



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2024 – 07:19 PM JST

PDB ID : 8H35
EMDB ID : EMD-34451
Title : Cryo-EM Structure of the KBTBD2-Cul3-Rbx1 octameric complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-08
Resolution : 7.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
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

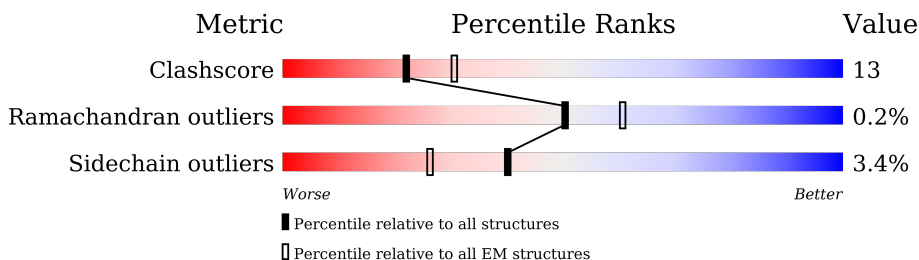
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.41 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	C	768	
1	F	768	
1	H	768	
1	I	768	
1	M	768	
1	O	768	
1	T	768	
1	V	768	

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Mol	Chain	Length	Quality of chain
2	A	623	 68% 22% 10%
2	B	623	 68% 22% 10%
2	G	623	 65% 25% 10%
2	J	623	 69% 21% 10%
2	N	623	 68% 22% 10%
2	P	623	 65% 24% 10%
2	S	623	 64% 26% 10%
2	U	623	 69% 21% 10%
3	D	108	 46% 32% 18%
3	E	108	 49% 33% 18%
3	K	108	 43% 38% 18%
3	L	108	 48% 33% 18%
3	Q	108	 48% 32% 18%
3	R	108	 49% 33% 18%
3	W	108	 49% 33% 18%
3	X	108	 5% 44% 37% 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 86872 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 Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	720	Total	C	N	O	S	0	0
			5654	3541	1003	1073	37		
1	F	720	Total	C	N	O	S	0	0
			5801	3645	1026	1092	38		
1	I	720	Total	C	N	O	S	0	0
			5764	3618	1021	1087	38		
1	H	720	Total	C	N	O	S	0	0
			5703	3581	1002	1084	36		
1	M	720	Total	C	N	O	S	0	0
			5708	3582	1003	1087	36		
1	O	720	Total	C	N	O	S	0	0
			5746	3608	1018	1082	38		
1	T	720	Total	C	N	O	S	0	0
			5770	3623	1024	1085	38		
1	V	720	Total	C	N	O	S	0	0
			5657	3549	1000	1072	36		

- Molecule 2 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	561	Total	C	N	O	S	0	0
			4380	2798	730	819	33		
2	B	563	Total	C	N	O	S	0	0
			4405	2810	736	824	35		
2	G	561	Total	C	N	O	S	0	0
			4424	2829	736	823	36		
2	J	563	Total	C	N	O	S	0	0
			4393	2808	730	818	37		
2	P	561	Total	C	N	O	S	0	0
			4387	2805	726	820	36		
2	N	563	Total	C	N	O	S	0	0
			4427	2828	736	827	36		
2	S	561	Total	C	N	O	S	0	0
			4435	2838	733	827	37		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	U	563	4398	2805	734	822	37	0	0

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	89	733	463	134	127	9	0	0
3	D	89	731	463	132	127	9	0	0
3	L	89	705	448	127	122	8	0	0
3	K	89	729	460	133	127	9	0	0
3	R	89	733	463	134	127	9	0	0
3	Q	89	695	442	123	122	8	0	0
3	W	89	737	466	135	127	9	0	0
3	X	89	733	463	134	127	9	0	0

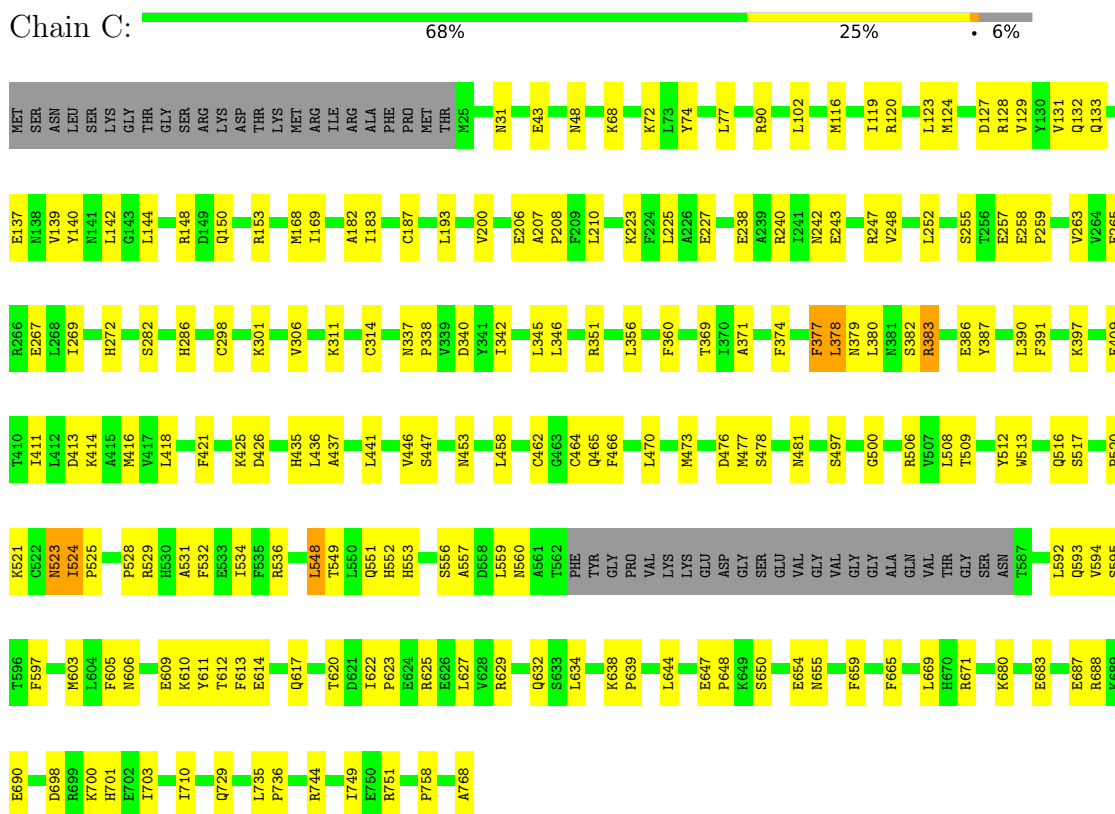
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	E	3	Total	Zn	0
			3	3	
4	D	3	Total	Zn	0
			3	3	
4	L	3	Total	Zn	0
			3	3	
4	K	3	Total	Zn	0
			3	3	
4	R	3	Total	Zn	0
			3	3	
4	Q	3	Total	Zn	0
			3	3	
4	W	3	Total	Zn	0
			3	3	
4	X	3	Total	Zn	0
			3	3	

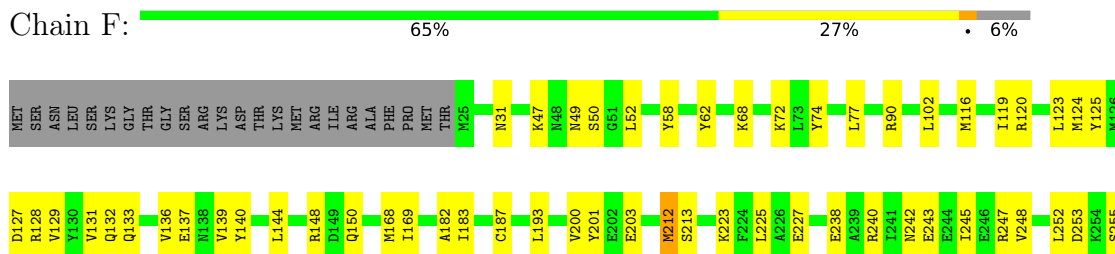
3 Residue-property plots [i](#)

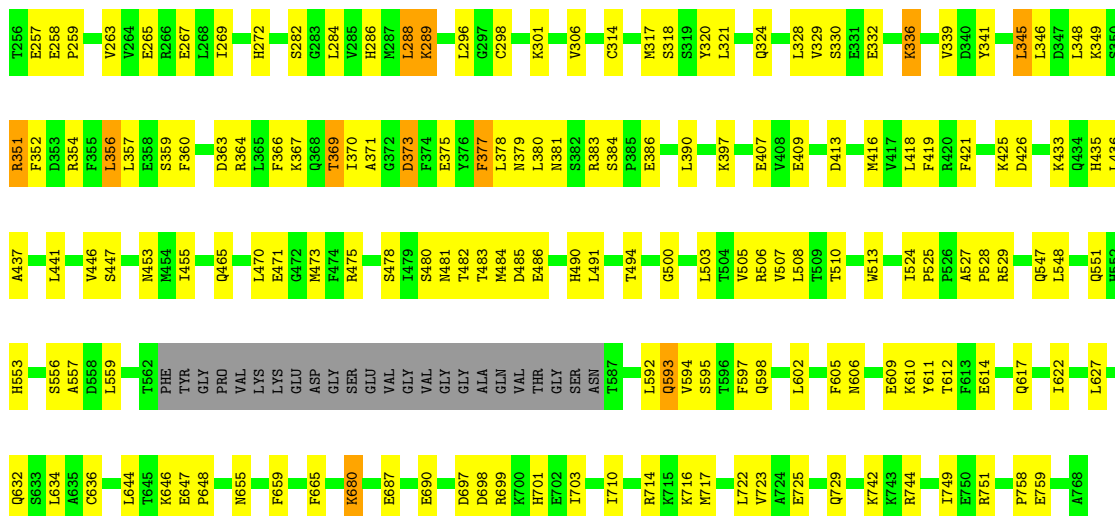
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Cullin-3

