



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 02:05 PM UTC

PDB ID : 7YI0 / pdb_00007yi0
EMDB ID : EMD-33845
Title : Cryo-EM structure of Rpd3S complex
Authors : Li, H.T.; Yan, C.Y.; Guan, H.P.; Wang, P.
Deposited on : 2022-07-14
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

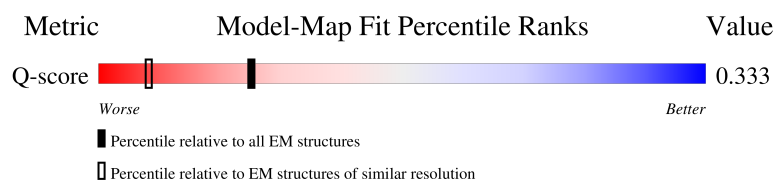
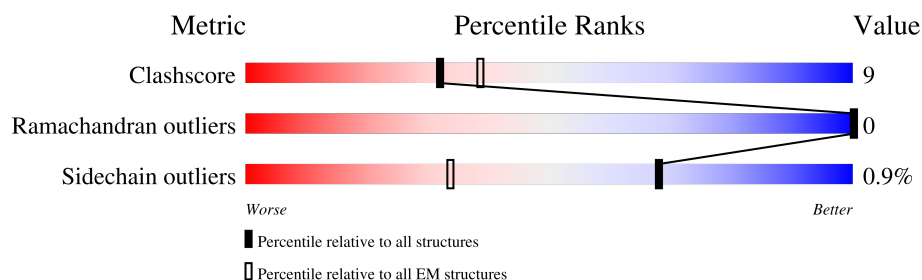
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	1536	
2	B	433	
3	C	401	
3	E	401	

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Mol	Chain	Length	Quality of chain
4	D	684	14% 35% 11% 55%
5	F	684	15% 13% 5% 82%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13430 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	503	Total	C	N	O	S	0	0
			4233	2722	708	790	13		

- Molecule 2 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	368	Total	C	N	O	S	0	0
			2923	1858	495	545	25		

- Molecule 3 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	182	Total	C	N	O	S	0	0
			1473	944	237	283	9		
3	E	154	Total	C	N	O	S	0	0
			1259	815	201	235	8		

- Molecule 4 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	311	Total	C	N	O	S	0	0
			2553	1625	441	469	18		

- Molecule 5 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	120	Total	C	N	O	S	0	0
			982	635	166	171	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	567	ALA	PHE	engineered mutation	UNP Q04779

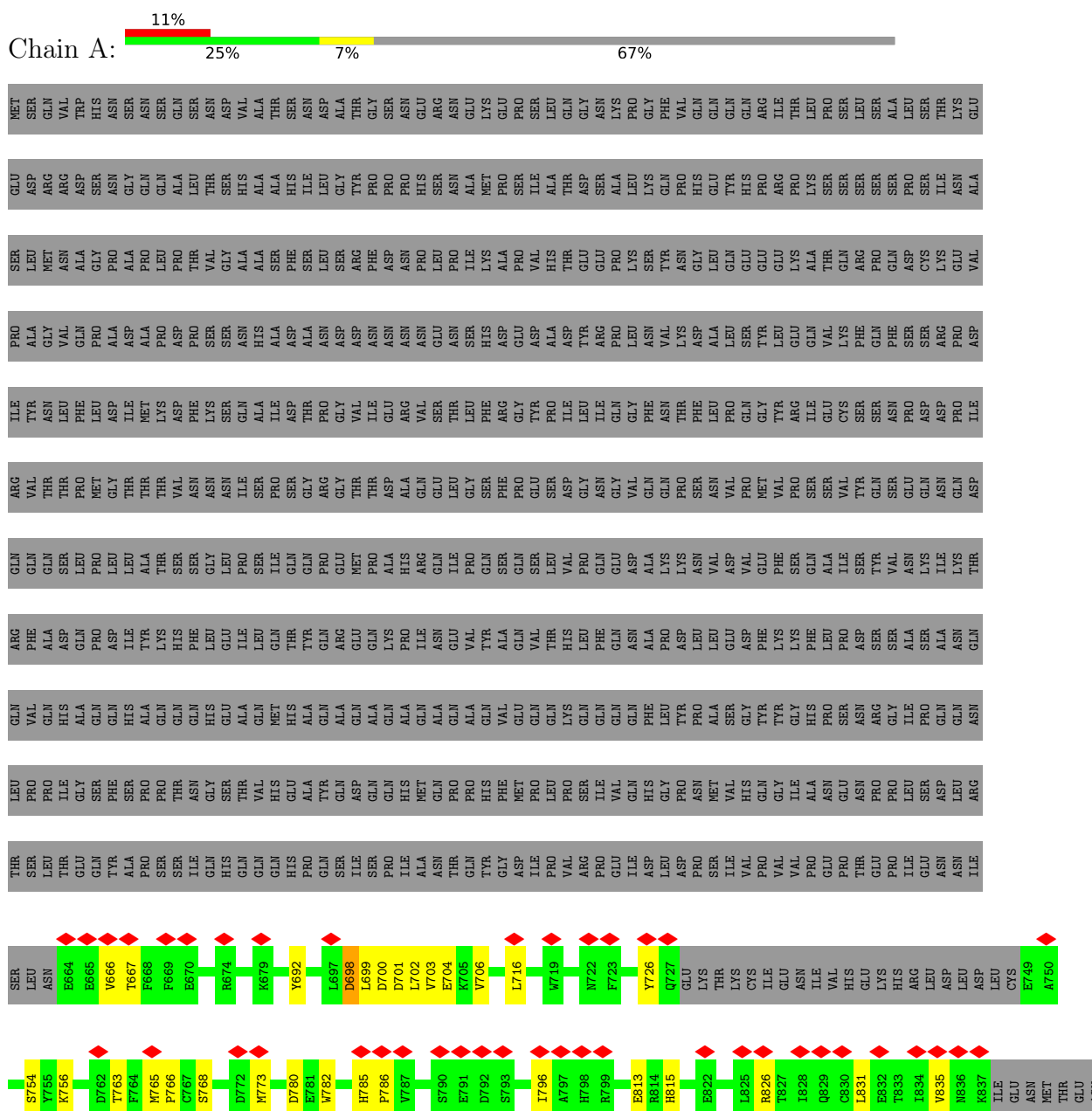
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

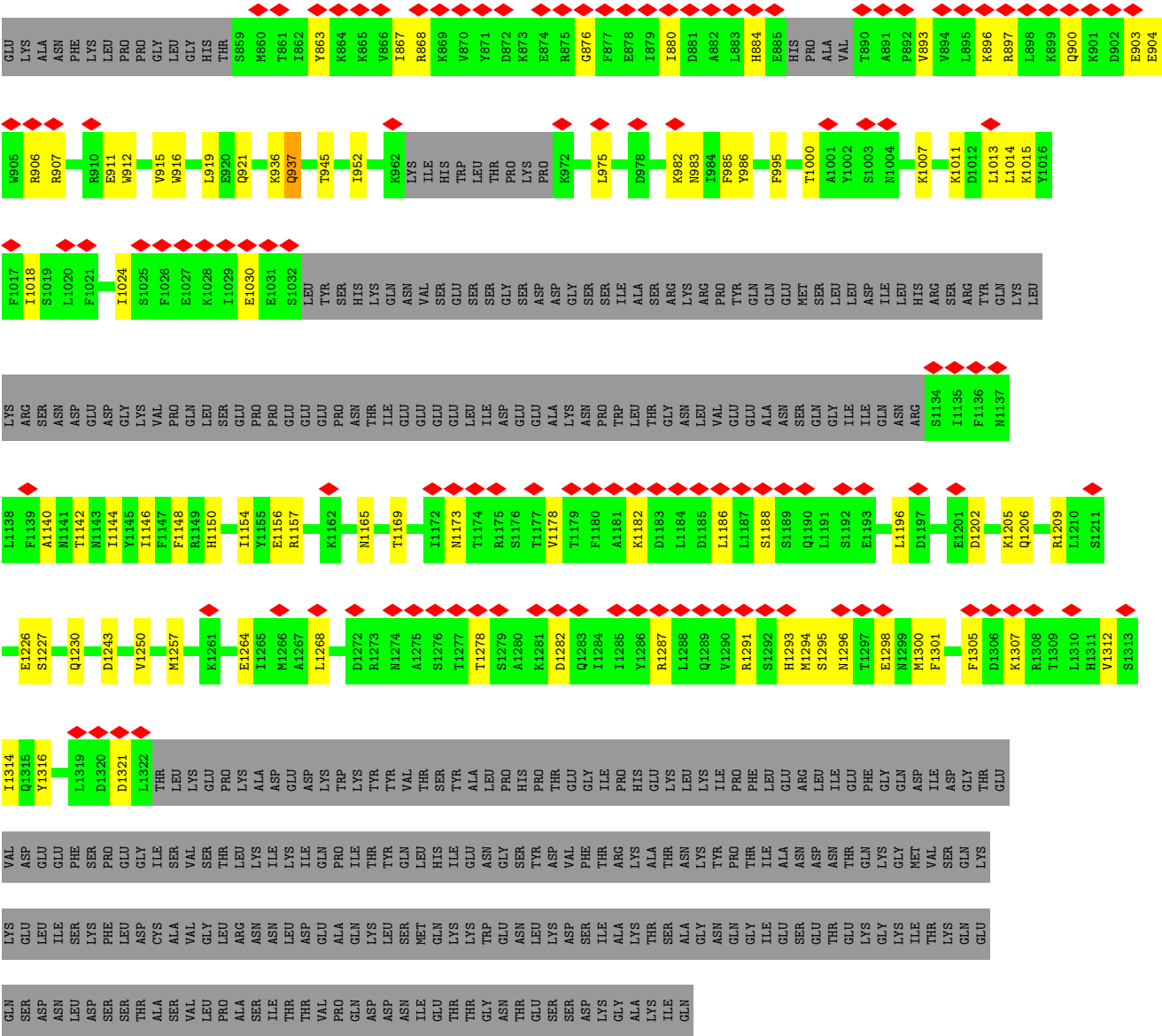
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total 1	Zn 1	0
6	D	4	Total 4	Zn 4	0
6	F	2	Total 2	Zn 2	0

3 Residue-property plots

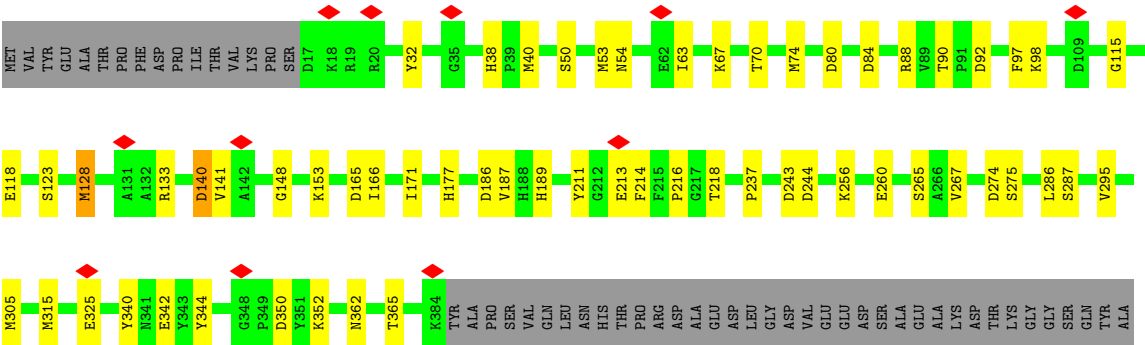
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transcriptional regulatory protein SIN3



