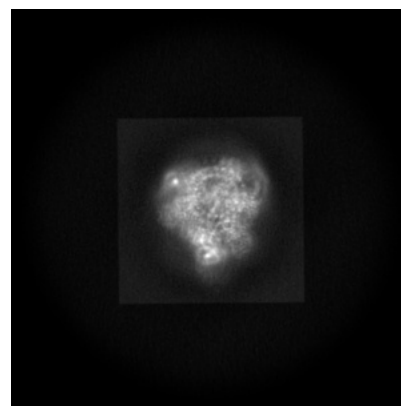
6.1.1 Primary map



X

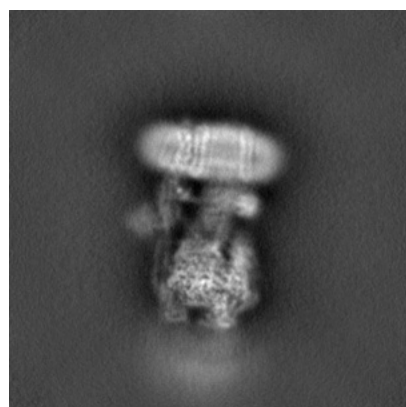


Y

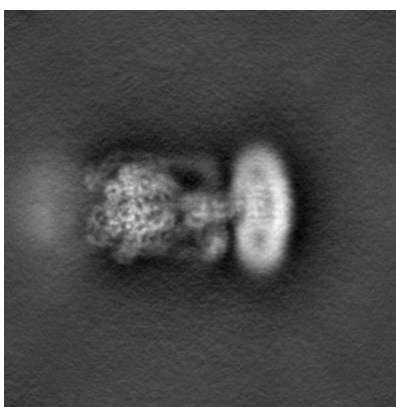


Z

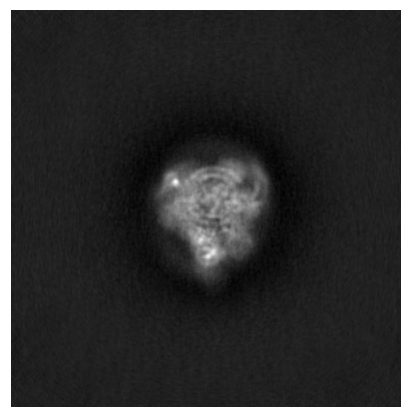
6.1.2 Raw map



X



Y

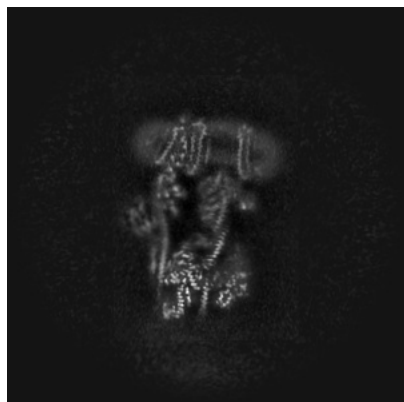


Z

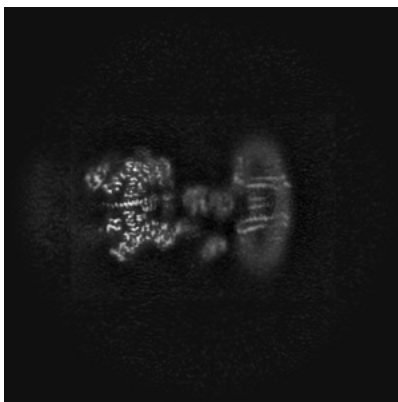
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

