



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:52 AM UTC

PDB ID : 8RS9 / pdb_00008rs9
EMDB ID : EMD-19473
Title : p97 (VCP) double mutant - F266A F539A
Authors : Arie, M.; Matzov, D.; Karmona, R.; Szenkier, N.; Stanhill, A.; Navon, A.
Deposited on : 2024-01-24
Resolution : 3.40 Å (reported)
Based on initial model : 5FTN

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

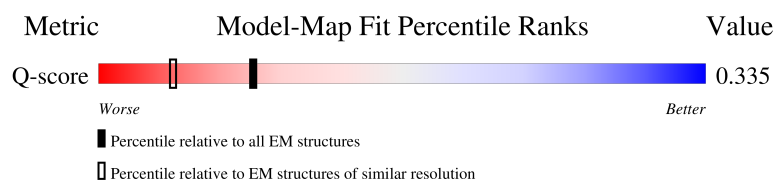
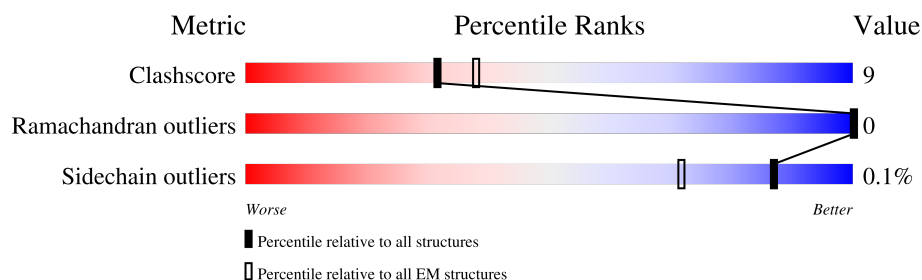
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	806	32% 79% 14% 8%
1	B	806	32% 77% 15% 8%
1	C	806	33% 78% 14% 8%
1	D	806	32% 79% 14% 8%

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Mol	Chain	Length	Quality of chain
1	E	806	33% 77% 15% 8%
1	F	806	32% 77% 15% 8%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 31359 atoms, of which 0 are hydrogens and 0 are deuteriums.

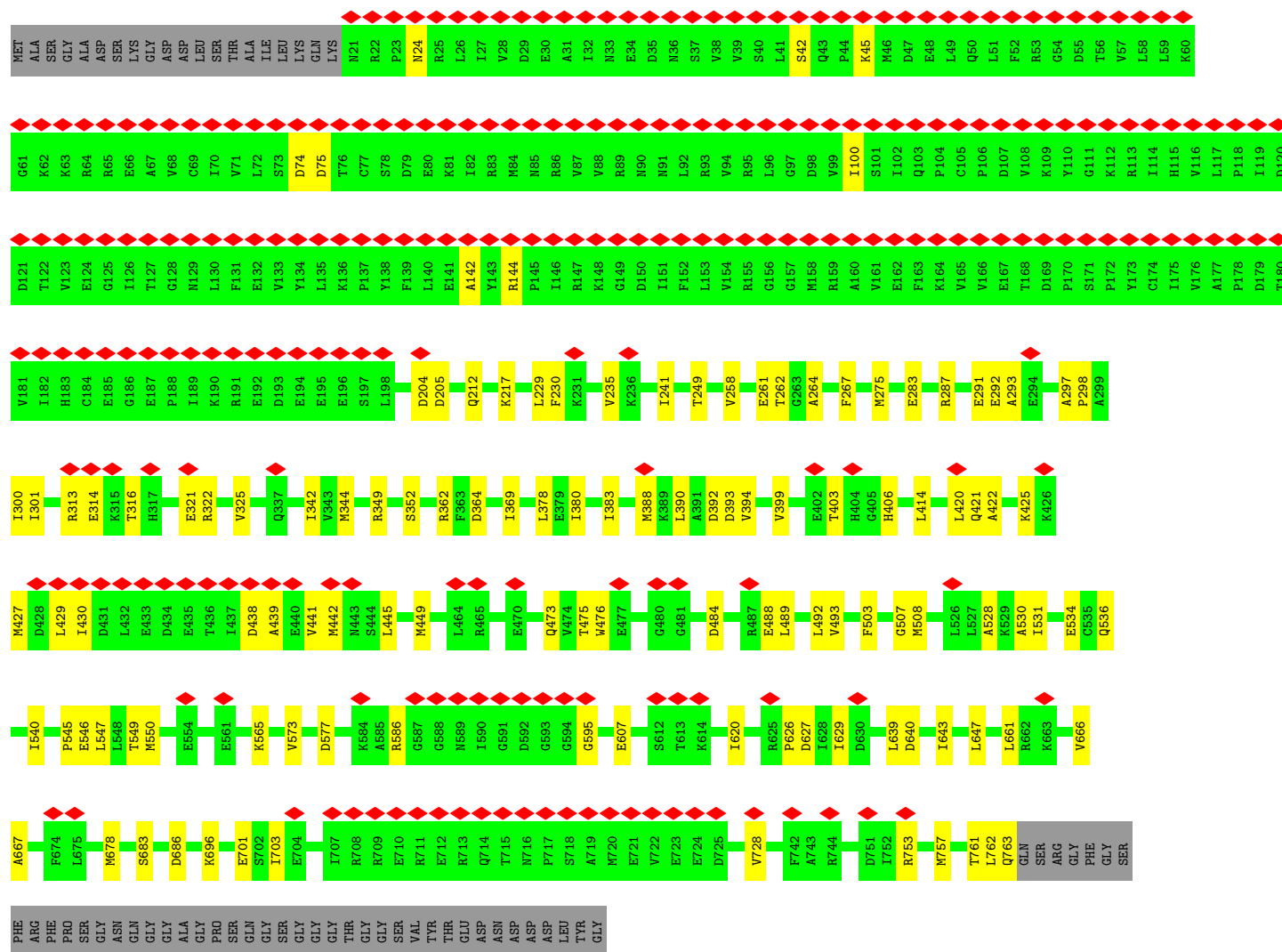
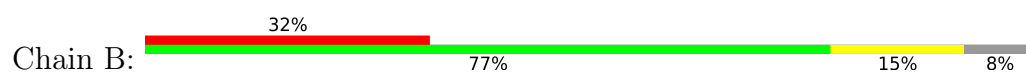
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

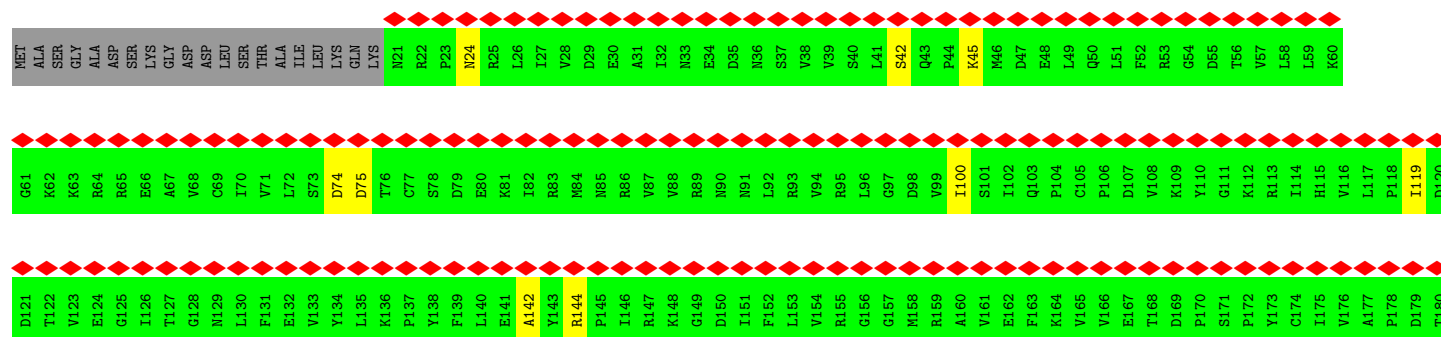
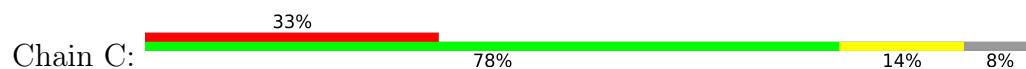
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	743	Total	C	N	O	S	0	0
			5248	3262	948	1015	23		
1	B	743	Total	C	N	O	S	0	0
			5242	3258	947	1014	23		
1	C	743	Total	C	N	O	S	0	0
			5244	3260	947	1014	23		
1	D	743	Total	C	N	O	S	0	0
			5131	3186	931	992	22		
1	E	743	Total	C	N	O	S	0	0
			5246	3260	948	1015	23		
1	F	743	Total	C	N	O	S	0	0
			5248	3262	948	1015	23		

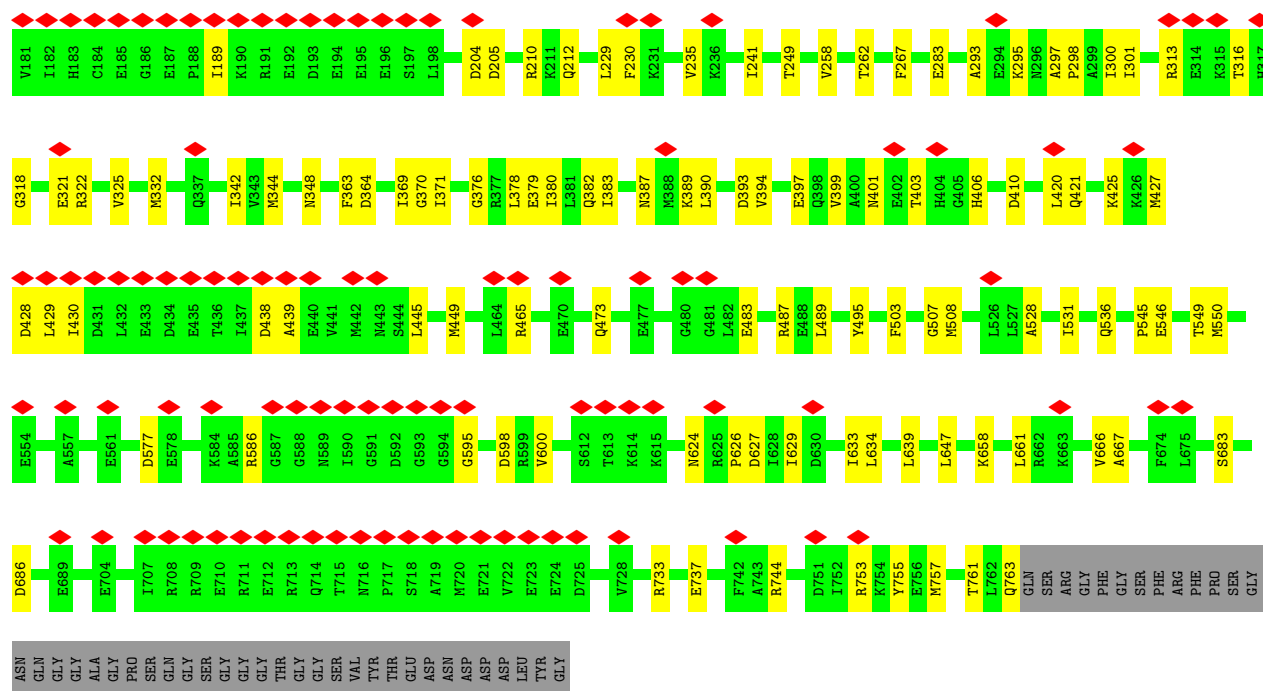
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	PHE	engineered mutation	UNP P55072
A	539	ALA	PHE	engineered mutation	UNP P55072
B	266	ALA	PHE	engineered mutation	UNP P55072
B	539	ALA	PHE	engineered mutation	UNP P55072
C	266	ALA	PHE	engineered mutation	UNP P55072
C	539	ALA	PHE	engineered mutation	UNP P55072
D	266	ALA	PHE	engineered mutation	UNP P55072
D	539	ALA	PHE	engineered mutation	UNP P55072
E	266	ALA	PHE	engineered mutation	UNP P55072
E	539	ALA	PHE	engineered mutation	UNP P55072
F	266	ALA	PHE	engineered mutation	UNP P55072
F	539	ALA	PHE	engineered mutation	UNP P55072

