



Full wwPDB EM Validation Report ⓘ

May 20, 2024 – 10:48 am BST

PDB ID : 8RS9
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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

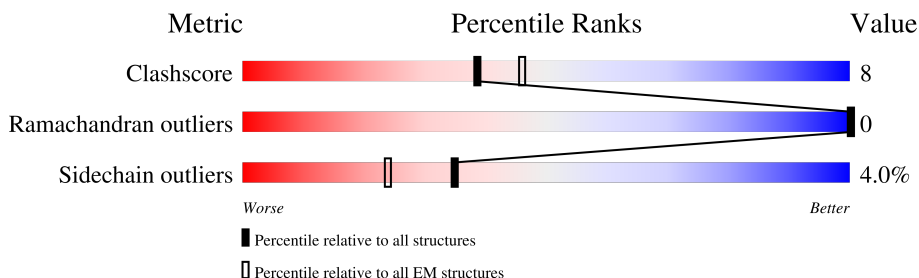
1 Overall quality at a glance i

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	806	
1	C	806	
1	D	806	
1	E	806	
1	F	806	

2 Entry composition

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

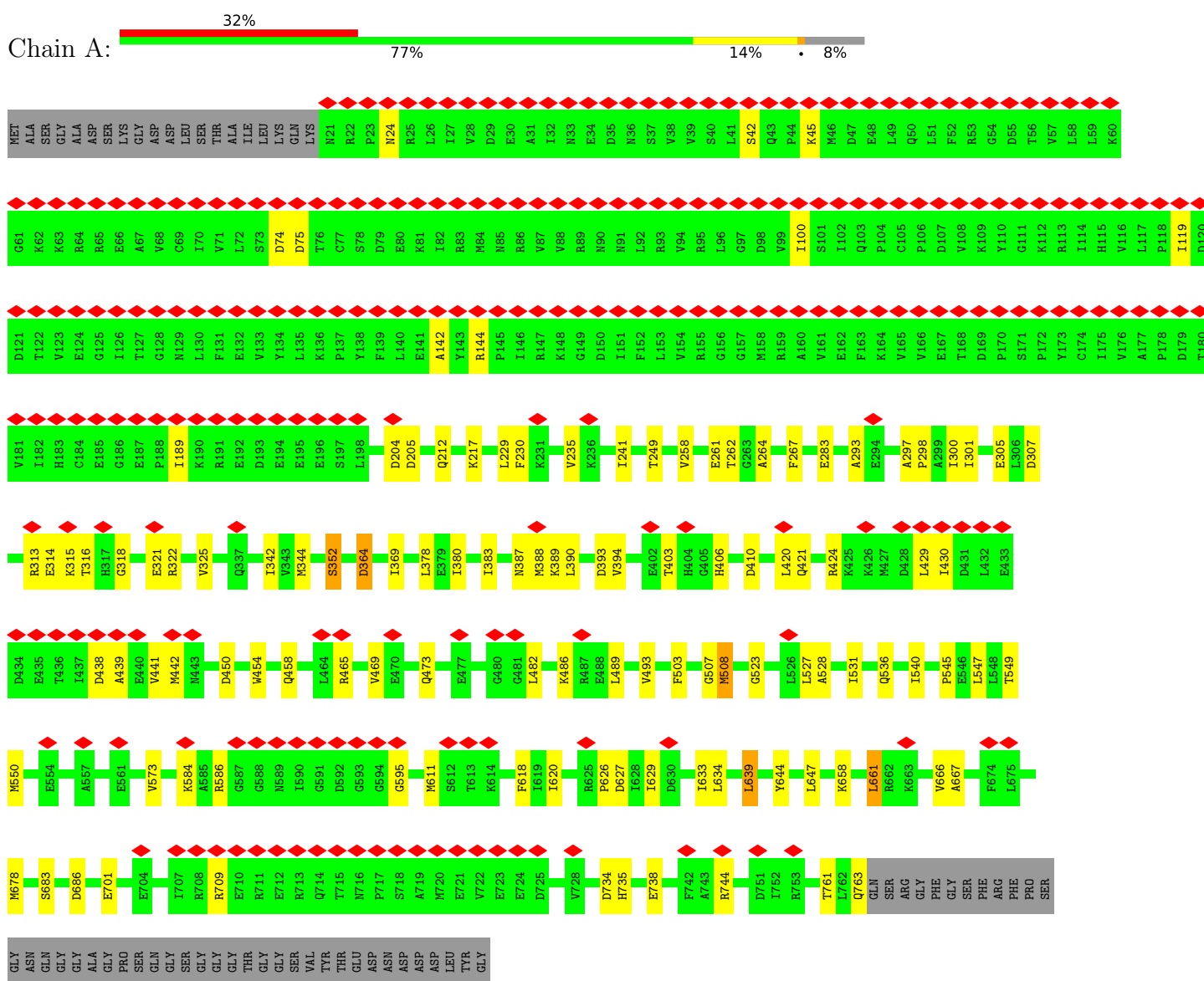
There are 12 discrepancies between the modelled and reference sequences:

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

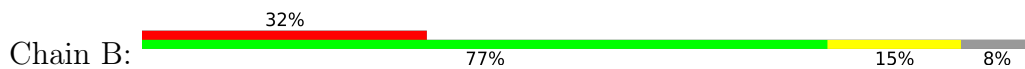
3 Residue-property plots

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: Transitional endoplasmic reticulum ATPase