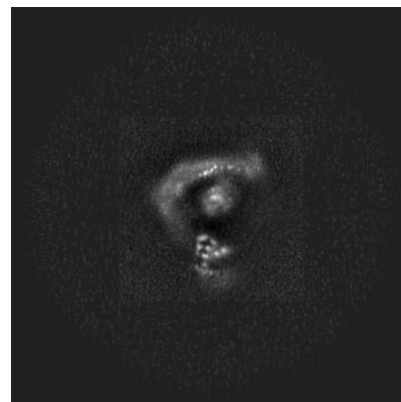
6.2.1 Primary map



X Index: 150



Y Index: 150

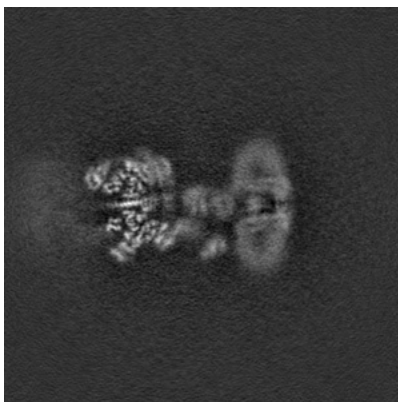


Z Index: 150

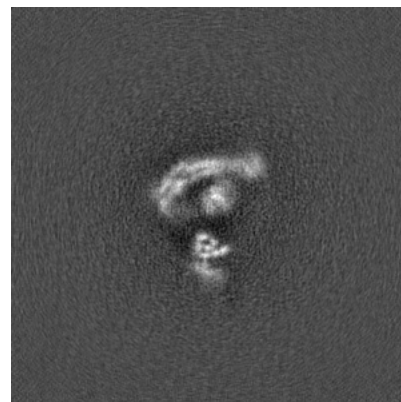
6.2.2 Raw map



X Index: 150



Y Index: 150

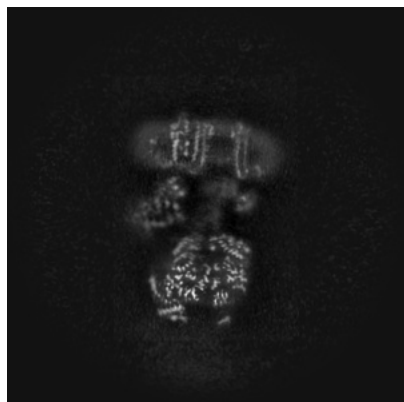


Z Index: 150

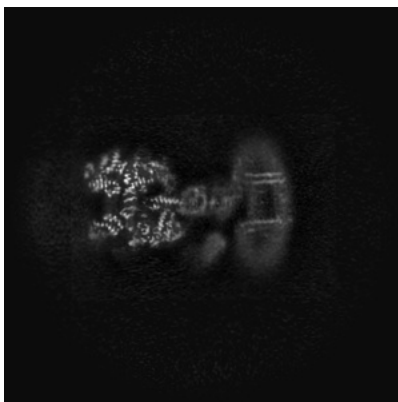
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

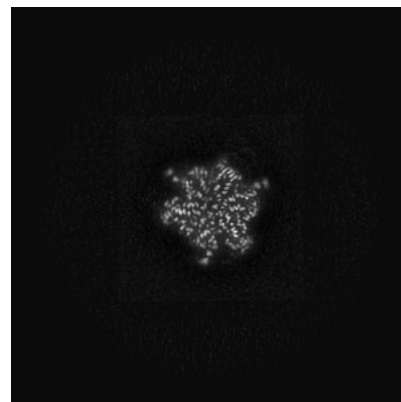
6.3.1 Primary map



X Index: 143

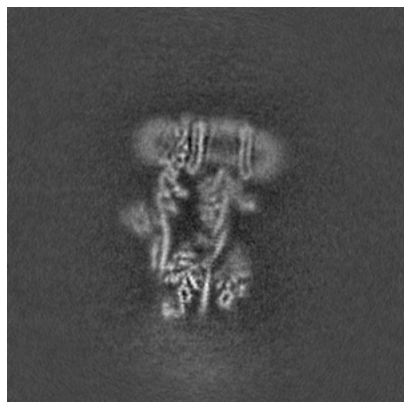


Y Index: 155

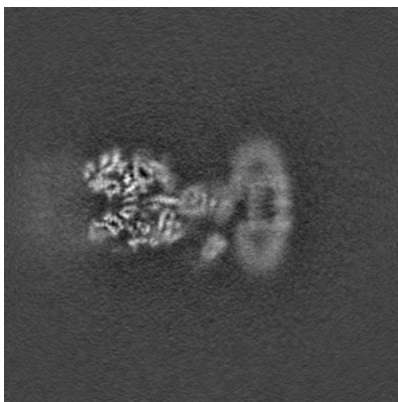


Z Index: 96

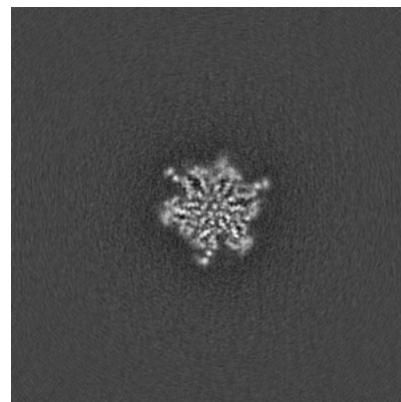
6.3.2 Raw map



X Index: 151



Y Index: 155

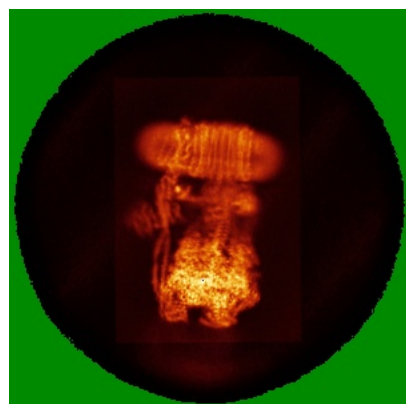


Z Index: 96

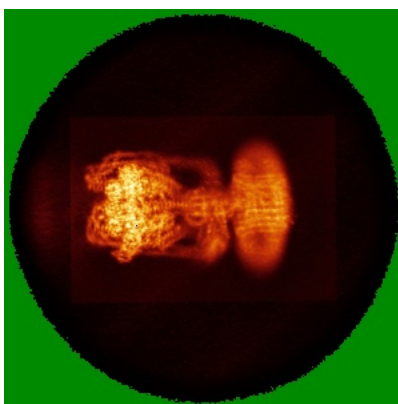
The images above show the largest variance slices of the map in three orthogonal directions.