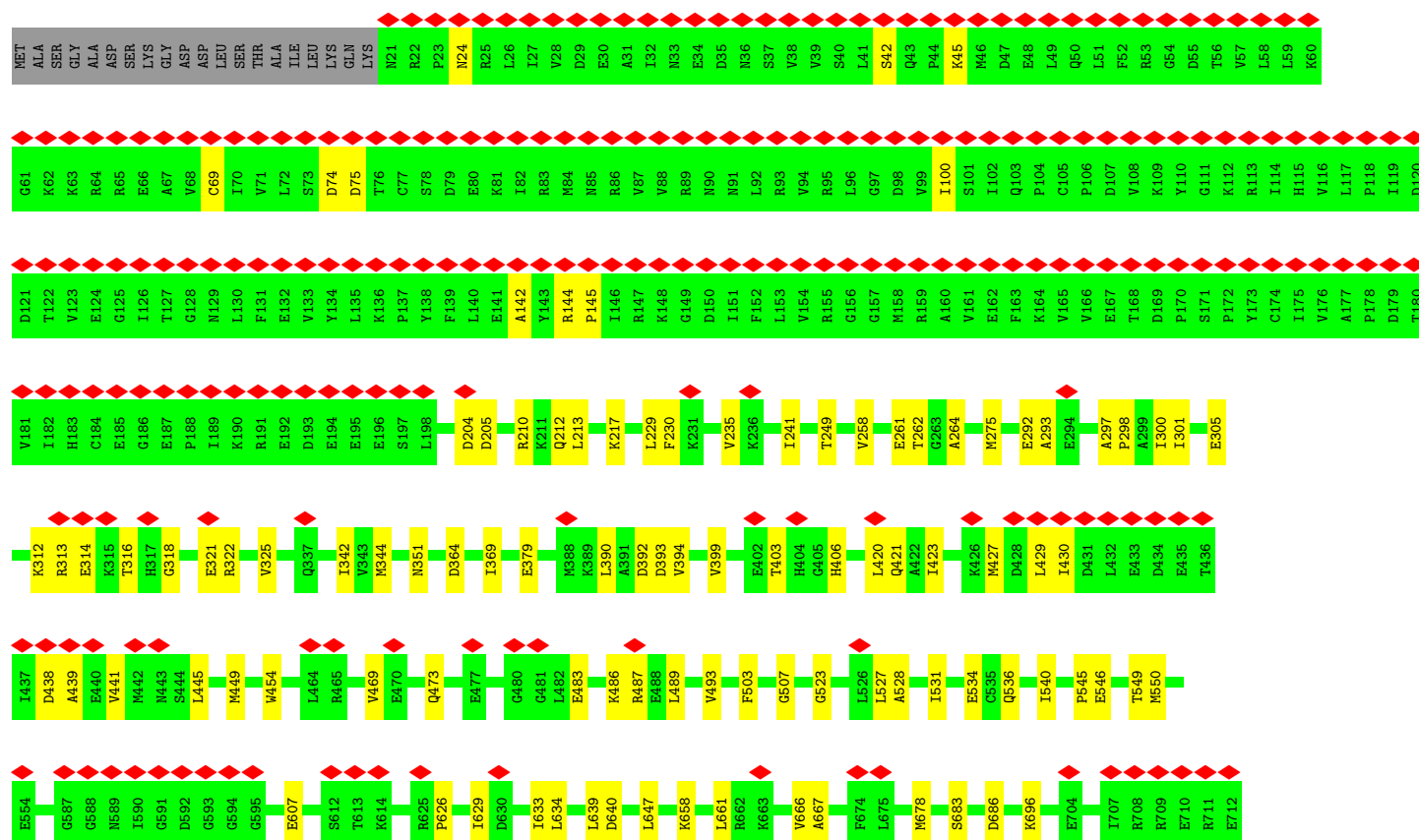
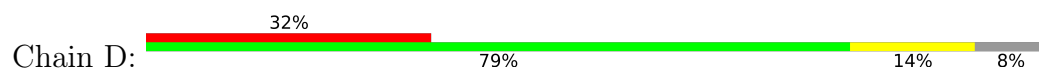


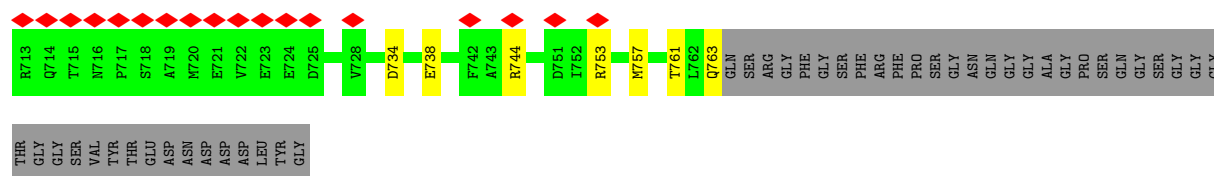
• Molecule 1: Transitional endoplasmic reticulum ATPase





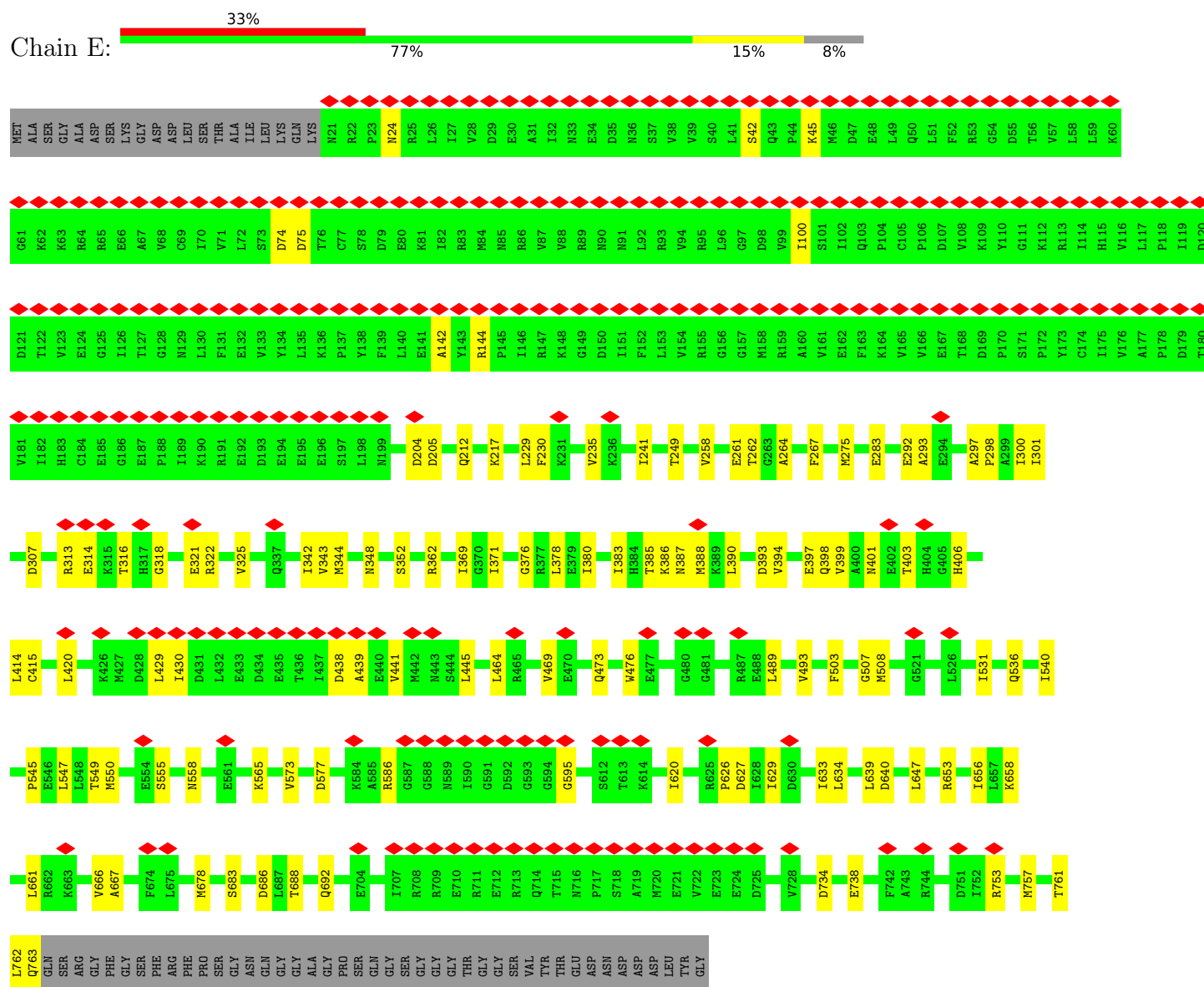
• Molecule 1: Transitional endoplasmic reticulum ATPase





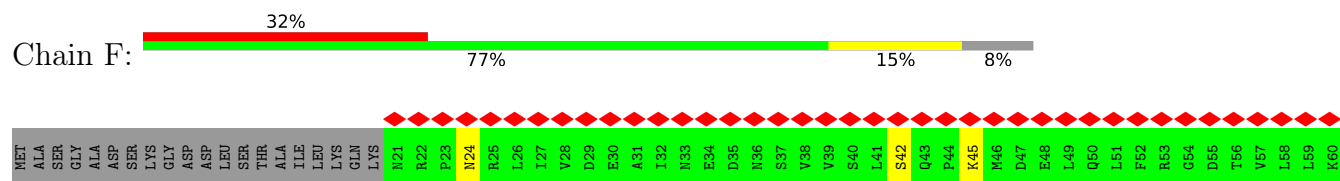
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



SER	V666	L547	K426	R313	V181	D121	G61
ARG	A667	L548	N427	E314	I182	T122	K62
GLY	K668	T549	D428	E315	H183	V123	K63
PHE	F674	E554	L429	T316	C184	E124	R64
GLY	L675	S555	I430	H517	E185	G125	R65
PHE	S683	E556	D431	G318	G186	I126	R66
ARG	A557	A557	L432	E321	E187	T127	A67
PHE	N558	N558	E433	R322	P188	G128	V68
PRO	D686	D686	D434	V325	I189	N129	C69
GLY	E701	E561	E435	M332	K190	L130	I70
ASN	E704	D577	T436	M332	R191	F131	V71
GLY	I707	K584	I437	Q337	E192	E132	L72
GLY	R708	G587	D438	T342	D193	V133	S73
ALA	R709	G588	A439	T342	E194	Y134	D74
PRO	E710	G589	E440	V343	E195	L135	D75
SER	R711	N589	V441	H344	E196	K136	T76
GLN	E712	I590	M442	F363	E197	P137	C77
GLY	E713	G591	M443	D364	Y138	Y138	S78
GLY	Q714	D592	S444	I369	F139	F139	D79
THR	T715	G593	A446	T369	L140	L140	E80
GLY	M716	G594	V447	G376	E141	E141	K81
SER	P717	G595	F452	R377	A142	A142	I82
VAL	S718	G612	R453	L378	Y143	Y143	R83
TYR	A719	T613	V454	E379	R144	R144	M84
THR	M720	K614	L464	I380	P145	P145	N85
ASP	E721	N624	R465	T383	I146	I146	N86
ASN	V722	R625	E470	M388	R147	R147	V87
ASP	E723	P626	Q473	V389	K148	K148	V88
ASP	E724	D627	Q477	L390	G149	G149	R89
LEU	D725	I628	E477	A391	D150	D150	N90
TYR	V728	I629	G480	D393	I151	I151	N91
GLY	R733	D630	G481	V394	F152	F152	L92
	D734	T633	G481	E397	L153	L153	R93
	H735	L634	L489	Q398	V154	V154	V94
	F736	L639	L489	V399	R155	R155	R95
	E737	D640	F503	A400	G156	G156	L96
	E738	T643	L504	M401	G157	G157	G97
	F742	Y644	K505	E402	M158	M158	D98
	A743	L647	F506	H404	R159	R159	V99
	R744	L647	G507	G405	A160	A160	I100
	D751	R653	M508	H406	F163	F163	S101
	I752	L656	L526	D410	K164	K164	I102
	R753	L657	T531	A419	V165	V165	Q103
	K754	K658	Q536	L420	V166	V166	P104
	Y755	L661	K543	Q421	E167	E167	C105
	E756	K662	G544	A422	T168	T168	P106
	M757	R663	P545	I423	D169	D169	D107
	T761	L762	E546		V170	V170	V108
	Q763				S171	S171	K109
GLN					P172	P172	Y110
					Y173	Y173	G111
					I174	I174	K112
					C174	C174	R113
					I175	I175	I114
					V176	V176	H115
					A177	A177	V116
					P178	P178	L117
					D179	D179	P118
					T180	T180	I119
							D120

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	79612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.979	Depositor
Minimum map value	-0.555	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.244	Depositor
Map size ($\text{\AA}$)	240.8, 240.8, 240.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/5318	0.38	0/7222
1	B	0.16	0/5312	0.40	0/7214
1	C	0.16	0/5314	0.39	0/7217
1	D	0.16	0/5197	0.40	0/7069
1	E	0.17	0/5316	0.40	0/7219
1	F	0.16	0/5318	0.40	0/7222
All	All	0.16	0/31775	0.39	0/43163

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](#)

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	5248	0	4751	85	0
1	B	5242	0	4738	101	0
1	C	5244	0	4745	86	0
1	D	5131	0	4543	88	0
1	E	5246	0	4744	94	0
1	F	5248	0	4751	94	0
All	All	31359	0	28272	516	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 9.