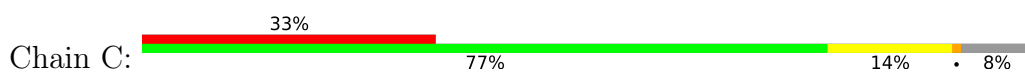


- Molecule 1: Transitional endoplasmic reticulum ATPase

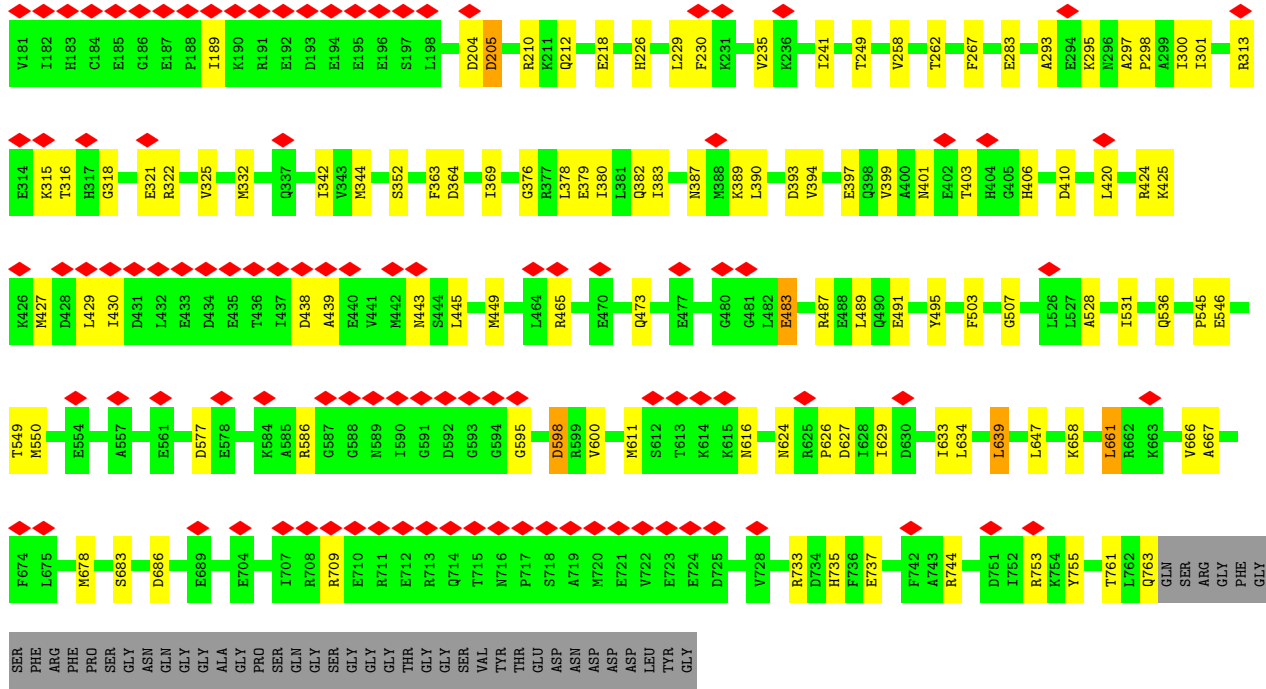


MET	ALA	SER	GLY	ALA	ASP	SER	LYS	GLY	ASP	ASP	LEU	SER	THR	ALA	LEU	LYS	GLN	LYS	N21	R22	P23	N24	R25	L26	I27	V28	D29	E30	A31	I32	N33	E34	D35	N36	S37	V38	V39	S40	L41	S42	Q43	P44	K45	M46	D47	E48	Q50	L51	F52	R53	G54	D55	T56	V57	L58	L59	K60	
G61	K62	K63	R64	R65	E66	A67	V68	C69	I70	V71	L72	S73	D74	D75	T76	C77	S78	D79	E80	K81	I82	R83	M84	N85	R86	V87	V88	R89	N90	N91	L92	R93	V94	R95	L96	G97	D98	V99	I100	S101	I102	Q103	P104	C105	P106	D107	V108	K109	G111	K112	R113	I114	H115	V116	L117	P118	I119	D120
D121	T122	V123	E124	G125	I126	T127	G128	M129	L130	F131	E132	V133	Y134	L135	K136	P137	Y138	F139	L140	E141	A142	Y143	R144	P145	I146	R147	K148	G149	D150	I151	F152	L153	V154	R155	G156	G157	M158	R159	A160	V161	E162	F163	K164	V165	V166	E167	T168	D169	P170	S171	P172	Y173	G174	I175	V176	A177	D178	T180
V181	I182	H183	C184	E185	G186	E187	P188	I189	K190	R191	E192	D193	E194	E195	E196	S197	L198	D204	D205	Q212	K217	E218	H226	L229	F230	K231	V235	K236	I241	T249	V258	E261	T262	G263	F265	A266	F267	E283	R287	E291	E292	A293	E294	A297														
P298	A299	I300	I301	R313	E314	K315	T316	H317	E321	R322	V325	Q337	I342	K343	K344	R349	S352	R362	F363	D364	I369	L378	E379	I380	I383	K388	K389	L390	A391	D392	D393	V394	V399	E402	T403	H404	G405	H406	L414	L420	Q421	A422	L423															
R424	K425	H426	H427	D428	L429	L430	D431	L432	E433	D434	E435	T436	L437	D438	A439	E440	V441	H442	H443	L464	R465	E470	Q473	V474	T475	H476	E477	G480	G481	D484	R487	E488	L489	L492	V493	F503	G507	H508	L526	L527	A528	I531	E534	G535	Q536	P545	E546											
T549	M550	E554	E561	V573	D577	K584	A585	R586	G587	G588	N589	I590	G591	D592	G593	G594	G595	E607	M611	S612	T613	K614	I620	R625	F626	D627	I628	I629	D630	L639	D640	I643	L647	L661	R662	K663	V666	G667	F674	L675	M678																	
S683	D686	E701	S702	I703	E704	I707	R708	R709	E710	R711	E712	R713	Q714	T715	N716	F717	S718	A719	M720	E721	V722	E723	E724	D725	V728	H735	F742	A743	R744	D751	I752	R753	M757	T761	L762	Q763	GLN	SER	ARG	GLY	PHE	GLY	SER	PHE	ARG	PRO	SER	GLY	ASN									

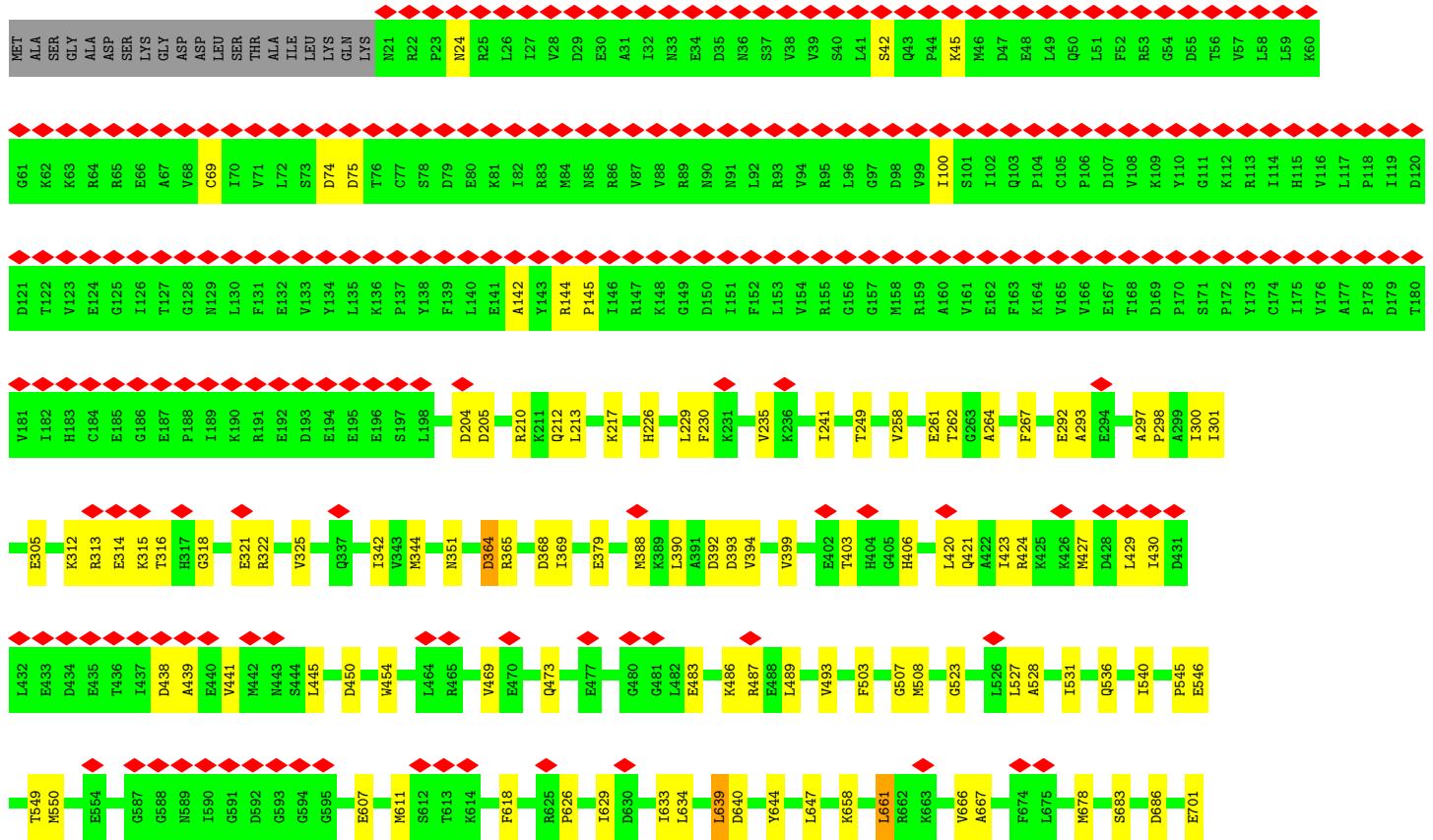
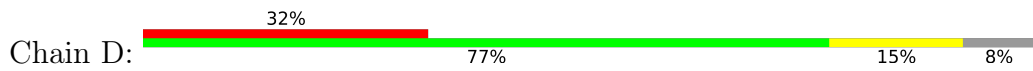
• Molecule 1: Transitional endoplasmic reticulum ATPase

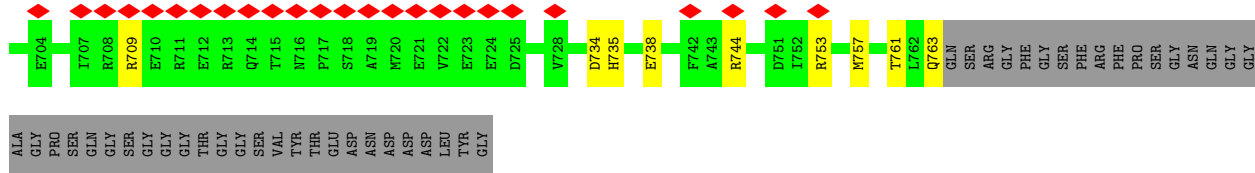


MET	ALA	SER	GLY	ALA	ASP	SER	LYS	GLY	ASP	ASP	LEU	SER	THR	ALA	LEU	LYS	GLN	LYS	N21	R22	P23	N24	R25	L26	I27	V28	D29	E30	A31	I32	N33	E34	D35	N36	S37	V38	V39	S40	L41	S42	Q43	P44	K45	M46	D47	E48	Q50	L51	F52	R53	G54	D55	T56	V57	L58	L59	K60	
G61	K62	K63	R64	R65	E66	A67	V68	C69	I70	V71	L72	S73	D74	D75	T76	C77	S78	D79	E80	K81	I82	R83	M84	N85	R86	V87	V88	R89	N90	N91	L92	R93	V94	R95	L96	G97	D98	V99	I100	S101	I102	Q103	P104	C105	P106	D107	V108	K109	G111	K112	R113	I114	H115	V116	L117	P118	I119	D120
D121	T122	V123	E124	G125	I126	T127	G128	M129	L130	F131	E132	V133	Y134	L135	K136	P137	Y138	F139	L140	E141	A142	Y143	R144	P145	I146	R147	K148	G149	D150	I151	F152	L153	V154	R155	G156	G157	M158	R159	A160	V161	E162	F163	K164	V165	V166	E167	T168	D169	P170	S171	P172	Y173	G174	I175	V176	A177	D178	T180