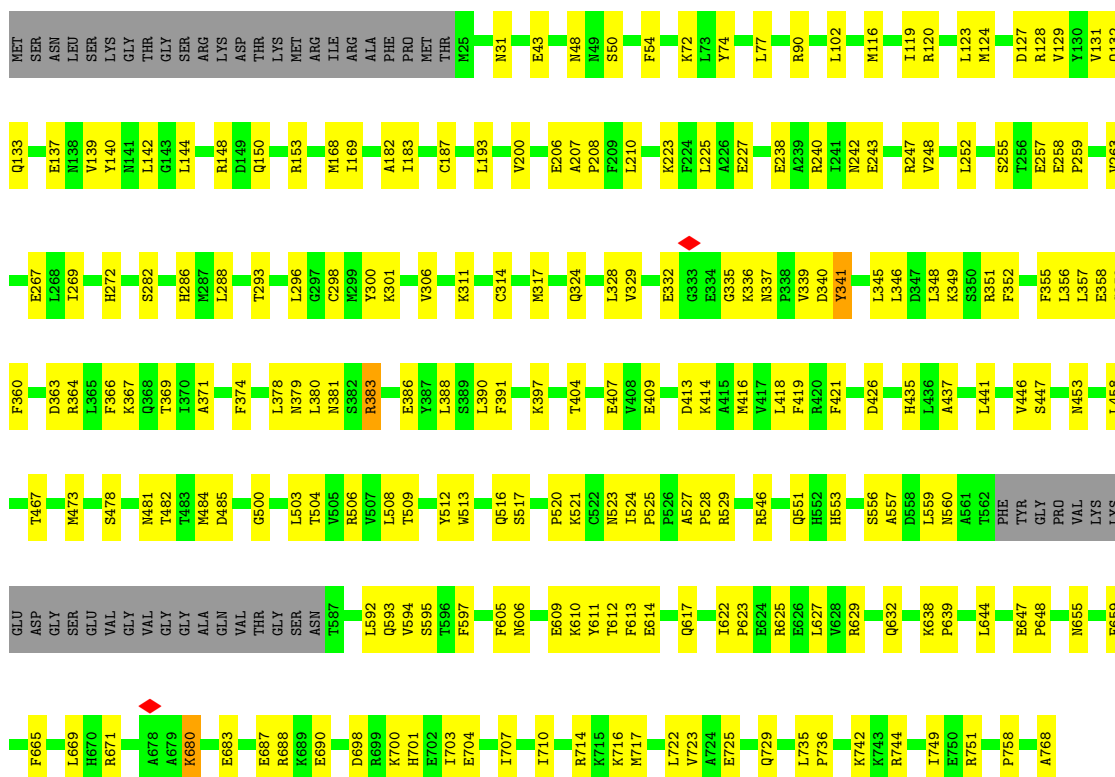


- Molecule 1: Cullin-3





• Molecule 1: Cullin-3



• Molecule 1: Cullin-3



V136	E137	M138	V139	Y140	L144	R148	D149	Q150	M168	I169	A182	I183	C187	L193	V200	Y201	E202	E203	M212	S213	K223	F224	L225	A226	E227	K236	R240	E243	E244	I245	E246	R247	V248	L252	D253	K254	S255	L256	E257	E258	P259	V263	V264	R266								
E267	L268	I269	H272	S282	H286	K289	C298	K301	V306	K311	C314	N337	P338	V339	D340	L345	L346	R351	L356	F360	T369	I370	A371	F374	F377	L378	N379	L380	E386	Y367	L380	E386	L390	E386	L390	K397	E407	V408	E409	D413	K414											
A415	M416	V417	L418	F419	R420	F421	M422	K425	D426	K433	G434	H435	L436	A437	L441	V446	S447	M453	M454	I455	Q465	L470	E471	G472	M473	R475	S478	I479	S480	M481	T482	T483	M484	D485	E486	F487	H490	L491	L498	G499	G500	V501	D502	V503	T504	V505	R506	E265	R266			
L508	T509	T510	W513	S517	P520	K521	P525	P528	I534	F535	R546	Q547	L548	Q551	H552	H553	S556	A557	D558	L559	T562	PHE	TYR	GLY	PRO	VAL	LYS	LYS	GLU	ASP	GLY	GLY	SER	GLU	VAL	VAL	VAL	ALA	GLN	VAL	THR	GLY	SER	ASN	T567	L592	Q593					
W594	S595	T596	F597	Q598	L602	F605	N606	E609	K610	Y611	T612	F613	E614	Q617	I622	L627	Q632	S633	L634	A635	C636	L644	T645	K646	N655	F659	F665	K680	K680	E687	E687	E690	D697	D698	R699	K700	H701	E702	I703	M717	V721	L722	V723									
K742	R743	R744	I749	E750	R751	P758	E759	A768																																												

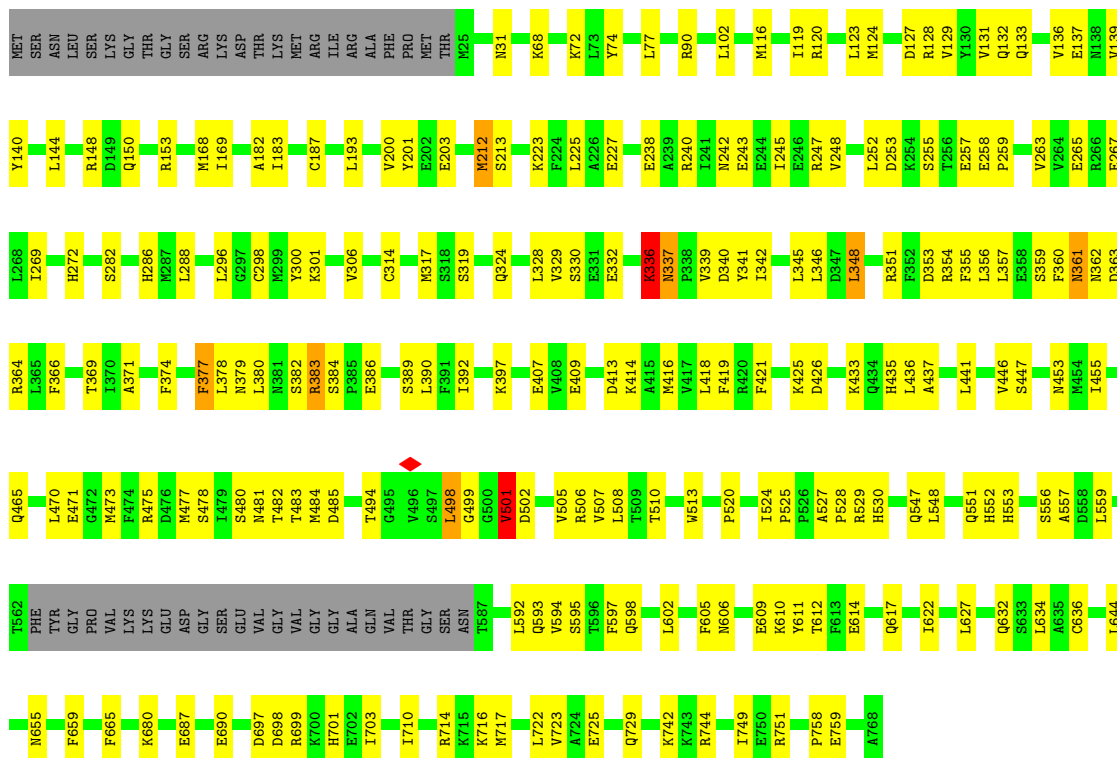
● Molecule 1: Cullin-3



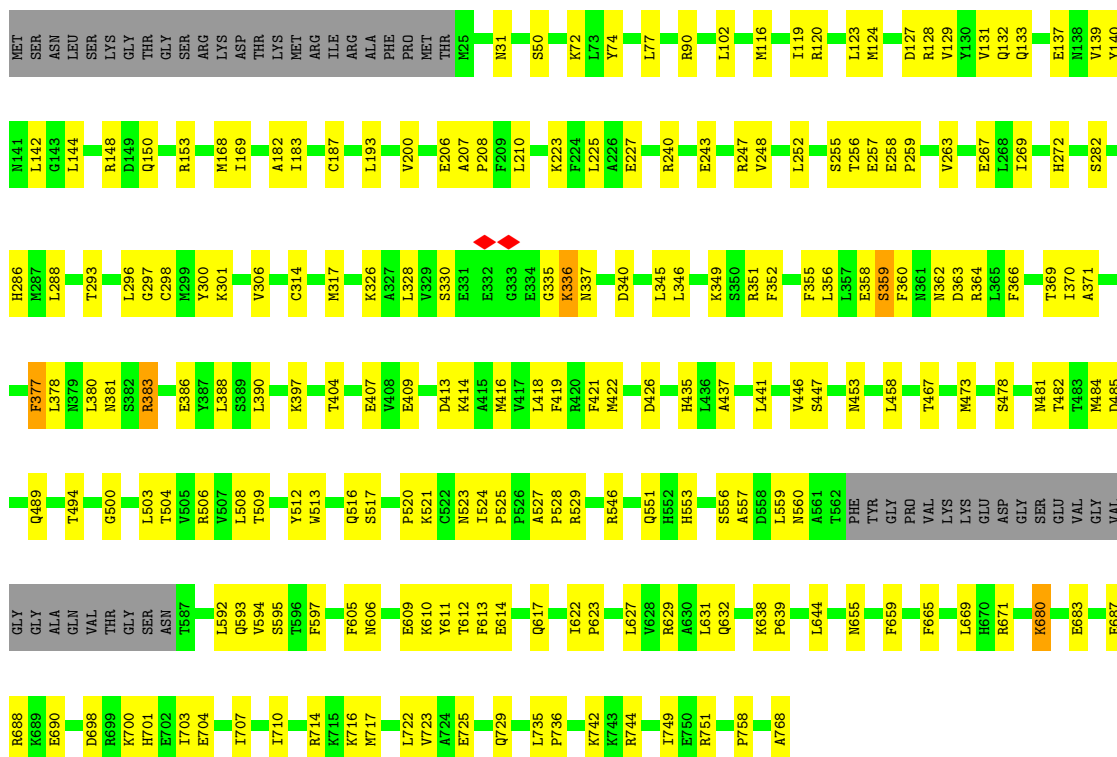
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E137	R138	V139	Y140	R141	L142	G143	L144	R148	D149	Q150	R153	I169	A182	C187	L193	V200	E206	A207	P208	F209	L210	K223	F224	L225	A226	E227	E238	A239	I241	E243	R247	V248	L252	S255	T256	E257	P259	V263	V264	R266	E267				
L268	I269	H272	S282	H286	C298	K301	V306	C314	N337	P338	V339	D340	I342	L345	L346	R351	L356	F360	T369	F377	L378	N379	L380	S381	R382	R383	E386	Y387	L388	L390	K397	T404	E407	V408	E409	D413	K414	A415							
M416	V417	F419	H435	L436	A437	L441	V446	S447	M453	L458	T467	M473	S478	M481	T482	D485	D485	Q492	V501	D502	L503	V505	L508	T509	Y512	W513	Q516	S517	P520	K521	C522	N523	I524	P525	P526	A527	P528	F532	R546	I622					
L550	Q551	H552	H553	S556	A557	D558	L559	N560	A561	T562	PHE	TYR	GLY	PRO	VAL	LYS	GLY	GLU	ASP	GLY	SER	GLU	VAL	GLY	VAL	VAL	L592	Q593	V594	S595	T596	F597	M603	L604	F605	N606	E609	K610	Y611	T612	F613	E614	Q617	R546	I622
P623	L627	V628	R629	Q632	K638	P639	L644	N655	F659	F665	L669	H670	R671	K680	E683	E687	R688	K689	E690	D698	R699	K700	H701	E702	I703	E704	I707	L735	P736	R744	I749	E750	R751	L754	P758	R761	K762	V763	Y764	T765					
A768																																													