All (516) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:LYS:NZ	1:E:387:ASN:OD1	2.01	0.93
1:A:465:ARG:NH2	1:B:607:GLU:OE2	2.05	0.89
1:B:442:MET:HE3	1:B:442:MET:O	1.75	0.85
1:C:744:ARG:NH1	1:D:763:GLN:OE1	2.10	0.84
1:C:763:GLN:N	1:C:763:GLN:OE1	2.10	0.84
1:A:458:GLN:OE1	1:A:458:GLN:N	2.11	0.83
1:A:387:ASN:OD1	1:A:389:LYS:NZ	2.14	0.81
1:C:378:LEU:HD23	1:C:382:GLN:NE2	1.98	0.78
1:D:210:ARG:NH2	1:D:379:GLU:OE1	2.16	0.78
1:B:390:LEU:HD23	1:B:394:VAL:HG11	1.64	0.78
1:C:119:ILE:O	1:C:189:ILE:N	2.18	0.77
1:E:390:LEU:HD23	1:E:394:VAL:HG11	1.66	0.76
1:C:318:GLY:O	1:C:322:ARG:NH1	2.18	0.76
1:C:465:ARG:NH2	1:D:607:GLU:OE2	2.19	0.76
1:F:119:ILE:O	1:F:189:ILE:N	2.18	0.76
1:A:119:ILE:O	1:A:189:ILE:N	2.18	0.75
1:D:318:GLY:O	1:D:322:ARG:NH1	2.20	0.75
1:A:258:VAL:O	1:A:262:THR:HG22	1.87	0.74
1:B:258:VAL:O	1:B:262:THR:HG22	1.86	0.74
1:E:318:GLY:O	1:E:322:ARG:NH1	2.20	0.74
1:A:421:GLN:OE1	1:A:454:TRP:NE1	2.21	0.74
1:F:318:GLY:O	1:F:322:ARG:NH1	2.21	0.74
1:A:318:GLY:O	1:A:322:ARG:NH1	2.20	0.73
1:A:212:GLN:N	1:A:212:GLN:OE1	2.20	0.73
1:A:744:ARG:NH1	1:B:763:GLN:OE1	2.21	0.73
1:C:624:ASN:OD1	1:C:755:TYR:OH	2.06	0.73
1:E:307:ASP:OD1	1:E:352:SER:OG	2.07	0.72
1:F:763:GLN:N	1:F:763:GLN:OE1	2.23	0.72
1:C:258:VAL:O	1:C:262:THR:HG23	1.91	0.70
1:C:293:ALA:HB2	1:C:301:ILE:HD11	1.72	0.70
1:D:392:ASP:OD1	1:D:393:ASP:N	2.25	0.70
1:F:212:GLN:N	1:F:212:GLN:OE1	2.25	0.69
1:D:212:GLN:N	1:D:212:GLN:OE1	2.24	0.69
1:A:683:SER:N	1:A:686:ASP:OD2	2.26	0.69
1:C:212:GLN:N	1:C:212:GLN:OE1	2.25	0.69
1:C:378:LEU:HD23	1:C:382:GLN:HE21	1.58	0.69
1:B:546:GLU:O	1:B:549:THR:OG1	2.09	0.69
1:A:763:GLN:N	1:A:763:GLN:OE1	2.26	0.68
1:C:489:LEU:HD22	1:C:531:ILE:HG21	1.75	0.68
1:F:206:ILE:HD11	1:F:213:LEU:HD21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:ILE:HD11	1:F:342:ILE:HD11	1.76	0.67
1:D:683:SER:N	1:D:686:ASP:OD2	2.28	0.67
1:F:489:LEU:HD22	1:F:531:ILE:HG21	1.77	0.67
1:F:300:ILE:HD11	1:F:344:MET:HE2	1.77	0.67
1:B:241:ILE:HD11	1:B:342:ILE:HD11	1.76	0.66
1:E:297:ALA:HB1	1:E:298:PRO:HD2	1.77	0.66
1:A:489:LEU:HD22	1:A:531:ILE:HG21	1.76	0.66
1:C:683:SER:N	1:C:686:ASP:OD2	2.28	0.66
1:E:683:SER:N	1:E:686:ASP:OD2	2.28	0.66
1:A:42:SER:O	1:A:45:LYS:N	2.28	0.66
1:B:42:SER:O	1:B:45:LYS:N	2.28	0.66
1:C:42:SER:O	1:C:45:LYS:N	2.28	0.66
1:D:640:ASP:OD1	1:D:640:ASP:O	2.14	0.66
1:E:42:SER:O	1:E:45:LYS:N	2.28	0.66
1:B:300:ILE:HD11	1:B:344:MET:SD	2.36	0.65
1:C:241:ILE:HD11	1:C:342:ILE:HD11	1.77	0.65
1:E:241:ILE:HD11	1:E:342:ILE:HD11	1.76	0.65
1:F:42:SER:O	1:F:45:LYS:N	2.28	0.65
1:F:683:SER:N	1:F:686:ASP:OD2	2.29	0.65
1:A:545:PRO:O	1:A:549:THR:HG23	1.96	0.65
1:F:545:PRO:O	1:F:549:THR:HG23	1.96	0.65
1:A:744:ARG:HH22	1:B:762:LEU:HD12	1.61	0.65
1:D:489:LEU:HD22	1:D:531:ILE:HG21	1.78	0.65
1:E:464:LEU:HD23	1:E:464:LEU:O	1.96	0.65
1:B:683:SER:N	1:B:686:ASP:OD2	2.30	0.65
1:D:42:SER:O	1:D:45:LYS:N	2.28	0.65
1:D:258:VAL:O	1:D:262:THR:HG22	1.97	0.65
1:C:297:ALA:HB1	1:C:298:PRO:HD2	1.78	0.64
1:E:258:VAL:O	1:E:262:THR:HG22	1.97	0.64
1:E:545:PRO:O	1:E:549:THR:HG23	1.96	0.64
1:A:275:MET:HE2	1:A:275:MET:HA	1.81	0.63
1:C:390:LEU:HD23	1:C:394:VAL:HG11	1.81	0.63
1:B:212:GLN:OE1	1:B:212:GLN:N	2.31	0.63
1:B:293:ALA:CB	1:B:301:ILE:HD11	2.29	0.63
1:A:307:ASP:OD2	1:A:352:SER:OG	2.11	0.62
1:A:421:GLN:OE1	1:A:454:TRP:CD1	2.53	0.62
1:F:488:GLU:OE1	1:F:643:ILE:HD11	2.00	0.62
1:F:624:ASN:OD1	1:F:755:TYR:OH	2.17	0.62
1:A:241:ILE:HD11	1:A:342:ILE:HD11	1.81	0.62
1:D:297:ALA:HB1	1:D:298:PRO:HD2	1.81	0.62
1:C:545:PRO:O	1:C:549:THR:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:NH2	1:C:379:GLU:OE2	2.33	0.61
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.83	0.61
1:D:293:ALA:CB	1:D:301:ILE:HD11	2.30	0.61
1:B:489:LEU:HD22	1:B:531:ILE:HG21	1.80	0.61
1:D:241:ILE:HD11	1:D:342:ILE:HD11	1.81	0.61
1:A:297:ALA:HB1	1:A:298:PRO:HD2	1.81	0.61
1:D:217:LYS:HZ1	1:D:261:GLU:CD	2.09	0.61
1:F:427:MET:HE3	1:F:445:LEU:HD12	1.82	0.61
1:C:387:ASN:OD1	1:C:389:LYS:NZ	2.34	0.61
1:E:212:GLN:N	1:E:212:GLN:OE1	2.32	0.60
1:E:753:ARG:O	1:E:757:MET:HE2	2.02	0.60
1:F:297:ALA:HB1	1:F:298:PRO:HD2	1.82	0.60
1:F:364:ASP:N	1:F:364:ASP:OD1	2.35	0.60
1:D:626:PRO:O	1:D:629:ILE:HG22	2.02	0.59
1:B:626:PRO:O	1:B:629:ILE:HG22	2.03	0.59
1:E:640:ASP:OD1	1:E:640:ASP:O	2.19	0.59
1:F:332:MET:HE3	1:F:363:PHE:CE1	2.38	0.59
1:D:545:PRO:O	1:D:549:THR:HG23	2.03	0.59
1:D:744:ARG:NH2	1:E:762:LEU:HD12	2.17	0.59
1:A:626:PRO:O	1:A:629:ILE:HG22	2.02	0.59
1:E:489:LEU:HD22	1:E:531:ILE:HG21	1.84	0.58
1:B:763:GLN:OE1	1:B:763:GLN:N	2.30	0.58
1:A:364:ASP:OD1	1:A:364:ASP:N	2.36	0.58
1:A:293:ALA:CB	1:A:301:ILE:HD11	2.34	0.58
1:B:545:PRO:O	1:B:549:THR:HG23	2.04	0.58
1:C:744:ARG:NH1	1:D:761:THR:O	2.34	0.58
1:A:313:ARG:HA	1:A:316:THR:HG22	1.86	0.58
1:D:321:GLU:O	1:D:325:VAL:HG23	2.04	0.58
1:D:546:GLU:O	1:D:550:MET:SD	2.62	0.58
1:A:321:GLU:O	1:A:325:VAL:HG23	2.04	0.57
1:F:626:PRO:O	1:F:629:ILE:HG22	2.04	0.57
1:B:349:ARG:O	1:B:352:SER:OG	2.22	0.57
1:D:421:GLN:OE1	1:D:454:TRP:NE1	2.38	0.57
1:A:142:ALA:O	1:A:144:ARG:N	2.36	0.57
1:B:627:ASP:N	1:B:627:ASP:OD1	2.38	0.57
1:C:473:GLN:OE1	1:C:473:GLN:N	2.38	0.57
1:B:421:GLN:OE1	1:B:422:ALA:N	2.37	0.57
1:B:488:GLU:OE1	1:B:643:ILE:HD11	2.04	0.57
1:E:626:PRO:O	1:E:629:ILE:HG22	2.05	0.57
1:A:627:ASP:OD1	1:A:627:ASP:N	2.37	0.56
1:B:473:GLN:N	1:B:473:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:GLN:N	1:D:473:GLN:OE1	2.39	0.56
1:F:283:GLU:OE2	1:F:283:GLU:N	2.32	0.56
1:F:473:GLN:N	1:F:473:GLN:OE1	2.37	0.56
1:C:283:GLU:OE2	1:C:283:GLU:N	2.33	0.56
1:C:639:LEU:HD12	1:C:639:LEU:H	1.70	0.56
1:D:142:ALA:O	1:D:144:ARG:N	2.36	0.56
1:E:678:MET:HE2	1:E:678:MET:HA	1.87	0.56
1:F:321:GLU:O	1:F:325:VAL:HG23	2.06	0.56
1:E:321:GLU:O	1:E:325:VAL:HG23	2.06	0.56
1:D:313:ARG:HA	1:D:316:THR:HG22	1.88	0.56
1:D:427:MET:HE3	1:D:445:LEU:HD12	1.87	0.56
1:D:744:ARG:HH21	1:E:762:LEU:HD12	1.69	0.56
1:F:421:GLN:OE1	1:F:454:TRP:NE1	2.39	0.56
1:A:473:GLN:N	1:A:473:GLN:OE1	2.38	0.56
1:B:313:ARG:HA	1:B:316:THR:HG22	1.87	0.56
1:E:473:GLN:OE1	1:E:473:GLN:N	2.39	0.56
1:B:321:GLU:O	1:B:325:VAL:HG23	2.05	0.55
1:F:293:ALA:HB2	1:F:301:ILE:HD11	1.88	0.55
1:B:275:MET:HE2	1:B:275:MET:HA	1.89	0.55
1:C:142:ALA:O	1:C:144:ARG:N	2.36	0.55
1:C:427:MET:HE3	1:C:445:LEU:HD12	1.88	0.55
1:C:483:GLU:OE2	1:C:487:ARG:NH2	2.40	0.55
1:D:364:ASP:OD1	1:D:364:ASP:N	2.36	0.55
1:C:321:GLU:O	1:C:325:VAL:HG23	2.06	0.55
1:D:275:MET:HE2	1:D:275:MET:N	2.21	0.55
1:B:701:GLU:OE2	1:B:728:VAL:HG11	2.07	0.55
1:E:313:ARG:HA	1:E:316:THR:HG22	1.88	0.55
1:B:392:ASP:OD1	1:B:393:ASP:N	2.40	0.55
1:E:142:ALA:O	1:E:144:ARG:N	2.36	0.55
1:B:142:ALA:O	1:B:144:ARG:N	2.36	0.55
1:E:275:MET:HA	1:E:275:MET:HE2	1.88	0.55
1:A:229:LEU:HD13	1:F:438:ASP:HB2	1.88	0.55
1:C:378:LEU:O	1:C:382:GLN:NE2	2.35	0.55
1:E:627:ASP:N	1:E:627:ASP:OD1	2.40	0.55
1:C:313:ARG:HA	1:C:316:THR:HG22	1.87	0.54
1:A:427:MET:HE3	1:A:445:LEU:HD12	1.89	0.54
1:B:427:MET:HE3	1:B:445:LEU:HD12	1.89	0.54
1:F:204:ASP:OD1	1:F:205:ASP:N	2.41	0.54
1:A:454:TRP:O	1:A:458:GLN:OE1	2.26	0.54
1:A:639:LEU:HD12	1:A:639:LEU:H	1.73	0.54
1:D:639:LEU:HD12	1:D:639:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:GLN:O	1:B:536:GLN:NE2	2.41	0.54
1:E:217:LYS:NZ	1:E:261:GLU:OE1	2.40	0.53
1:F:313:ARG:HA	1:F:316:THR:HG22	1.88	0.53
1:B:425:LYS:HD2	1:B:425:LYS:C	2.34	0.53
1:D:661:LEU:HD22	1:D:666:VAL:HG21	1.91	0.53
1:B:546:GLU:O	1:B:550:MET:SD	2.67	0.53
1:B:639:LEU:H	1:B:639:LEU:HD12	1.73	0.53
1:B:661:LEU:HD22	1:B:666:VAL:HG21	1.90	0.53
1:C:761:THR:O	1:C:761:THR:HG23	2.09	0.53
1:B:438:ASP:HB2	1:C:229:LEU:HD13	1.90	0.52
1:A:205:ASP:C	1:A:205:ASP:OD1	2.52	0.52
1:B:761:THR:HG23	1:B:761:THR:O	2.10	0.52
1:A:314:GLU:N	1:A:314:GLU:OE1	2.38	0.52
1:D:438:ASP:HB2	1:E:229:LEU:HD13	1.91	0.52
1:F:761:THR:HG23	1:F:761:THR:O	2.09	0.52
1:F:733:ARG:O	1:F:737:GLU:OE2	2.26	0.52