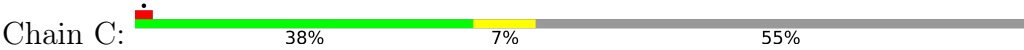


● Molecule 2: Histone deacetylase RPD3



ARG
ASP
LEU
HIS
VAL
GLU
HIS
ASP
ASN
GLU
PHE
TYR

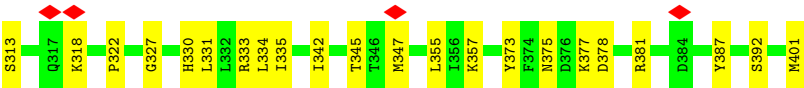
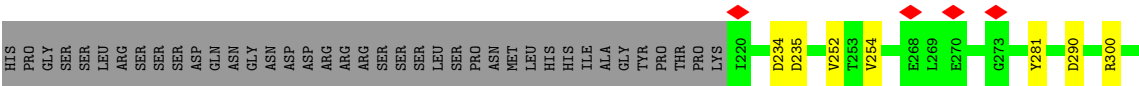
• Molecule 3: Chromatin modification-related protein EAF3



MET VAL ASP LEU ASP LEU GLU GLN GLU PHE GLU ALA GLY GLY ARG CYS LEU ALA PHE HIS GLY PRO LEU TYR MET GLN TRP GLU LYS ALA LYS ILE ASP LEU TRP ASP ILE TRP ASP PRO SER SER LYS MET ILE TYR THR SER GLN ILE ASN PRO GLU ASN LYS ASP THR

LEU GLY GLU ASP LEU SER ILE PRO GLU LEU ILE GLY ILE ASN GLY LYS CYS PHE PHE HIS GLY PRO ARG HIS GLY TYR GLN TRP LYS LYS TRP GLU LYS SER SER TRP ASP ILE TRP ASP VAL GLY TYR SER SER LYS ILE TRP THR ARG ALA TYR ASN GLU ASN LYS ILE THR

SER LEU LEU GLU SER GLN LYS LYS LYS LEU ILE GLY ILE ASN THR SER THR SER GLY GLY ASN GLY ASP GLY PHE PRO ARG ARG SER ARG SER GLY SER LYS LYS GLY SER PRO ASP MET LEU ASP ILE HIS HIS ILE ALA SER ILE TYR LYS THR PRO THR SER GLN PHE ASN ILE THR LEU THR ASP THR



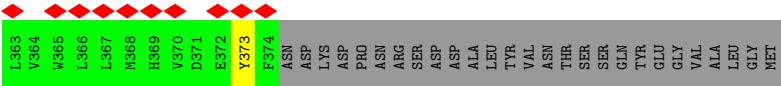
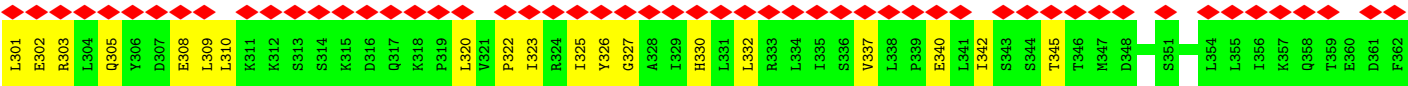
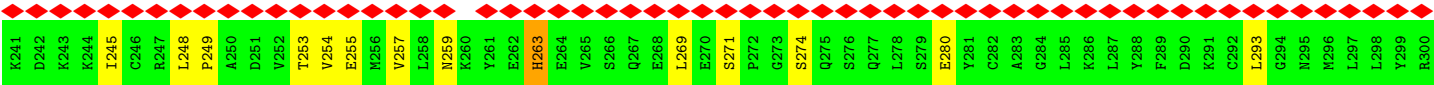
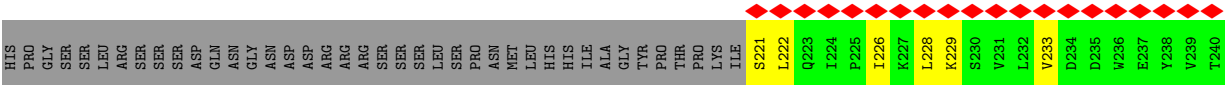
• Molecule 3: Chromatin modification-related protein EAF3



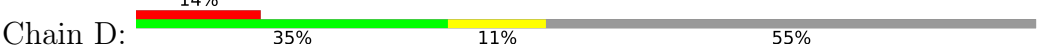
MET VAL ASP LEU ASP LEU GLU GLN GLU PHE GLU ALA GLY GLY ARG CYS LEU ALA PHE HIS GLY PRO LEU TYR MET GLN TRP GLU LYS ALA LYS ILE ASP LEU TRP ASP ILE TRP ASP PRO SER SER LYS MET ILE TYR THR SER GLN ILE ASN PRO GLU ASN LYS ASP THR

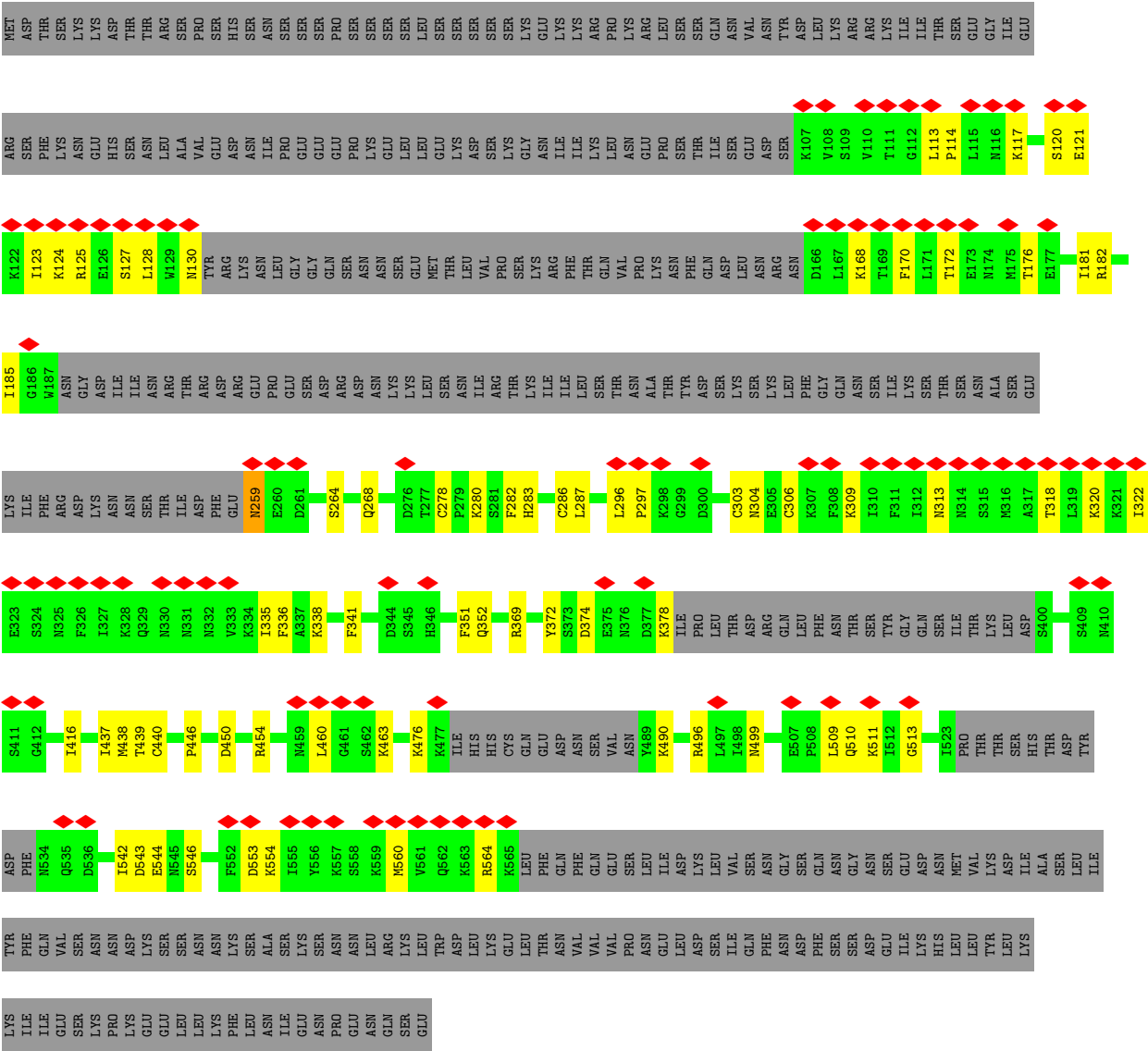
LEU GLY GLU ASP LEU SER ILE PRO GLU LEU ILE GLY ILE ASN GLY LYS CYS PHE PHE HIS GLY PRO ARG HIS GLY TYR GLN TRP LYS LYS TRP GLU LYS SER SER TRP ASP VAL GLY TYR SER ASP ARG LYS MET ILE ARG ALA TYR THR SER GLN TYR ASN ILE THR LEU THR ASP THR

SER LEU LEU GLU SER GLN LYS LYS LYS LEU ILE GLY ILE ASN THR SER THR SER GLY GLY ASN GLY PHE GLU GLU GLU LYS ILE THR SER GLN ILE THR LEU THR ASP THR