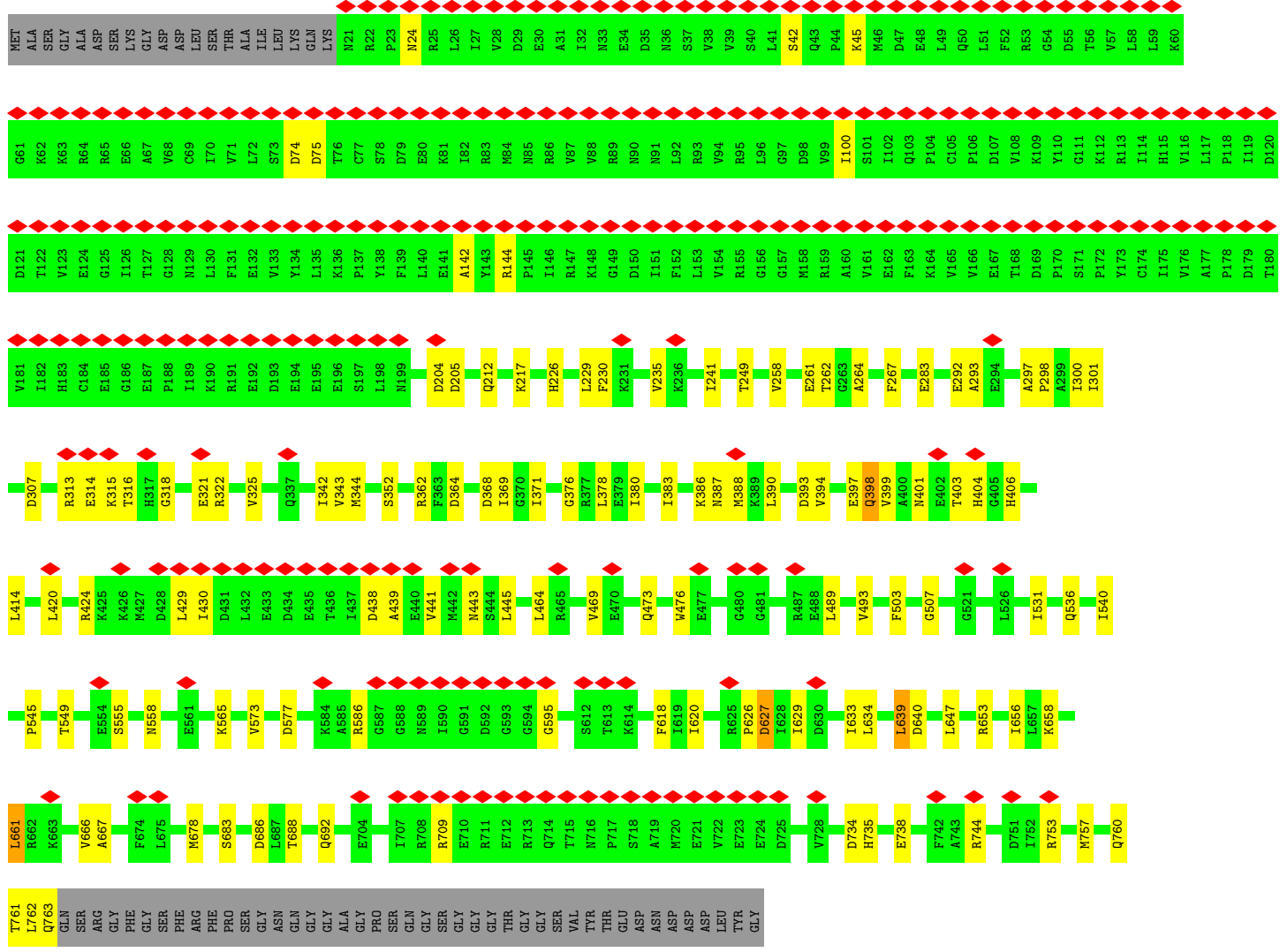
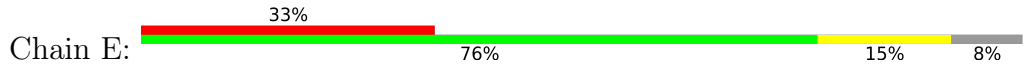


• Molecule 1: Transitional endoplasmic reticulum ATPase

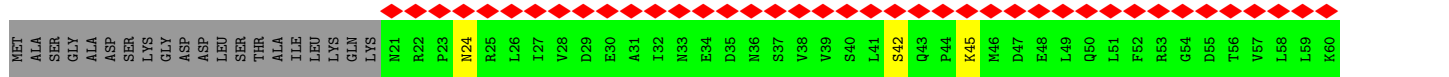
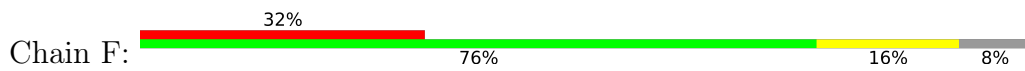




• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



G61	K62	K63	R64	R65	E66	A67	V68	C69	I70	V71	L72	S73	D74	D75	T76	C77	S78	D79	E80	K81	I82	R83	M84	N85	R86	V87	V88	R89	N90	N91	L92	R93	V94	R95	L96	G97	D98	V99	I100	S101	I102	Q103	P104	C105	P106	D107	V108	K109	Y110	F163	K164	V165	V166	E167	T168	D169	P170	S171	P172	C174	I175	V176	A177	P178	D179	T180																																																																				
V181	I182	H183	C184	E185	G186	E187	P188	I189	K190	R191	E192	D193	E194	E195	E196	S197	L198	D204	D205	I206	Q212	L213	A214	Q215	M219	H226	L229	F230	K231	V235	K236	I241	T249	V258	T262	F265	A266	F267	E283	A293	E294	A297	P298	I301	R313	E314	K315	T316	H317	G318	E321	R322	V325	M332	Q337	I342	S352	F363	D364	I369	G376	R377	L378	E379	I380	I383	M388	K389	L390	D393	V394	E397	Q398	V399	A400	N401	E402	T403	H404	G405	H406	D410	C415	A419	L420	Q421	A422	L423	R424	K426	M427	D428	L429	I430	D431	L432	E433	D434	E435	T436	L437	D438	A439	E440	V441	M442	N443	S444	L445	A446	V447	D450	D451	F452	R453	W454	L464	R465	E470	Q473	E477	G480	G481	E488	L489	F503	L504	K505	F506	G507	M508	L526	I531	Q536
K543	G544	P545	T549	M550	E554	S555	E556	A557	N558	E561	D577	K584	G587	G588	N589	I590	G591	D592	G593	G594	G595	M611	S612	T613	K614	F618	N624	R625	D627	I628	D630	L633	L634	L639	D640	L643	Y644	L647	R653	T656	L657	K658																																																																																												
L661	R662	K663	V666	A667	K668	F674	L675	S683	D686	Q692	E701	E704	I707	R708	R709	E710	R711	E712	R713	Q714	T715	N716	F717	S718	A719	M720	E721	V722	E723	E724	D725	V726	R733	D734	H735	F736	E737	E738	F742	A743	R744	D751	I752	R753	K754	Y755																																																																																								
E756	H757	T761	L762	Q763	GLN	SER	ARG	GLY	PHE	ARG	PHE	PRO	SER	GLY	ASN	GLN	GLY	GLY	ALA	GLY	PRO	SER	GLN	GLY	SER	GLY	GLY	THR	GLY	GLY	VAL	TYR	THR	GLU	ASP	ASN	ASP	ASP	ASP	ASP	LEU	TYR	GLY																																																																																											

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 (\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 (\AA)	0.86, 0.86, 0.86	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	0.26	0/5318	0.53	0/7222
1	B	0.26	0/5312	0.53	0/7214
1	C	0.26	0/5314	0.53	0/7217
1	D	0.26	0/5197	0.53	0/7069
1	E	0.26	0/5316	0.54	0/7219
1	F	0.26	0/5318	0.54	0/7222
All	All	0.26	0/31775	0.53	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

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	81	0
1	B	5242	0	4738	89	0
1	C	5244	0	4745	79	0
1	D	5131	0	4543	81	0
1	E	5246	0	4744	85	0
1	F	5248	0	4751	85	0
All	All	31359	0	28272	471	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 (471) 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: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
1:F:241:ILE:HD11	1:F:342:ILE:HD11	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:F:321:GLU:O	1:F:325:VAL:HG23	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:142:ALA:O	1:C:144:ARG:N	2.36	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: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: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: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
1:B:536:GLN:O	1:B:536:GLN:NE2	2.41	0.54
1:F:313:ARG:HA	1:F:316:THR:HG22	1.88	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:E:217:LYS:NZ	1:E:261:GLU:OE1	2.40	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:217:LYS:HZ1	1:B:261:GLU:CD	2.13	0.51
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: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
1:D:213:LEU:O	1:D:217:LYS:HG2	2.11	0.50
1:A:744:ARG:HH12	1:B:762:LEU:HA	1.77	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: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: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:C:438:ASP:OD1	1:C:439:ALA:N	2.42	0.49
1:D:292:GLU:HA	1:D:292:GLU:OE2	2.13	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:C:364:ASP:OD1	1:C:364:ASP:N	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:HD2	1:B:425:LYS:C	2.34	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: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
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: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:A:205:ASP:C	1:A:205:ASP:OD1	2.52	0.47
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: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:332:MET:HE3	1:F:363:PHE:CE1	2.50	0.47
1:F:734:ASP:HA	1:F:737:GLU:OE2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:503:PHE:O	1:A:507:GLY:N	2.48	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:CG	1:C:536:GLN:O	2.64	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: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:D:217:LYS:HZ1	1:D:261:GLU:CD	2.18	0.46
1:A:429:LEU:C	1:A:430:ILE:HD12	2.36	0.45
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLN:CG	1:A:536:GLN:O	2.64	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:420:LEU:HD21	1:E:235:VAL:HG21	1.99	0.45
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:C:429:LEU:C	1:C:430:ILE:HD12	2.37	0.45
1:C:577:ASP:OD1	1:C:577:ASP:N	2.48	0.45
1:D:429:LEU:C	1:D:430:ILE:HD12	2.37	0.45
1:A:403:THR:HG22	1:A:406:HIS:CG	2.52	0.45
1:E:429:LEU:C	1:E:430:ILE:HD12	2.38	0.44
1:E:586:ARG:NH2	1:E:595:GLY:O	2.49	0.44
1:D:393:ASP:N	1:D:393:ASP:OD1	2.47	0.44
1:F:403:THR:HG22	1:F:406:HIS:CG	2.53	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:429:LEU:C	1:F:430:ILE:HD12	2.37	0.44
1:F:447:VAL:HG11	1:F:452:PHE:HE1	1.83	0.44
1:A:536:GLN:O	1:A:536:GLN:HG2	2.16	0.44
1:F:314:GLU:H	1:F:314:GLU:CD	2.20	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:E:205:ASP:OD1	1:E:205:ASP:C	2.56	0.44
1:E:403:THR:HG22	1:E:406:HIS:CG	2.53	0.44
1:B:586:ARG:NH2	1:B:595:GLY:O	2.51	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:CG	1:E:536:GLN:O	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:314:GLU:H	1:E:314:GLU:CD	2.21	0.43
1:A:283:GLU:OE2	1:A:283:GLU:N	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:MET:HE1	1:F:692:GLN:O	2.19	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
1:E:445:LEU:C	1:E:445:LEU:HD23	2.39	0.43
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:C:425:LYS:HD2	1:C:425:LYS:C	2.39	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: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: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:B:429:LEU:C	1:B:430:ILE:HD12	2.39	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: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:E:469:VAL:CG1	1:E:565:LYS:HZ1	2.32	0.42
1:F:427:MET:CE	1:F:445:LEU:HD12	2.48	0.42
1:A:573:VAL:CG1	1:A:620:ILE:HD12	2.50	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:E:390:LEU:HD12	1:E:390:LEU:H	1.84	0.42

Continued on next page...