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

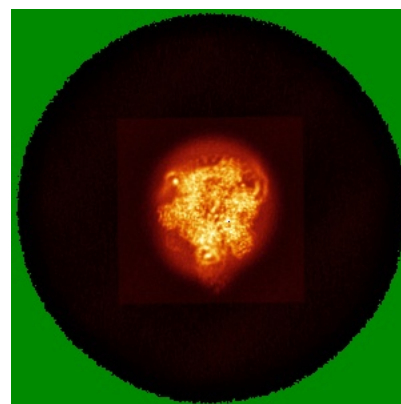
6.4.1 Primary map



X



Y

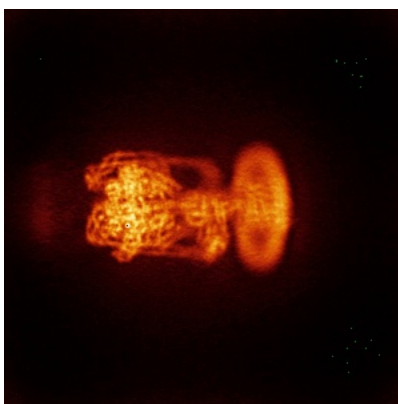


Z

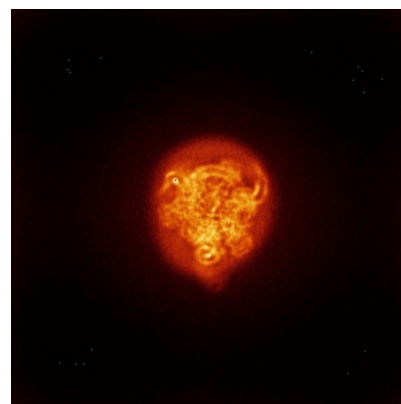
6.4.2 Raw map



X



Y

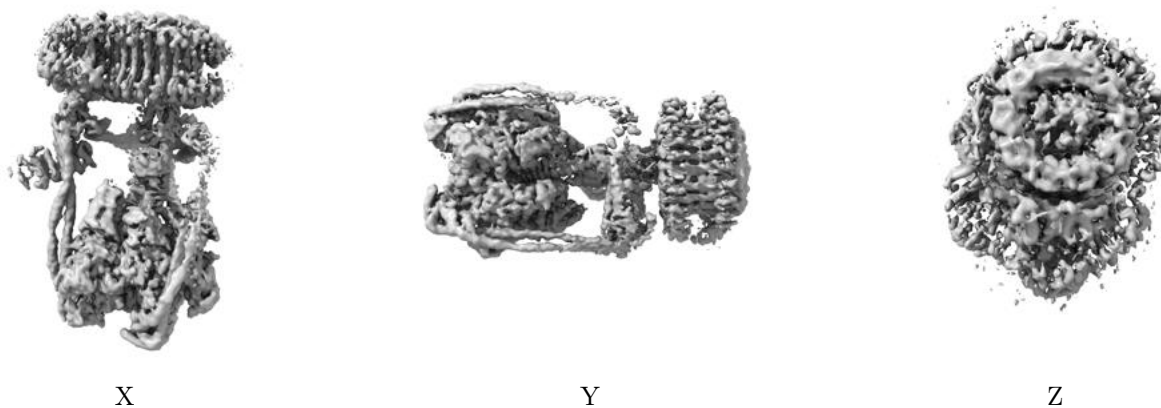


Z

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

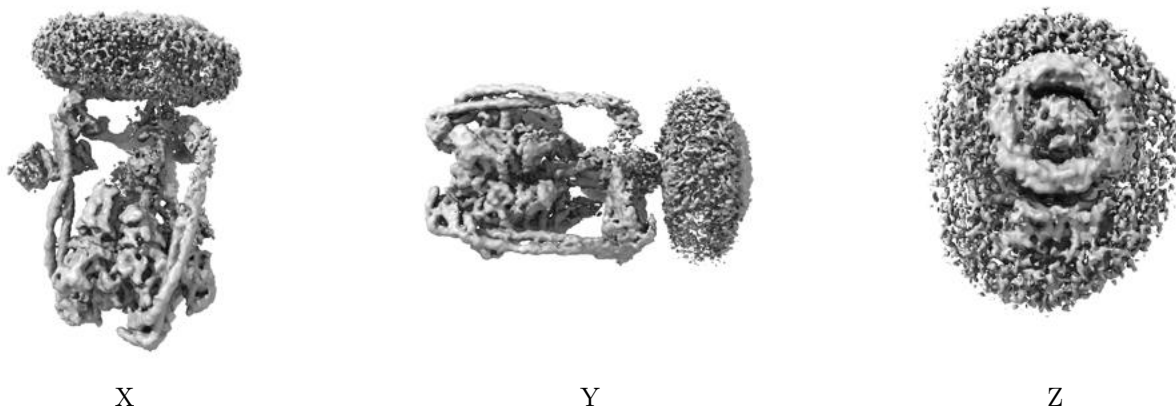
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