1:C:503:PHE:O	1:C:507:GLY:N	2.43	0.52
1:F:275:MET:HE2	1:F:275:MET:HA	1.91	0.52
1:A:300:ILE:HD11	1:A:344:MET:SD	2.49	0.52
1:E:283:GLU:OE2	1:E:283:GLU:N	2.33	0.52
1:F:142:ALA:O	1:F:144:ARG:N	2.36	0.52
1:A:438:ASP:HB2	1:B:229:LEU:HD13	1.91	0.52
1:B:484:ASP:N	1:B:484:ASP:OD1	2.43	0.52
1:E:388:MET:HE2	1:E:415:CYS:SG	2.49	0.52
1:B:241:ILE:CD1	1:B:342:ILE:HD11	2.39	0.51
1:A:661:LEU:HD22	1:A:666:VAL:HG21	1.93	0.51
1:E:438:ASP:OD1	1:E:439:ALA:N	2.41	0.51
1:D:483:GLU:OE2	1:D:487:ARG:NH2	2.43	0.51
1:C:626:PRO:O	1:C:629:ILE:HG22	2.11	0.51
1:E:388:MET:HB2	1:E:390:LEU:HD11	1.93	0.51
1:F:640:ASP:OD1	1:F:640:ASP:O	2.28	0.51
1:F:215:GLN:O	1:F:219:MET:HG3	2.11	0.51
1:D:438:ASP:OD1	1:D:439:ALA:N	2.42	0.50
1:F:661:LEU:HD22	1:F:666:VAL:HG21	1.93	0.50
1:D:314:GLU:H	1:D:314:GLU:CD	2.20	0.50
1:E:241:ILE:CD1	1:E:342:ILE:HD11	2.42	0.50
1:F:423:ILE:HG12	1:F:445:LEU:HD11	1.91	0.50
1:D:761:THR:O	1:D:761:THR:HG23	2.11	0.50
1:E:555:SER:O	1:E:558:ASN:OD1	2.28	0.50
1:C:393:ASP:OD1	1:C:393:ASP:N	2.44	0.50
1:C:661:LEU:HD22	1:C:666:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:LEU:O	1:D:217:LYS:HG2	2.11	0.50
1:A:429:LEU:C	1:A:430:ILE:HD12	2.36	0.49
1:A:744:ARG:HH12	1:B:762:LEU:HA	1.77	0.49
1:E:385:THR:HG22	1:E:388:MET:HE3	1.94	0.49
1:F:258:VAL:O	1:F:262:THR:HG22	2.12	0.49
1:F:438:ASP:OD1	1:F:439:ALA:N	2.42	0.49
1:F:734:ASP:O	1:F:738:GLU:HG2	2.11	0.49
1:B:438:ASP:O	1:B:441:VAL:HG22	2.12	0.49
1:C:429:LEU:C	1:C:430:ILE:HD12	2.37	0.49
1:D:300:ILE:HD11	1:D:344:MET:SD	2.52	0.49
1:E:438:ASP:HB2	1:F:229:LEU:HD13	1.94	0.49
1:A:230:PHE:CE1	1:A:235:VAL:HG23	2.47	0.49
1:A:393:ASP:N	1:A:393:ASP:OD1	2.45	0.49
1:D:429:LEU:C	1:D:430:ILE:HD12	2.37	0.49
1:E:429:LEU:C	1:E:430:ILE:HD12	2.38	0.49
1:C:528:ALA:O	1:C:531:ILE:HG12	2.13	0.49
1:D:230:PHE:CE1	1:D:235:VAL:HG23	2.47	0.49
1:F:429:LEU:C	1:F:430:ILE:HD12	2.37	0.49
1:C:438:ASP:OD1	1:C:439:ALA:N	2.42	0.49
1:D:744:ARG:NH2	1:E:761:THR:O	2.45	0.49
1:E:230:PHE:CE1	1:E:235:VAL:HG23	2.48	0.49
1:B:753:ARG:O	1:B:757:MET:HE2	2.13	0.49
1:C:364:ASP:OD1	1:C:364:ASP:N	2.45	0.49
1:D:678:MET:HA	1:D:678:MET:HE2	1.95	0.49
1:F:314:GLU:H	1:F:314:GLU:CD	2.20	0.49
1:D:204:ASP:OD1	1:D:205:ASP:N	2.46	0.48
1:F:733:ARG:O	1:F:736:PHE:N	2.46	0.48
1:B:753:ARG:O	1:B:757:MET:HG2	2.13	0.48
1:C:230:PHE:CE1	1:C:235:VAL:HG23	2.48	0.48
1:C:390:LEU:CD2	1:C:394:VAL:HG11	2.43	0.48
1:E:639:LEU:HD12	1:E:639:LEU:H	1.77	0.48
1:E:661:LEU:HD22	1:E:666:VAL:HG21	1.94	0.48
1:F:393:ASP:N	1:F:393:ASP:OD1	2.45	0.48
1:E:205:ASP:OD1	1:E:205:ASP:C	2.56	0.48
1:E:753:ARG:O	1:E:757:MET:HG2	2.14	0.48
1:A:438:ASP:OD1	1:A:439:ALA:N	2.42	0.48
1:A:528:ALA:O	1:A:531:ILE:HG12	2.12	0.48
1:B:283:GLU:OE2	1:B:283:GLU:N	2.33	0.48
1:C:380:ILE:O	1:C:383:ILE:HG12	2.13	0.48
1:F:503:PHE:O	1:F:507:GLY:N	2.47	0.48
1:C:438:ASP:HB2	1:D:229:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:OD1	1:A:205:ASP:N	2.47	0.48
1:C:241:ILE:CD1	1:C:342:ILE:HD11	2.43	0.48
1:D:230:PHE:HE1	1:D:235:VAL:HG23	1.79	0.48
1:E:314:GLU:H	1:E:314:GLU:CD	2.21	0.48
1:F:230:PHE:CE1	1:F:235:VAL:HG23	2.48	0.48
1:A:249:THR:HB	1:A:369:ILE:HG21	1.95	0.48
1:C:204:ASP:OD1	1:C:205:ASP:N	2.47	0.48
1:A:230:PHE:HE1	1:A:235:VAL:HG23	1.79	0.48
1:E:292:GLU:OE2	1:E:292:GLU:HA	2.13	0.48
1:A:420:LEU:HD21	1:B:235:VAL:HG21	1.96	0.48
1:B:230:PHE:CE1	1:B:235:VAL:HG23	2.48	0.48
1:D:292:GLU:HA	1:D:292:GLU:OE2	2.13	0.48
1:C:425:LYS:C	1:C:425:LYS:HD2	2.39	0.48
1:E:445:LEU:C	1:E:445:LEU:HD23	2.39	0.48
1:A:241:ILE:CD1	1:A:342:ILE:HD11	2.44	0.47
1:B:287:ARG:O	1:B:291:GLU:HG3	2.14	0.47
1:A:761:THR:HG23	1:A:761:THR:O	2.14	0.47
1:E:393:ASP:OD1	1:E:393:ASP:N	2.46	0.47
1:B:438:ASP:OD1	1:B:439:ALA:N	2.43	0.47
1:D:305:GLU:OE2	1:E:362:ARG:NH2	2.46	0.47
1:F:230:PHE:HE1	1:F:235:VAL:HG23	1.80	0.47
1:E:230:PHE:HE1	1:E:235:VAL:HG23	1.80	0.47
1:B:316:THR:O	1:B:322:ARG:NH2	2.47	0.47
1:C:633:ILE:HG23	1:C:634:LEU:HD12	1.97	0.47
1:D:390:LEU:HD23	1:D:394:VAL:HG11	1.96	0.47
1:B:678:MET:HA	1:B:678:MET:HE2	1.95	0.47
1:F:249:THR:HB	1:F:369:ILE:HG21	1.97	0.47
1:B:703:ILE:HG21	1:C:495:TYR:CE1	2.50	0.47
1:C:300:ILE:HD11	1:C:344:MET:SD	2.55	0.47
1:F:734:ASP:HA	1:F:737:GLU:OE2	2.15	0.47
1:F:390:LEU:HD23	1:F:394:VAL:HG11	1.96	0.47
1:F:753:ARG:O	1:F:757:MET:HG2	2.15	0.47
1:F:241:ILE:CD1	1:F:342:ILE:HD11	2.43	0.47
1:F:380:ILE:O	1:F:383:ILE:HG12	2.14	0.47
1:C:230:PHE:HE1	1:C:235:VAL:HG23	1.80	0.47
1:C:332:MET:HE3	1:C:363:PHE:CE1	2.49	0.47
1:A:235:VAL:HG21	1:F:420:LEU:HD21	1.97	0.46
1:A:489:LEU:O	1:A:493:VAL:HG22	2.15	0.46
1:B:230:PHE:HE1	1:B:235:VAL:HG23	1.80	0.46
1:B:414:LEU:HD23	1:B:414:LEU:O	2.15	0.46
1:D:528:ALA:O	1:D:531:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ASP:OD1	1:B:205:ASP:C	2.58	0.46
1:A:503:PHE:O	1:A:507:GLY:N	2.48	0.46
1:B:429:LEU:C	1:B:430:ILE:HD12	2.39	0.46
1:F:733:ARG:O	1:F:734:ASP:C	2.58	0.46
1:A:380:ILE:O	1:A:383:ILE:HG12	2.15	0.46
1:C:425:LYS:HD2	1:C:425:LYS:O	2.15	0.46
1:C:627:ASP:OD1	1:C:627:ASP:N	2.48	0.46
1:B:380:ILE:O	1:B:383:ILE:HG12	2.16	0.46
1:B:425:LYS:HD2	1:B:425:LYS:O	2.16	0.46
1:C:536:GLN:O	1:C:536:GLN:CG	2.64	0.46
1:F:300:ILE:CD1	1:F:344:MET:HE2	2.43	0.46
1:A:647:LEU:H	1:A:647:LEU:HD22	1.80	0.46
1:B:314:GLU:OE1	1:B:314:GLU:N	2.36	0.46
1:B:378:LEU:HD23	1:B:378:LEU:O	2.15	0.46
1:B:393:ASP:N	1:B:393:ASP:OD1	2.48	0.46
1:B:204:ASP:OD1	1:B:205:ASP:N	2.48	0.46
1:B:217:LYS:HZ2	1:B:261:GLU:CD	2.24	0.46
1:A:390:LEU:HD23	1:A:394:VAL:HG11	1.98	0.46
1:E:633:ILE:HG23	1:E:634:LEU:HD12	1.98	0.46
1:E:734:ASP:O	1:E:738:GLU:HG2	2.15	0.46
1:F:536:GLN:CG	1:F:536:GLN:O	2.64	0.46
1:B:403:THR:HG22	1:B:406:HIS:CG	2.51	0.46
1:B:292:GLU:OE2	1:B:292:GLU:HA	2.15	0.45
1:D:351:ASN:OD1	1:D:351:ASN:O	2.33	0.45
1:E:420:LEU:HD21	1:F:235:VAL:HG21	1.98	0.45
1:F:647:LEU:H	1:F:647:LEU:HD22	1.81	0.45
1:C:403:THR:HG22	1:C:406:HIS:CG	2.51	0.45
1:D:536:GLN:CG	1:D:536:GLN:O	2.65	0.45
1:F:639:LEU:HD12	1:F:639:LEU:H	1.81	0.45
1:B:536:GLN:O	1:B:536:GLN:CG	2.64	0.45
1:D:403:THR:HG22	1:D:406:HIS:CG	2.52	0.45
1:E:414:LEU:O	1:E:414:LEU:HD23	2.17	0.45
1:E:647:LEU:HD22	1:E:647:LEU:H	1.81	0.45
1:F:668:LYS:HD3	1:F:668:LYS:N	2.31	0.45
1:A:536:GLN:CG	1:A:536:GLN:O	2.64	0.45
1:A:547:LEU:HA	1:A:550:MET:HE3	1.99	0.45
1:C:449:MET:SD	1:C:449:MET:C	2.99	0.45
1:B:249:THR:HB	1:B:369:ILE:HG21	1.97	0.45
1:B:420:LEU:HD21	1:C:235:VAL:HG21	1.98	0.45
1:D:205:ASP:OD1	1:D:205:ASP:C	2.60	0.45
1:D:420:LEU:HD21	1:E:235:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:555:SER:O	1:F:558:ASN:ND2	2.50	0.45
1:C:733:ARG:O	1:C:737:GLU:HG2	2.16	0.45
1:D:312:LYS:HB3	1:D:314:GLU:OE1	2.16	0.45
1:D:647:LEU:H	1:D:647:LEU:HD22	1.82	0.45
1:B:547:LEU:HD23	1:B:550:MET:HE1	1.99	0.45
1:C:577:ASP:OD1	1:C:577:ASP:N	2.48	0.45
1:A:403:THR:HG22	1:A:406:HIS:CG	2.52	0.45
1:F:753:ARG:HB3	1:F:757:MET:HE2	1.99	0.45
1:E:586:ARG:NH2	1:E:595:GLY:O	2.49	0.44
1:F:403:THR:HG22	1:F:406:HIS:CG	2.53	0.44
1:D:393:ASP:N	1:D:393:ASP:OD1	2.47	0.44
1:E:264:ALA:HB1	1:E:298:PRO:O	2.18	0.44
1:E:577:ASP:OD1	1:E:577:ASP:N	2.48	0.44
1:F:447:VAL:HG11	1:F:452:PHE:HE1	1.83	0.44
1:F:547:LEU:HA	1:F:550:MET:HE3	1.99	0.44
1:A:536:GLN:O	1:A:536:GLN:HG2	2.16	0.44
1:C:249:THR:HB	1:C:369:ILE:HG21	1.98	0.44
1:C:546:GLU:O	1:C:550:MET:HG3	2.18	0.44
1:F:543:LYS:HA	1:F:577:ASP:OD1	2.18	0.44
1:B:503:PHE:O	1:B:507:GLY:N	2.51	0.44
1:D:249:THR:HB	1:D:369:ILE:HG21	1.99	0.44
1:E:658:LYS:HA	1:E:661:LEU:HD11	2.00	0.44
1:A:305:GLU:OE2	1:B:362:ARG:NH2	2.50	0.44
1:A:678:MET:HE2	1:A:678:MET:HA	1.98	0.44
1:D:486:LYS:NZ	1:D:534:GLU:OE2	2.48	0.44
1:E:403:THR:HG22	1:E:406:HIS:CG	2.53	0.44
1:E:692:GLN:HB3	1:F:508:MET:HE1	2.00	0.44
1:B:586:ARG:NH2	1:B:595:GLY:O	2.51	0.44
1:D:696:LYS:HG3	1:E:508:MET:HE2	2.00	0.44
1:E:489:LEU:O	1:E:493:VAL:HG12	2.17	0.44
1:C:666:VAL:HG12	1:C:667:ALA:O	2.18	0.43
1:D:738:GLU:OE1	1:D:738:GLU:HA	2.18	0.43
1:E:536:GLN:O	1:E:536:GLN:CG	2.65	0.43