Continued from previous page...

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: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:442:MET:CE	1:B:442:MET:O	2.68	0.42
1:C:295:LYS:O	1:C:295:LYS:HG2	2.18	0.42
1:D:489:LEU:O	1:D:493:VAL:HG12	2.20	0.42
1:F:332:MET:CE	1:F:363:PHE:CE1	3.03	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:205:ASP:OD1	1:B:205:ASP:C	2.58	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:N	1:C:410:ASP:OD1	2.53	0.41
1:E:217:LYS:HZ1	1:E:261:GLU:CD	2.23	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:F:733:ARG:O	1:F:734:ASP:C	2.58	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: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: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

Continued on next page...

Continued from previous page...

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:D:314:GLU:H	1:D:314:GLU:CD	2.20	0.41
1:A:547:LEU:HA	1:A:550:MET:HE3	2.03	0.41
1:A:666:VAL:HG12	1:A:667:ALA:O	2.20	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:A:235:VAL:CG2	1:F:420:LEU:HD21	2.51	0.41
1:B:74:ASP:O	1:B:75:ASP:CB	2.68	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:217:LYS:NZ	1:D:261:GLU:OE1	2.51	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: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:A:438:ASP:O	1:A:441:VAL:HG22	2.20	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: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
1:C:449:MET:SD	1:C:449:MET:C	2.99	0.40
1:D:69:CYS:HA	1:D:145:PRO:O	2.22	0.40
1:D:427:MET:CE	1:D:445:LEU:HD12	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:442:MET:O	1:B:442:MET:HE3	2.22	0.40
1:C:399:VAL:O	1:C:403:THR:OG1	2.39	0.40
1:C:427:MET:CE	1:C:445:LEU:HD12	2.52	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: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:D:205:ASP:OD1	1:D:205:ASP:C	2.60	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:427:MET:HE3	1:F:445:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/806 (92%)	670 (90%)	71 (10%)	0	100	100
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	463/676 (68%)	444 (96%)	19 (4%)	30	59
1	B	461/676 (68%)	445 (96%)	16 (4%)	36	65
1	C	462/676 (68%)	444 (96%)	18 (4%)	32	61
1	D	430/676 (64%)	410 (95%)	20 (5%)	26	57
1	E	462/676 (68%)	443 (96%)	19 (4%)	30	59
1	F	463/676 (68%)	444 (96%)	19 (4%)	30	59
All	All	2741/4056 (68%)	2630 (96%)	111 (4%)	35	60

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	PHE
1	A	315	LYS
1	A	352	SER
1	A	364	ASP
1	A	388	MET
1	A	424	ARG
1	A	442	MET
1	A	450	ASP
1	A	508	MET
1	A	584	LYS
1	A	611	MET
1	A	618	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	639	LEU
1	A	644	TYR
1	A	661	LEU
1	A	678	MET
1	A	701	GLU
1	A	709	ARG
1	A	735	HIS
1	B	218	GLU
1	B	226	HIS
1	B	265	PHE
1	B	267	PHE
1	B	315	LYS
1	B	388	MET
1	B	424	ARG
1	B	584	LYS
1	B	611	MET
1	B	627	ASP
1	B	639	LEU
1	B	661	LEU
1	B	678	MET
1	B	709	ARG
1	B	735	HIS
1	B	744	ARG
1	C	205	ASP
1	C	218	GLU
1	C	226	HIS
1	C	267	PHE
1	C	315	LYS
1	C	352	SER
1	C	424	ARG
1	C	443	ASN
1	C	483	GLU
1	C	491	GLU
1	C	598	ASP
1	C	611	MET
1	C	616	ASN
1	C	639	LEU
1	C	661	LEU
1	C	678	MET
1	C	709	ARG
1	C	735	HIS
1	D	226	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	267	PHE
1	D	315	LYS
1	D	364	ASP
1	D	365	ARG
1	D	368	ASP
1	D	388	MET
1	D	424	ARG
1	D	450	ASP
1	D	486	LYS
1	D	508	MET
1	D	611	MET
1	D	618	PHE
1	D	639	LEU
1	D	644	TYR
1	D	661	LEU
1	D	678	MET
1	D	701	GLU
1	D	709	ARG
1	D	735	HIS
1	E	226	HIS
1	E	267	PHE
1	E	315	LYS
1	E	364	ASP
1	E	368	ASP
1	E	398	GLN
1	E	404	HIS
1	E	424	ARG
1	E	443	ASN
1	E	476	TRP
1	E	618	PHE
1	E	627	ASP
1	E	639	LEU
1	E	661	LEU
1	E	678	MET
1	E	709	ARG
1	E	735	HIS
1	E	744	ARG
1	E	760	GLN
1	F	205	ASP
1	F	226	HIS
1	F	267	PHE
1	F	315	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	352	SER
1	F	364	ASP
1	F	388	MET
1	F	415	CYS
1	F	424	ARG
1	F	450	ASP
1	F	508	MET
1	F	584	LYS
1	F	611	MET
1	F	618	PHE
1	F	639	LEU
1	F	644	TYR
1	F	661	LEU
1	F	674	PHE
1	F	709	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

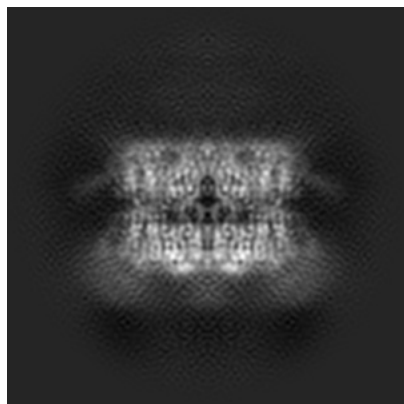
6 Map visualisation [i](#)

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.

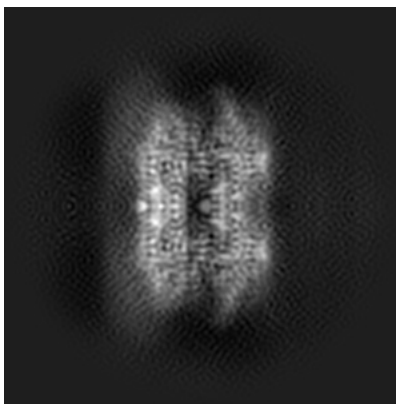
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

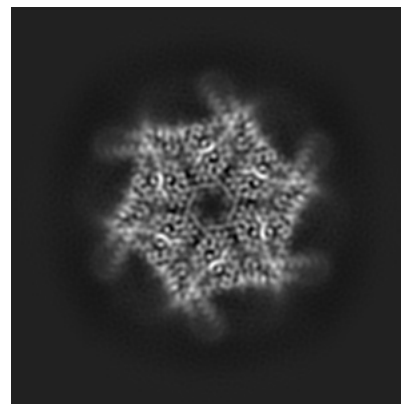
6.1.1 Primary map



X

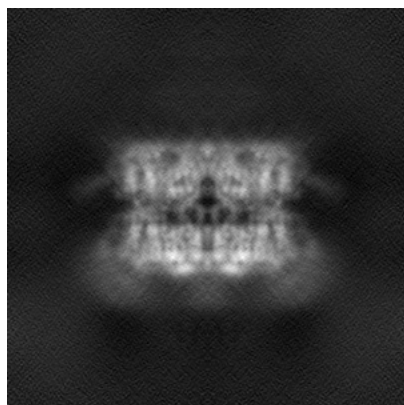


Y

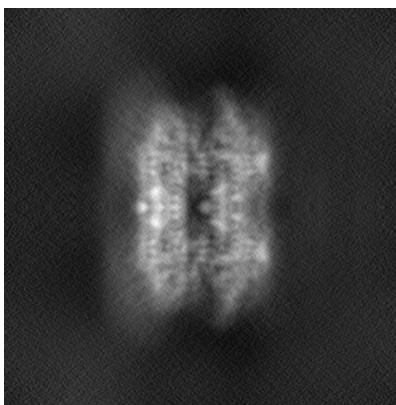


Z

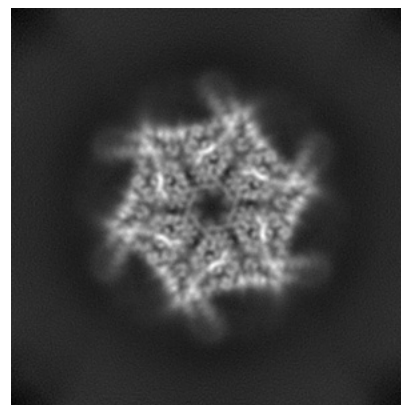
6.1.2 Raw map



X



Y

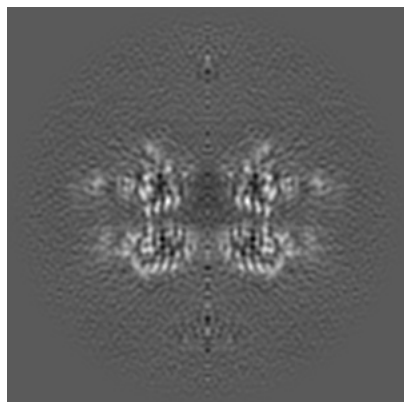


Z

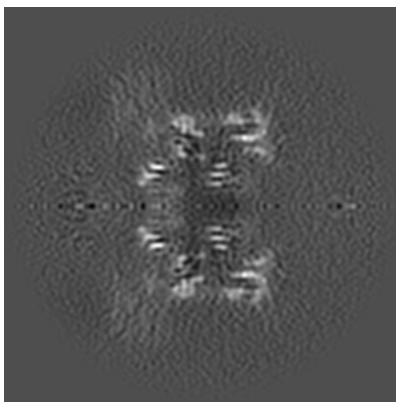
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