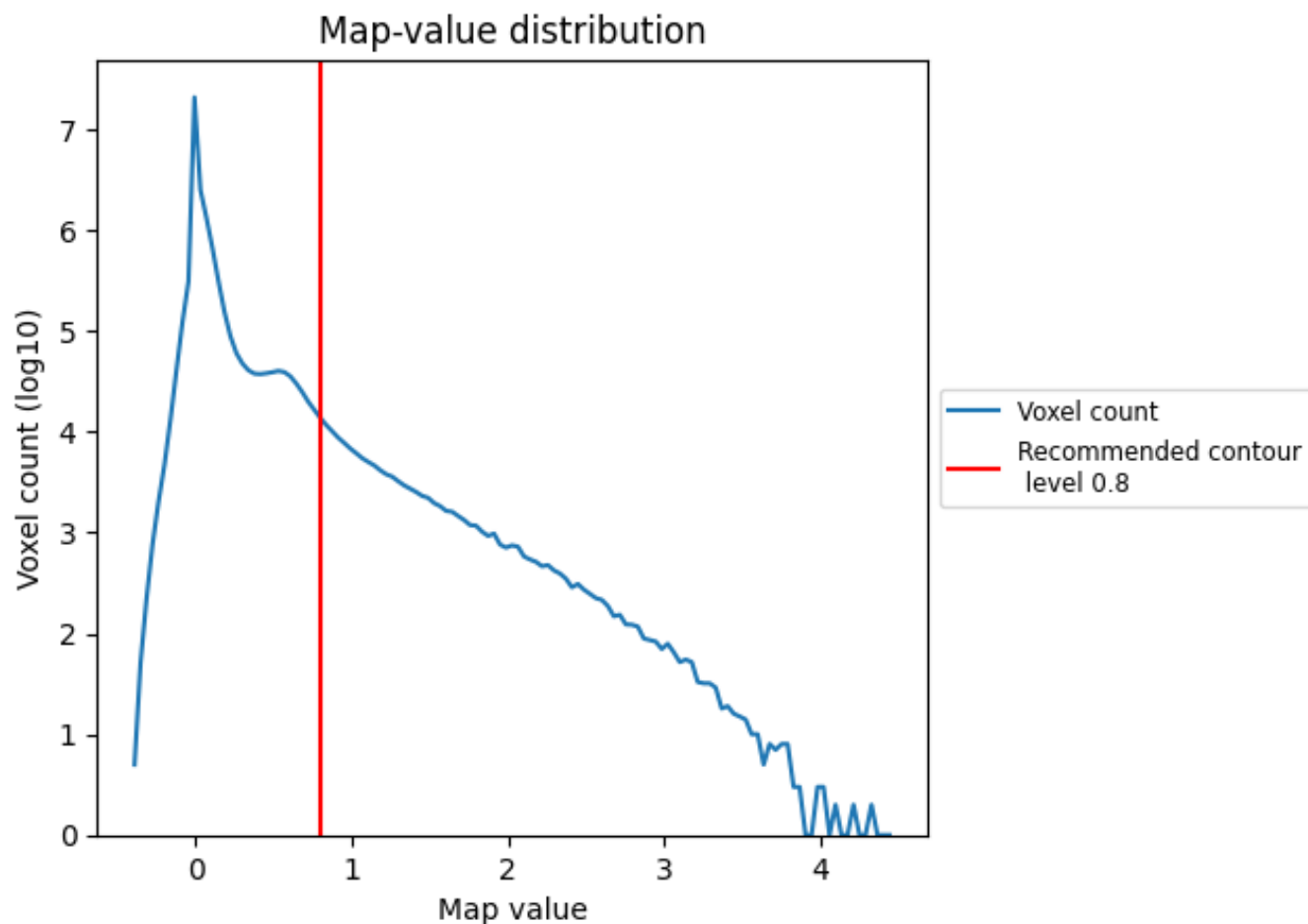
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