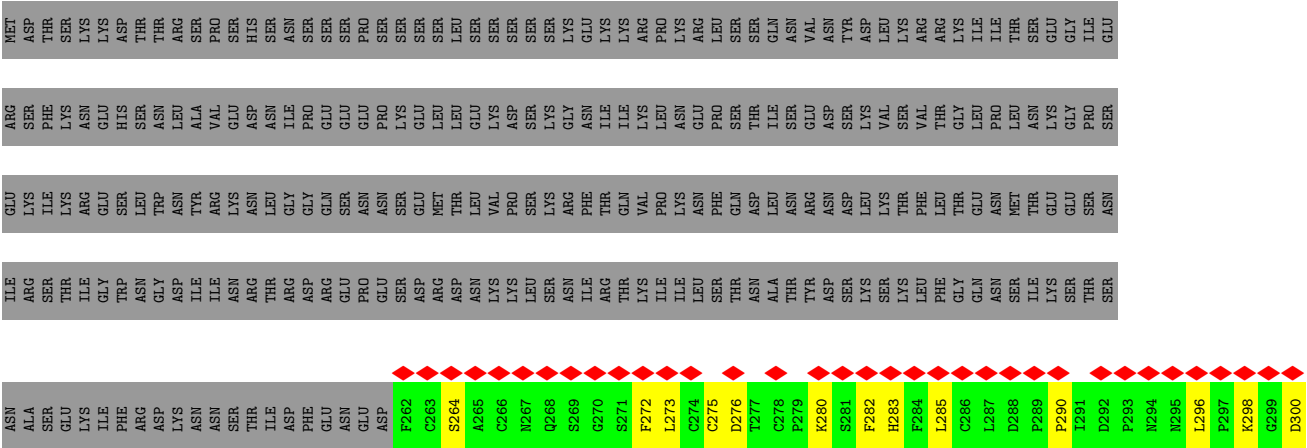


• Molecule 4: Transcriptional regulatory protein RCO1





● Molecule 5: Transcriptional regulatory protein RCO1



LYS PRO PRO LYS GLU GLU LEU LEU LYS PHE LEU ASN ILE GLU ASN PRO GLU ASN GLN SER GLU	ASN	N545	ASN	LEU	LYS	W301
	ASP	S546	SER	GLY	THR	H302
	LYS	I547	ASN	TRP	SER	N303
	SER	K549	LYS	SER	ARG	N304
	ASN	Y549	VAL	HIS	GLY	E305
	ASN	D550	TRP	PRO	GLN	C306
	LYS	F551	LYS	ASN	TYR	K307
	SER	F552	LYS	SER	ASP	F308
	ALA	D553	GLN	ARG	GLU	K309
	SER	K554	LEU	LEU	ASN	I310
ASN ASN VAL VAL VAL PRO ASN GLU ASP LEU GLU LEU THR THR ASN ASN VAL VAL VAL PRO ASN GLU ASP ASP TLE GLN PHE ASN SER ASP GLU TLE LYS LYS TLE GLU SER	LYS	I555	ILE	ILE	ASP	F311
	ASN	Y556	LYS	THR	ILE	I312
	ASN	K557	LYS	CYS	PRO	N313
	LEU	S558	LYS	ASP	LEU	N314
	ARG	K559	ASN	TYR	THR	N315
	LYS	M560	GLN	CYS	ASP	S316
	TRP	V561	TYR	THR	GLN	A317
	ASP	Q562	GLU	PRO	LEU	T318
	LEU	K563	LEU	HIS	ASN	L319
	GLU	R564	LEU	LEU	THR	K320
PHE ASN ASP PHE PHE SER SER ASP GLU ILE LYS HIS LEU LEU TYR LEU LYS LYS TLE GLU SER	THR	L565	GLN	ASP	SER	K321
	VAL	A567	VAL	CYS	TYR	I322
	VAL	G568	VAL	ARG	SER	E323
	PRO	PHE	GLN	ALA	ILE	Q329
	ASN	GLN	ASN	SER	THR	N330
	GLU	SER	GLY	PHE	LYS	N331
	LEU	LEU	ASN	LYS	LEU	N332
	ASP	ILE	ILE	LEU	ASP	V333
	SER	ASP	GLN	GLY	SER	T334
	TLE	LYS	ILE	SER	ASN	K334
LYS LEU LEU PHE GLN VAL SER SER ASP GLU ILE LYS HIS LEU LEU TYR LEU LYS LYS TLE GLU SER	PRO	LEU	LYS	PRO	I335	
	PHE	VAL	TRP	TRP	ASP	F336
	ASN	ASN	LYS	LYS	THR	A337
	ASP	ASN	CYS	CYS	HIS	K338
	PHE	GLY	PRO	PRO	ILE	L339
	SER	SER	LEU	HIS	SER	N340
	ASP	ASN	SER	SER	ASN	F341
	GLU	GLY	THR	PRO	SER	N342
	ILE	ASN	PHE	LYS	LYS	I343
	LYS	SER	VAL	VAL	PHE	D344
HIS LEU LEU TYR LEU LYS LYS TLE GLU TLE GLU SER	HIS	GLU	ASN	TYR	LEU	S345
	LEU	ASP	GLN	TYR	LEU	S346
	LEU	ASN	ASP	LYS	ILE	H346
	TYR	MET	PHE	LYS	TYR	N347
	LEU	VAL	LYS	ILE	LYS	F348
	LYS	LYS	ILE	HIS	CYS	K349
	LYS	ASP	THR	GLN	ASN	Q350
	TLE	ILE	ILE	GLN	GLN	F351
	GLU	ALA	SER	ASP	THR	Q352
	GLU	SER	LEU	GLU	ARG	P354
LYS LEU LEU PHE GLN VAL SER	VAL	VAL	VAL	N355	Y356	
	SER	SER	SER	I357	K358	
				GLU	THR	
				PRO	PHE	
				ALA	VAL	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	670000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	A	0.13	0/4321	0.33	1/5814 (0.0%)
2	B	0.13	0/2997	0.27	0/4051
3	C	0.12	0/1499	0.29	0/2028
3	E	0.14	0/1282	0.38	0/1733
4	D	0.13	0/2614	0.32	0/3517
5	F	0.11	0/1007	0.35	0/1351
All	All	0.13	0/13720	0.32	1/18494 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	937	GLN	N-CA-C	-6.25	107.49	114.62