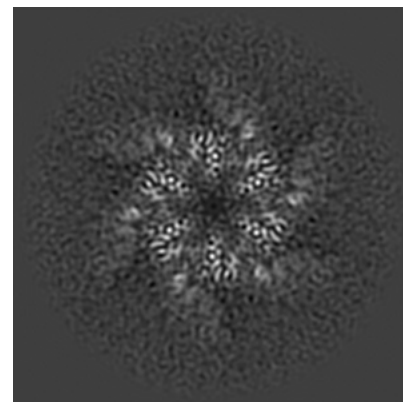
6.2.1 Primary map



X Index: 140

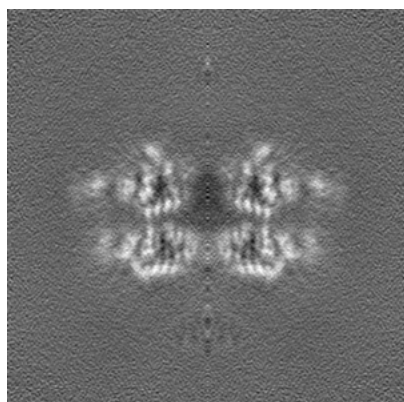


Y Index: 140

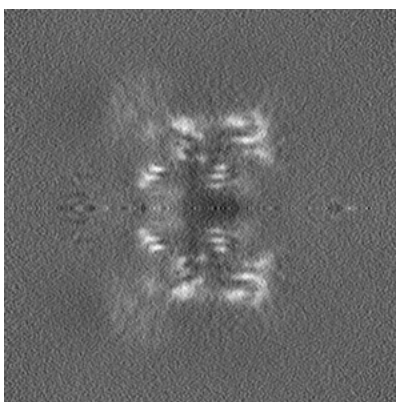


Z Index: 140

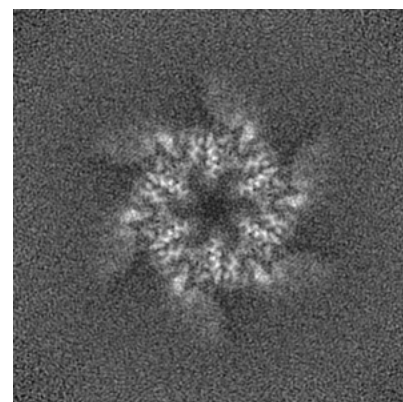
6.2.2 Raw map



X Index: 140



Y Index: 140

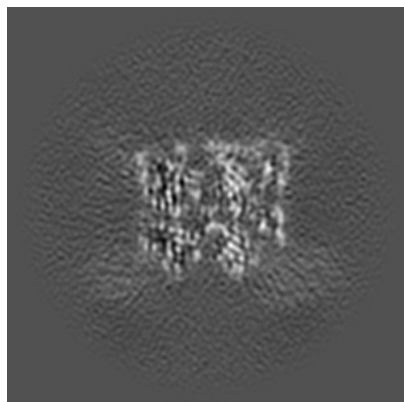


Z Index: 140

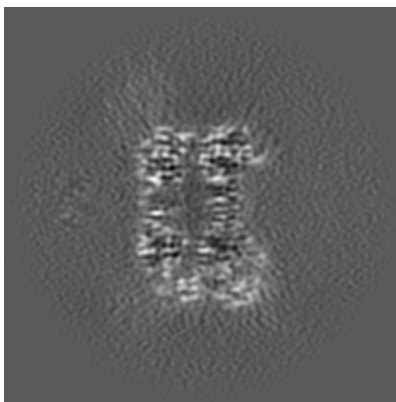
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

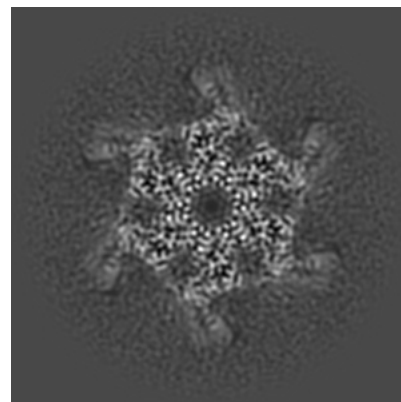
6.3.1 Primary map



X Index: 104

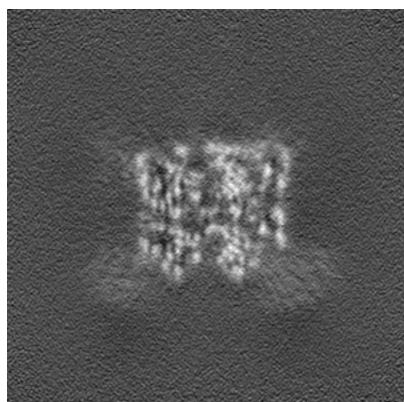


Y Index: 123

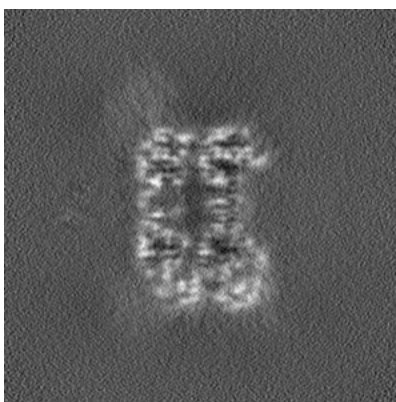


Z Index: 152

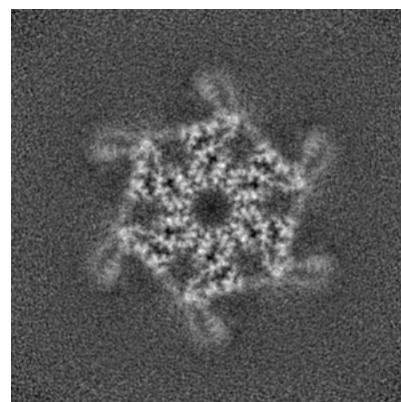
6.3.2 Raw map



X Index: 104



Y Index: 123

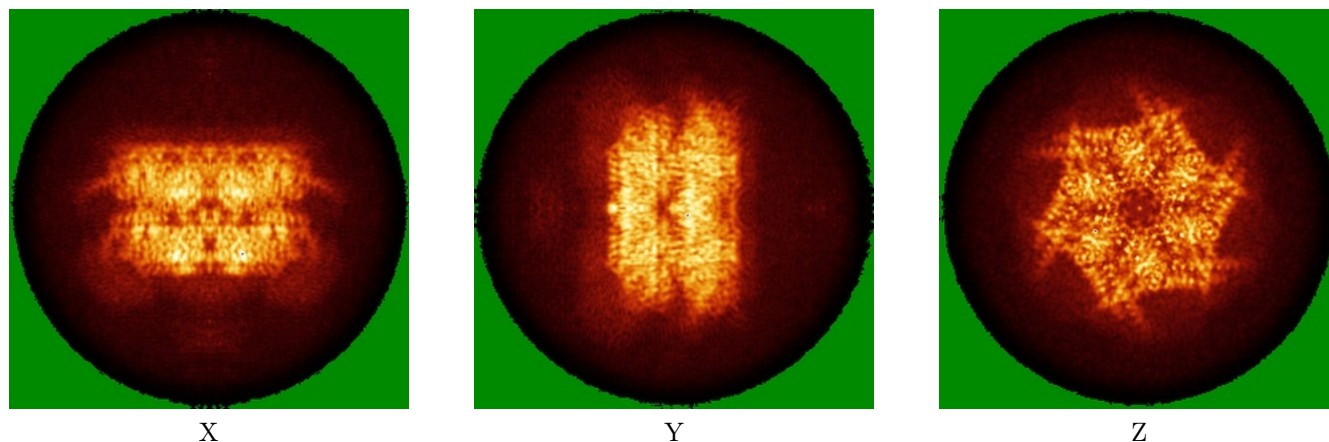


Z Index: 152

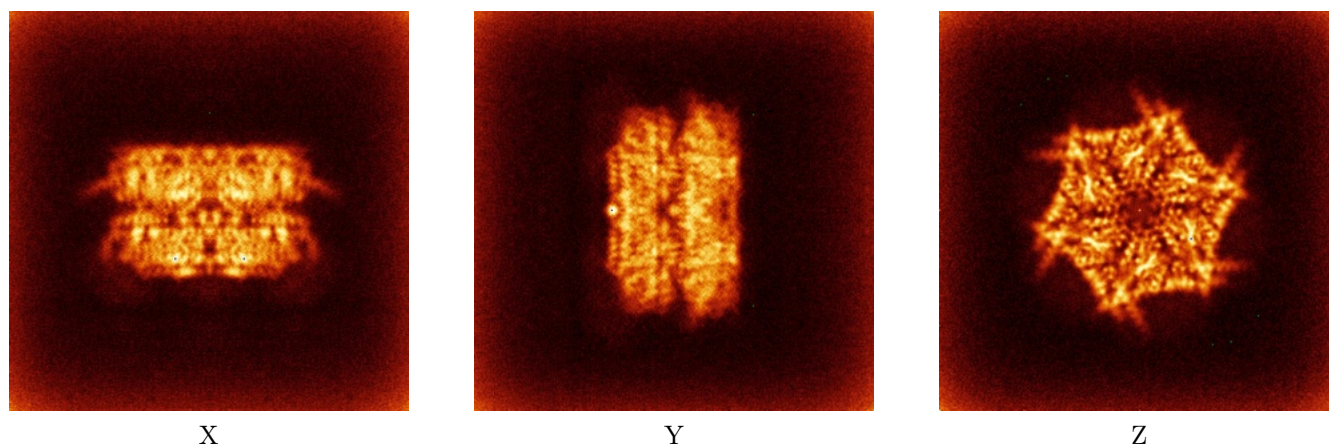
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