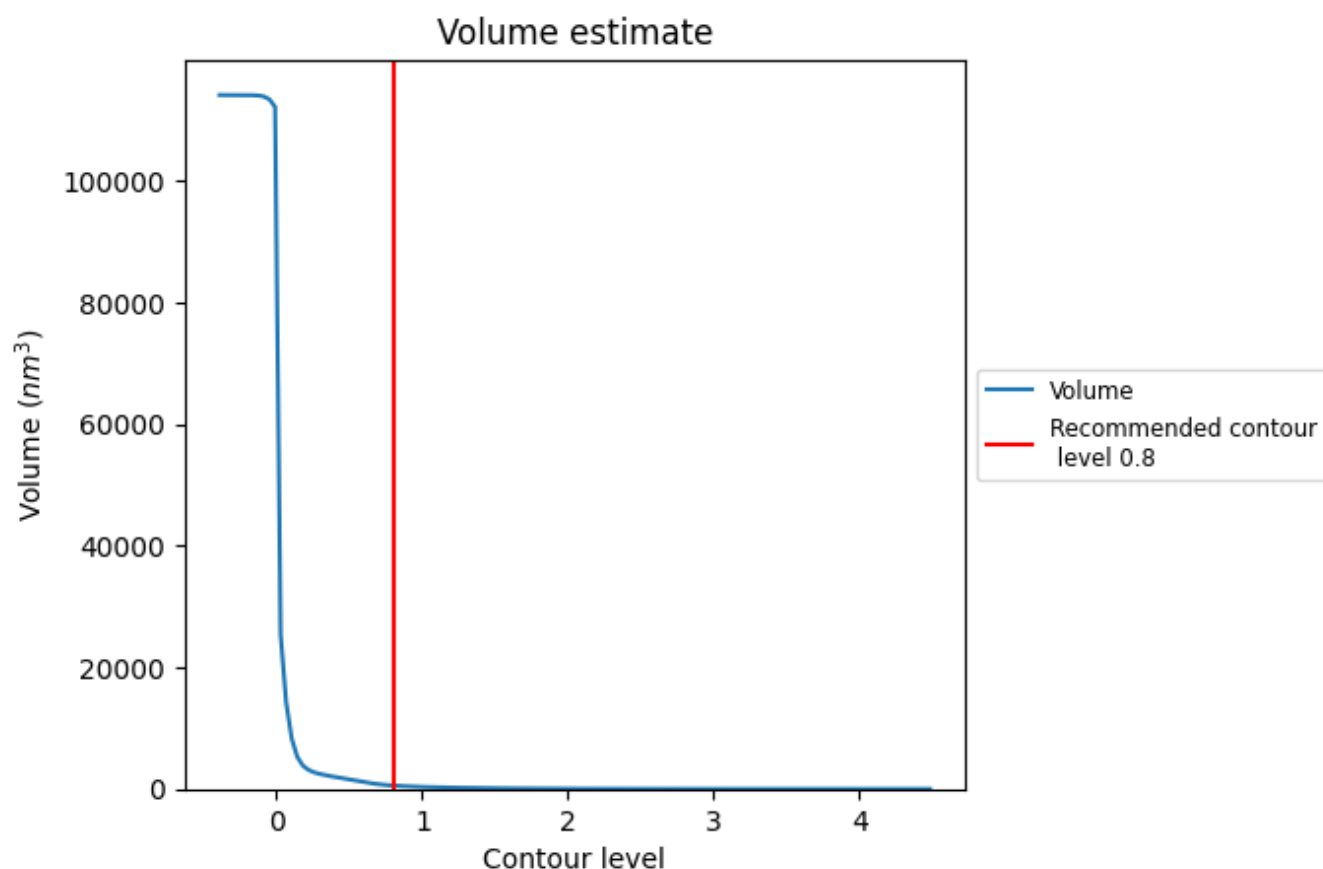
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

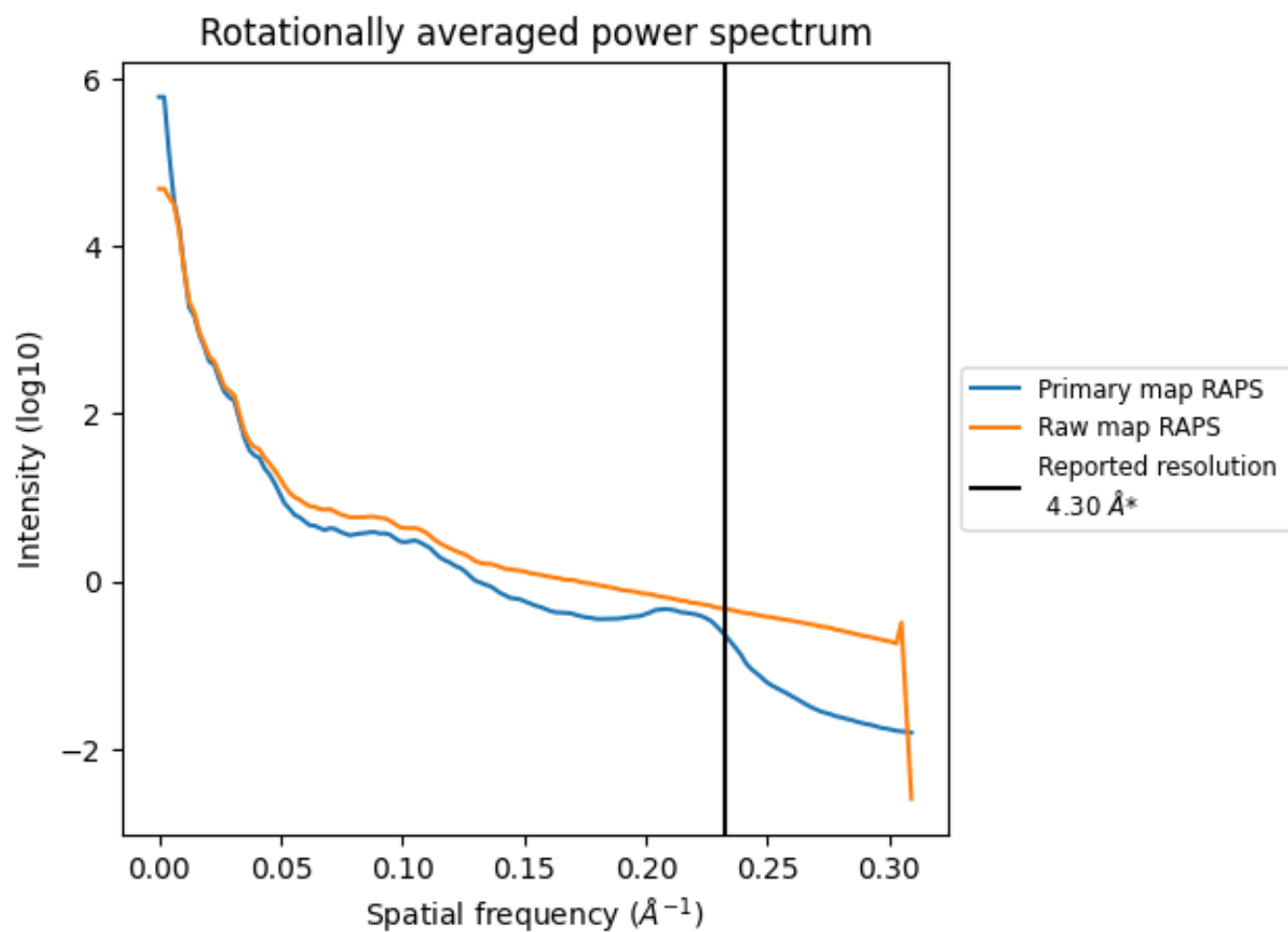
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 560 nm^3 ; this corresponds to an approximate mass of 506 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