● Molecule 1: Cullin-3



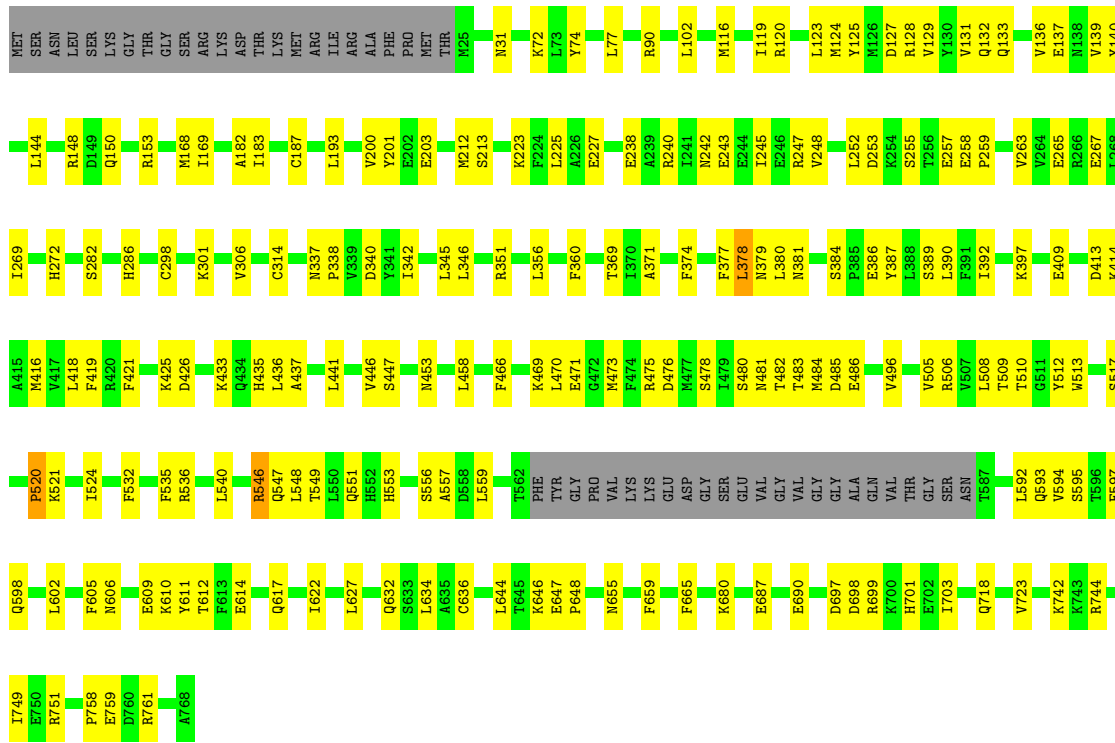


• Molecule 1: Cullin-3



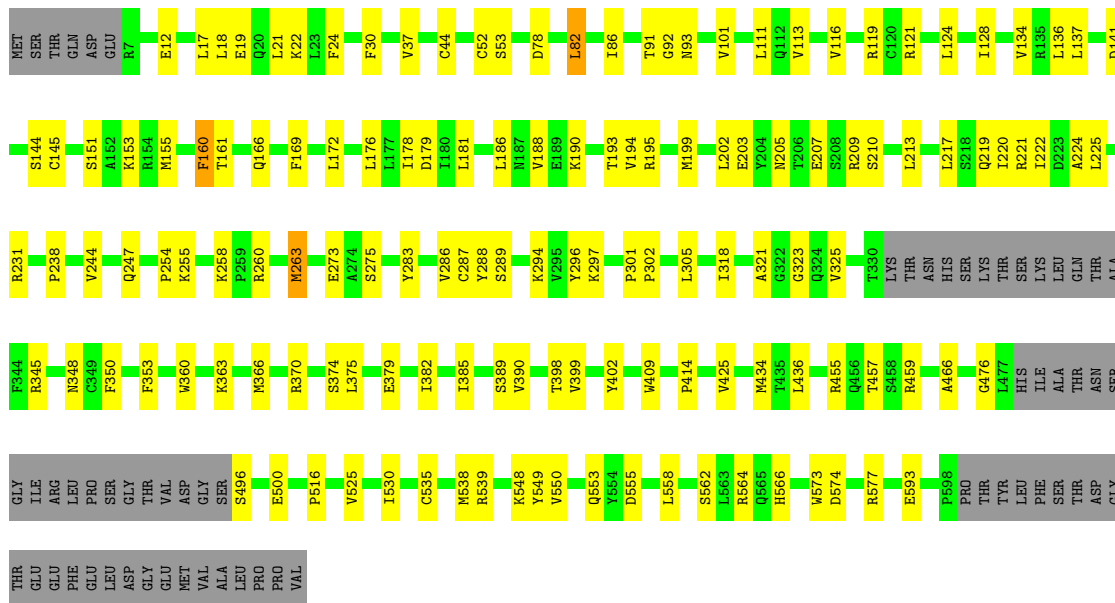
• Molecule 1: Cullin-3

Chain V: 69% 24% 6%



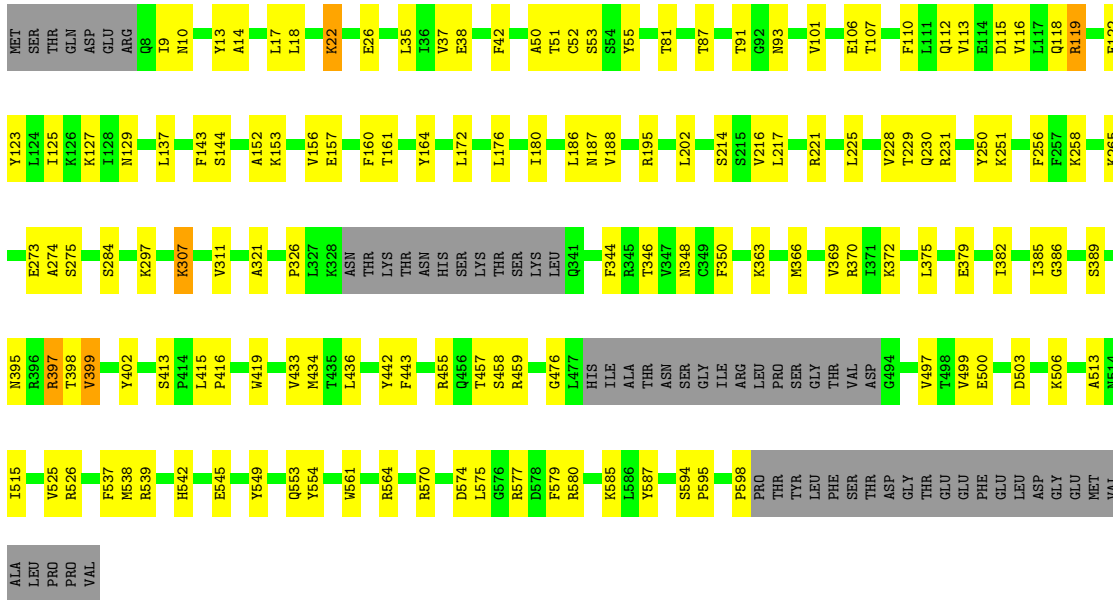
• Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain A: 68% 22% 10%

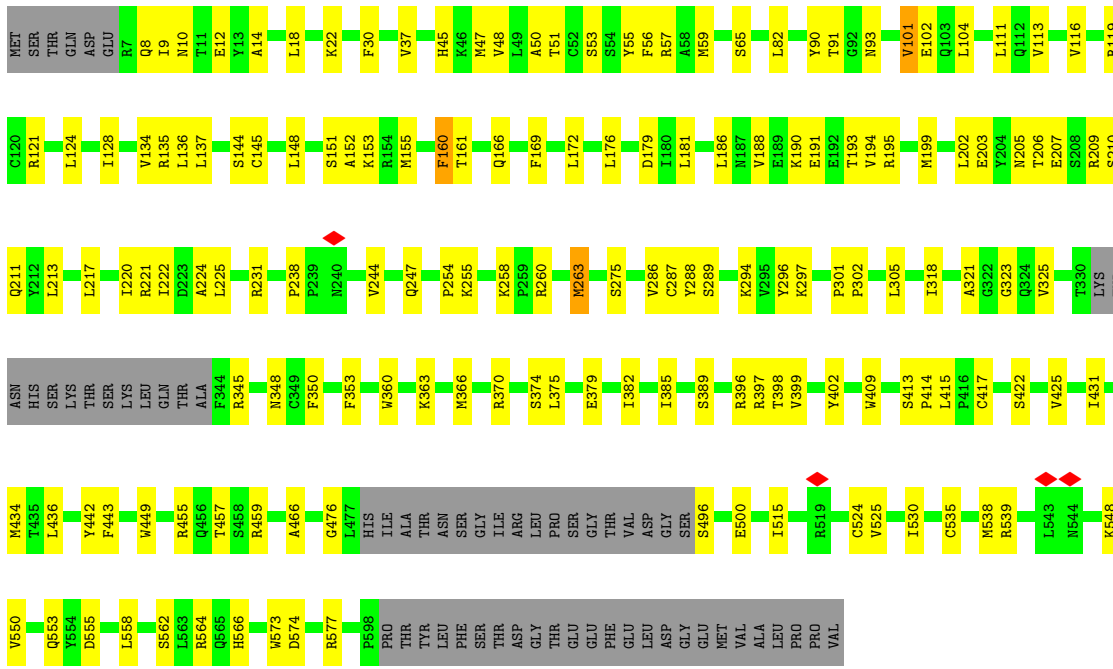


• Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain B: 68% 22% 10%

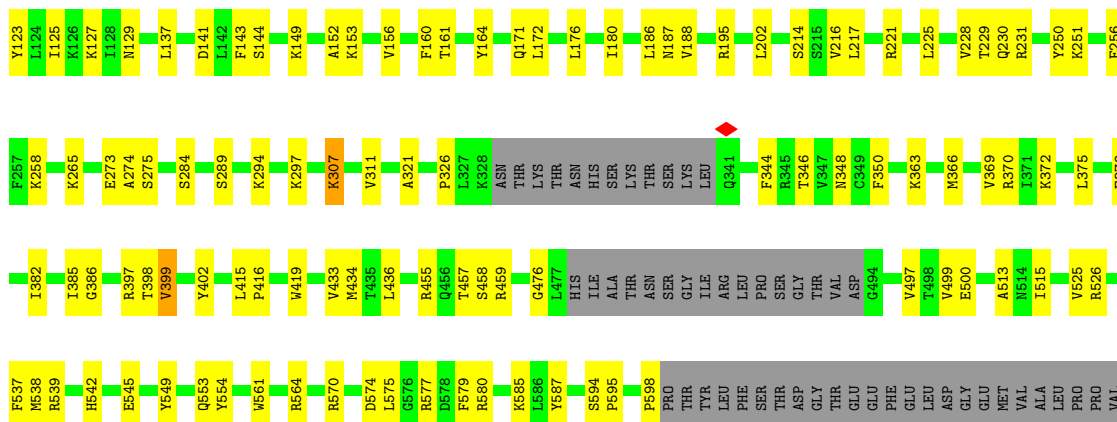


• Molecule 2: Kelch repeat and BTB domain-containing protein 2



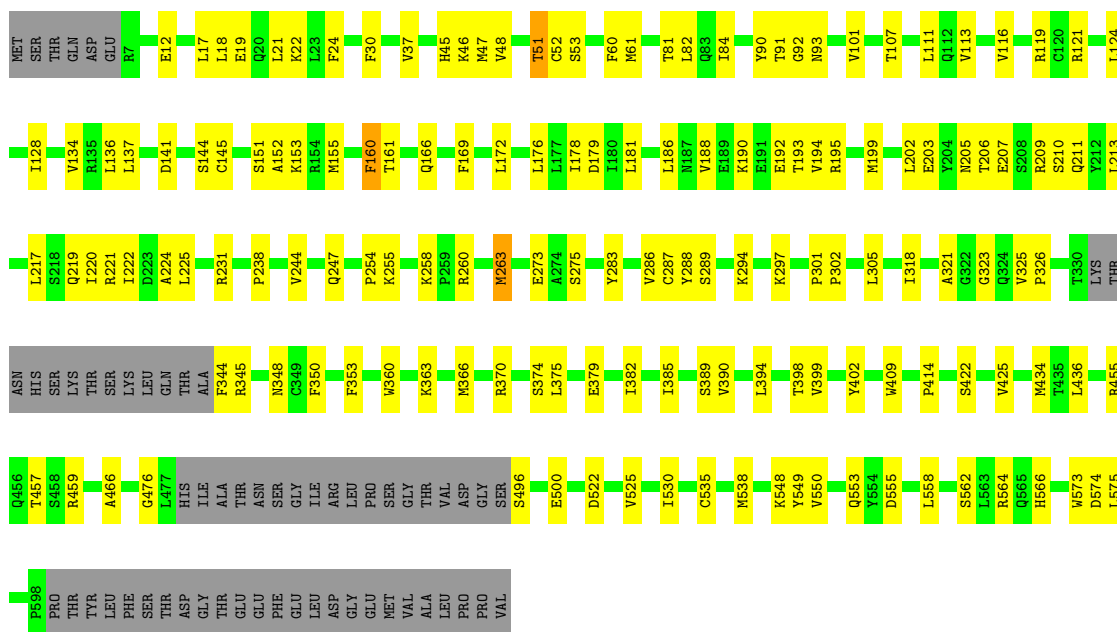
• Molecule 2: Kelch repeat and BTB domain-containing protein 2