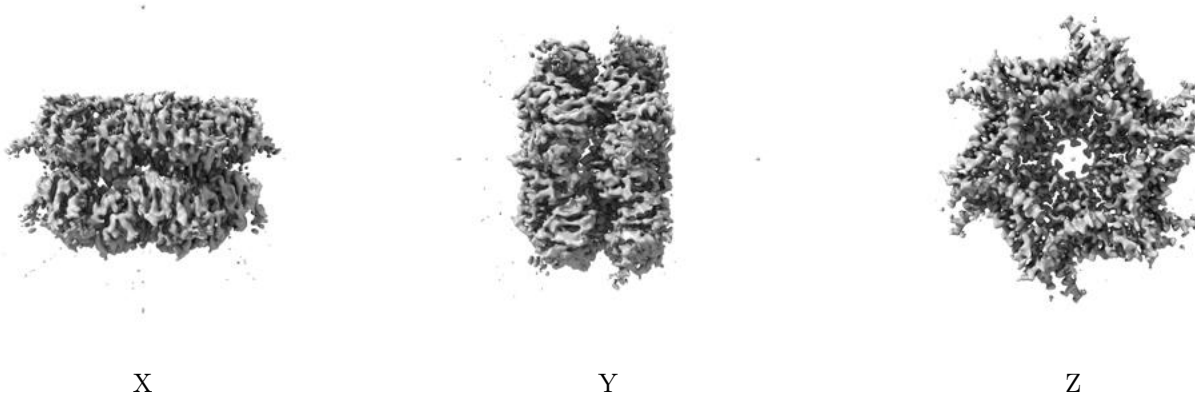
6.4.2 Raw map



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.

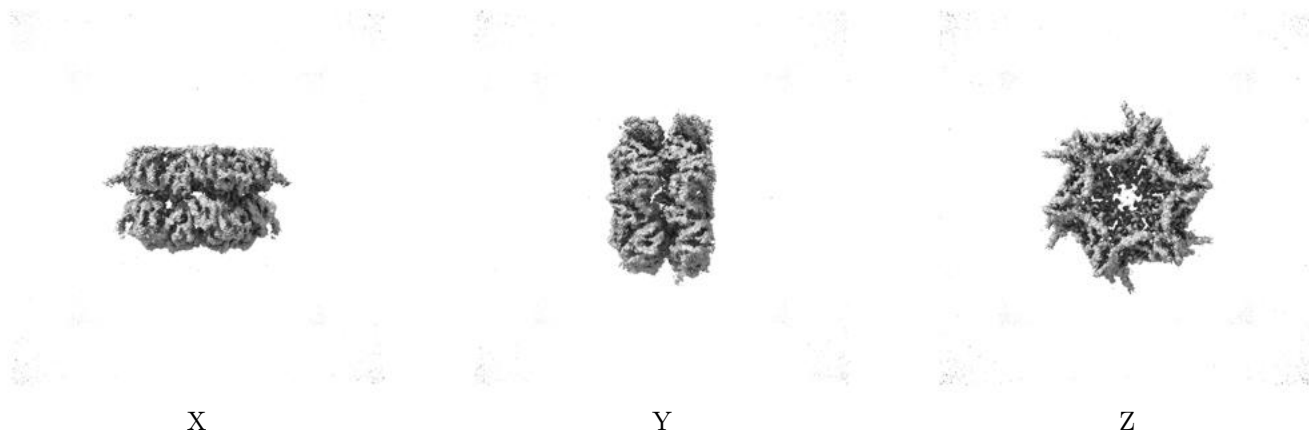
6.5 Orthogonal surface views [i](#)

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.

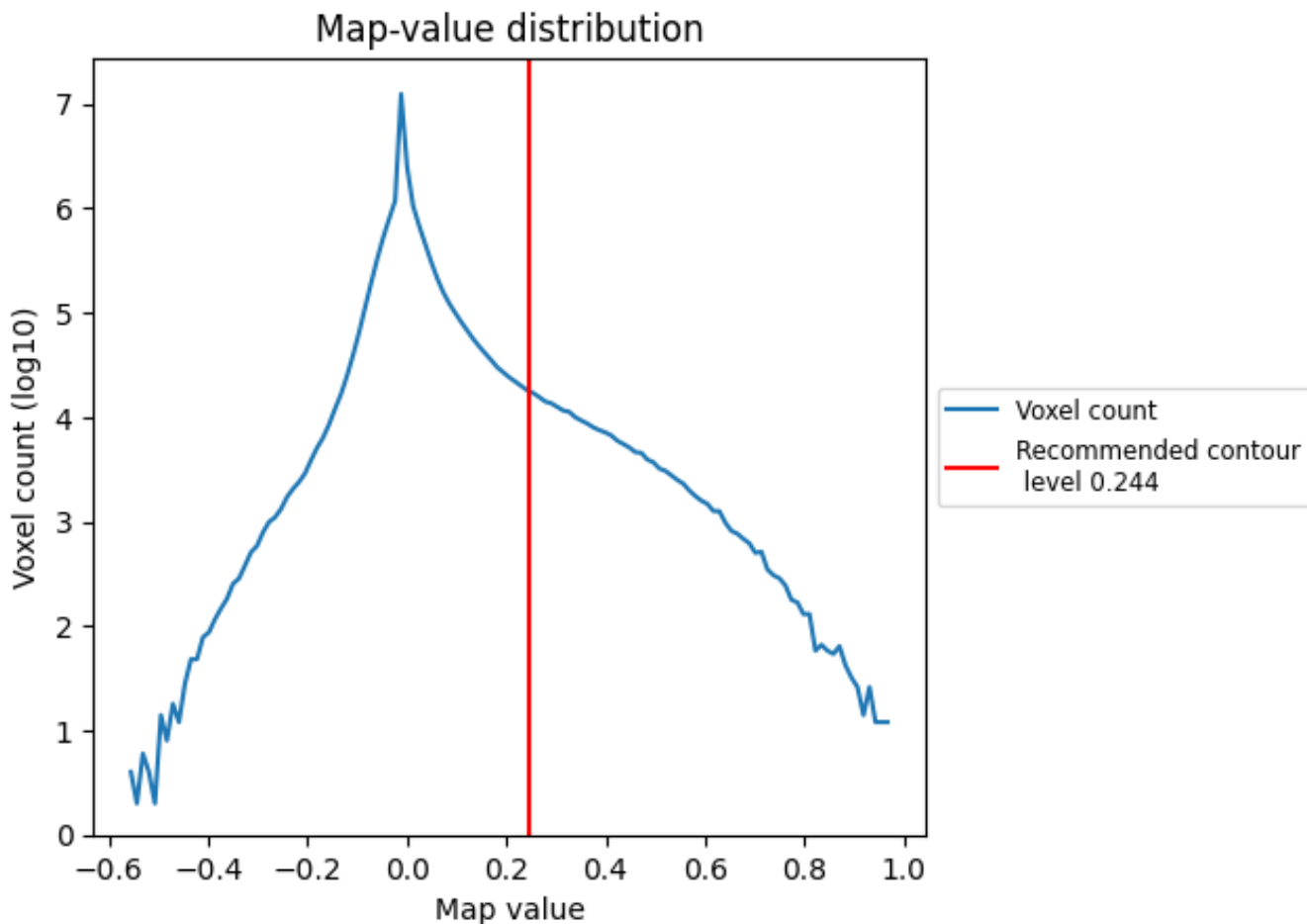
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