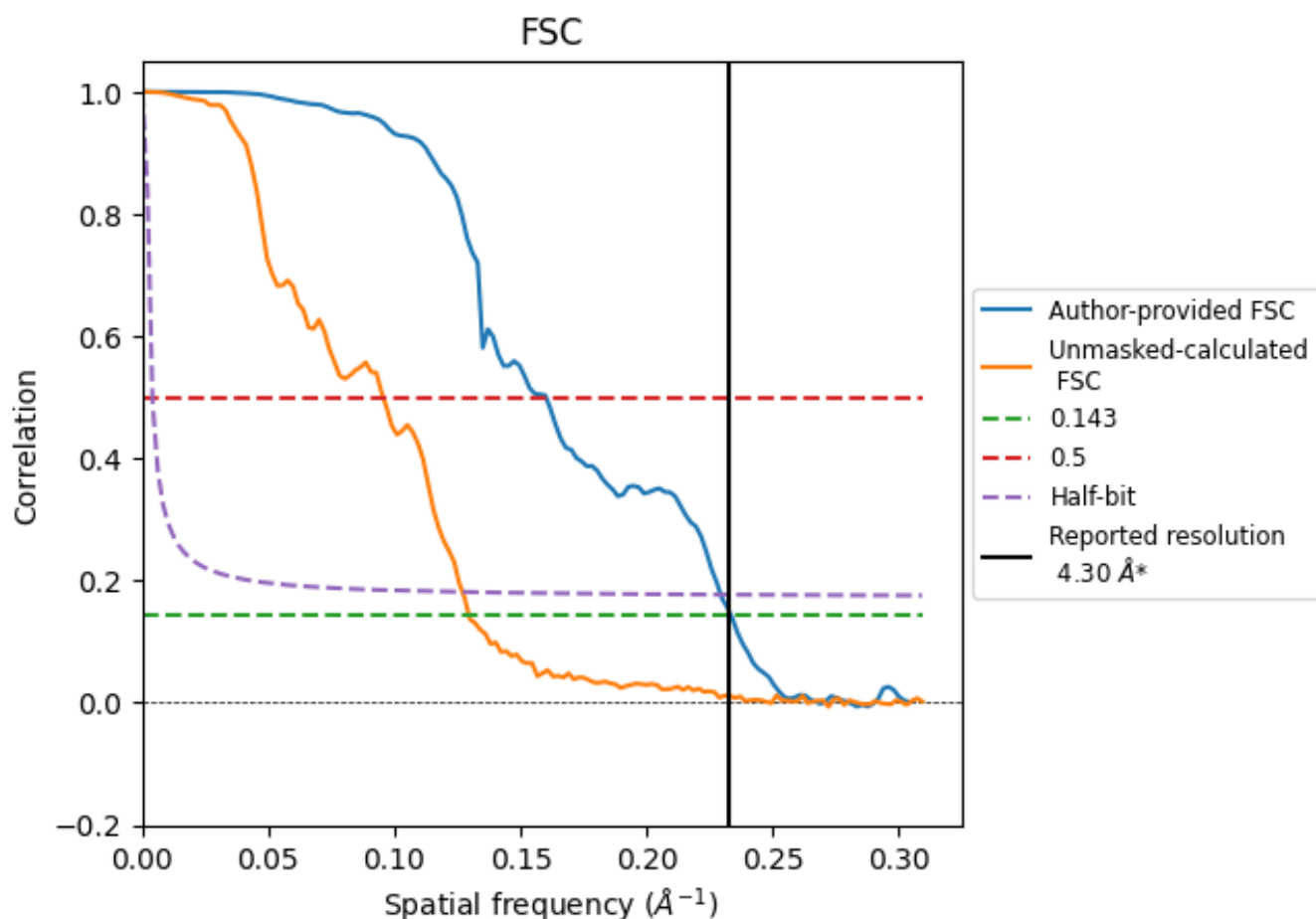


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

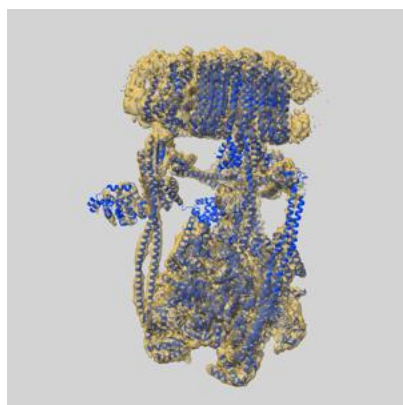
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.28	6.25	4.36
Unmasked-calculated*	7.72	10.46	7.87