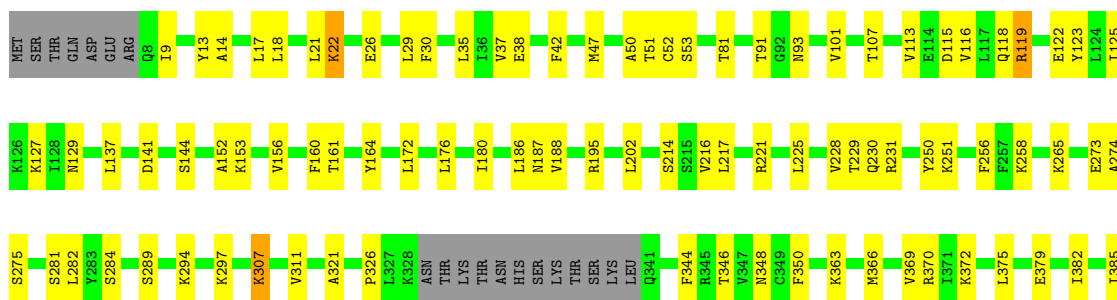
• Molecule 2: Kelch repeat and BTB domain-containing protein 2

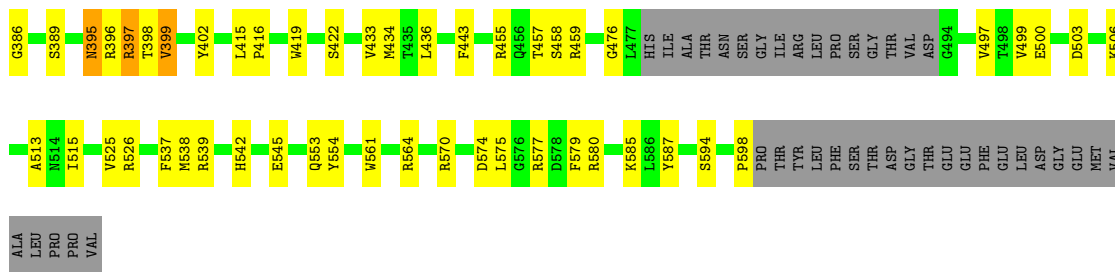
Chain P: 65% 24% 10%



• Molecule 2: Kelch repeat and BTB domain-containing protein 2

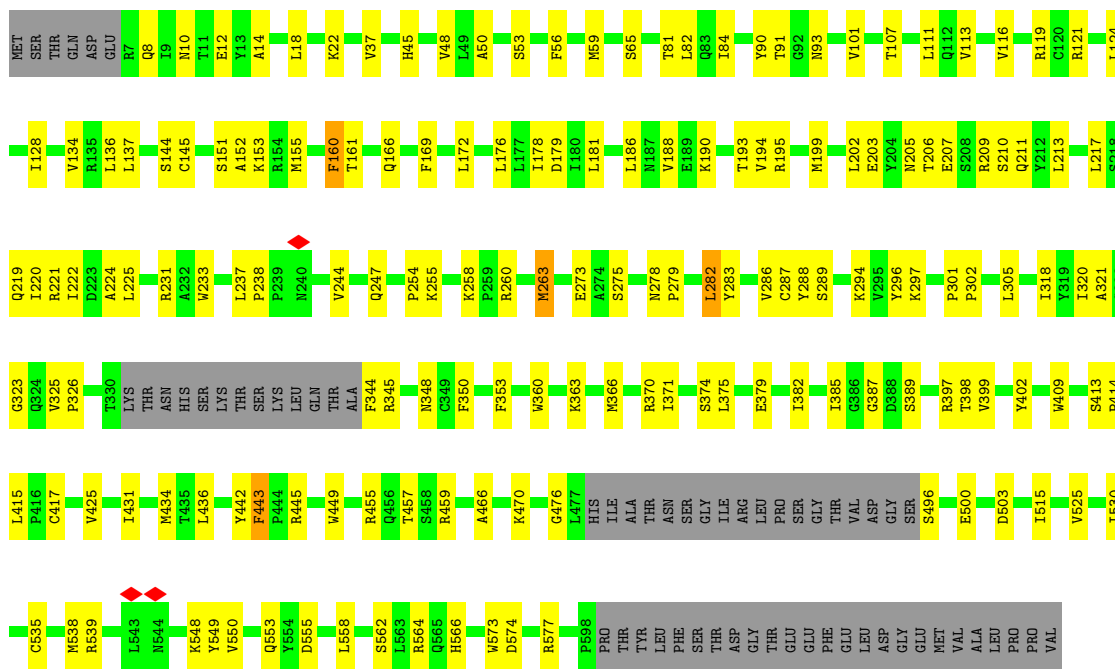
Chain N: 68% 22% 10%





• Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain S: 64% 26% 10%



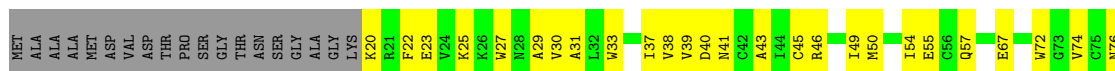
• Molecule 2: Kelch repeat and BTB domain-containing protein 2

Chain U: 69% 21% 10%

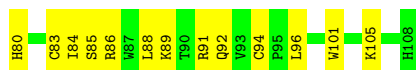




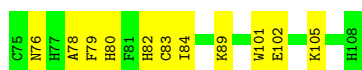
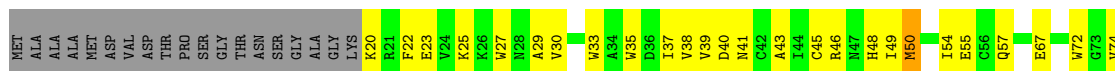
- Molecule 3: E3 ubiquitin-protein ligase RBX1



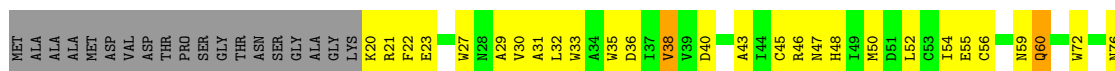
- Molecule 3: E3 ubiquitin-protein ligase RBX1



- Molecule 3: E3 ubiquitin-protein ligase RBX1

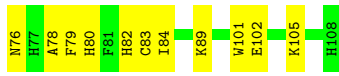
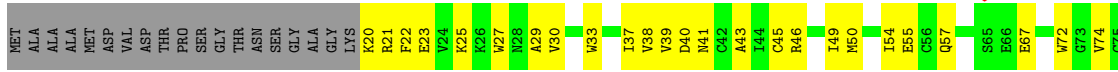


- Molecule 3: E3 ubiquitin-protein ligase RBX1

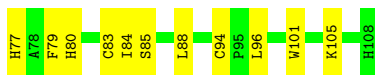
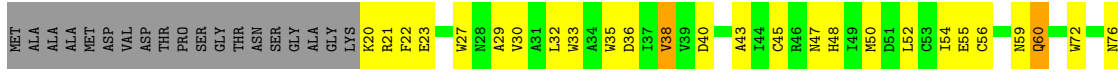


- Molecule 3: E3 ubiquitin-protein ligase RBX1

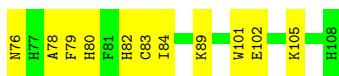
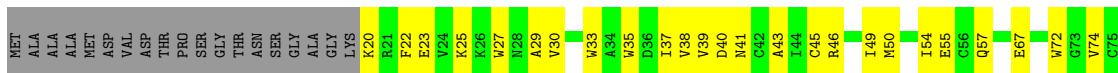




• Molecule 3: E3 ubiquitin-protein ligase RBX1



• Molecule 3: E3 ubiquitin-protein ligase RBX1



• Molecule 3: E3 ubiquitin-protein ligase RBX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30204	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.454	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	511.488, 511.488, 511.488	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.664, 2.664, 2.664	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	C	0.30	0/5736	0.49	0/7726
1	F	0.32	0/5891	0.51	0/7919
1	H	0.29	0/5788	0.49	0/7793
1	I	0.28	0/5850	0.48	0/7865
1	M	0.29	0/5793	0.48	0/7799
1	O	0.31	0/5832	0.50	0/7843
1	T	0.27	0/5858	0.48	0/7875
1	V	0.30	0/5742	0.50	0/7735
2	A	0.30	0/4476	0.50	0/6083
2	B	0.28	0/4503	0.47	0/6117
2	G	0.28	0/4524	0.49	0/6143
2	J	0.28	0/4491	0.48	0/6100
2	N	0.27	0/4526	0.47	0/6146
2	P	0.28	0/4485	0.48	0/6095
2	S	0.26	0/4537	0.48	0/6161
2	U	0.29	0/4493	0.48	0/6100
3	D	0.33	0/753	0.50	0/1022
3	E	0.24	0/755	0.49	0/1025
3	K	0.23	0/751	0.49	0/1021
3	L	0.24	0/726	0.47	0/986
3	Q	0.22	0/716	0.45	0/975
3	R	0.24	0/755	0.49	0/1025
3	W	0.23	0/759	0.49	0/1029
3	X	0.23	0/755	0.49	0/1025
All	All	0.29	0/88495	0.49	0/119608

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	C	5654	0	5513	147	0
1	F	5801	0	5790	144	0
1	H	5703	0	5614	130	0
1	I	5764	0	5731	172	0
1	M	5708	0	5611	121	0
1	O	5746	0	5703	200	0
1	T	5770	0	5727	214	0
1	V	5657	0	5503	139	0
2	A	4380	0	4183	115	0
2	B	4405	0	4201	111	0
2	G	4424	0	4237	119	0
2	J	4393	0	4189	107	0
2	N	4427	0	4256	123	0
2	P	4387	0	4183	140	0
2	S	4435	0	4253	117	0
2	U	4398	0	4205	89	0
3	D	731	0	675	27	0
3	E	733	0	675	26	0
3	K	729	0	664	34	0
3	L	705	0	623	27	0
3	Q	695	0	601	30	0
3	R	733	0	675	26	0
3	W	737	0	686	28	0
3	X	733	0	675	33	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
4	Q	3	0	0	0	0
4	R	3	0	0	0	0
4	W	3	0	0	0	0
4	X	3	0	0	0	0
All	All	86872	0	84173	2193	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 13.