1:B:528:ALA:O	1:B:531:ILE:HG12	2.17	0.43
1:B:647:LEU:HD22	1:B:647:LEU:H	1.83	0.43
1:A:469:VAL:HG12	1:A:540:ILE:HD11	2.00	0.43
1:E:547:LEU:HA	1:E:550:MET:HE3	1.99	0.43
1:A:283:GLU:OE2	1:A:283:GLU:N	2.30	0.43
1:B:449:MET:SD	1:B:449:MET:C	3.02	0.43
1:B:640:ASP:OD1	1:B:640:ASP:O	2.37	0.43
1:D:503:PHE:O	1:D:507:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:LEU:O	1:F:378:LEU:HD23	2.18	0.43
1:F:658:LYS:HA	1:F:661:LEU:HD11	2.01	0.43
1:B:264:ALA:HB1	1:B:298:PRO:O	2.18	0.43
1:C:378:LEU:O	1:C:382:GLN:HG2	2.19	0.43
1:E:378:LEU:HD12	1:E:378:LEU:O	2.18	0.43
1:B:421:GLN:OE1	1:B:421:GLN:C	2.62	0.43
1:C:598:ASP:OD1	1:C:600:VAL:HG22	2.19	0.43
1:C:647:LEU:HD22	1:C:647:LEU:H	1.83	0.43
1:F:265:PHE:CD1	1:F:265:PHE:C	2.96	0.43
1:F:410:ASP:N	1:F:410:ASP:OD1	2.50	0.43
1:A:420:LEU:HD21	1:B:235:VAL:CG2	2.48	0.43
1:A:449:MET:SD	1:A:449:MET:C	3.01	0.43
1:D:763:GLN:OE1	1:D:763:GLN:N	2.43	0.43
1:E:763:GLN:OE1	1:E:763:GLN:N	2.38	0.43
1:F:653:ARG:O	1:F:656:ILE:HG22	2.18	0.43
1:E:376:GLY:O	1:E:380:ILE:HG13	2.18	0.43
1:E:761:THR:O	1:E:761:THR:HG23	2.18	0.43
1:F:376:GLY:O	1:F:380:ILE:HG13	2.19	0.43
1:A:734:ASP:O	1:A:738:GLU:HG2	2.18	0.43
1:C:428:ASP:OD1	1:C:428:ASP:C	2.61	0.43
1:A:696:LYS:HG3	1:B:508:MET:HE2	2.01	0.42
1:B:399:VAL:O	1:B:403:THR:OG1	2.37	0.42
1:B:666:VAL:HG12	1:B:667:ALA:O	2.19	0.42
1:C:420:LEU:HD21	1:D:235:VAL:HG21	2.01	0.42
1:B:314:GLU:H	1:B:314:GLU:CD	2.25	0.42
1:A:573:VAL:CG1	1:A:620:ILE:HD12	2.50	0.42
1:B:421:GLN:C	1:B:421:GLN:CD	2.87	0.42
1:B:577:ASP:OD1	1:B:577:ASP:N	2.48	0.42
1:D:666:VAL:HG12	1:D:667:ALA:O	2.19	0.42
1:E:503:PHE:O	1:E:507:GLY:N	2.53	0.42
1:E:653:ARG:O	1:E:656:ILE:HG22	2.20	0.42
1:E:688:THR:O	1:E:692:GLN:HG2	2.19	0.42
1:F:397:GLU:O	1:F:401:ASN:OD1	2.37	0.42
1:C:376:GLY:O	1:C:380:ILE:HG13	2.20	0.42
1:D:423:ILE:HG12	1:D:445:LEU:HD11	2.01	0.42
1:E:380:ILE:O	1:E:383:ILE:HG22	2.20	0.42
1:E:399:VAL:O	1:E:403:THR:OG1	2.38	0.42
1:A:229:LEU:O	1:A:229:LEU:HD12	2.19	0.42
1:E:249:THR:HB	1:E:369:ILE:HG21	2.01	0.42
1:D:449:MET:SD	1:D:449:MET:C	3.02	0.42
1:E:390:LEU:HD12	1:E:390:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:ASP:O	1:E:441:VAL:HG22	2.19	0.42
1:A:658:LYS:HA	1:A:661:LEU:HD11	2.01	0.42
1:C:74:ASP:O	1:C:75:ASP:CB	2.68	0.42
1:D:264:ALA:HB1	1:D:298:PRO:O	2.20	0.42
1:E:297:ALA:O	1:E:298:PRO:C	2.62	0.42
1:E:666:VAL:HG12	1:E:667:ALA:O	2.19	0.42
1:B:24:ASN:O	1:B:100:ILE:O	2.38	0.42
1:B:696:LYS:HG3	1:C:508:MET:HE2	2.02	0.42
1:C:295:LYS:O	1:C:295:LYS:HG2	2.18	0.42
1:C:753:ARG:HB3	1:C:757:MET:HE2	2.01	0.42
1:D:489:LEU:O	1:D:493:VAL:HG12	2.20	0.42
1:A:74:ASP:O	1:A:75:ASP:CB	2.68	0.42
1:A:410:ASP:N	1:A:410:ASP:OD1	2.52	0.42
1:A:482:LEU:O	1:A:486:LYS:HG3	2.20	0.42
1:C:332:MET:CE	1:C:363:PHE:CE1	3.03	0.42
1:C:586:ARG:NH2	1:C:595:GLY:O	2.53	0.42
1:D:523:GLY:O	1:D:527:LEU:HD23	2.20	0.42
1:D:536:GLN:O	1:D:536:GLN:HG2	2.19	0.42
1:E:74:ASP:O	1:E:75:ASP:CB	2.68	0.42
1:F:399:VAL:O	1:F:403:THR:OG1	2.38	0.42
1:B:476:TRP:HE3	1:B:476:TRP:H	1.67	0.42
1:E:301:ILE:HB	1:E:343:VAL:HG12	2.02	0.42
1:E:371:ILE:N	1:E:371:ILE:HD13	2.35	0.42
1:A:217:LYS:NZ	1:A:261:GLU:OE1	2.51	0.41
1:C:410:ASP:OD1	1:C:410:ASP:N	2.53	0.41
1:E:293:ALA:HB2	1:E:301:ILE:HD11	2.02	0.41
1:F:701:GLU:OE2	1:F:728:VAL:HG11	2.20	0.41
1:A:24:ASN:O	1:A:100:ILE:O	2.38	0.41
1:B:364:ASP:OD1	1:B:364:ASP:N	2.51	0.41
1:B:540:ILE:HD11	1:B:565:LYS:HZ1	1.84	0.41
1:E:397:GLU:O	1:E:401:ASN:OD1	2.38	0.41
1:F:74:ASP:O	1:F:75:ASP:CB	2.68	0.41
1:A:378:LEU:O	1:A:378:LEU:HD23	2.19	0.41
1:A:633:ILE:HG23	1:A:634:LEU:HD23	2.02	0.41
1:C:370:GLY:C	1:C:371:ILE:HD13	2.45	0.41
1:D:241:ILE:CD1	1:D:342:ILE:HD11	2.48	0.41
1:D:483:GLU:OE2	1:D:487:ARG:NH1	2.52	0.41
1:F:505:LYS:HD2	1:F:505:LYS:O	2.19	0.41
1:F:627:ASP:N	1:F:627:ASP:OD1	2.53	0.41
1:A:264:ALA:HB1	1:A:298:PRO:O	2.20	0.41
1:A:523:GLY:O	1:A:527:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASN:O	1:C:100:ILE:O	2.38	0.41
1:A:666:VAL:HG12	1:A:667:ALA:O	2.20	0.41
1:C:421:GLN:C	1:C:421:GLN:OE1	2.64	0.41
1:D:275:MET:HE2	1:D:275:MET:CA	2.51	0.41
1:D:438:ASP:O	1:D:441:VAL:HG22	2.21	0.41
1:E:204:ASP:OD1	1:E:205:ASP:N	2.54	0.41
1:F:392:ASP:OD1	1:F:392:ASP:C	2.63	0.41
1:A:235:VAL:CG2	1:F:420:LEU:HD21	2.51	0.41
1:B:390:LEU:HD12	1:B:390:LEU:H	1.86	0.41
1:C:397:GLU:O	1:C:401:ASN:OD1	2.38	0.41
1:C:536:GLN:O	1:C:536:GLN:HG2	2.21	0.41
1:D:753:ARG:O	1:D:757:MET:HG2	2.20	0.41
1:E:24:ASN:O	1:E:100:ILE:O	2.38	0.41
1:F:419:ALA:O	1:F:423:ILE:HG13	2.20	0.41
1:C:430:ILE:HD12	1:C:430:ILE:N	2.36	0.41
1:C:658:LYS:HA	1:C:661:LEU:HD11	2.03	0.41
1:D:633:ILE:HG23	1:D:634:LEU:HD23	2.02	0.41
1:F:24:ASN:O	1:F:100:ILE:O	2.38	0.41
1:A:390:LEU:HB3	1:A:394:VAL:HG21	2.03	0.41
1:B:573:VAL:CG1	1:B:620:ILE:HD12	2.51	0.41
1:D:74:ASP:O	1:D:75:ASP:CB	2.68	0.41
1:D:297:ALA:O	1:D:298:PRO:C	2.63	0.41
1:D:734:ASP:O	1:D:738:GLU:HG2	2.21	0.41
1:E:493:VAL:HG11	1:E:531:ILE:HD12	2.03	0.41
1:F:265:PHE:CD1	1:F:266:ALA:N	2.89	0.41
1:F:427:MET:CE	1:F:445:LEU:HD12	2.48	0.41
1:A:438:ASP:O	1:A:441:VAL:HG22	2.20	0.41
1:B:74:ASP:O	1:B:75:ASP:CB	2.68	0.41
1:B:430:ILE:HD12	1:B:430:ILE:N	2.36	0.41
1:B:488:GLU:O	1:B:492:LEU:HD23	2.21	0.41
1:B:489:LEU:O	1:B:493:VAL:HG12	2.21	0.41
1:D:24:ASN:O	1:D:100:ILE:O	2.38	0.41
1:D:469:VAL:HG12	1:D:540:ILE:HD11	2.03	0.41
1:D:658:LYS:HA	1:D:661:LEU:HD11	2.03	0.41
1:E:229:LEU:HD12	1:E:229:LEU:O	2.21	0.41
1:E:300:ILE:HD11	1:E:344:MET:SD	2.61	0.41
1:E:469:VAL:CG1	1:E:540:ILE:HD11	2.50	0.41
1:E:469:VAL:CG1	1:E:565:LYS:HZ1	2.34	0.41
1:F:438:ASP:O	1:F:441:VAL:HG22	2.21	0.41
1:F:633:ILE:HG23	1:F:634:LEU:HD23	2.03	0.41
1:E:573:VAL:HG11	1:E:620:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:CYS:HA	1:D:145:PRO:O	2.22	0.40
1:D:430:ILE:HD12	1:D:430:ILE:N	2.36	0.40
1:F:536:GLN:O	1:F:536:GLN:HG2	2.21	0.40
1:F:550:MET:SD	1:F:558:ASN:ND2	2.92	0.40
1:A:573:VAL:HG11	1:A:620:ILE:HD12	2.03	0.40
1:C:399:VAL:O	1:C:403:THR:OG1	2.39	0.40
1:D:390:LEU:CD2	1:D:394:VAL:HG11	2.52	0.40
1:D:399:VAL:O	1:D:403:THR:OG1	2.39	0.40
1:D:753:ARG:O	1:D:757:MET:HE2	2.21	0.40
1:E:420:LEU:HD21	1:F:235:VAL:CG2	2.52	0.40
1:A:586:ARG:NH2	1:A:595:GLY:O	2.54	0.40
1:B:229:LEU:HD12	1:B:229:LEU:O	2.20	0.40
1:B:476:TRP:CZ3	1:B:534:GLU:OE2	2.74	0.40
1:F:644:TYR:CD1	1:F:644:TYR:C	2.97	0.40
1:B:476:TRP:CH2	1:B:530:ALA:C	3.00	0.40
1:C:348:ASN:C	1:C:348:ASN:OD1	2.64	0.40
1:E:348:ASN:OD1	1:E:348:ASN:C	2.65	0.40
1:F:430:ILE:HD12	1:F:430:ILE:N	2.36	0.40
1:B:388:MET:HB2	1:B:390:LEU:HD11	2.03	0.40
1:B:475:THR:HG22	1:B:476:TRP:H	1.87	0.40
1:C:753:ARG:HB2	1:C:753:ARG:NH1	2.37	0.40
1:E:398:GLN:H	1:E:398:GLN:HG2	1.74	0.40
1:F:69:CYS:HA	1:F:145:PRO:O	2.22	0.40
1:F:297:ALA:O	1:F:298:PRO:C	2.64	0.40
1:F:332:MET:CE	1:F:363:PHE:CE1	3.03	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	741/806 (92%)	670 (90%)	71 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	741/806 (92%)	670 (90%)	71 (10%)	0	100	100
1	C	741/806 (92%)	672 (91%)	69 (9%)	0	100	100
1	D	741/806 (92%)	671 (91%)	70 (9%)	0	100	100
1	E	741/806 (92%)	671 (91%)	70 (9%)	0	100	100
1	F	741/806 (92%)	667 (90%)	74 (10%)	0	100	100
All	All	4446/4836 (92%)	4021 (90%)	425 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	463/676 (68%)	463 (100%)	0	100	100
1	B	461/676 (68%)	460 (100%)	1 (0%)	87	85
1	C	462/676 (68%)	461 (100%)	1 (0%)	87	85
1	D	430/676 (64%)	430 (100%)	0	100	100
1	E	462/676 (68%)	460 (100%)	2 (0%)	84	83
1	F	463/676 (68%)	463 (100%)	0	100	100
All	All	2741/4056 (68%)	2737 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	267	PHE
1	C	267	PHE
1	E	267	PHE
1	E	476	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	GLN
1	A	616	ASN
1	B	270	ASN
1	B	327	GLN
1	B	536	GLN
1	B	616	ASN
1	C	602	ASN
1	D	382	GLN
1	D	490	GLN
1	E	285	ASN
1	E	351	ASN
1	E	382	GLN
1	E	490	GLN
1	E	602	ASN
1	F	460	ASN
1	F	602	ASN
1	F	603	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 ⓘ