*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 7.72 differs from the reported value 4.3 by more than 10 %

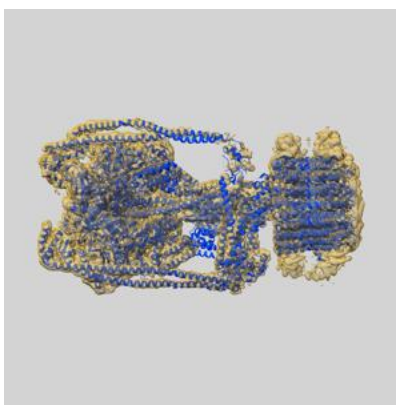
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26826 and PDB model 7UWA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

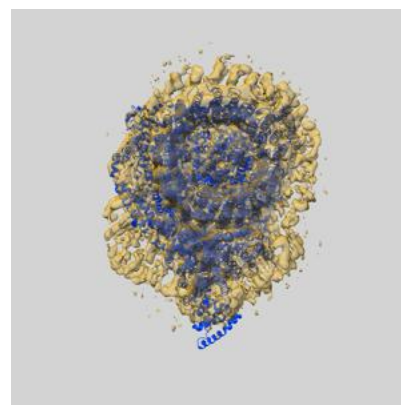
9.1 Map-model overlay [i](#)



X



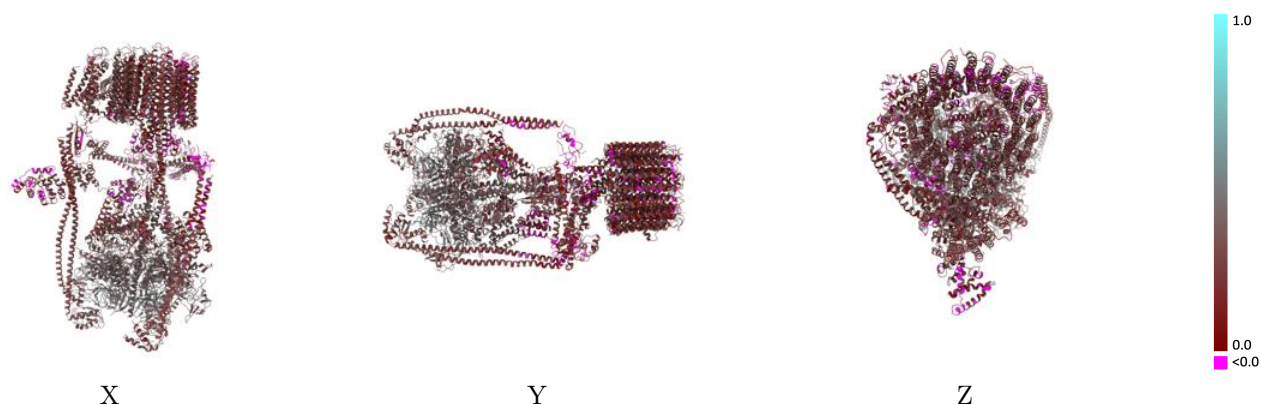
Y



Z

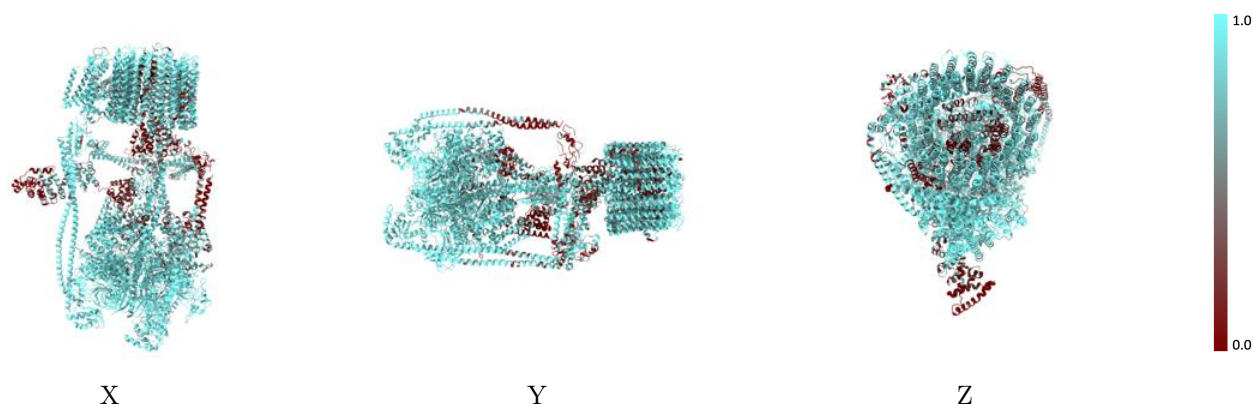
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