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	4233	0	4188	77	0
2	B	2923	0	2805	43	0
3	C	1473	0	1497	20	0
3	E	1259	0	1300	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2553	0	2507	60	0
5	F	982	0	976	27	0
6	B	1	0	0	0	0
6	D	4	0	0	0	0
6	F	2	0	0	0	0
All	All	13430	0	13273	229	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 (229) 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:A:921:GLN:HE21	1:A:1188:SER:HB2	1.26	0.96
4:D:259:ASN:N	4:D:259:ASN:HD22	1.70	0.89
2:B:140:ASP:OD1	2:B:140:ASP:N	2.19	0.76
1:A:985:PHE:HB3	1:A:1018:ILE:HD11	1.68	0.75
2:B:187:VAL:HG22	2:B:274:ASP:HB3	1.71	0.72
4:D:113:LEU:HD11	4:D:120:SER:HB2	1.71	0.72
4:D:510:GLN:NE2	4:D:513:GLY:O	2.22	0.72
3:E:248:LEU:HB3	3:E:249:PRO:HD2	1.72	0.71
2:B:123:SER:OG	2:B:165:ASP:OD1	2.11	0.69
3:C:313:SER:OG	3:C:318:LYS:O	2.11	0.69
1:A:815:HIS:HB2	2:B:315:MET:HE1	1.74	0.69
2:B:213:GLU:HG2	4:D:460:LEU:HD12	1.73	0.69
3:C:234:ASP:OD1	4:D:496:ARG:NH1	2.26	0.68
5:F:357:ILE:HG23	3:E:229:LYS:HG2	1.76	0.68
1:A:921:GLN:NE2	1:A:1188:SER:HB2	2.07	0.65
2:B:84:ASP:OD2	2:B:88:ARG:NH1	2.30	0.65
1:A:982:LYS:HD2	1:A:1024:ILE:HG23	1.80	0.64
3:C:300:ARG:NH1	4:D:268:GLN:OE1	2.30	0.64
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.80	0.63
3:E:249:PRO:HB3	3:E:325:ILE:HA	1.79	0.63
4:D:560:MET:HE1	5:F:562:GLN:CD	2.24	0.63
1:A:701:ASP:HA	1:A:704:GLU:HG2	1.80	0.62
2:B:118:GLU:CD	2:B:118:GLU:H	2.07	0.62
2:B:256:LYS:O	2:B:260:GLU:HG2	1.99	0.62
1:A:765:MET:HE3	1:A:766:PRO:HD2	1.79	0.62
4:D:114:PRO:HD2	4:D:117:LYS:HG2	1.81	0.61
3:E:253:THR:HA	3:E:327:GLY:HA3	1.81	0.61
3:E:342:ILE:O	3:E:345:THR:OG1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:VAL:HG11	3:C:373:TYR:HE1	1.65	0.61
2:B:128:MET:HB3	4:D:182:ARG:HD2	1.83	0.61
1:A:863:TYR:O	1:A:867:ILE:HG12	2.00	0.60
4:D:543:ASP:OD1	4:D:544:GLU:N	2.34	0.60
2:B:342:GLU:N	2:B:342:GLU:OE1	2.33	0.59
4:D:259:ASN:N	4:D:259:ASN:ND2	2.44	0.59
5:F:290:PRO:HD2	3:E:310:LEU:HD12	1.84	0.59
5:F:319:LEU:HD22	5:F:320:LYS:H	1.68	0.59
3:C:235:ASP:OD2	3:C:333:ARG:NH2	2.35	0.58
2:B:189:HIS:H	2:B:216:PRO:HG2	1.67	0.58
3:C:375:ASN:HD22	3:C:377:LYS:HE2	1.69	0.58
4:D:437:ILE:HD11	4:D:446:PRO:HB2	1.86	0.58
2:B:88:ARG:HH21	2:B:97:PHE:HE1	1.50	0.58
1:A:919:LEU:HB2	4:D:127:SER:HB3	1.86	0.57
2:B:365:THR:OG1	4:D:450:ASP:OD2	2.21	0.57
1:A:698:ASP:OD1	1:A:698:ASP:N	2.33	0.57
4:D:509:LEU:HD11	5:F:338:LYS:HE3	1.87	0.57
4:D:309:LYS:HA	4:D:313:ASN:HB2	1.86	0.57
1:A:786:PRO:HB3	2:B:216:PRO:O	2.05	0.56
3:C:375:ASN:ND2	3:C:377:LYS:HE2	2.20	0.56
1:A:975:LEU:HB2	1:A:1314:ILE:HB	1.86	0.56
2:B:244:ASP:OD2	2:B:287:SER:OG	2.22	0.56
5:F:264:SER:O	5:F:264:SER:OG	2.20	0.56
3:C:342:ILE:HD11	3:C:355:LEU:HD23	1.89	0.55
5:F:556:TYR:CE1	5:F:560:MET:HE1	2.41	0.55
4:D:542:ILE:O	4:D:546:SER:OG	2.19	0.55
2:B:50:SER:OG	2:B:342:GLU:OE1	2.25	0.55
4:D:372:TYR:OH	4:D:496:ARG:NH2	2.40	0.55
2:B:243:ASP:OD1	2:B:362:ASN:ND2	2.41	0.53
1:A:1300:MET:HG2	1:A:1301:PHE:N	2.23	0.53
5:F:282:PHE:HE1	5:F:347:ASN:HB3	1.74	0.53
4:D:511:LYS:HD3	5:F:334:LYS:HD3	1.91	0.53
2:B:90:THR:HG22	2:B:92:ASP:H	1.73	0.53
5:F:275:CYS:SG	5:F:276:ASP:N	2.82	0.53
1:A:945:THR:HG22	1:A:1146:ILE:HG13	1.92	0.52
5:F:273:LEU:N	5:F:282:PHE:O	2.42	0.52
1:A:826:ARG:HG3	1:A:826:ARG:HH11	1.74	0.52
1:A:1169:THR:O	1:A:1173:ASN:ND2	2.43	0.52
4:D:318:THR:O	4:D:322:ILE:HG13	2.10	0.52
1:A:1007:LYS:O	1:A:1011:LYS:HG3	2.10	0.52
3:E:228:LEU:HD13	3:E:332:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:GLY:O	1:A:880:ILE:HG13	2.10	0.51
1:A:1264:GLU:OE1	1:A:1293:HIS:ND1	2.43	0.51
2:B:177:HIS:HB3	2:B:265:SER:HB2	1.91	0.51
2:B:53:MET:HE2	4:D:172:THR:HB	1.92	0.51
5:F:322:ILE:HD12	5:F:322:ILE:H	1.76	0.51
3:E:226:ILE:HA	3:E:229:LYS:HE3	1.92	0.51
4:D:283:HIS:HB2	4:D:286:CYS:HB2	1.92	0.51
4:D:296:LEU:HD12	4:D:297:PRO:HD2	1.93	0.51
1:A:785:HIS:CE1	3:C:392:SER:HB3	2.46	0.51
3:E:245:ILE:HD11	3:E:301:LEU:HD13	1.92	0.51
2:B:243:ASP:OD1	2:B:243:ASP:N	2.44	0.51
3:C:378:ASP:HB3	3:C:381:ARG:HG3	1.93	0.51
5:F:280:LYS:NZ	5:F:347:ASN:OD1	2.44	0.51
3:C:281:TYR:HA	4:D:335:ILE:HD11	1.93	0.51
3:E:263:HIS:ND1	3:E:263:HIS:C	2.69	0.50
1:A:768:SER:OG	2:B:80:ASP:OD2	2.25	0.50
1:A:896:LYS:HD2	1:A:897:ARG:N	2.26	0.50
2:B:133:ARG:HG2	4:D:181:ILE:HD11	1.93	0.50
3:E:305:GLN:O	3:E:308:GLU:HG3	2.12	0.50
3:C:342:ILE:O	3:C:345:THR:OG1	2.29	0.49
5:F:357:ILE:HD12	3:E:229:LYS:HG2	1.94	0.49
3:E:221:SER:OG	3:E:222:LEU:N	2.45	0.49
5:F:300:ASP:OD2	5:F:302:HIS:NE2	2.45	0.49
1:A:983:ASN:HA	1:A:986:TYR:CD1	2.47	0.49
1:A:893:VAL:HA	1:A:896:LYS:HE3	1.95	0.49
3:C:235:ASP:OD1	3:C:387:TYR:OH	2.30	0.49
4:D:125:ARG:NH1	4:D:130:ASN:O	2.42	0.49
1:A:826:ARG:HG3	1:A:826:ARG:NH1	2.27	0.49
3:E:255:GLU:HG2	3:E:259:ASN:HD21	1.78	0.49
1:A:1305:PHE:CE2	1:A:1307:LYS:HG2	2.48	0.48
2:B:186:ASP:OD1	2:B:187:VAL:N	2.47	0.48
2:B:295:VAL:HG21	2:B:325:GLU:HG2	1.95	0.48
1:A:1278:THR:HB	1:A:1282:ASP:HB2	1.95	0.48
3:C:331:LEU:HD12	3:C:334:LEU:HD23	1.95	0.48
4:D:120:SER:O	4:D:123:ILE:N	2.47	0.48
4:D:351:PHE:O	4:D:352:GLN:NE2	2.41	0.48
4:D:278:CYS:SG	4:D:280:LYS:NZ	2.87	0.48
5:F:296:LEU:O	5:F:298:LYS:HD2	2.14	0.48
3:C:254:VAL:HG23	3:C:327:GLY:HA2	1.95	0.48
4:D:476:LYS:HG3	4:D:490:LYS:HB2	1.94	0.48
1:A:1287:ARG:HG3	1:A:1300:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:ASN:O	1:A:1169:THR:OG1	2.24	0.47
5:F:276:ASP:N	5:F:276:ASP:OD1	2.43	0.47
1:A:1206:GLN:OE1	1:A:1209:ARG:NH2	2.38	0.47
2:B:216:PRO:C	2:B:218:THR:H	2.22	0.47
4:D:542:ILE:HG13	4:D:546:SER:OG	2.14	0.47
2:B:32:TYR:CD1	2:B:115:GLY:HA3	2.50	0.47
5:F:556:TYR:CZ	5:F:560:MET:HE1	2.50	0.47
1:A:702:LEU:O	1:A:706:VAL:HG23	2.15	0.47
1:A:831:LEU:O	1:A:835:VAL:HG23	2.15	0.47
1:A:754:SER:HB2	2:B:218:THR:HG22	1.97	0.46
4:D:553:ASP:OD1	3:E:271:SER:HB3	2.15	0.46
3:E:303:ARG:HE	3:E:303:ARG:HB3	1.59	0.46
3:C:357:LYS:HE3	3:C:357:LYS:HB3	1.67	0.46
4:D:378:LYS:HB3	4:D:463:LYS:HG3	1.97	0.46
5:F:305:GLU:H	5:F:347:ASN:HD21	1.63	0.46
4:D:121:GLU:HA	4:D:124:LYS:HG3	1.97	0.46
2:B:70:THR:O	2:B:74:MET:HG3	2.16	0.46
2:B:350:ASP:HB2	2:B:352:LYS:HD3	1.98	0.46
1:A:1000:THR:O	1:A:1000:THR:HG23	2.16	0.46
1:A:1202:ASP:HB3	1:A:1205:LYS:HE2	1.96	0.46
1:A:773:MET:HE1	2:B:171:ILE:HG23	1.98	0.45
2:B:38:HIS:CE1	2:B:40:MET:HB3	2.51	0.45
3:E:255:GLU:O	3:E:259:ASN:ND2	2.49	0.45
1:A:700:ASP:OD1	1:A:700:ASP:N	2.48	0.45
1:A:1142:THR:O	1:A:1146:ILE:HG12	2.16	0.45
1:A:703:VAL:HG21	1:A:726:TYR:CD1	2.52	0.45
4:D:124:LYS:O	4:D:128:LEU:HB2	2.17	0.45
3:E:253:THR:O	3:E:257:VAL:HG23	2.17	0.45
3:E:254:VAL:HG23	3:E:327:GLY:HA2	1.98	0.45
4:D:511:LYS:NZ	3:E:280:GLU:OE1	2.50	0.45
1:A:900:GLN:O	1:A:904:GLU:HG2	2.17	0.45
4:D:335:ILE:HG13	4:D:336:PHE:CD1	2.51	0.45
3:E:326:TYR:HD2	3:E:330:HIS:CD2	2.35	0.45
1:A:868:ARG:HG3	1:A:868:ARG:HH11	1.81	0.45
1:A:1014:LEU:O	1:A:1018:ILE:HG22	2.16	0.45
1:A:1178:VAL:HB	1:A:1182:LYS:HB3	1.98	0.45
2:B:148:GLY:HA2	2:B:166:ILE:HD11	1.98	0.45
3:E:337:VAL:HG22	3:E:340:GLU:HB3	1.97	0.45
1:A:906:ARG:HG2	1:A:906:ARG:HH11	1.82	0.45
2:B:275:SER:HB2	2:B:286:LEU:HD12	1.99	0.45
5:F:322:ILE:HD12	5:F:322:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:264:SER:HB2	4:D:282:PHE:CE1	2.52	0.45
5:F:272:PHE:CD1	5:F:283:HIS:CE1	3.05	0.45
1:A:1015:LYS:HD3	1:A:1030:GLU:HG2	1.99	0.44
4:D:564:ARG:HA	4:D:564:ARG:HD3	1.77	0.44
1:A:936:LYS:O	1:A:937:GLN:HG3	2.17	0.44
1:A:1013:LEU:HD12	1:A:1257:MET:HG3	1.99	0.44
4:D:499:ASN:OD1	4:D:499:ASN:N	2.50	0.44
2:B:50:SER:O	2:B:54:ASN:ND2	2.47	0.44
3:E:229:LYS:O	3:E:233:VAL:HG23	2.18	0.44
3:C:290:ASP:HA	3:C:322:PRO:HG2	1.99	0.44
4:D:439:THR:HG23	4:D:439:THR:O	2.18	0.44
1:A:756:LYS:O	1:A:782:TRP:HA	2.18	0.44
1:A:1294:MET:HG2	1:A:1298:GLU:OE2	2.18	0.44
3:E:257:VAL:HG22	3:E:373:TYR:CE1	2.53	0.44
3:E:320:LEU:HD12	3:E:322:PRO:HD3	1.99	0.44
2:B:67:LYS:HD3	4:D:185:ILE:HD11	2.00	0.43
3:E:293:LEU:HD21	3:E:326:TYR:CD1	2.53	0.43
1:A:1156:GLU:HG3	1:A:1157:ARG:N	2.34	0.43
1:A:1243:ASP:OD1	1:A:1243:ASP:N	2.50	0.43
3:E:309:LEU:HD12	3:E:309:LEU:HA	1.85	0.43
2:B:340:TYR:HA	2:B:344:TYR:CD1	2.54	0.43
2:B:63:ILE:HG22	4:D:176:THR:HG22	2.00	0.43
3:C:330:HIS:HA	3:C:333:ARG:HG2	1.99	0.43
3:C:331:LEU:O	3:C:335:ILE:HG12	2.18	0.43
4:D:306:CYS:HA	4:D:309:LYS:HG2	2.00	0.43
1:A:1295:SER:OG	1:A:1296:ASN:N	2.50	0.43
4:D:168:LYS:HB2	4:D:170:PHE:CE1	2.54	0.43
1:A:666:VAL:HG23	1:A:667:THR:HG23	1.99	0.43
1:A:915:VAL:HA	4:D:128:LEU:HD11	2.01	0.42
4:D:438:MET:HE1	4:D:454:ARG:NE	2.34	0.42
1:A:1148:PHE:CZ	1:A:1312:VAL:HG11	2.54	0.42
4:D:338:LYS:HE2	4:D:338:LYS:HB2	1.88	0.42
4:D:369:ARG:NH1	4:D:369:ARG:HB2	2.35	0.42
1:A:1226:GLU:OE2	1:A:1230:GLN:NE2	2.36	0.42
2:B:267:VAL:O	2:B:305:MET:HA	2.18	0.42
4:D:374:ASP:N	4:D:374:ASP:OD1	2.52	0.42
1:A:1150:HIS:O	1:A:1154:ILE:HG13	2.19	0.42
4:D:438:MET:HE1	4:D:454:ARG:HE	1.84	0.42
1:A:699:LEU:O	1:A:703:VAL:HG23	2.19	0.42
2:B:244:ASP:OD1	2:B:244:ASP:N	2.53	0.42
5:F:285:LEU:HD23	5:F:285:LEU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:349:LYS:HE3	5:F:349:LYS:HB2	1.78	0.42
4:D:320:LYS:HD3	4:D:320:LYS:HA	1.84	0.41
5:F:340:LEU:O	5:F:343:ILE:HG22	2.20	0.41
1:A:1268:LEU:HD11	1:A:1293:HIS:CD2	2.55	0.41
1:A:1169:THR:HG22	1:A:1173:ASN:ND2	2.36	0.41
1:A:763:THR:HG23	1:A:780:ASP:HB3	2.03	0.41
1:A:785:HIS:HA	1:A:786:PRO:HD2	1.86	0.41
1:A:716:LEU:HD23	1:A:716:LEU:HA	1.91	0.41
1:A:796:ILE:H	2:B:213:GLU:HB3	1.85	0.41
3:E:255:GLU:CG	3:E:259:ASN:HD21	2.33	0.41
1:A:995:PHE:HD2	1:A:1250:VAL:HG21	1.86	0.41
4:D:322:ILE:HG12	4:D:341:PHE:CE1	2.56	0.41
1:A:912:TRP:HB3	1:A:916:TRP:CH2	2.56	0.41
2:B:141:VAL:HG22	2:B:305:MET:HG2	2.03	0.41
3:C:401:MET:HE2	3:C:401:MET:HB3	1.78	0.41
4:D:335:ILE:HG13	4:D:336:PHE:HD1	1.86	0.41
5:F:551:PHE:HE1	5:F:555:ILE:HD11	1.86	0.41
1:A:1196:LEU:HB3	1:A:1227:SER:HB3	2.03	0.41
5:F:305:GLU:C	5:F:307:LYS:H	2.29	0.41
1:A:952:ILE:HG12	1:A:1316:TYR:HB2	2.03	0.40
1:A:831:LEU:HD23	1:A:831:LEU:HA	1.90	0.40
1:A:907:ARG:O	1:A:911:GLU:HG2	2.21	0.40
1:A:912:TRP:HH2	4:D:123:ILE:HD12	1.86	0.40
5:F:308:PHE:HA	5:F:311:PHE:HB3	2.02	0.40
1:A:692:TYR:O	4:D:554:LYS:NZ	2.52	0.40
1:A:813:GLU:OE1	1:A:916:TRP:NE1	2.55	0.40
1:A:867:ILE:HD12	1:A:880:ILE:HG12	2.03	0.40
3:E:245:ILE:HG12	3:E:302:GLU:HG2	2.02	0.40
3:E:269:LEU:HD13	3:E:274:SER:HB2	2.03	0.40
1:A:880:ILE:HG22	1:A:884:HIS:CE1	2.57	0.40
2:B:211:TYR:CB	2:B:237:PRO:HB3	2.52	0.40
4:D:287:LEU:HD12	4:D:287:LEU:HA	1.98	0.40
4:D:304:ASN:OD1	4:D:304:ASN:N	2.53	0.40
4:D:416:ILE:O	4:D:446:PRO:HG2	2.21	0.40
1:A:1291:ARG:HD3	1:A:1321:ASP:OD2	2.21	0.40
4:D:130:ASN:OD1	4:D:130:ASN:N	2.54	0.40
3:E:255:GLU:N	3:E:323:ILE:HG22	2.37	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	491/1536 (32%)	472 (96%)	19 (4%)	0	100	100
2	B	366/433 (84%)	350 (96%)	16 (4%)	0	100	100
3	C	180/401 (45%)	171 (95%)	9 (5%)	0	100	100
3	E	152/401 (38%)	141 (93%)	11 (7%)	0	100	100
4	D	299/684 (44%)	272 (91%)	27 (9%)	0	100	100
5	F	116/684 (17%)	106 (91%)	10 (9%)	0	100	100
All	All	1604/4139 (39%)	1512 (94%)	92 (6%)	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	469/1391 (34%)	466 (99%)	3 (1%)	78	84
2	B	311/367 (85%)	306 (98%)	5 (2%)	55	75
3	C	171/359 (48%)	170 (99%)	1 (1%)	78	84
3	E	147/359 (41%)	146 (99%)	1 (1%)	76	83
4	D	294/653 (45%)	291 (99%)	3 (1%)	68	80
5	F	114/652 (18%)	113 (99%)	1 (1%)	70	81
All	All	1506/3781 (40%)	1492 (99%)	14 (1%)	68	81