The worst 5 of 2193 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:T:288:LEU:HD21	1:T:352:PHE:CZ	1.45	1.52
1:T:378:LEU:CD2	1:T:422:MET:HG2	1.43	1.47
1:O:346:LEU:HD21	1:O:414:LYS:CB	1.41	1.47
1:O:346:LEU:CD2	1:O:414:LYS:HB3	1.53	1.38
1:T:288:LEU:HD21	1:T:352:PHE:CE2	1.60	1.34

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	C	716/768 (93%)	655 (92%)	61 (8%)	0	100	100
1	F	716/768 (93%)	655 (92%)	60 (8%)	1 (0%)	51	86
1	H	716/768 (93%)	654 (91%)	61 (8%)	1 (0%)	51	86
1	I	716/768 (93%)	657 (92%)	58 (8%)	1 (0%)	51	86
1	M	716/768 (93%)	656 (92%)	60 (8%)	0	100	100
1	O	716/768 (93%)	650 (91%)	61 (8%)	5 (1%)	22	63
1	T	716/768 (93%)	656 (92%)	59 (8%)	1 (0%)	51	86
1	V	716/768 (93%)	647 (90%)	67 (9%)	2 (0%)	41	77
2	A	555/623 (89%)	521 (94%)	32 (6%)	2 (0%)	34	72
2	B	557/623 (89%)	532 (96%)	25 (4%)	0	100	100
2	G	555/623 (89%)	520 (94%)	34 (6%)	1 (0%)	47	81
2	J	557/623 (89%)	533 (96%)	24 (4%)	0	100	100
2	N	557/623 (89%)	534 (96%)	23 (4%)	0	100	100
2	P	555/623 (89%)	516 (93%)	39 (7%)	0	100	100
2	S	555/623 (89%)	520 (94%)	32 (6%)	3 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U	557/623 (89%)	531 (95%)	25 (4%)	1 (0%)	47	81
3	D	87/108 (81%)	67 (77%)	19 (22%)	1 (1%)	14	52
3	E	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	14	52
3	K	87/108 (81%)	70 (80%)	16 (18%)	1 (1%)	14	52
3	L	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	14	52
3	Q	87/108 (81%)	70 (80%)	16 (18%)	1 (1%)	14	52
3	R	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	14	52
3	W	87/108 (81%)	75 (86%)	11 (13%)	1 (1%)	14	52
3	X	87/108 (81%)	70 (80%)	16 (18%)	1 (1%)	14	52
All	All	10872/11992 (91%)	10014 (92%)	832 (8%)	26 (0%)	50	81

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	279	PRO
2	S	515	ILE
1	O	501	VAL
2	U	388	ASP
2	G	144	SER

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	C	596/693 (86%)	574 (96%)	22 (4%)	34	58
1	F	636/693 (92%)	593 (93%)	43 (7%)	16	41
1	H	613/693 (88%)	599 (98%)	14 (2%)	50	70
1	I	626/693 (90%)	605 (97%)	21 (3%)	37	60
1	M	613/693 (88%)	590 (96%)	23 (4%)	33	57
1	O	621/693 (90%)	588 (95%)	33 (5%)	22	47
1	T	624/693 (90%)	603 (97%)	21 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	595/693 (86%)	572 (96%)	23 (4%)	32	56
2	A	461/560 (82%)	451 (98%)	10 (2%)	52	71
2	B	464/560 (83%)	452 (97%)	12 (3%)	46	66
2	G	469/560 (84%)	456 (97%)	13 (3%)	43	65
2	J	460/560 (82%)	450 (98%)	10 (2%)	52	71
2	N	472/560 (84%)	455 (96%)	17 (4%)	35	59
2	P	462/560 (82%)	453 (98%)	9 (2%)	57	75
2	S	473/560 (84%)	464 (98%)	9 (2%)	57	75
2	U	463/560 (83%)	452 (98%)	11 (2%)	49	69
3	D	77/90 (86%)	69 (90%)	8 (10%)	7	24
3	E	77/90 (86%)	76 (99%)	1 (1%)	69	81
3	K	76/90 (84%)	73 (96%)	3 (4%)	32	56
3	L	68/90 (76%)	67 (98%)	1 (2%)	65	80
3	Q	66/90 (73%)	65 (98%)	1 (2%)	65	80
3	R	77/90 (86%)	76 (99%)	1 (1%)	69	81
3	W	78/90 (87%)	77 (99%)	1 (1%)	69	81
3	X	77/90 (86%)	74 (96%)	3 (4%)	32	56
All	All	9244/10744 (86%)	8934 (97%)	310 (3%)	40	60

5 of 310 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	384	SER
1	V	213	SER
1	O	697	ASP
1	T	665	PHE
1	V	547	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	163	GLN
1	T	718	GLN
1	O	606	ASN
3	Q	47	ASN

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Mol	Chain	Res	Type
2	U	187	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

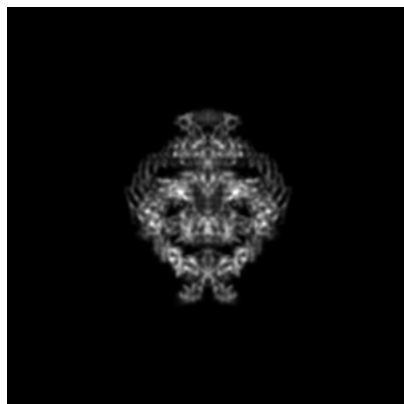
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34451. These allow visual inspection of the internal detail of the map and identification of artifacts.

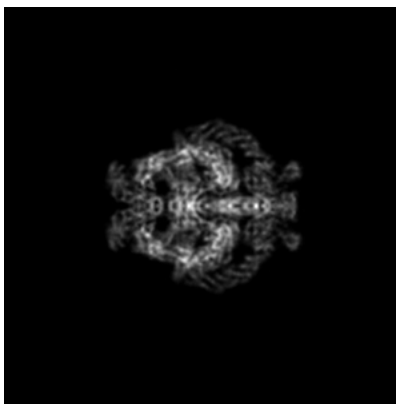
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

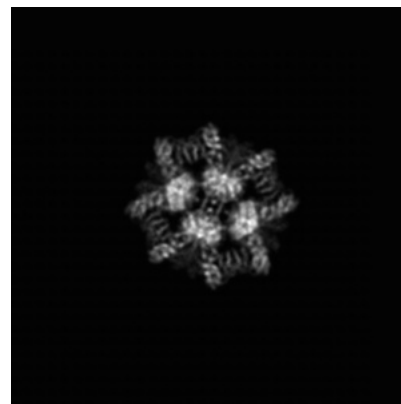
6.1.1 Primary map



X

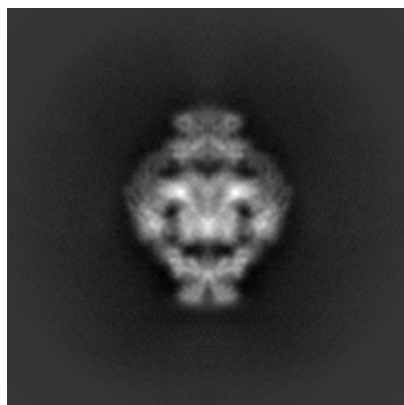


Y

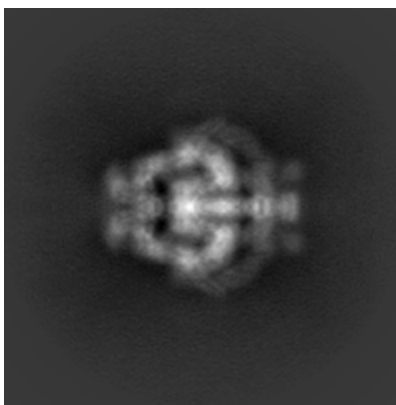


Z

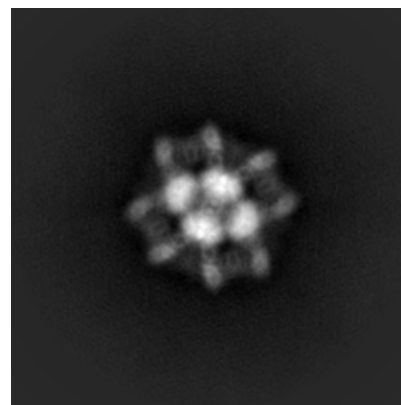
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