There are no chain breaks in this entry.

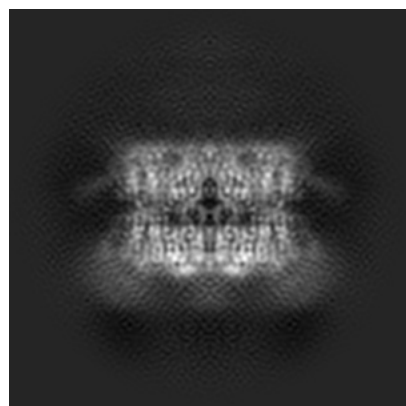
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19473. These allow visual inspection of the internal detail of the map and identification of artifacts.

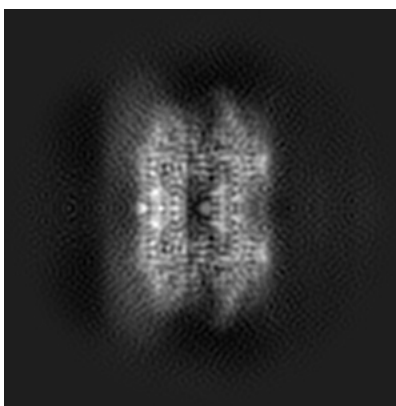
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

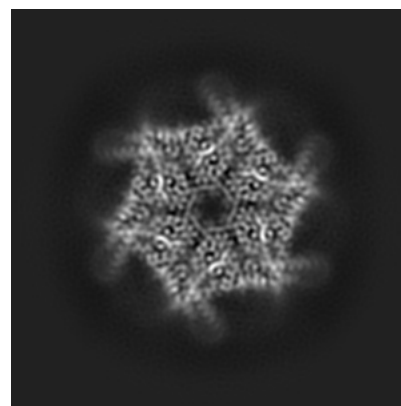
6.1.1 Primary map



X

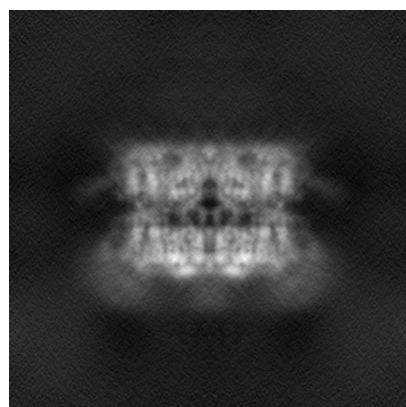


Y

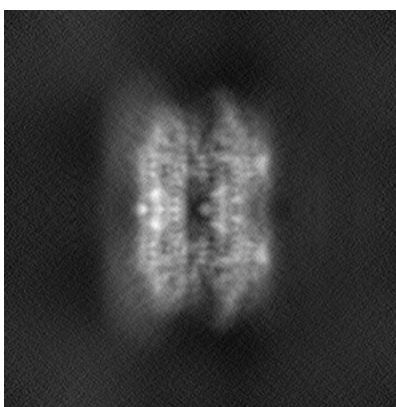


Z

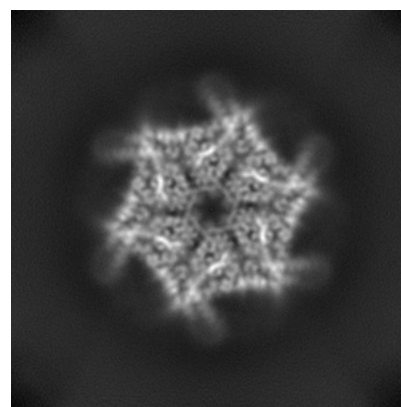
6.1.2 Raw map



X



Y

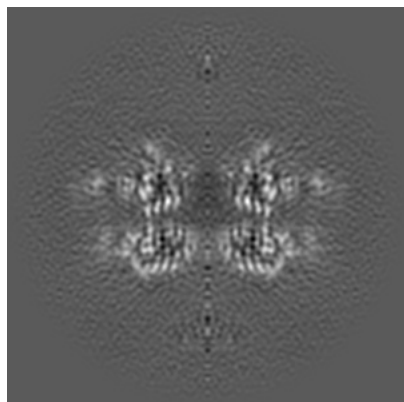


Z

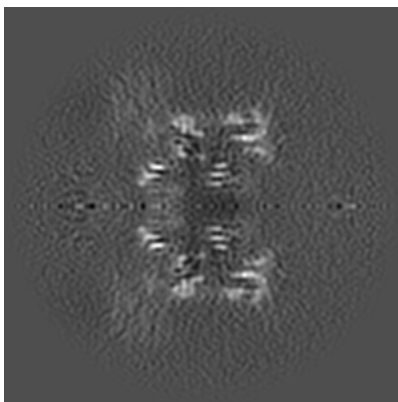
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

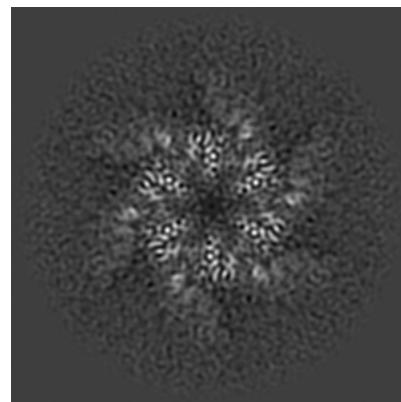
6.2.1 Primary map



X Index: 140

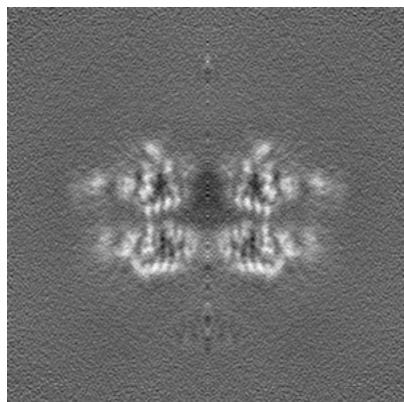


Y Index: 140

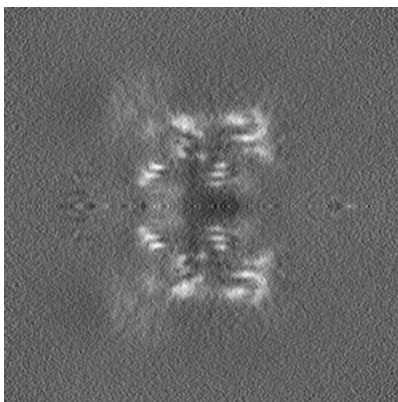


Z Index: 140

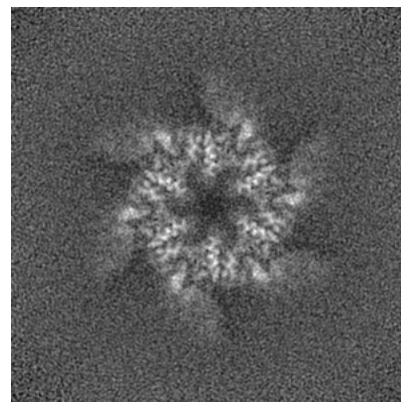
6.2.2 Raw map



X Index: 140



Y Index: 140

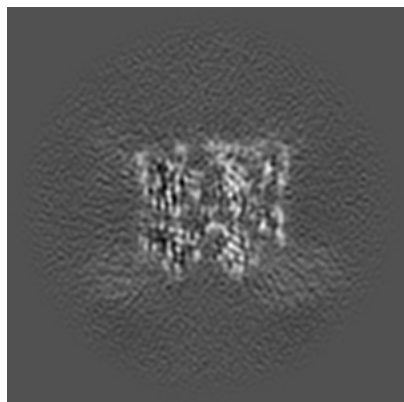


Z Index: 140

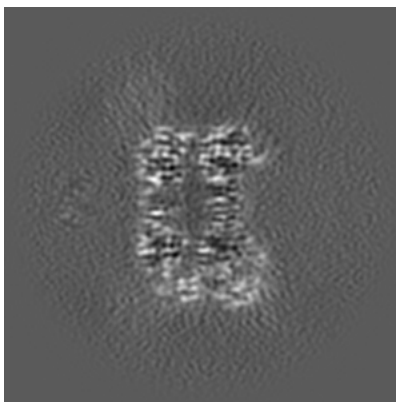
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

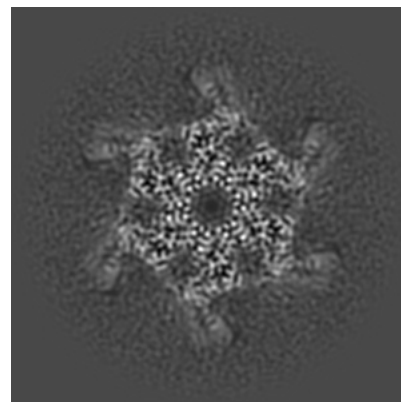
6.3.1 Primary map



X Index: 104

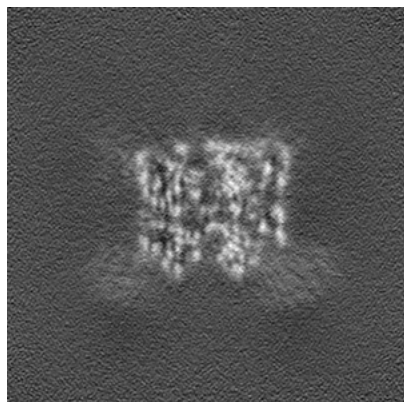


Y Index: 123

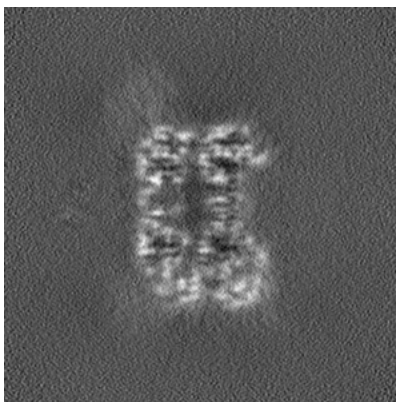


Z Index: 152

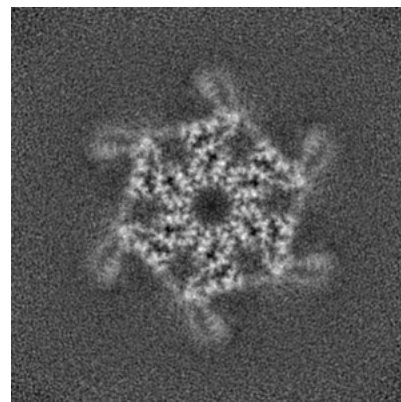
6.3.2 Raw map



X Index: 104



Y Index: 123

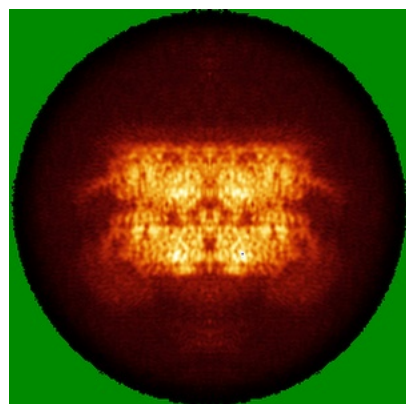


Z Index: 152

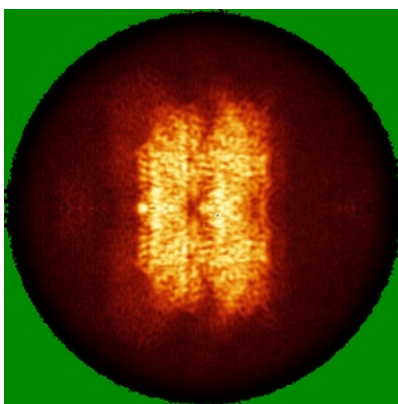
The images above show the largest variance slices of the map in three orthogonal directions.