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	698	ASP
1	A	903	GLU
1	A	1186	LEU
2	B	98	LYS
2	B	128	MET
2	B	140	ASP
2	B	153	LYS
2	B	214	PHE
3	C	347	MET
4	D	259	ASN
4	D	303	CYS
4	D	440	CYS
5	F	547	ILE
3	E	263	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	909	GLN
1	A	921	GLN
1	A	983	ASN
1	A	1173	ASN
4	D	302	HIS
4	D	459	ASN
4	D	510	GLN
4	D	545	ASN
5	F	283	HIS
5	F	331	ASN
3	E	317	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 7 ligands modelled in this entry, 7 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-33845. These allow visual inspection of the internal detail of the map and identification of artifacts.

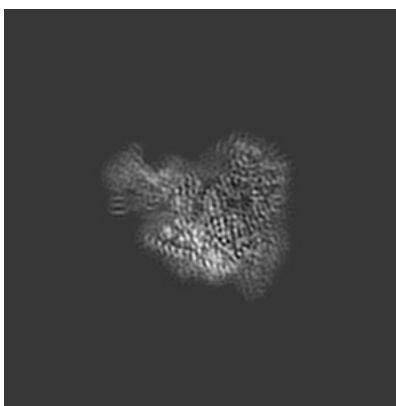
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

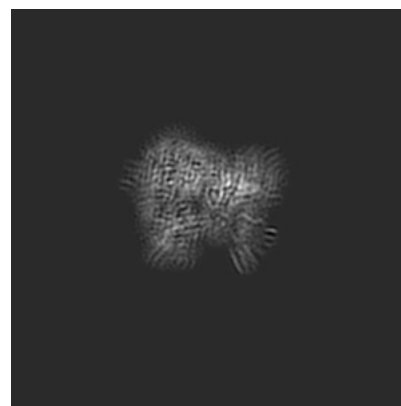
6.1.1 Primary map



X

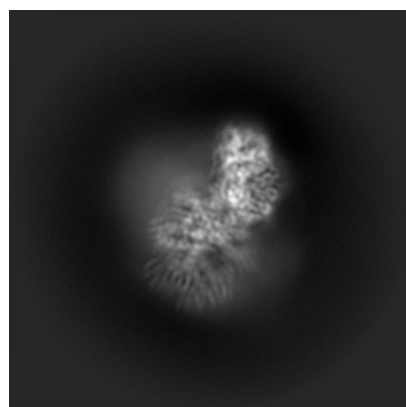


Y

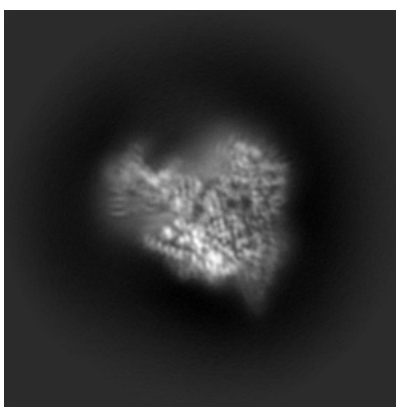


Z

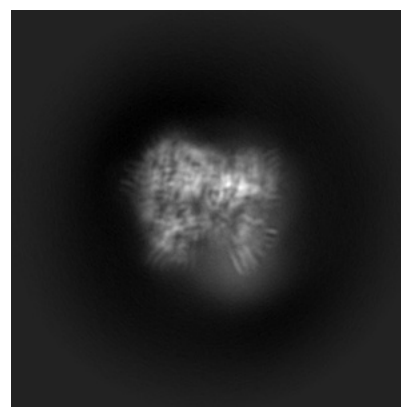
6.1.2 Raw map



X



Y

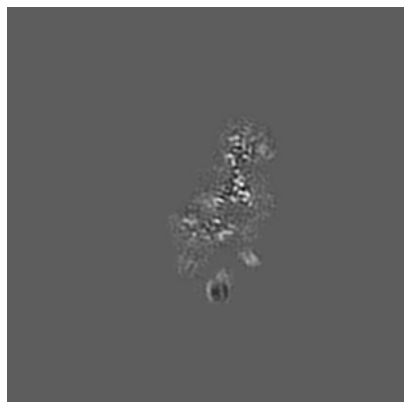


Z

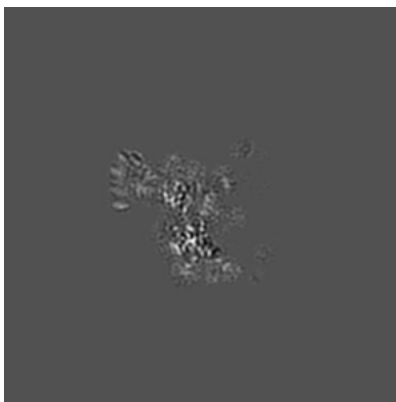
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

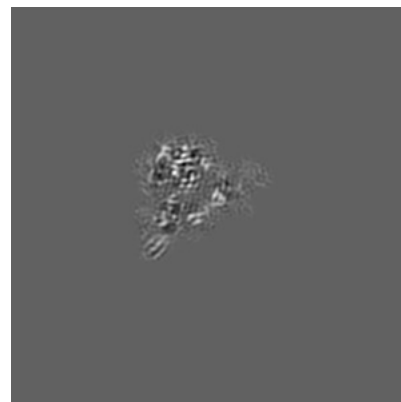
6.2.1 Primary map



X Index: 128

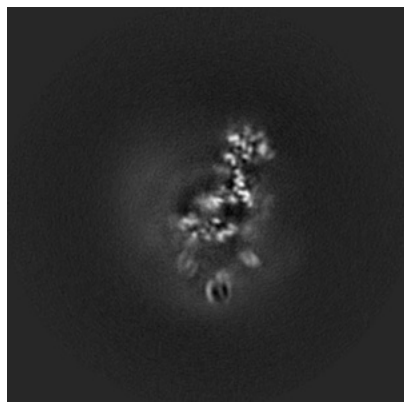


Y Index: 128

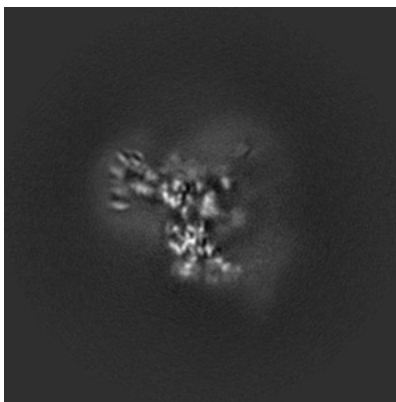


Z Index: 128

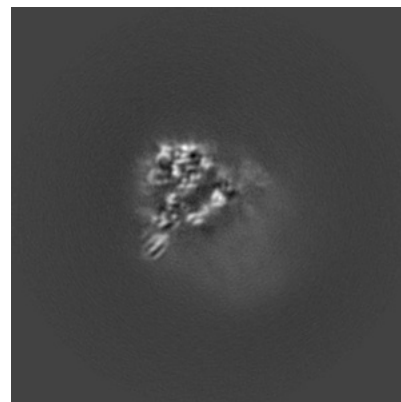
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

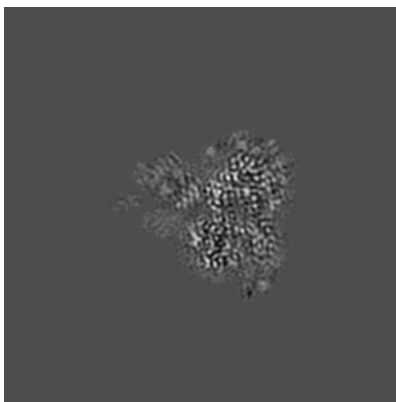
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