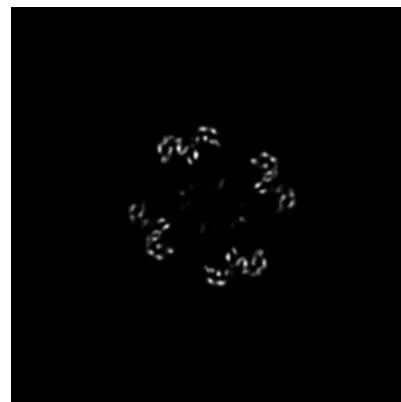
6.2.1 Primary map



X Index: 96

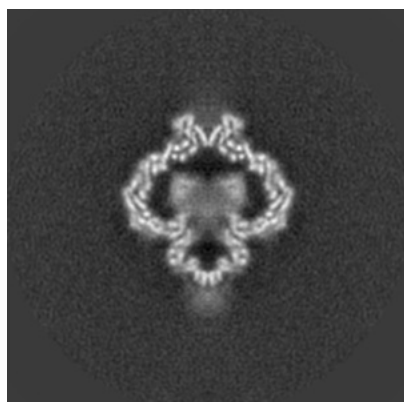


Y Index: 96

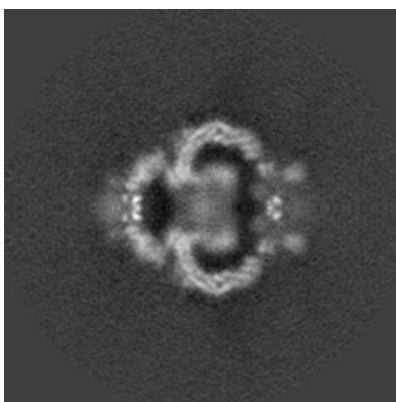


Z Index: 96

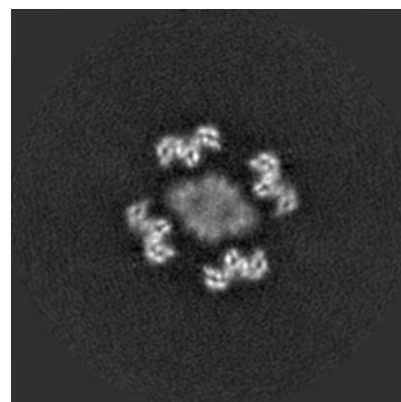
6.2.2 Raw map



X Index: 96



Y Index: 96



Z Index: 96

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

6.3 Largest variance slices [i](#)

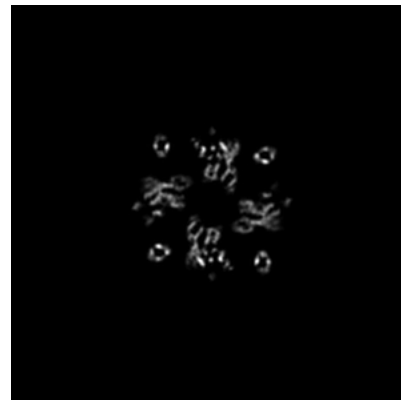
6.3.1 Primary map



X Index: 96

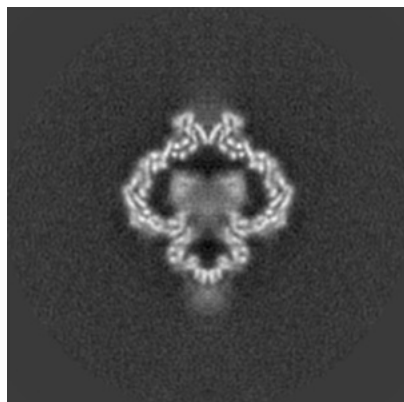


Y Index: 83

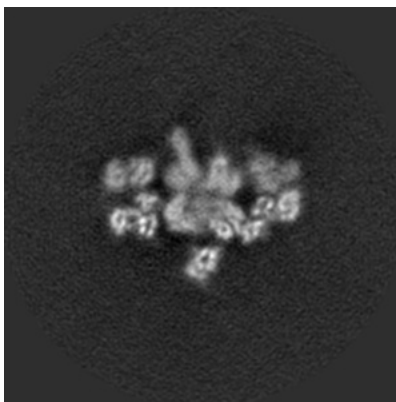


Z Index: 87

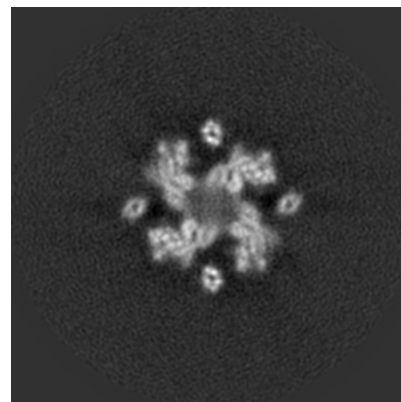
6.3.2 Raw map



X Index: 96



Y Index: 86

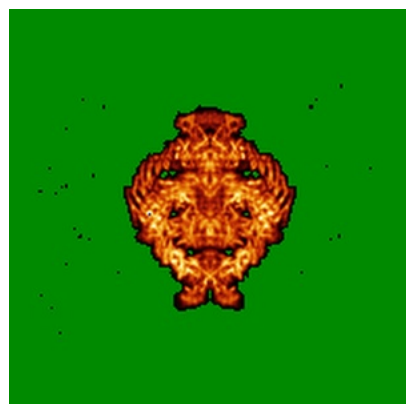


Z Index: 103

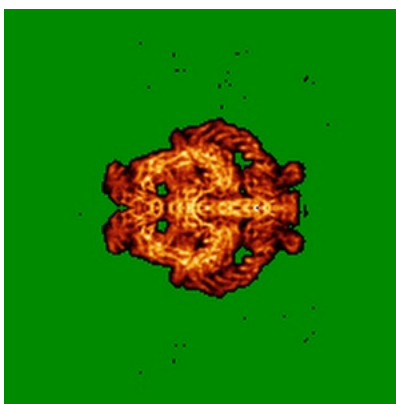
The images above show the largest variance slices of the map in three orthogonal directions.

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

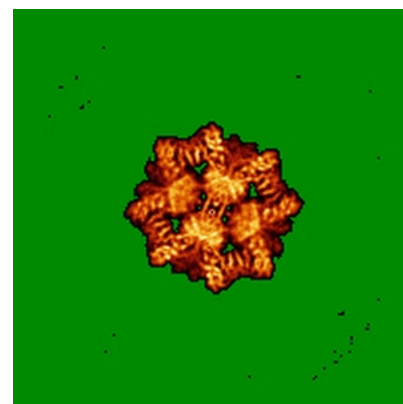
6.4.1 Primary map



X

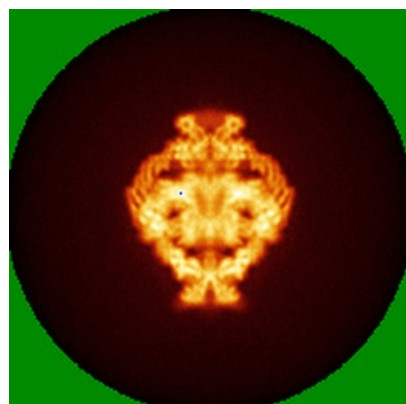


Y

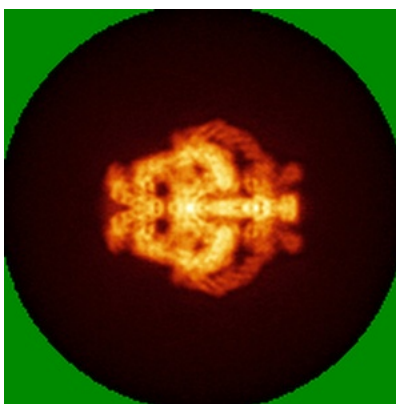


Z

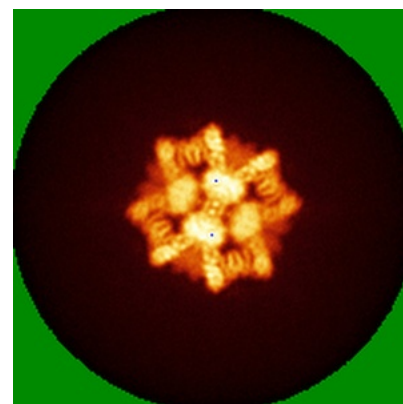
6.4.2 Raw map



X



Y

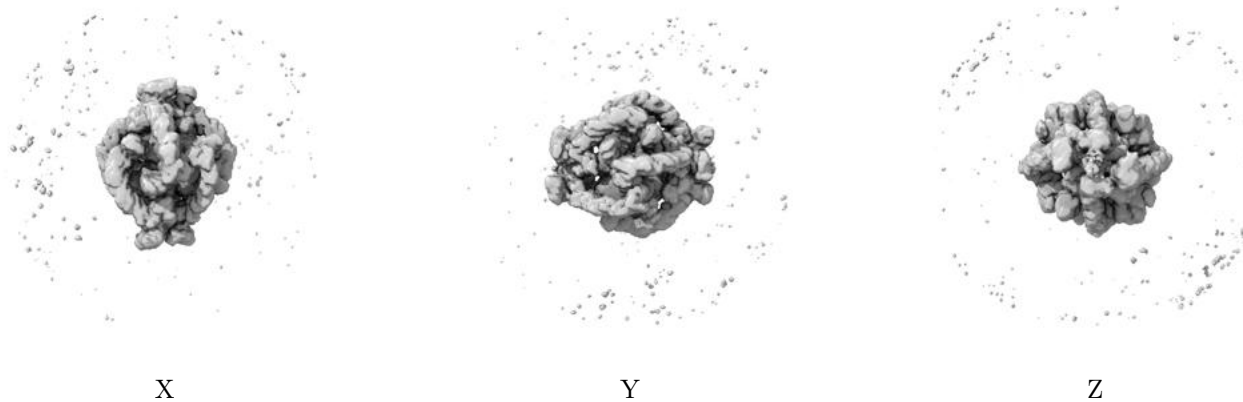


Z

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.

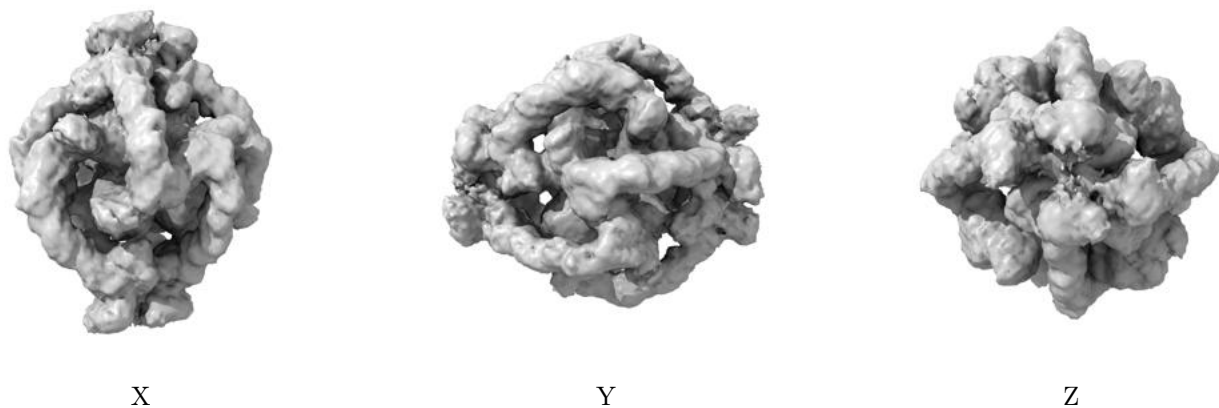
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. 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.

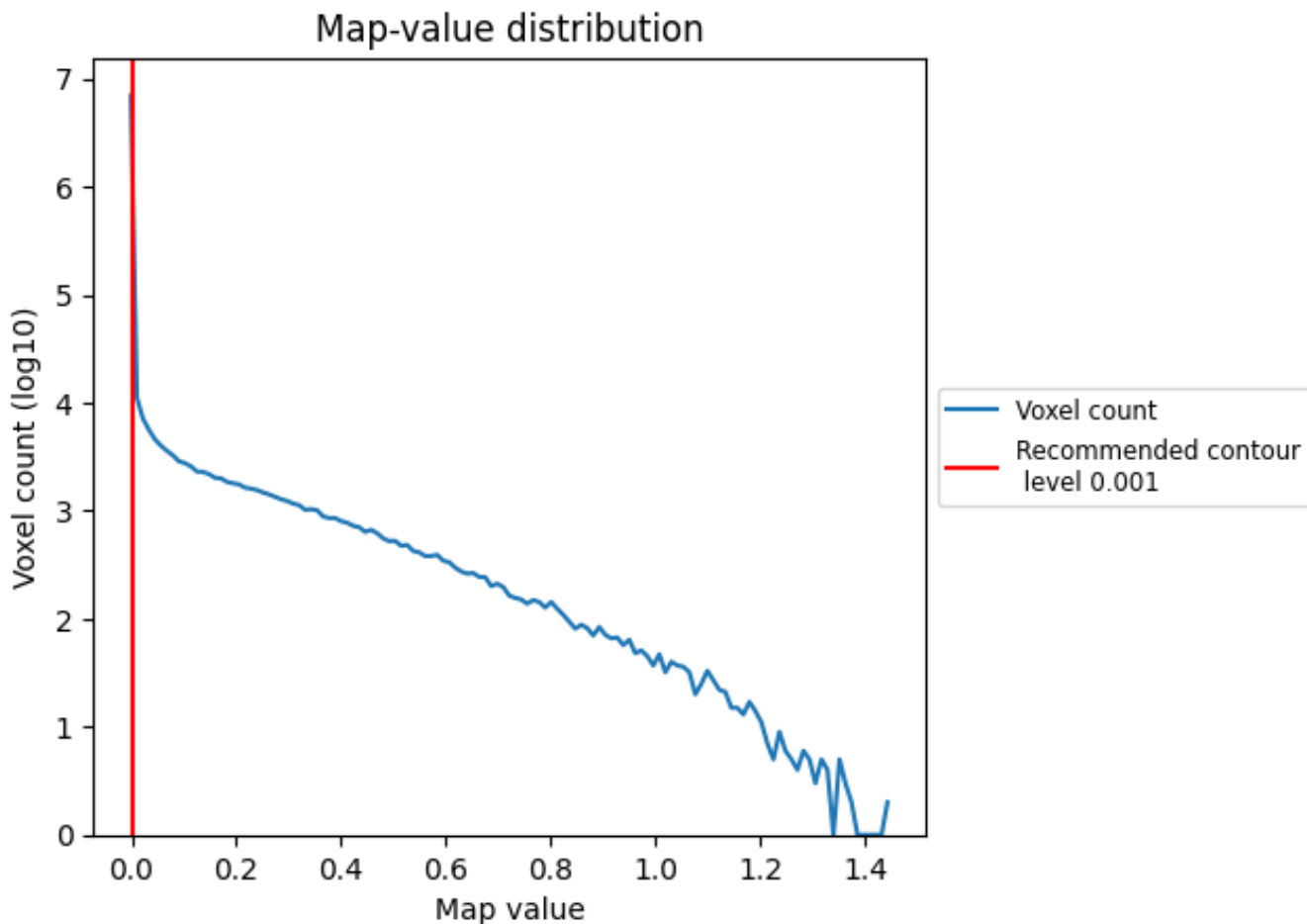
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