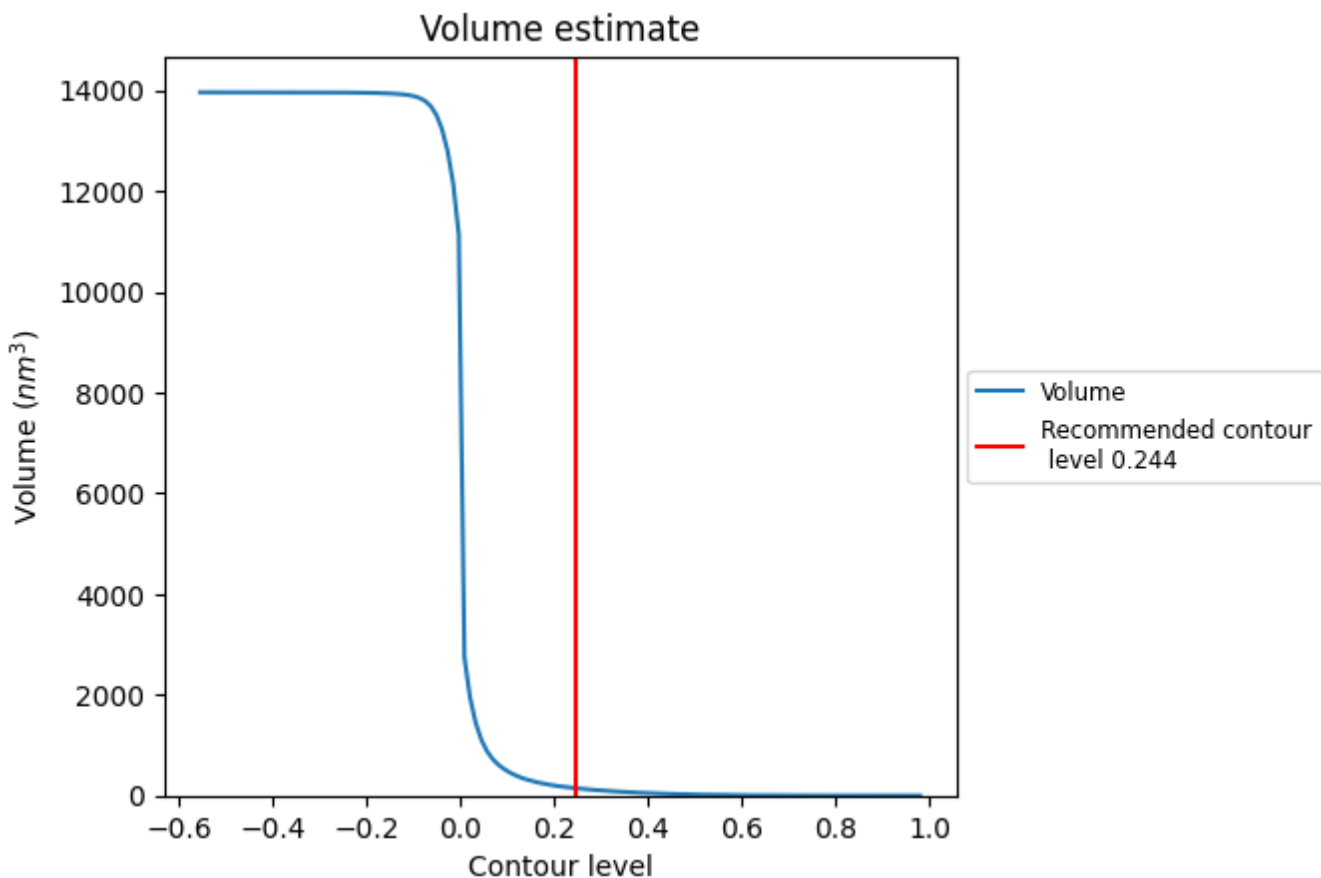
This section contains the results of statistical analysis of the map.

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.

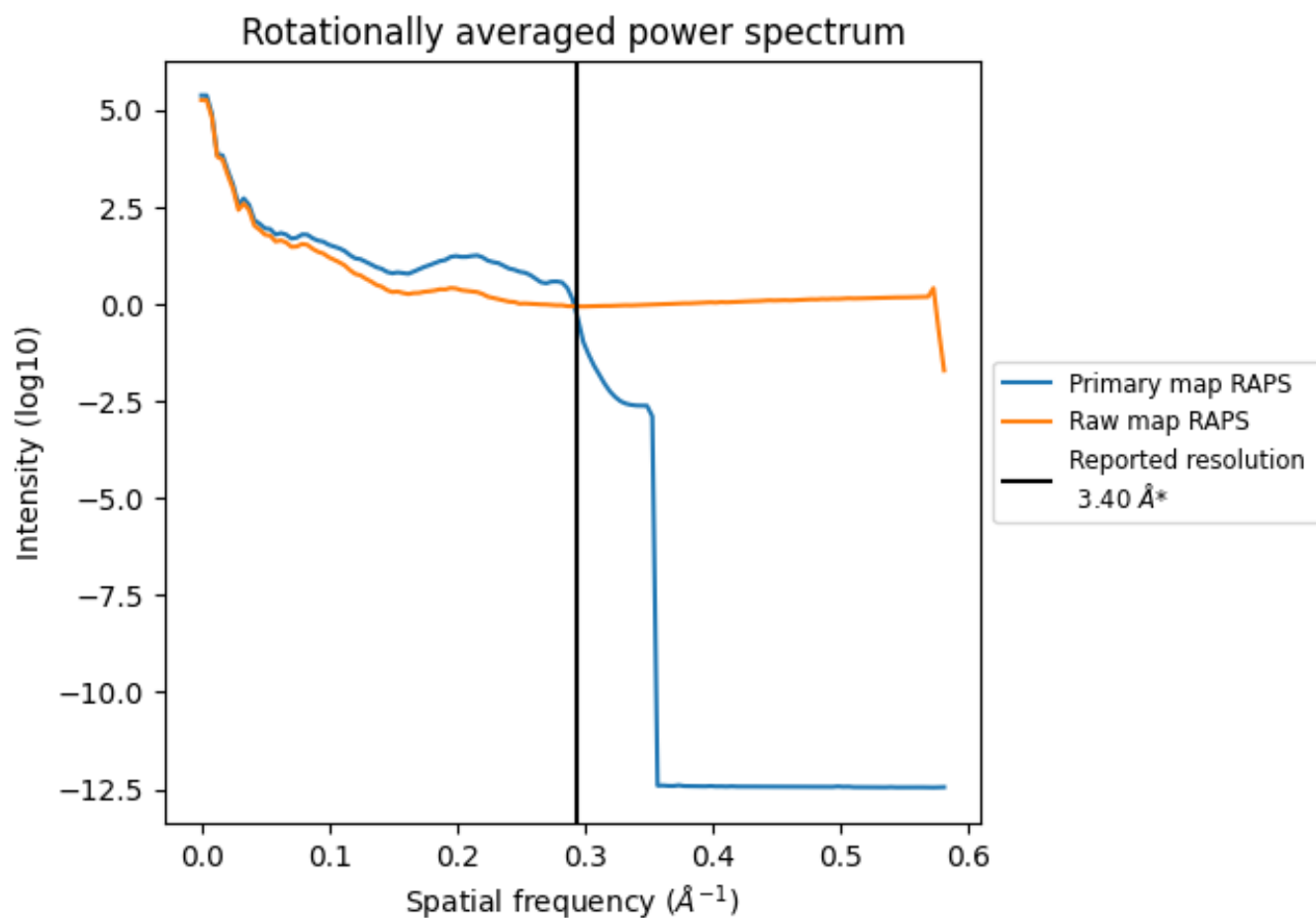
7.2 Volume estimate [i](#)



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 [i](#)

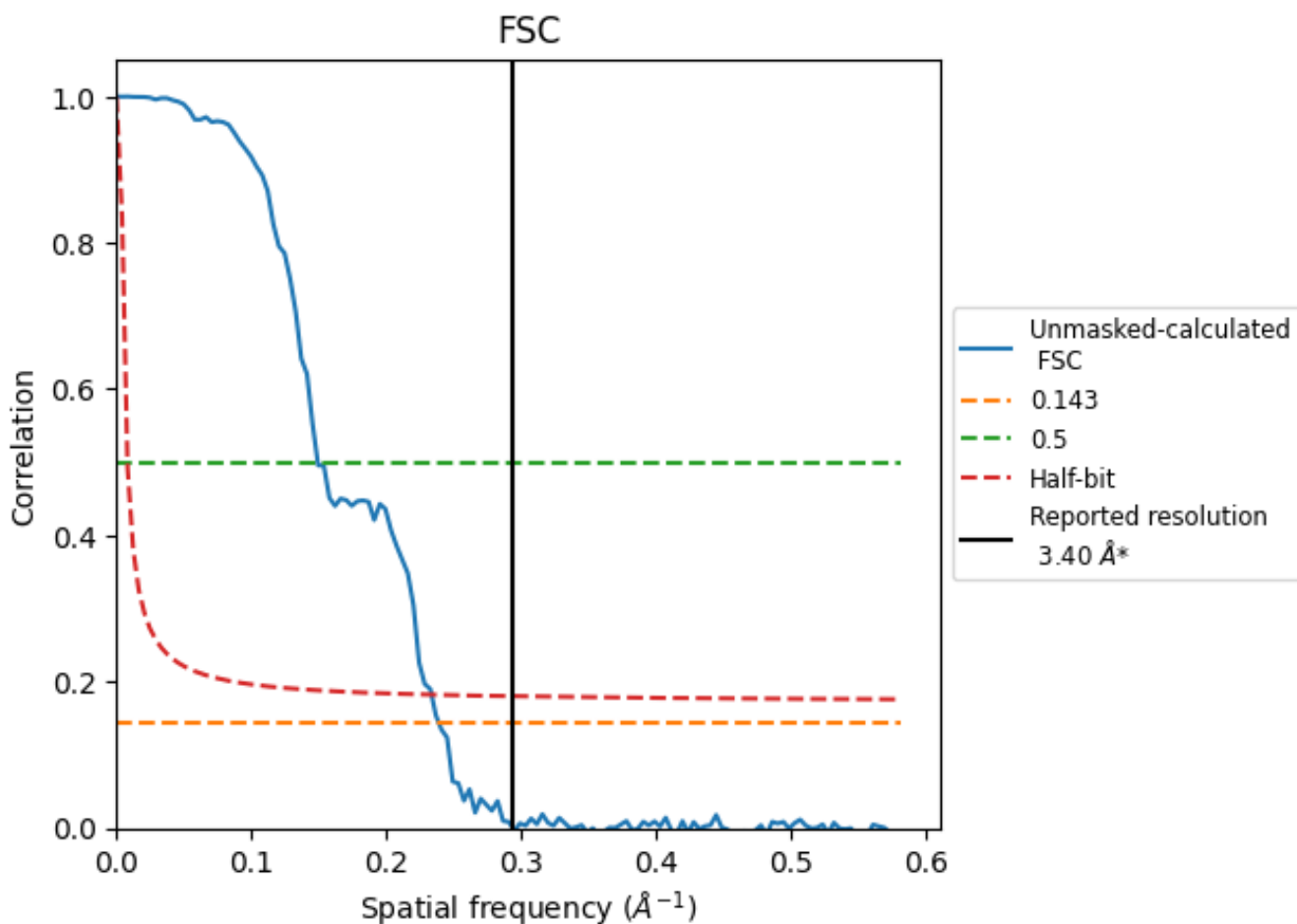


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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](#)