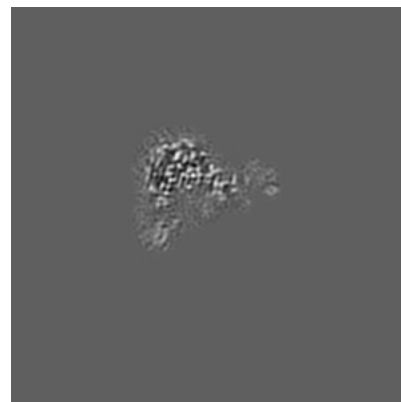
6.3.1 Primary map



X Index: 108

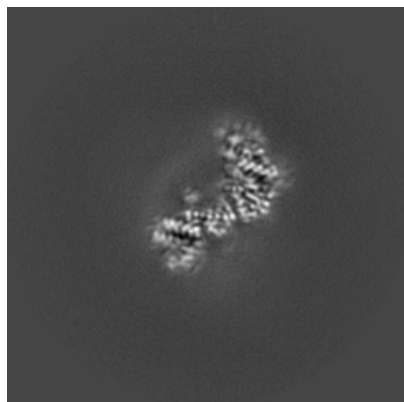


Y Index: 143

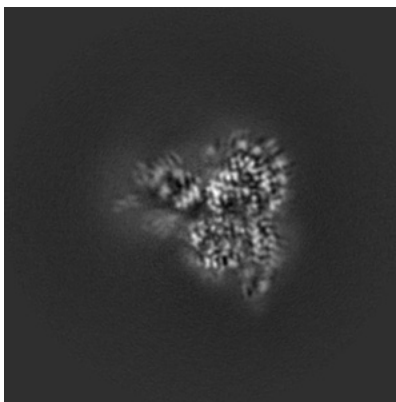


Z Index: 136

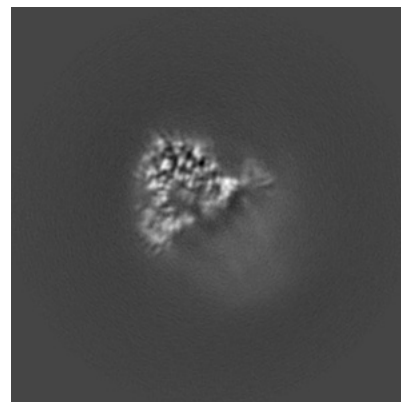
6.3.2 Raw map



X Index: 108



Y Index: 143

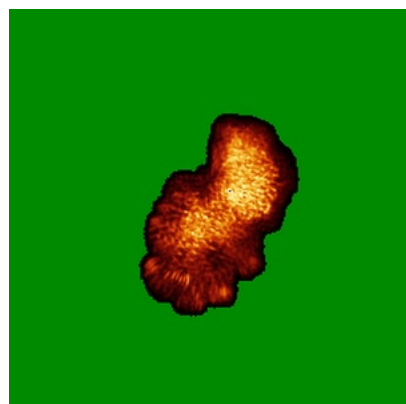


Z Index: 134

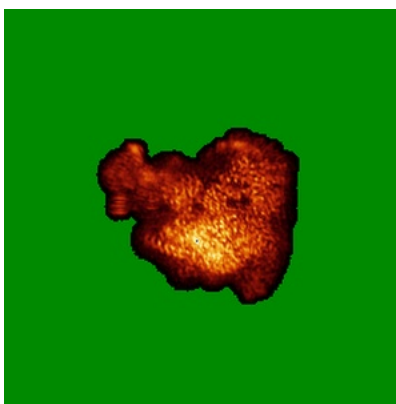
The images above show the largest variance slices of the map in three orthogonal directions.

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

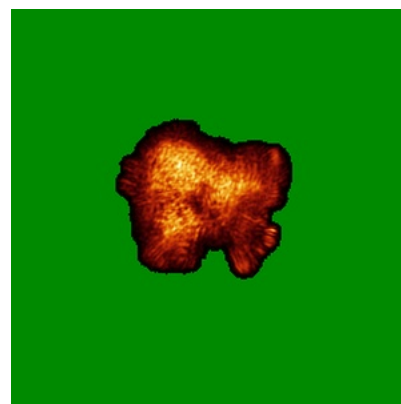
6.4.1 Primary map



X

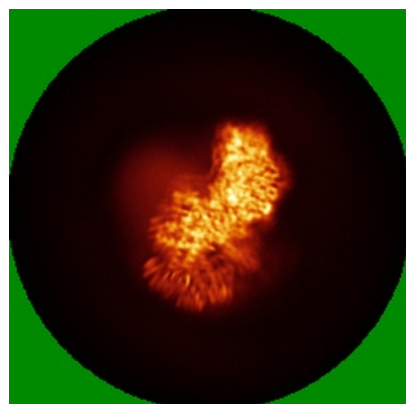


Y

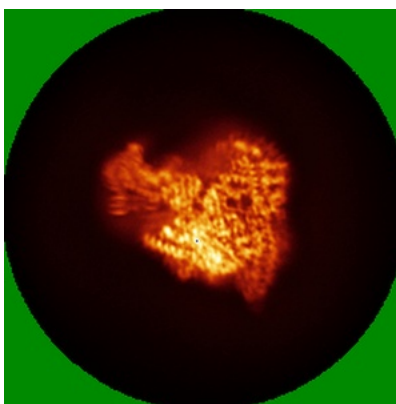


Z

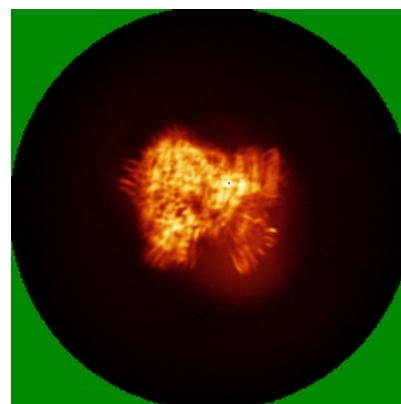
6.4.2 Raw map



X



Y

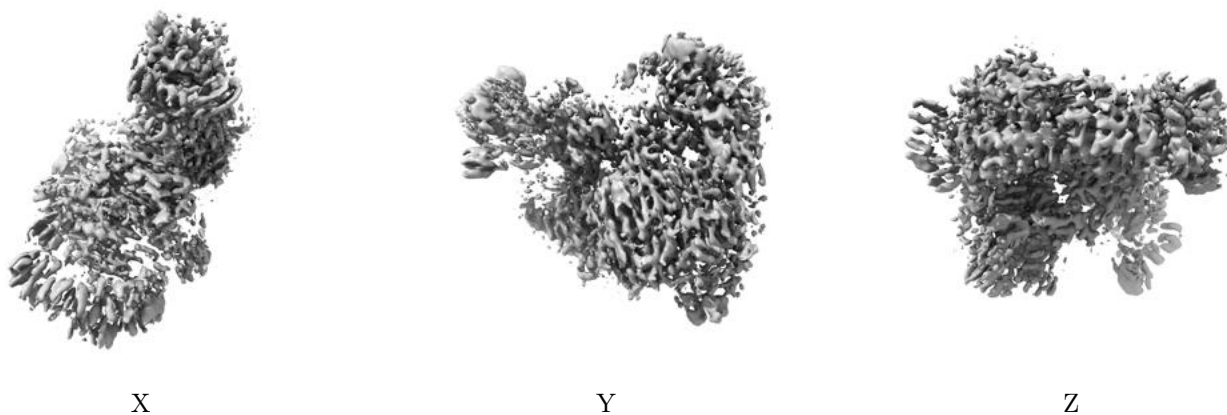


Z

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.

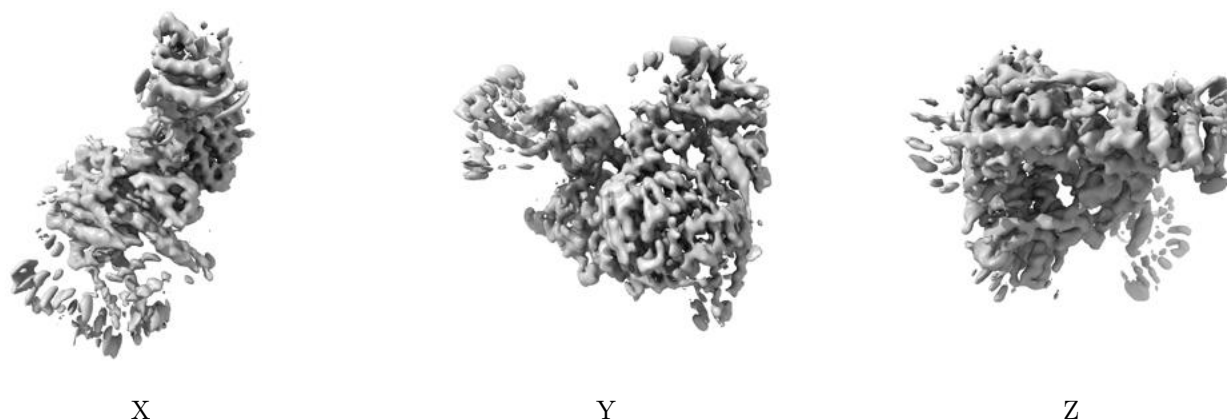
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

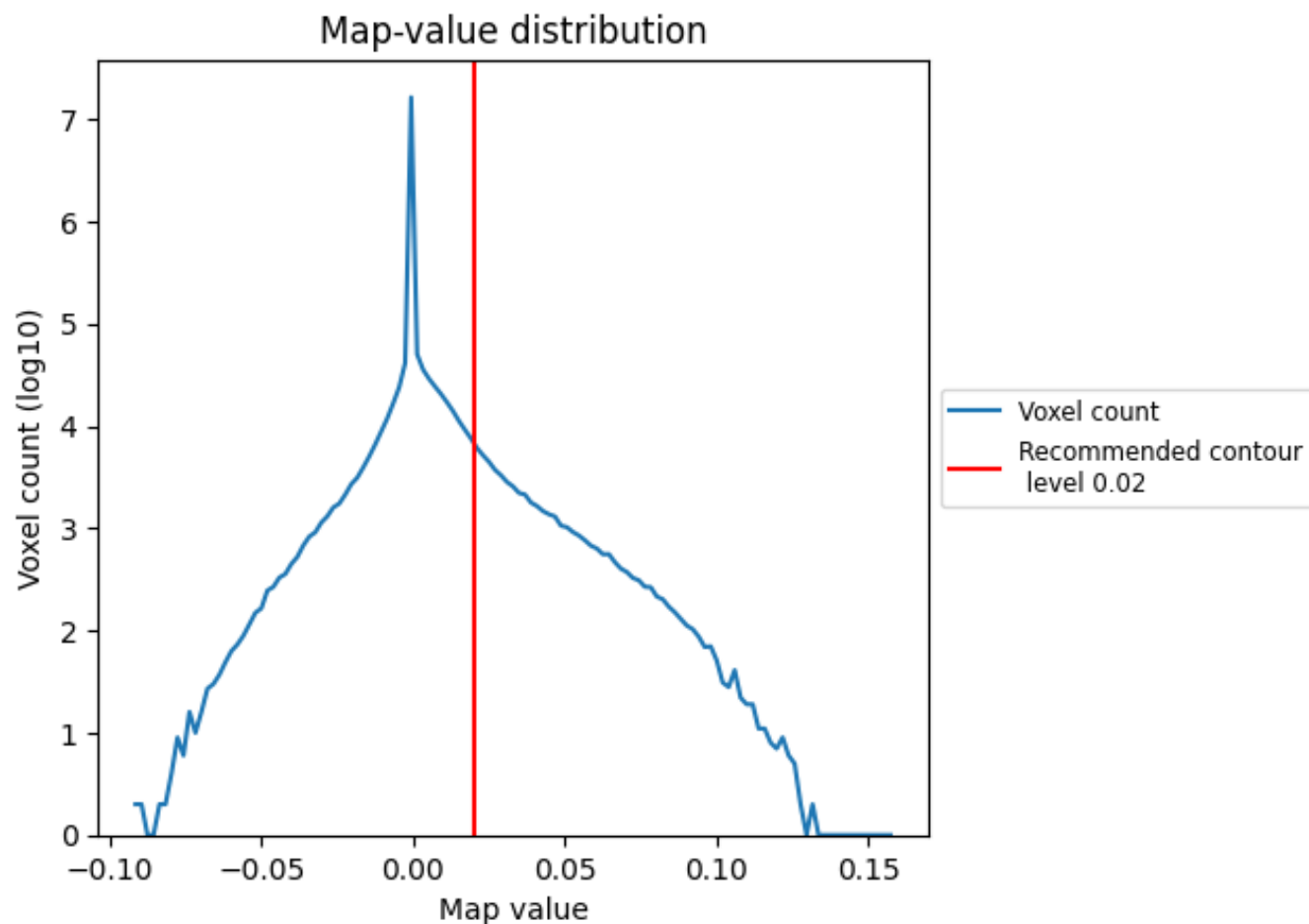
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

