



wwPDB EM Validation Summary Report ⓘ

Mar 2, 2024 – 06:58 pm GMT

PDB ID : 8CED
EMDB ID : EMD-16606
Title : Rnase R bound to a 30S degradation intermediate (State I - head-turning)
Authors : Paternoga, H.; Dimitrova-Paternoga, L.; Wilson, D.N.
Deposited on : 2023-02-01
Resolution : 4.15 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

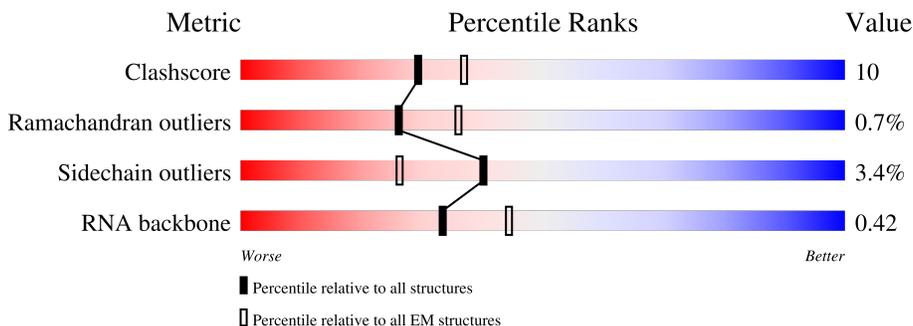
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.15 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
RNA backbone	4643	859

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	1554	34% (Poor fit) 28% (0 outliers) 41% (1 outlier) 16% (2 outliers) 14% (3+ outliers) 0% (Not modelled)
2	B	7	100% (0 outliers) 14% (1 outlier) 29% (2 outliers) 29% (3+ outliers) 0% (Not modelled)
3	C	779	91% (0 outliers) 85% (1 outlier) 5% (2 outliers) 9% (3+ outliers) 0% (Not modelled)
4	D	246	79% (0 outliers) 77% (1 outlier) 10% (2 outliers) 11% (3+ outliers) 0% (Not modelled)
5	F	200	45% (0 outliers) 64% (1 outlier) 26% (2 outliers) 8% (3+ outliers) 0% (Not modelled)
6	G	166	30% (0 outliers) 65% (1 outlier) 28% (2 outliers) 5% (3+ outliers) 0% (Not modelled)
7	I	132	30% (0 outliers) 69% (1 outlier) 26% (2 outliers) 0% (3+ outliers) 0% (Not modelled)

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Mol	Chain	Length	Quality of chain
8	L	138	
9	O	89	
10	P	90	
11	Q	87	
12	S	88	
13	T	95	
14	U	79	
15	V	131	
16	E	218	
17	H	156	
18	J	130	
19	K	102	
20	M	121	
21	N	61	
22	R	92	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 51964 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1333	28597	12753	5245	9266	1333	0	0

- Molecule 2 is a RNA chain called RNA Substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	7	154	70	35	42	7	0	0

- Molecule 3 is a protein called RNase R.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	708	5650	3559	962	1102	27	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	218	1757	1119	309	323	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	185	1490	942	276	270	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	158	1170	736	216	216	2	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	131	1036	655	191	187	3	0	0

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	136	1052	653	211	186	2	0	0

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O	85	710	436	144	129	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	88	695	441	128	124	2	0	0

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	84	691	435	128	126	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	S	83	637	390	130	116	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	T	95	784	492	138	152	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	101	Total	C	N	O	S	0	0
			730	450	136	143	1		

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	205	Total	C	N	O	S	0	0
			1615	1009	303	300	3		

- Molecule 17 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 18 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	108	Total	C	N	O	S	0	0
			826	510	160	155	1		

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	M	108	Total	C	N	O	0	0
			868	534	176	158		

- Molecule 21 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	49	409	263	79	63	4	0	0