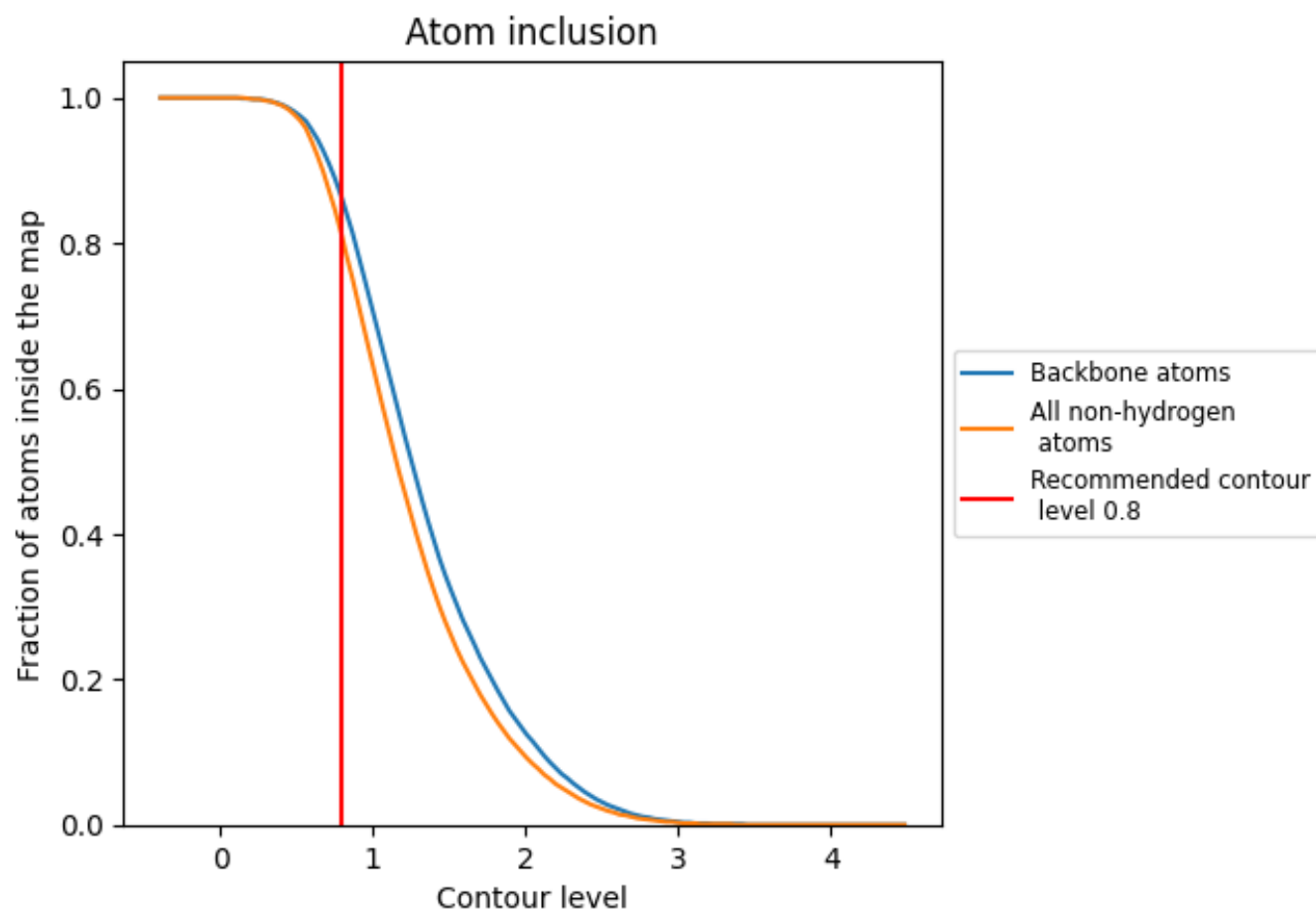
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.3110
A	 0.9160	 0.3960
B	 0.8770	 0.3740
C	 0.9090	 0.3920
D	 0.8640	 0.3840
E	 0.8220	 0.3620
F	 0.9290	 0.4080
G	 0.7980	 0.2930
H	 0.6020	 0.2420
I	 0.8440	 0.2800
J	 0.8030	 0.2500
K	 0.9110	 0.3100
L	 0.9140	 0.2790
M	 0.8760	 0.3260
N	 0.7350	 0.2340
O	 0.5260	 0.1700
P	 0.3390	 0.1840
a	 0.8510	 0.2480
b	 0.2440	 0.2260
c	 0.8220	 0.2250
d	 0.3160	 0.1820
e	 0.8960	 0.2850
g	 0.8320	 0.2530
h	 0.8730	 0.2790
i	 0.9050	 0.3060
j	 0.8170	 0.2580
k	 0.7980	 0.2490
l	 0.8430	 0.2370
m	 0.8800	 0.2090
n	 0.7830	 0.1800
o	 0.7950	 0.2150
r	 0.3580	 0.2530