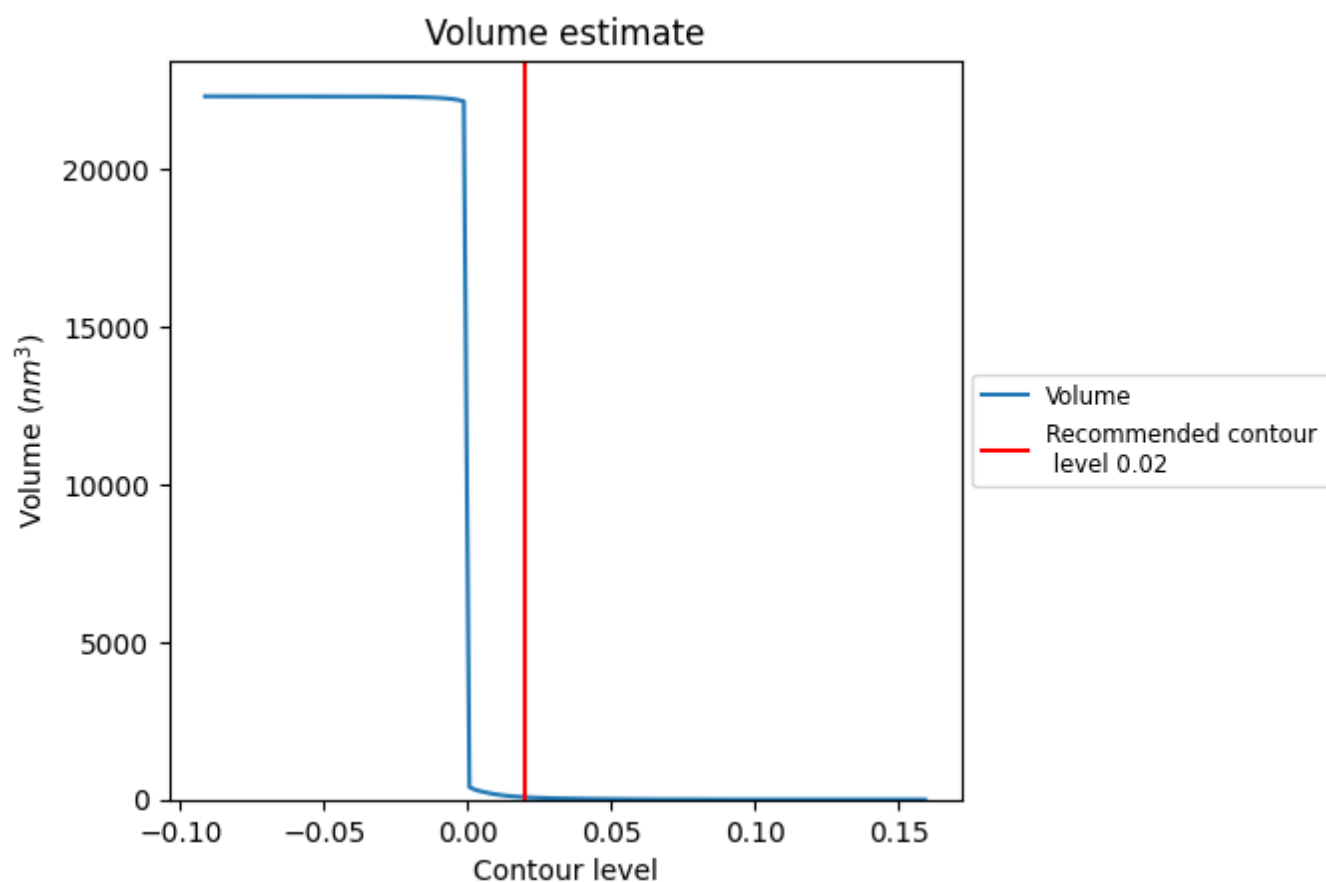
This section contains the results of statistical analysis of the map.

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.

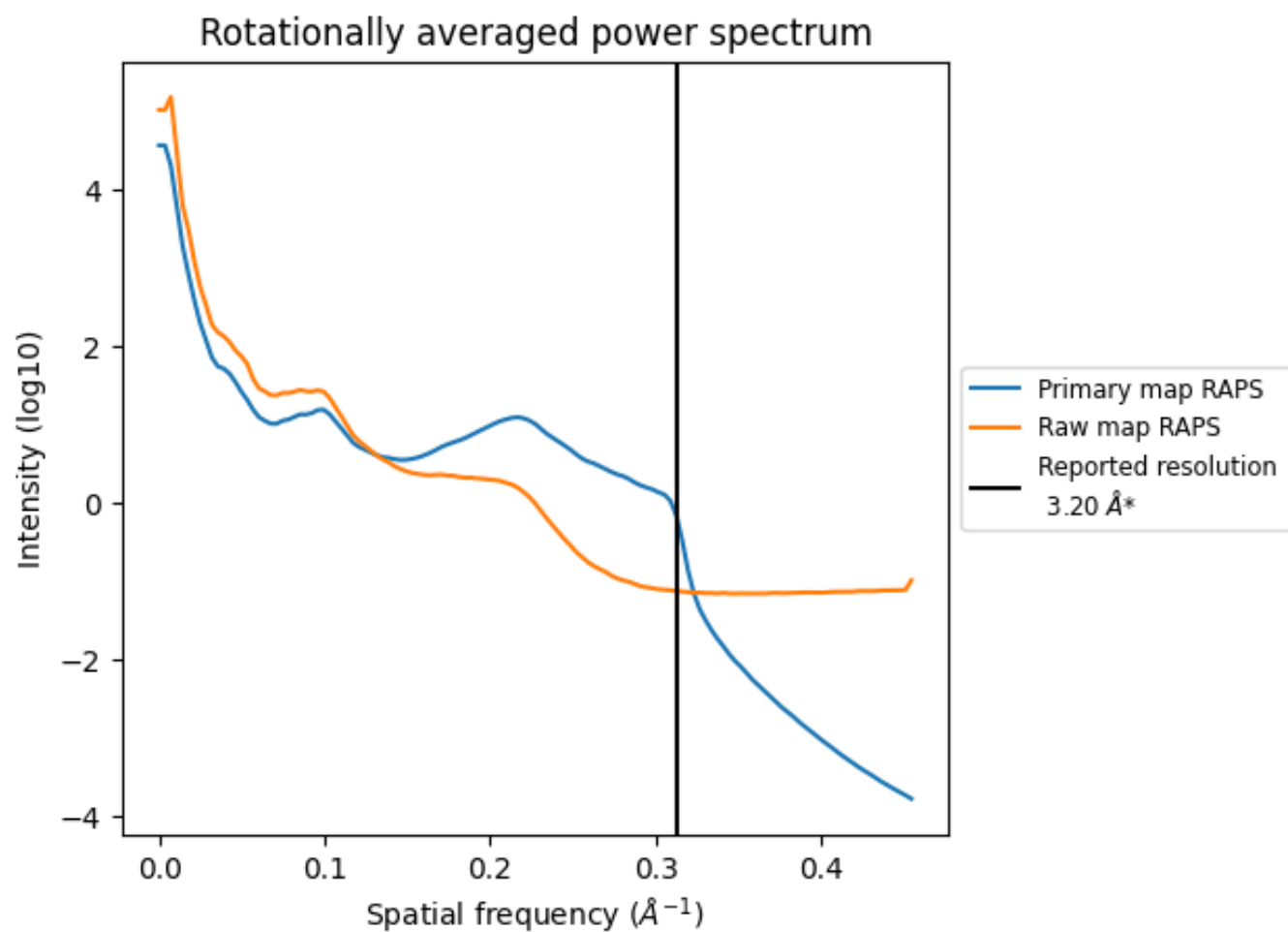
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm^3 ; this corresponds to an approximate mass of 66 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 ⓘ