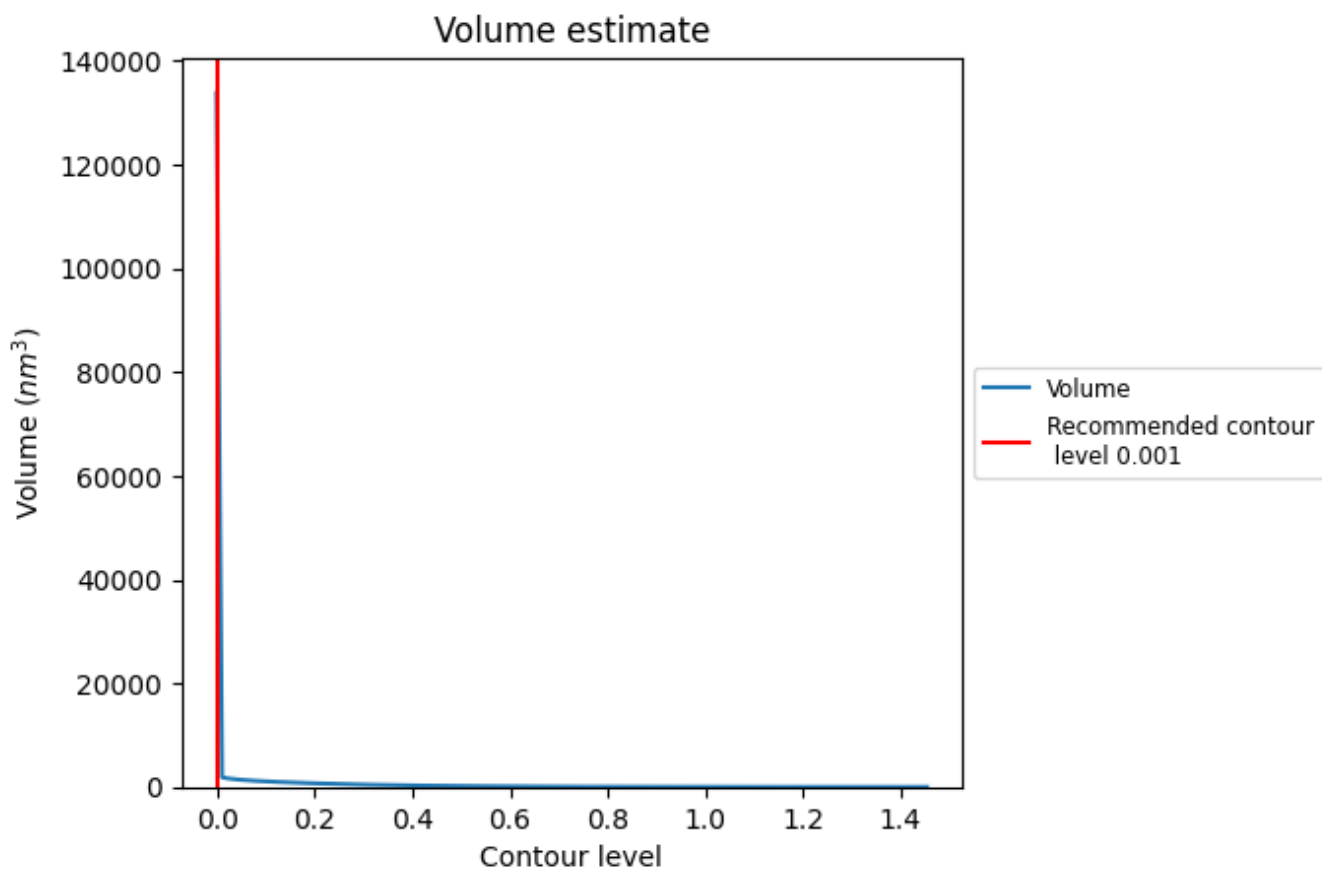
This section contains the results of statistical analysis of the map.

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.

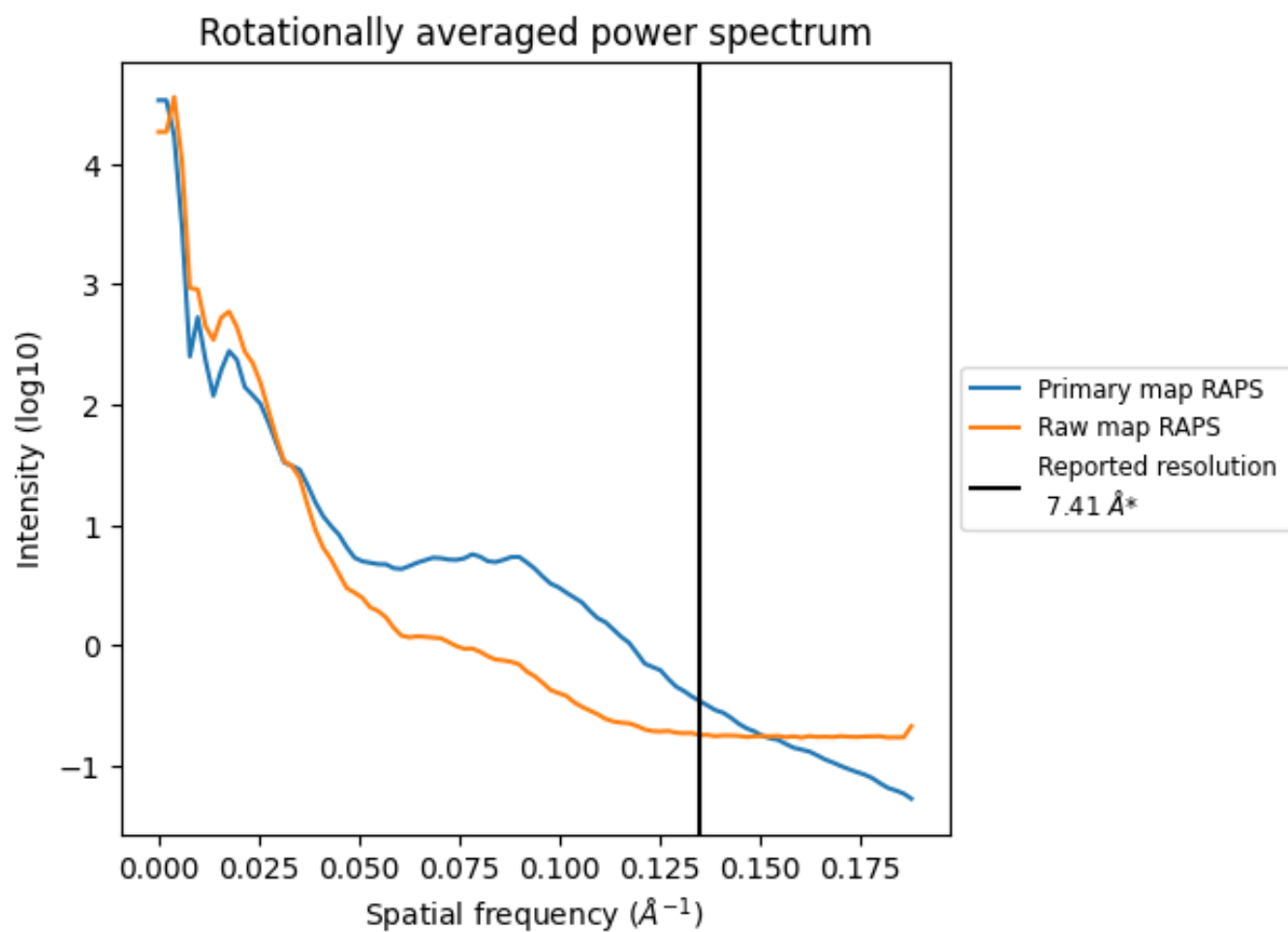
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106431 nm^3 ; this corresponds to an approximate mass of 96142 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