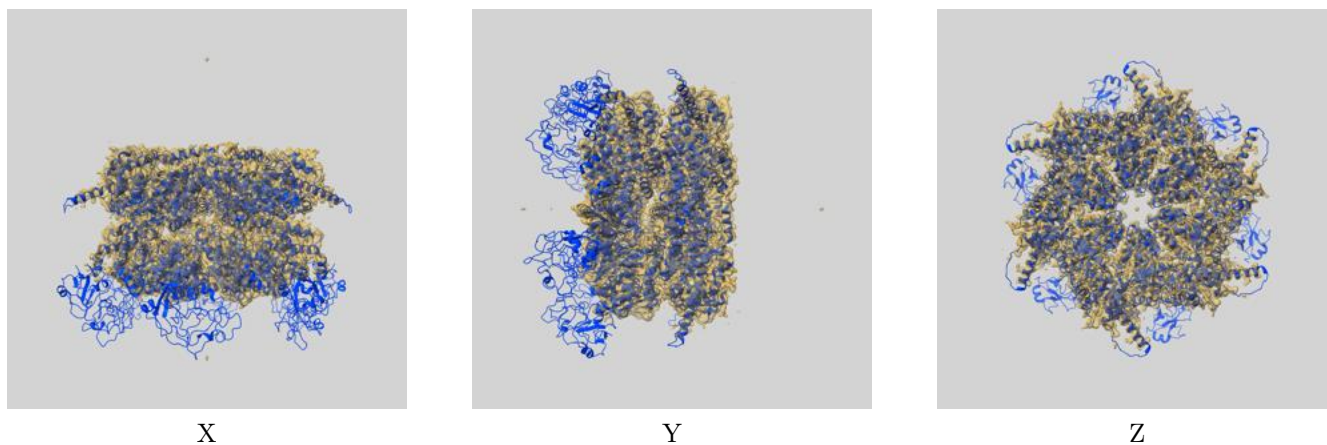
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	6.70	4.28

*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](#)

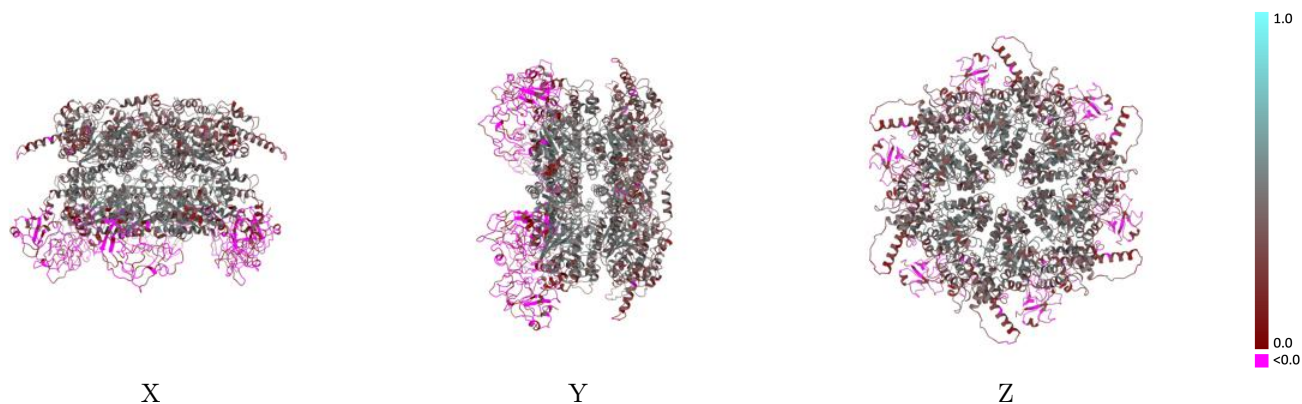
This section contains information regarding the fit between EMDB map EMD-19473 and PDB model 8RS9. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



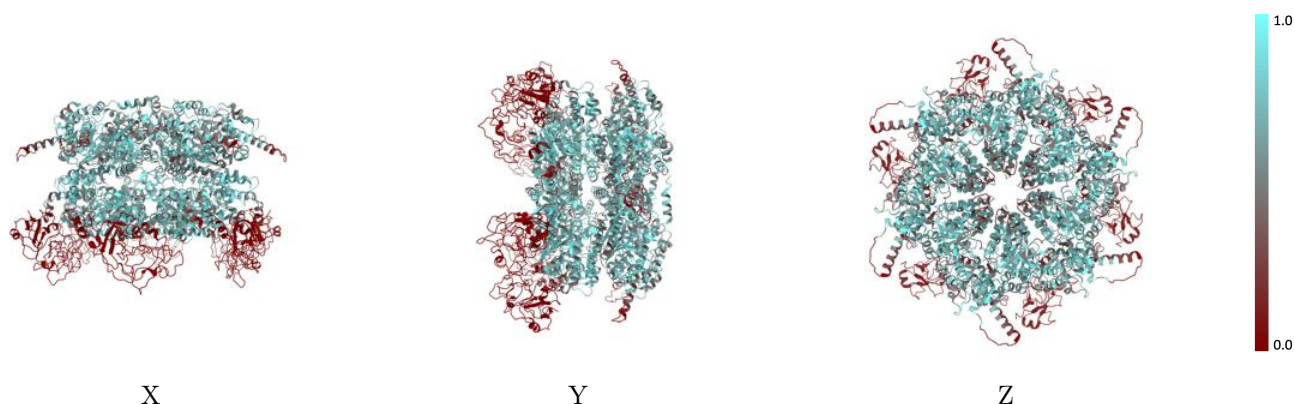
The images above show the 3D surface view of the map at the recommended contour level 0.244 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



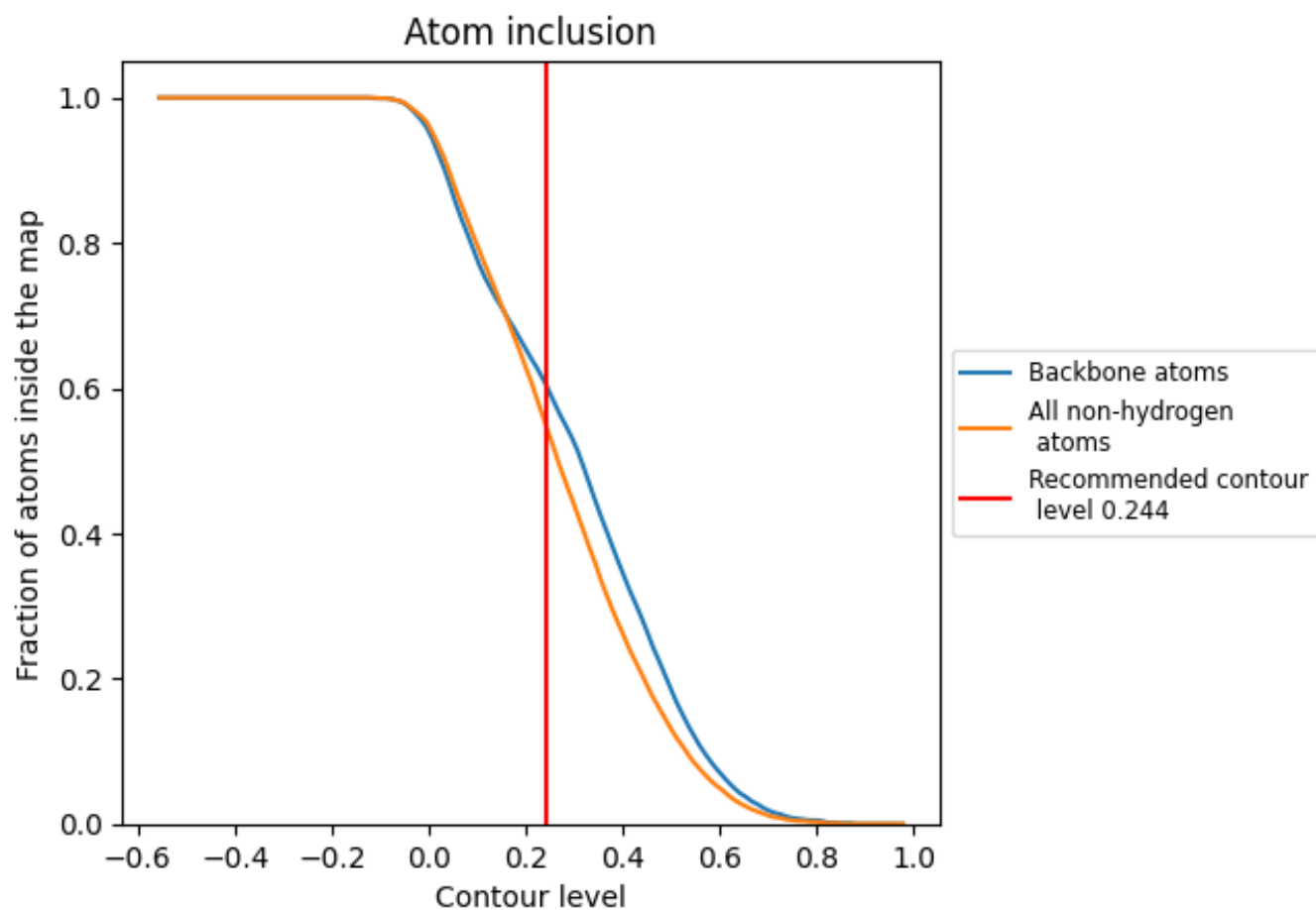
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.244).















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 [i](#)

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