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

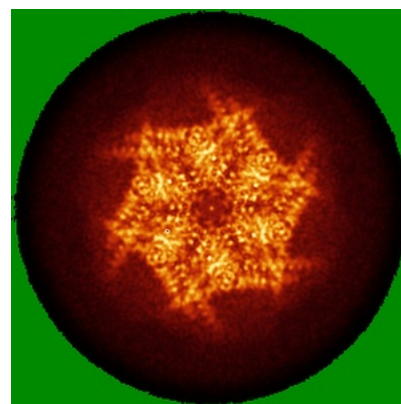
6.4.1 Primary map



X

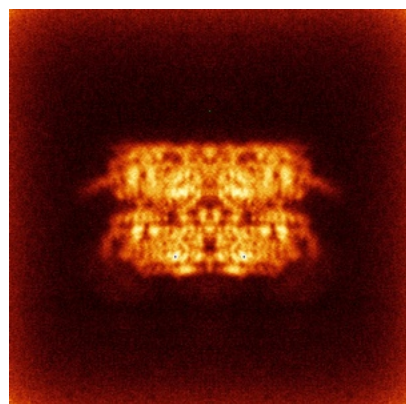


Y

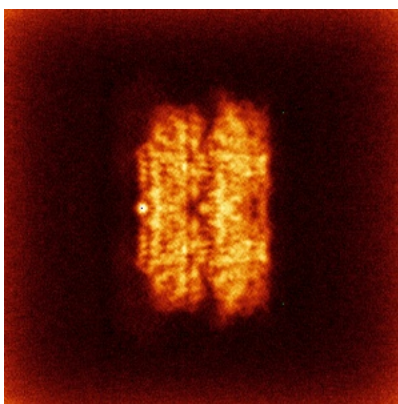


Z

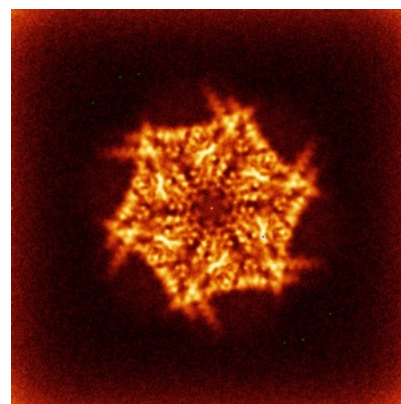
6.4.2 Raw map



X



Y

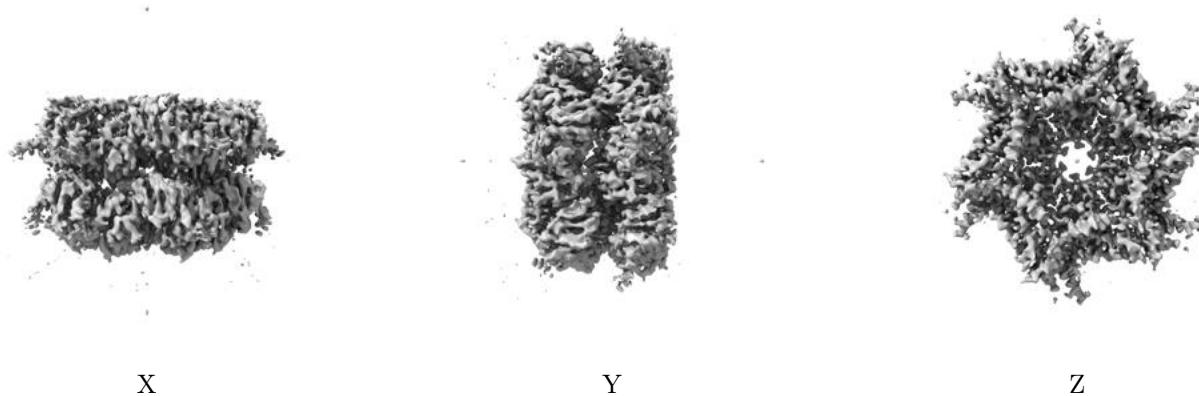


Z

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.

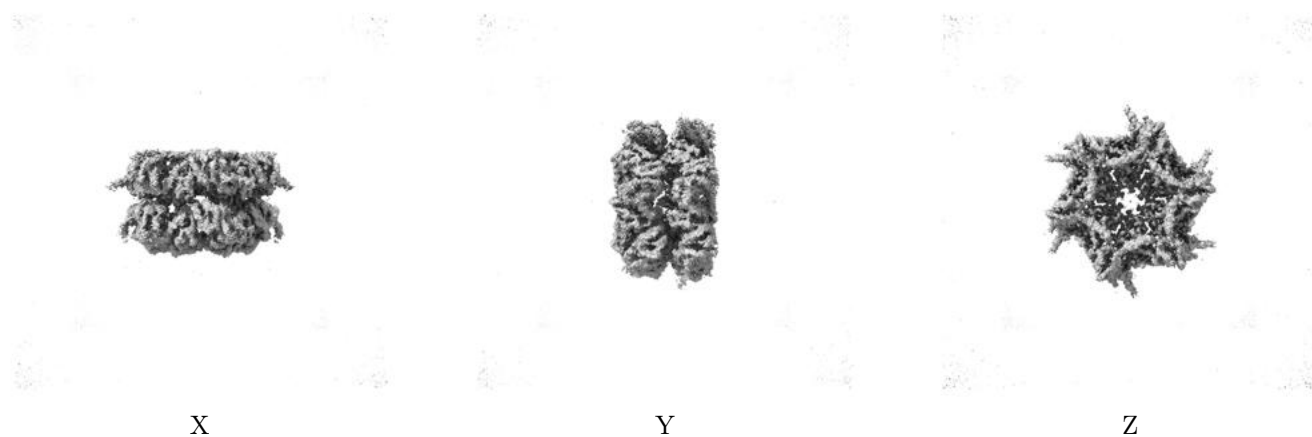
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.244. 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.

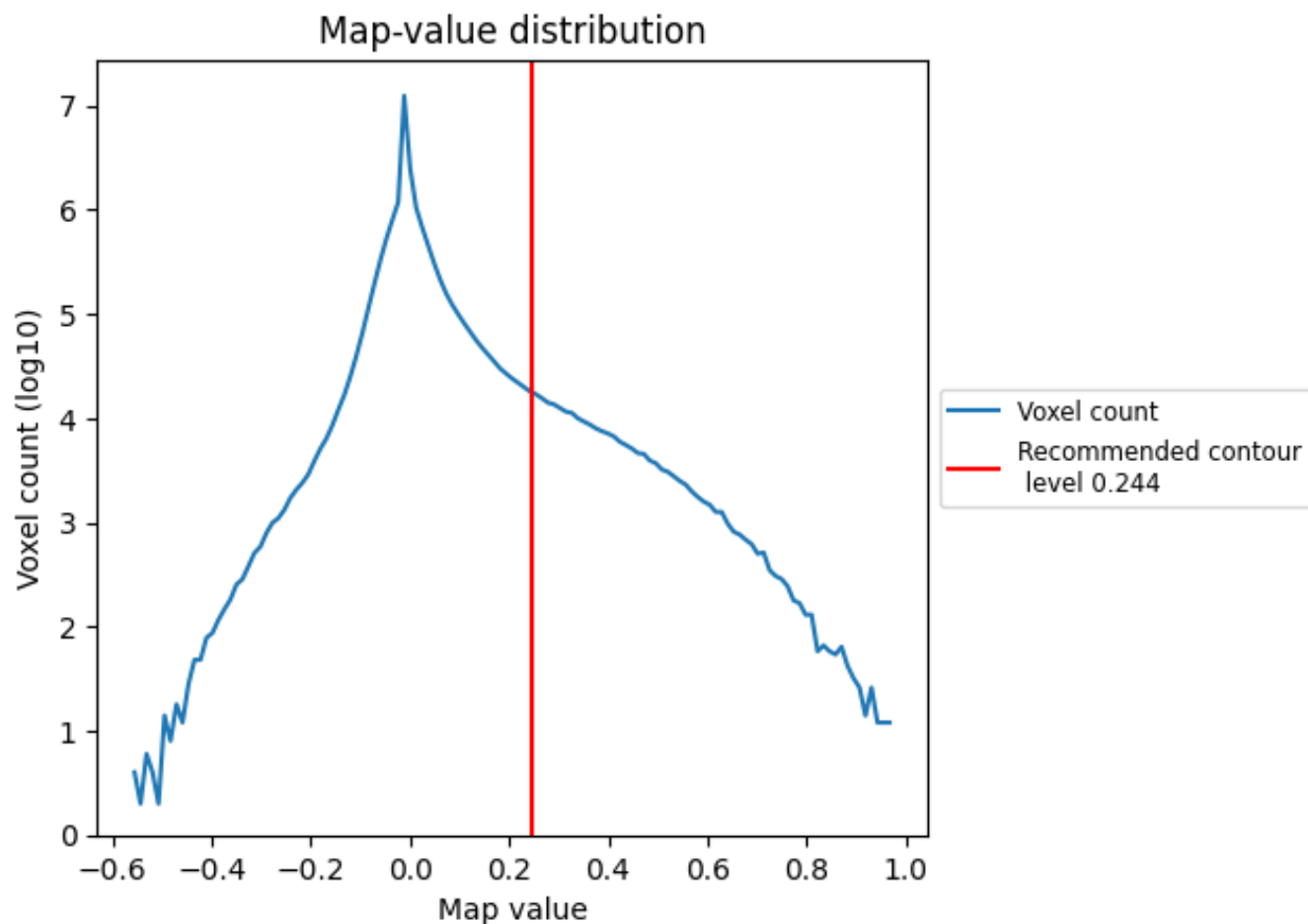
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

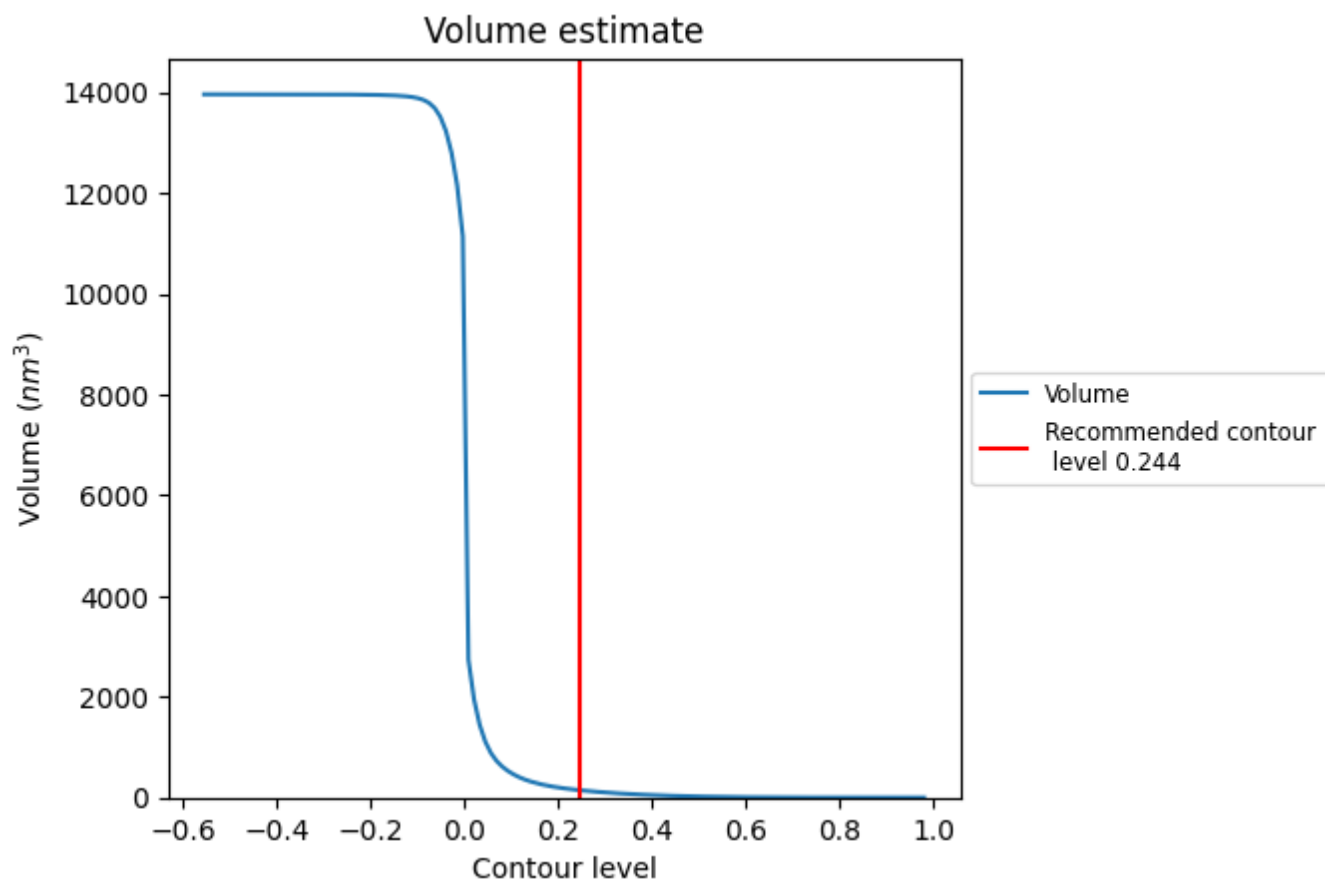
This section contains the results of statistical analysis of the map.

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.