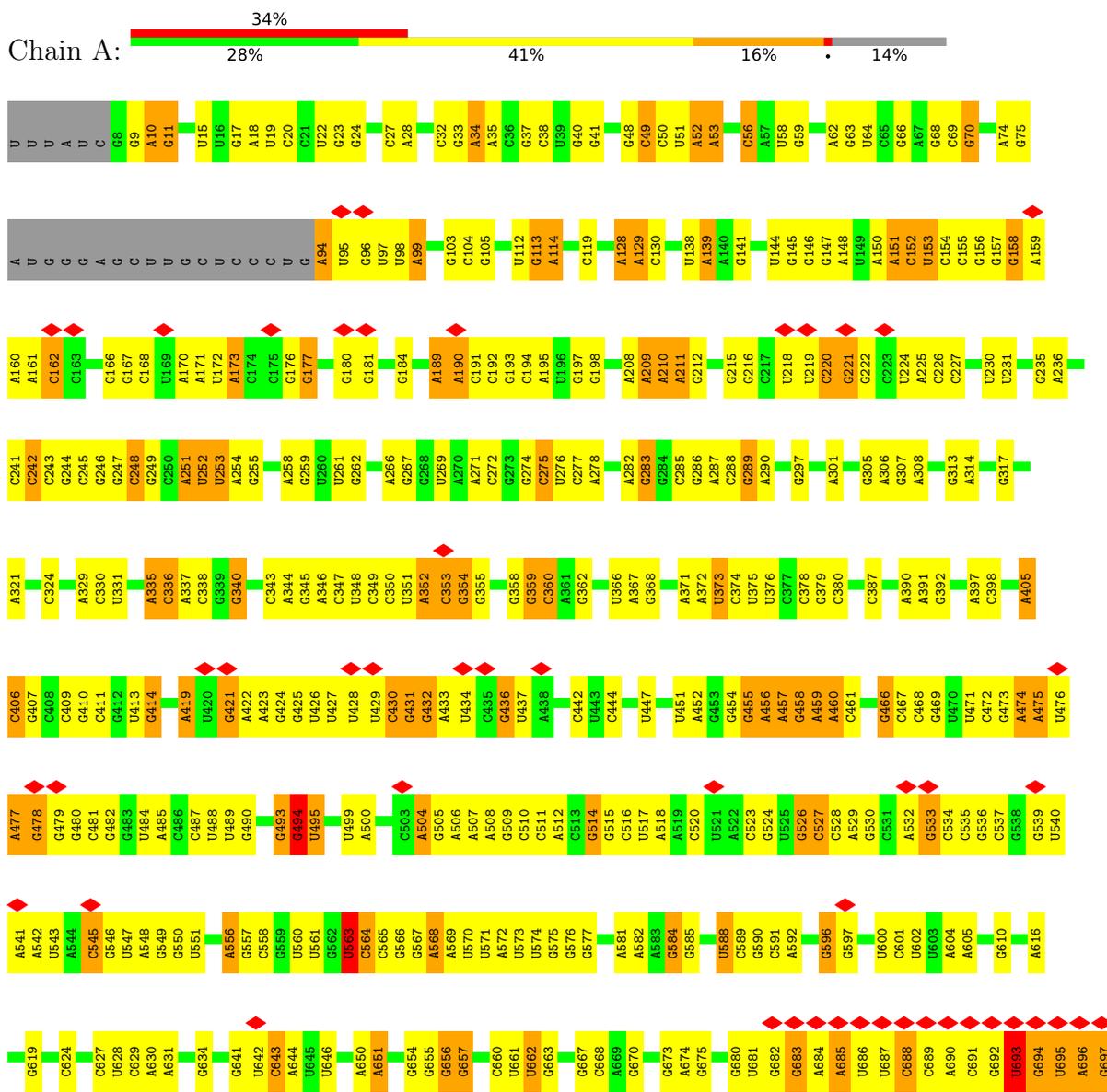
- Molecule 22 is a protein called 30S ribosomal protein S19.

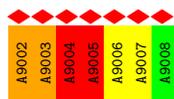
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	78	633	409	112	110	2	0	0

3 Residue-property plots

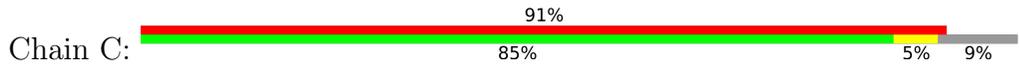
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