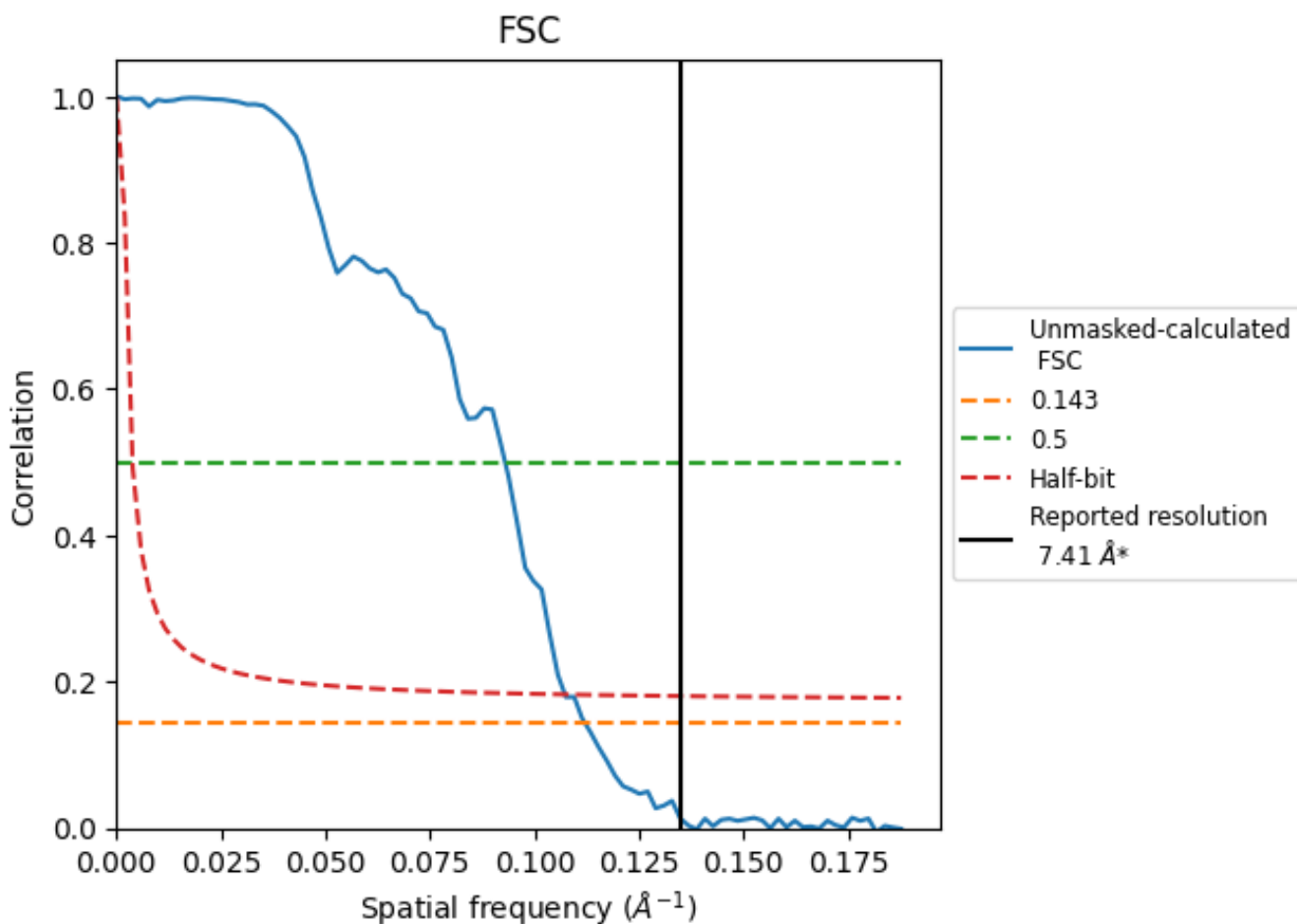


*Reported resolution corresponds to spatial frequency of 0.135 Å⁻¹

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 0.135 Å⁻¹

8.2 Resolution estimates

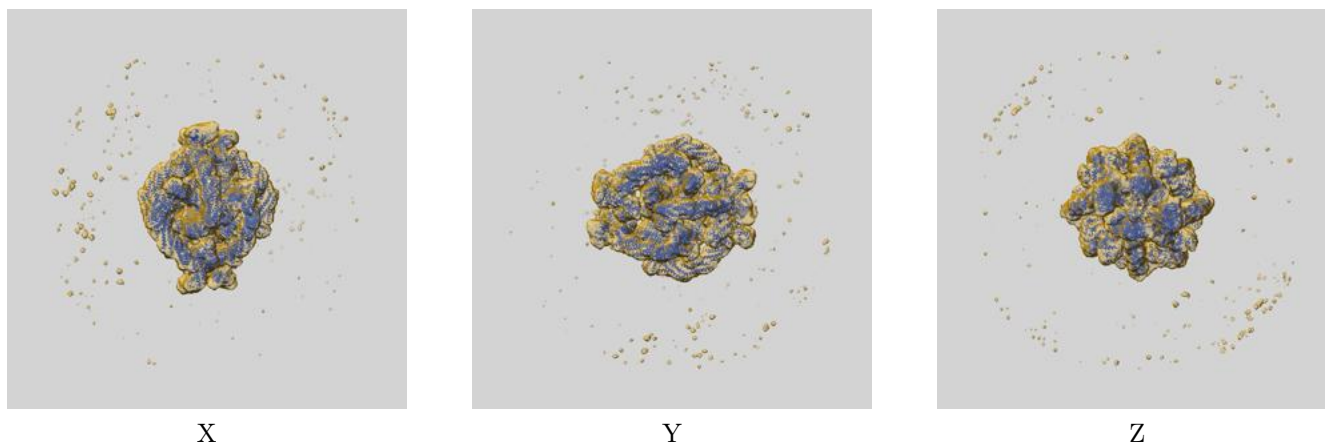
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.41	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.92	10.75	9.32

*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 8.92 differs from the reported value 7.41 by more than 10 %

9 Map-model fit [i](#)

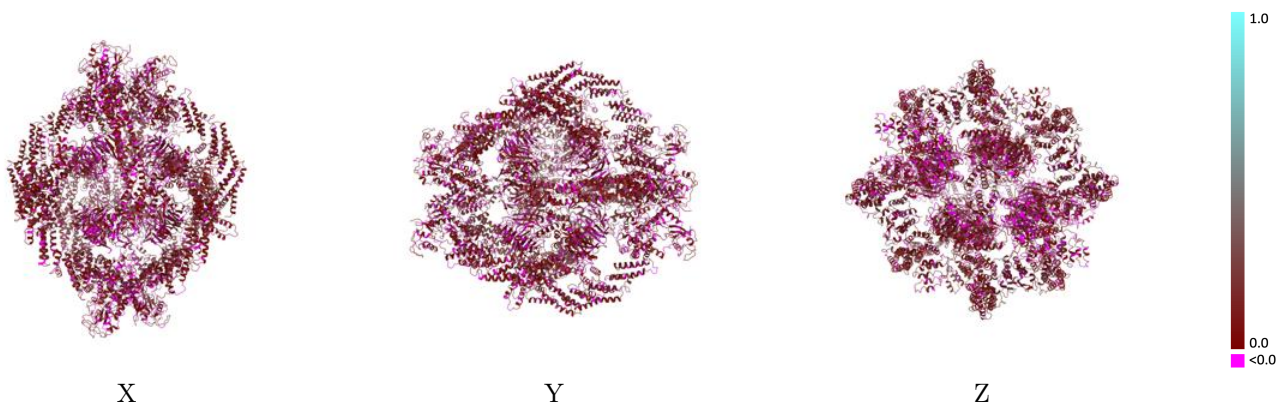
This section contains information regarding the fit between EMDB map EMD-34451 and PDB model 8H35. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



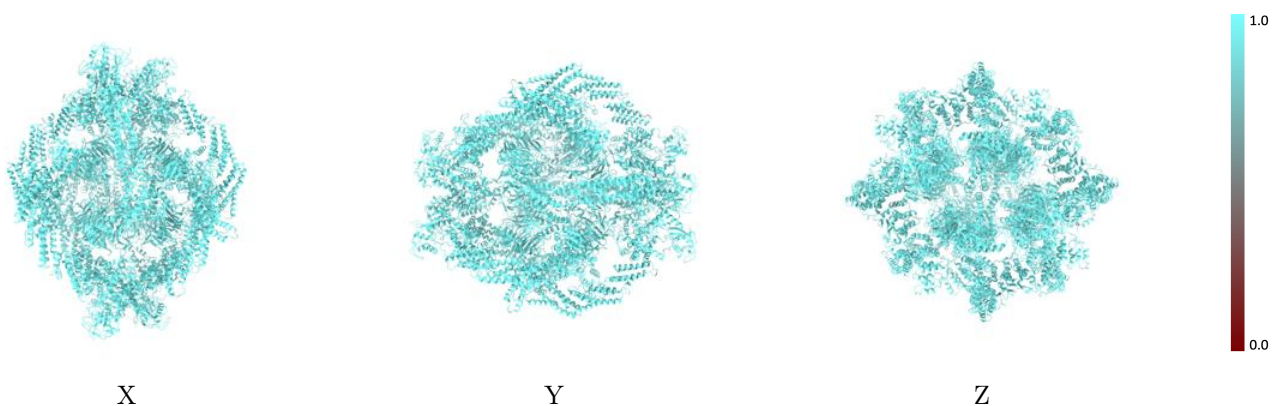
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



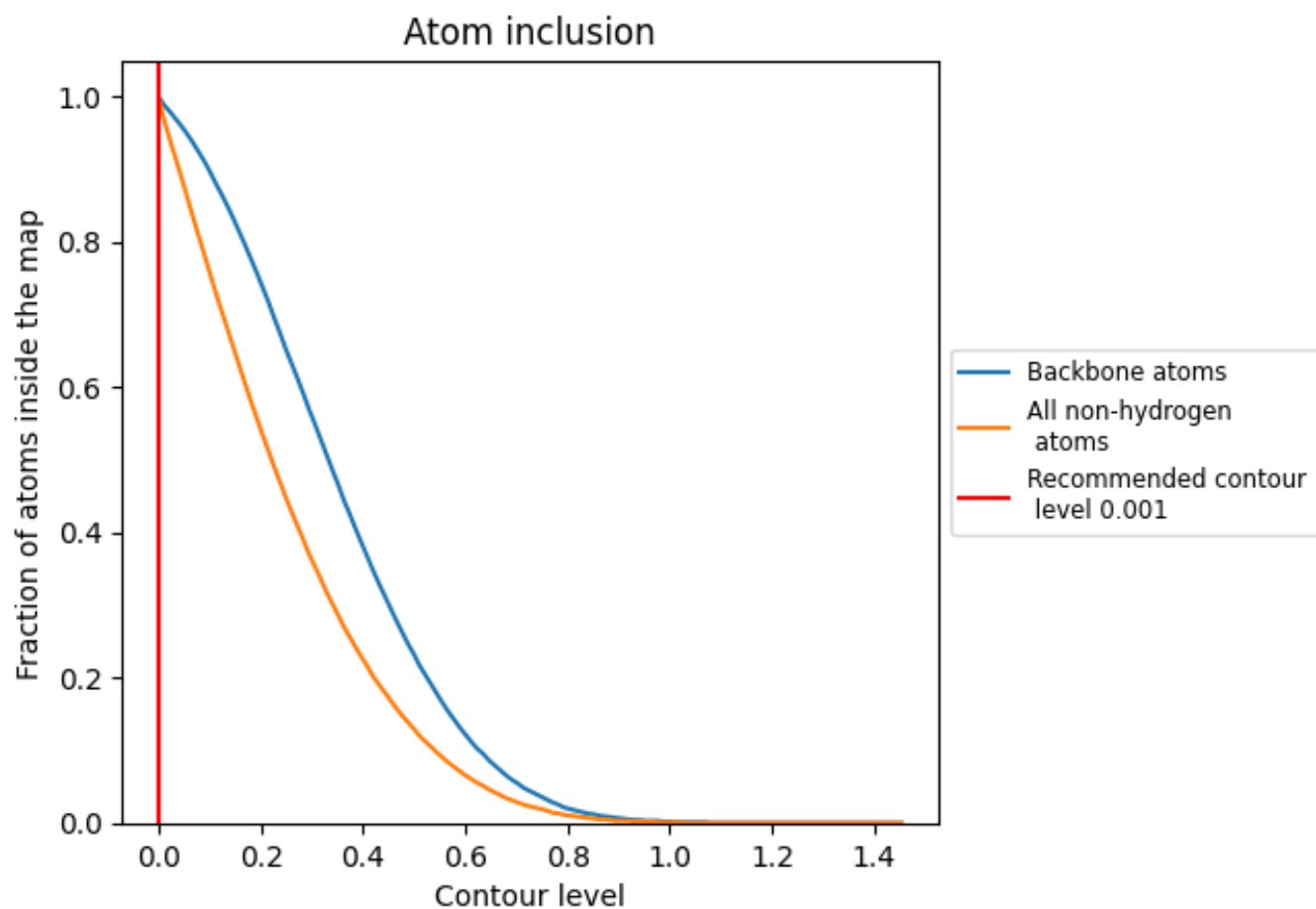
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.001).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9940	 0.0910
A	 0.9960	 0.1030
B	 0.9910	 0.0770
C	 0.9980	 0.1100
D	 0.9830	 0.0370
E	 0.9900	 0.0710
F	 0.9990	 0.0950
G	 0.9900	 0.0720
H	 0.9980	 0.1060
I	 0.9940	 0.0900
J	 0.9930	 0.0960
K	 0.9820	 0.0840
L	 0.9900	 0.0380
M	 0.9970	 0.1080
N	 0.9920	 0.0760
O	 0.9980	 0.0970
P	 0.9950	 0.1020
Q	 0.9900	 0.0380
R	 0.9790	 0.0640
S	 0.9890	 0.0690
T	 0.9940	 0.0910
U	 0.9930	 0.0930
V	 0.9970	 0.1050
W	 0.9860	 0.0380
X	 0.9430	 0.0710