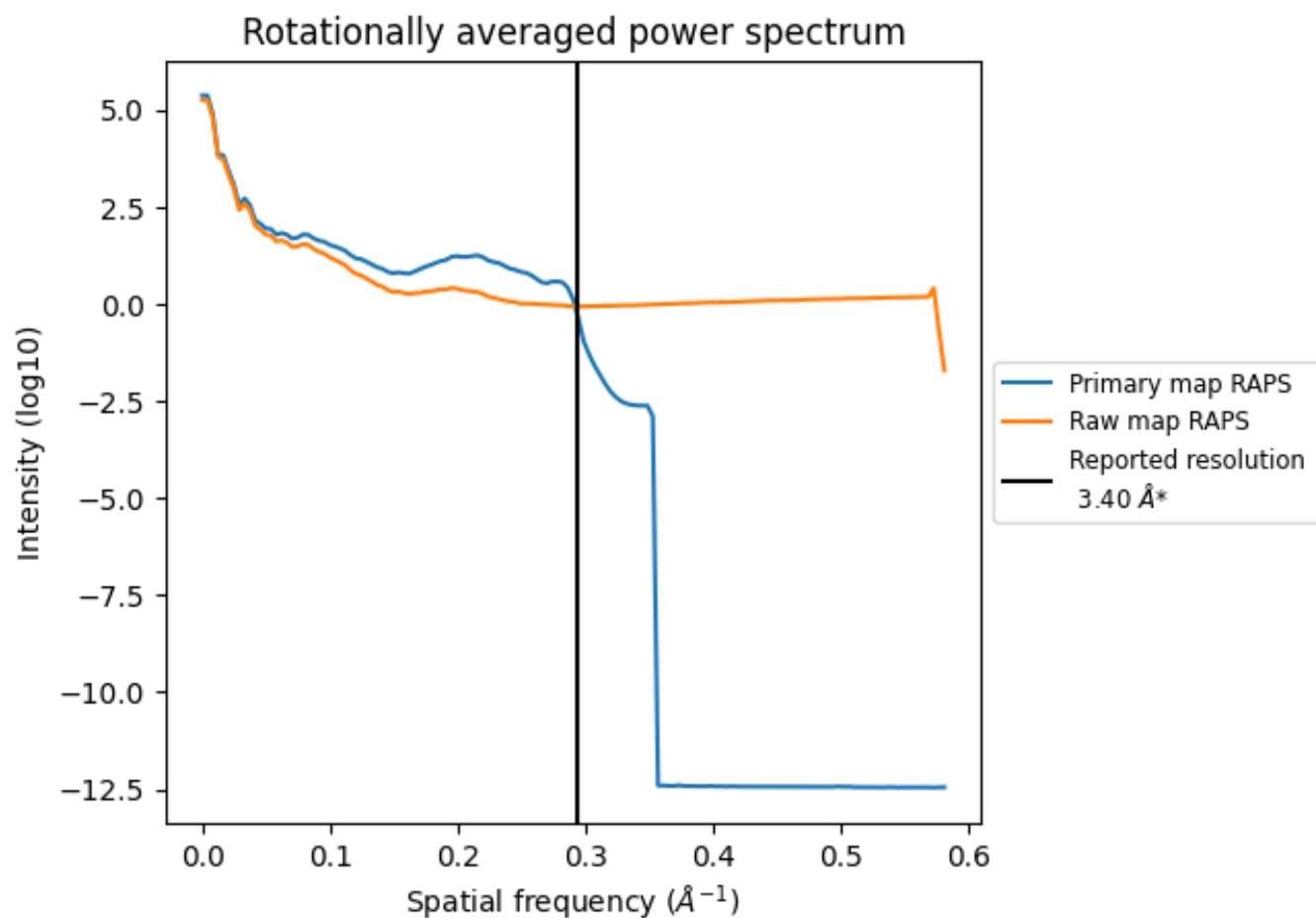
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 ⓘ

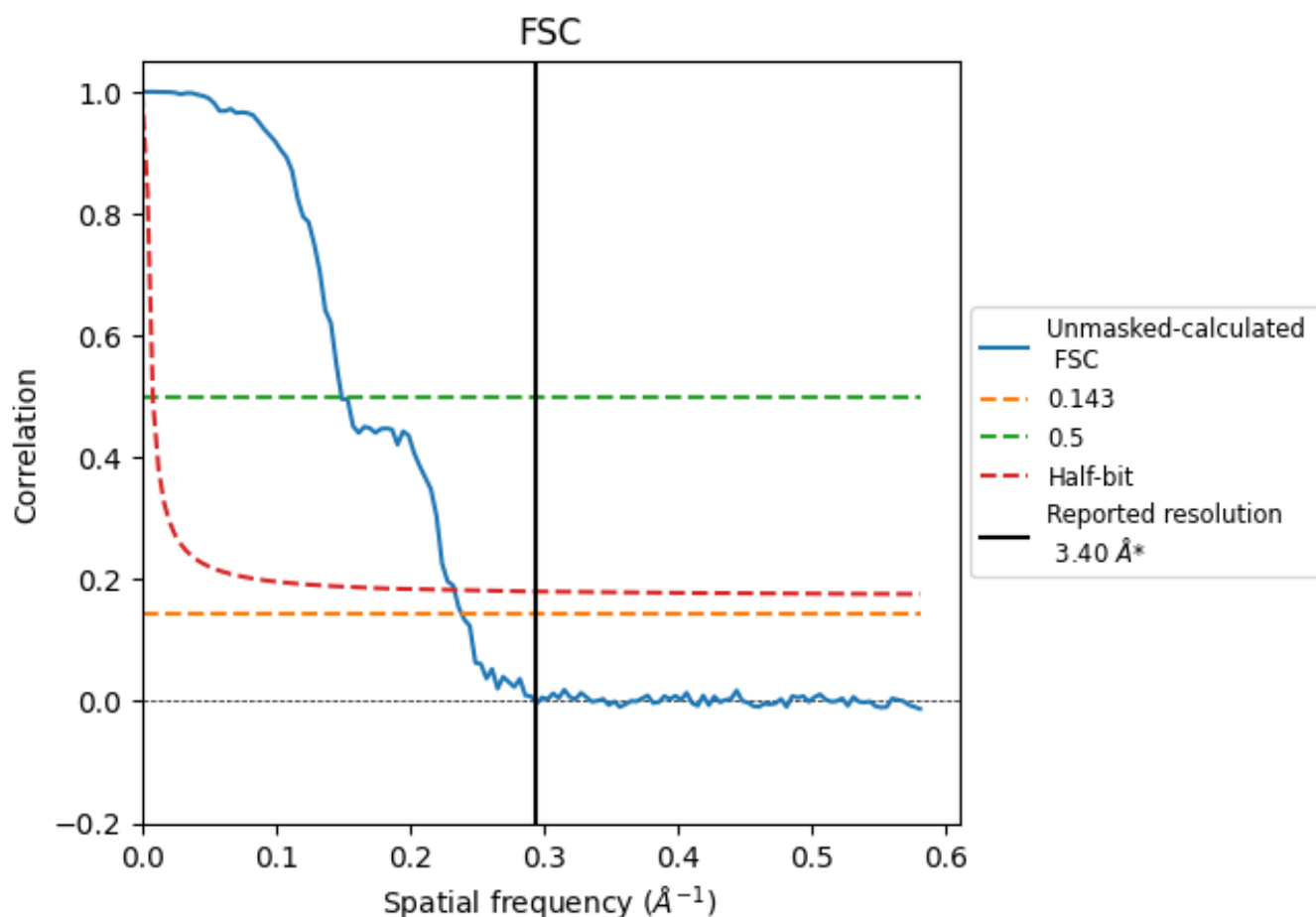


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	6.70	4.28

*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 4.18 differs from the reported value 3.4 by more than 10 %

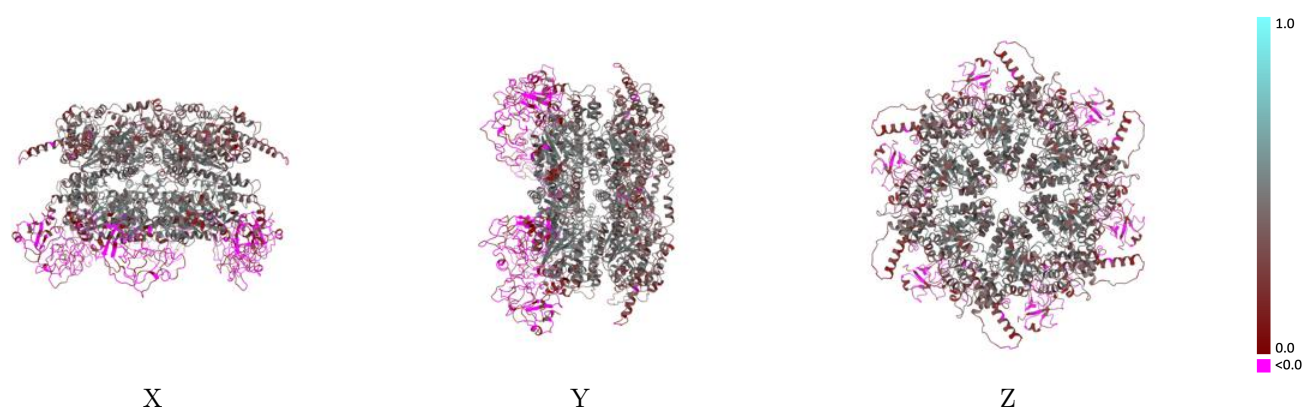
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-19473 and PDB model 8RS9. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

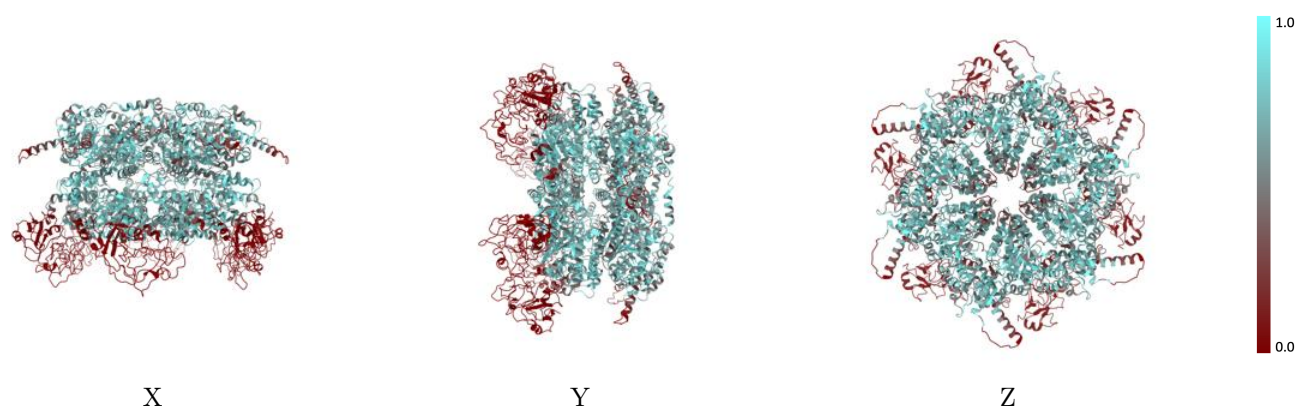
This section was not generated.

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



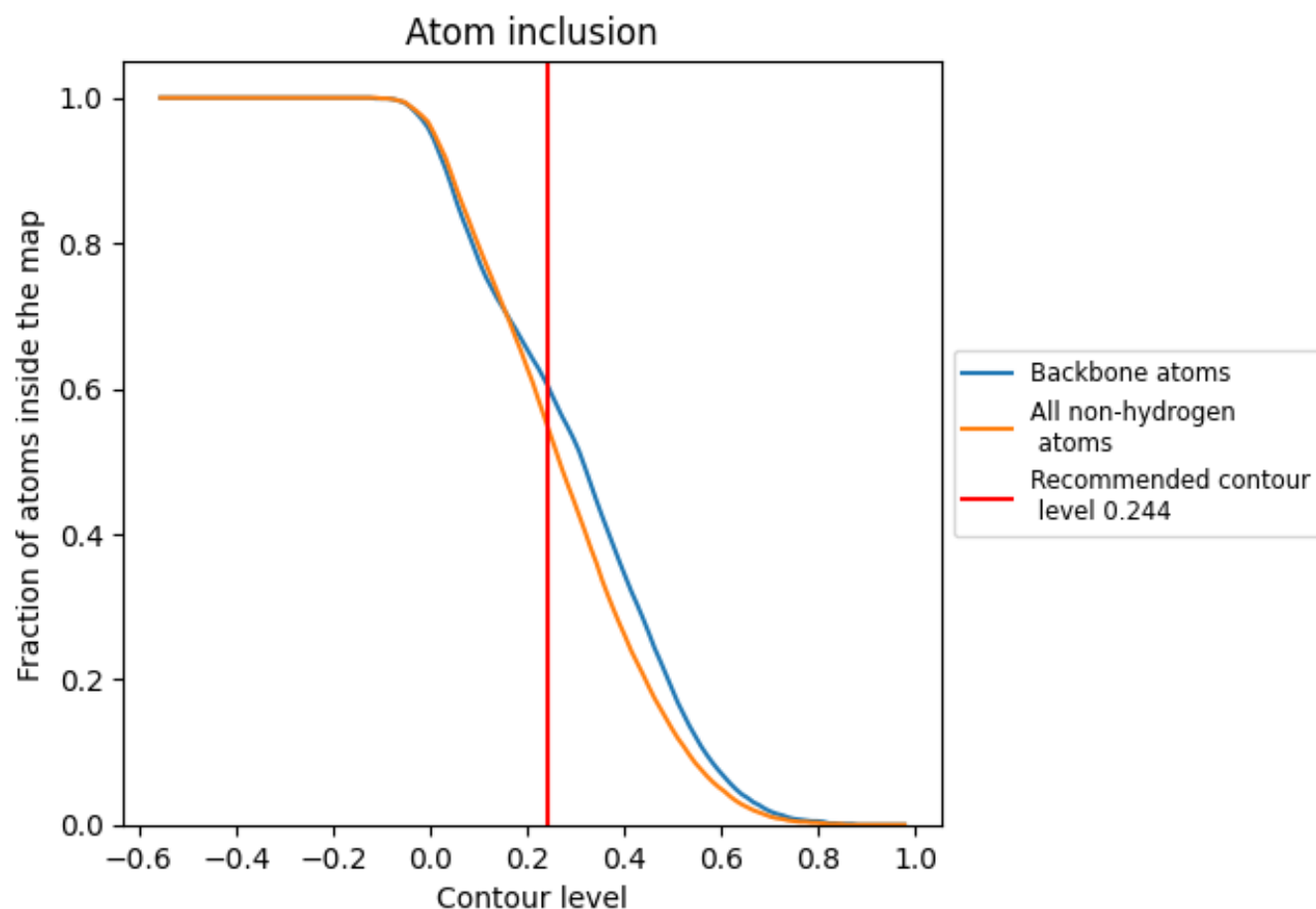
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.244).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 55% 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 (0.244) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5460	0.3350
A	0.5460	0.3350
B	0.5450	0.3340
C	0.5440	0.3360
D	0.5500	0.3340
E	0.5460	0.3360
F	0.5460	0.3340

1.0

0.0

<0.0