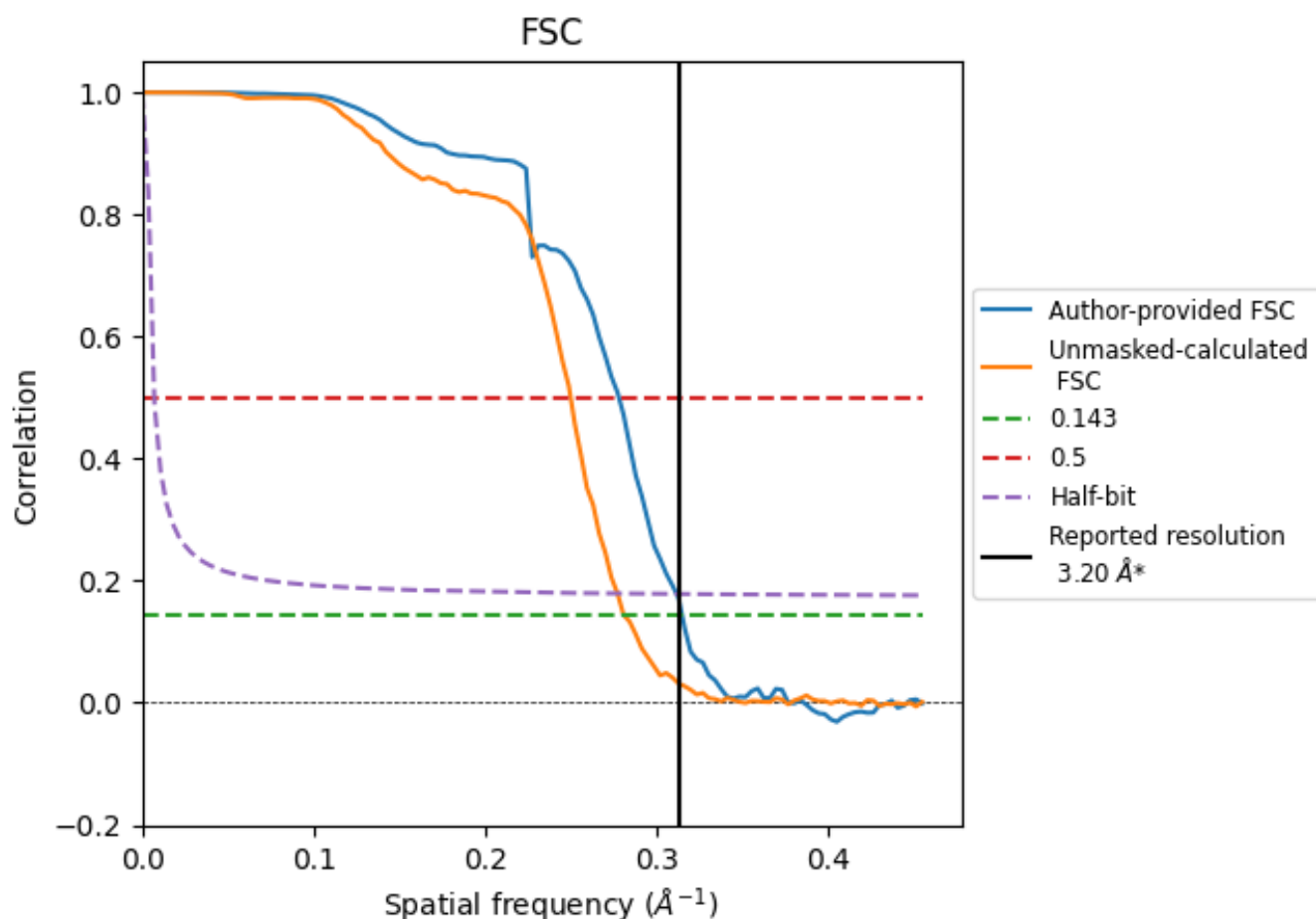


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

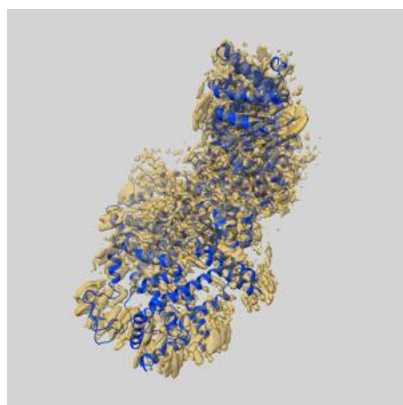
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.60	3.21
Unmasked-calculated*	3.56	4.00	3.61

*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 3.56 differs from the reported value 3.2 by more than 10 %

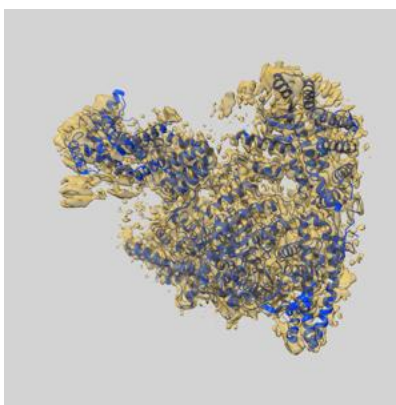
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33845 and PDB model 7YI0. Per-residue inclusion information can be found in section 3 on page 6.

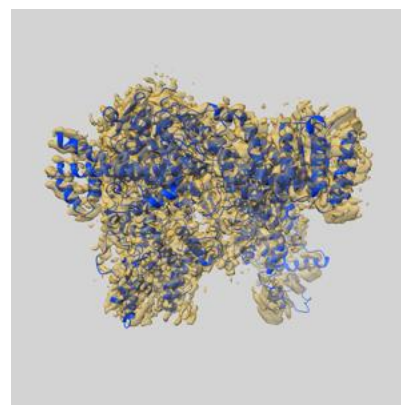
9.1 Map-model overlay [i](#)



X



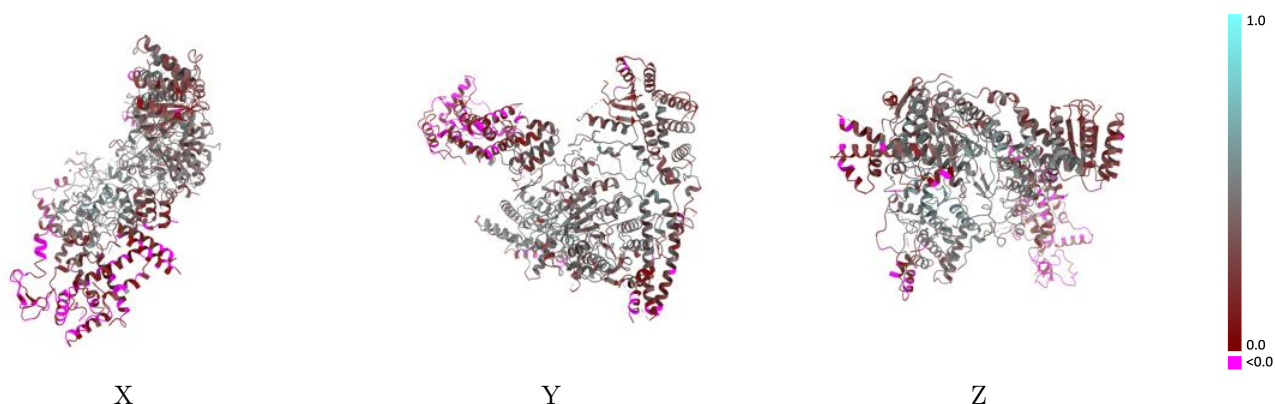
Y



Z

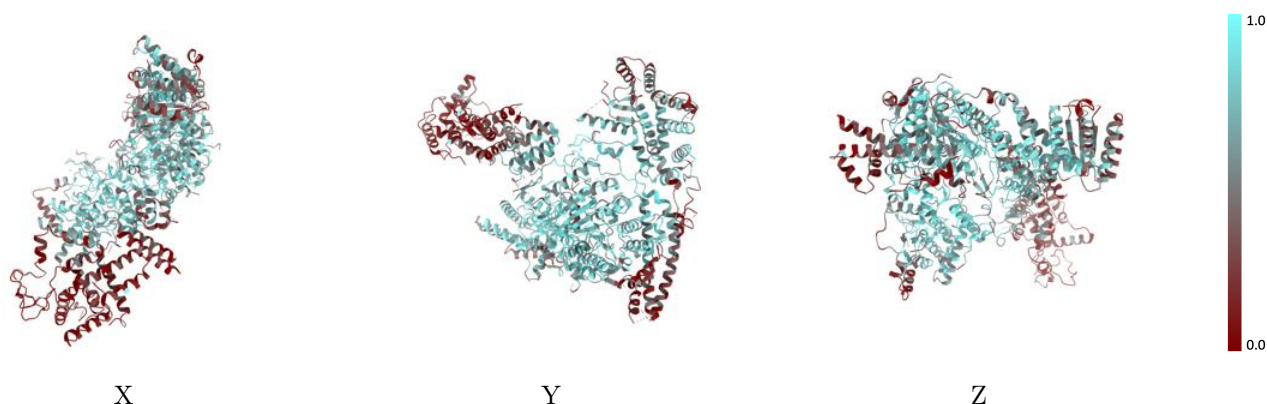
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



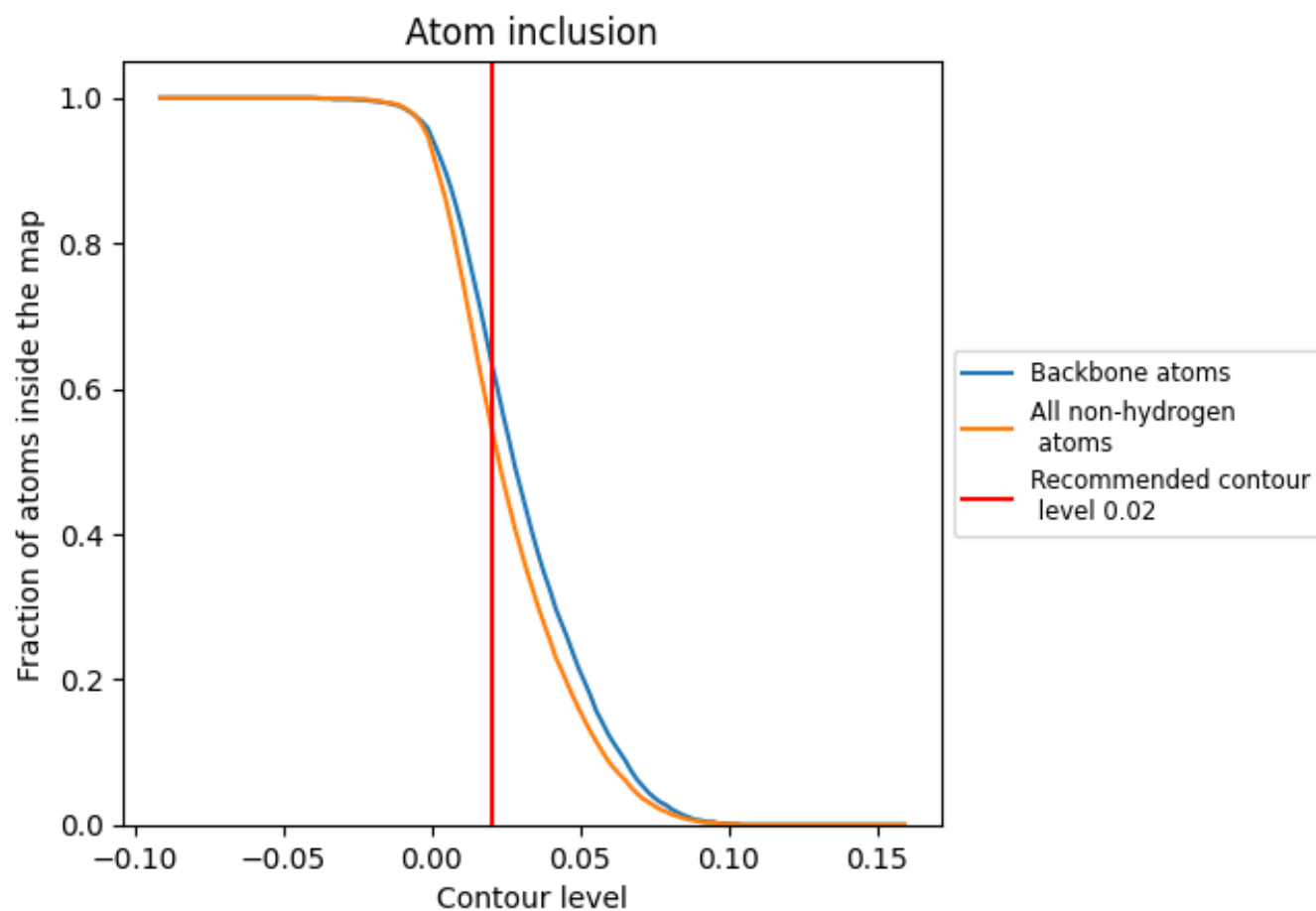
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 64% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.3330
A	0.5340	0.3410
B	0.7650	0.4400
C	0.7620	0.4700
D	0.5580	0.3490
E	0.1440	0.0800
F	0.1460	0.0650

1.0

0.0

<0.0