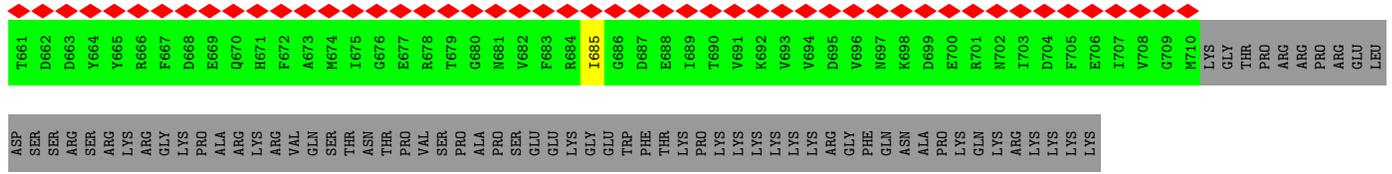




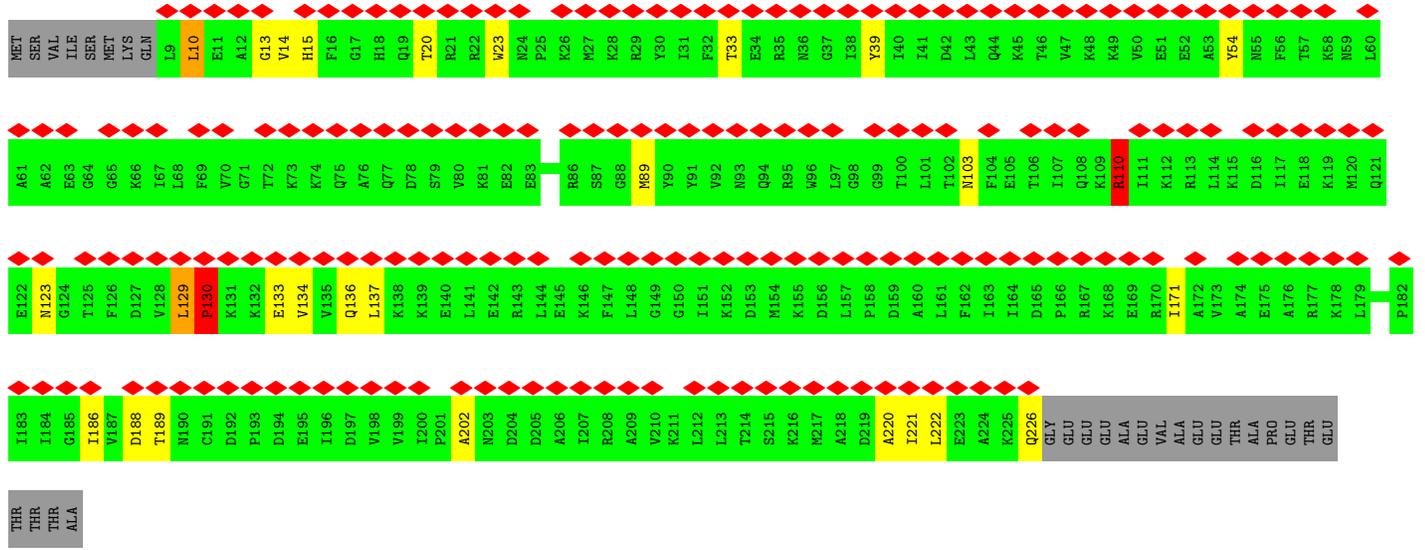
● Molecule 3: RNase R



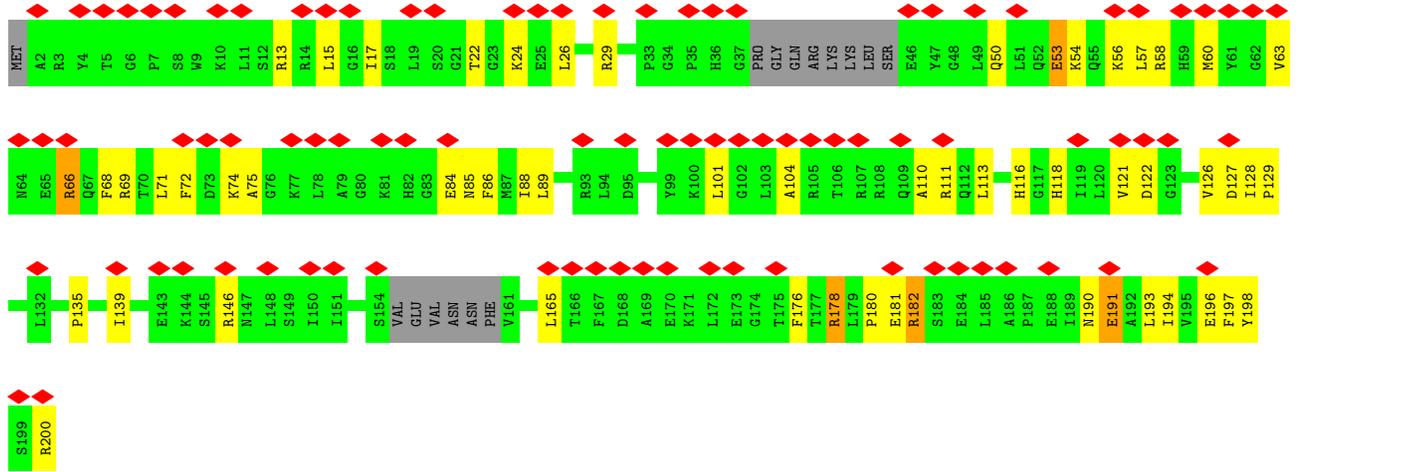
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D61	R62	Y63	G64	I65	O66	E67	K68	M69	V70	L71	I72	K73	G74	K75	I76	S77	A78	H79	A80	K81	L82	G83	F84	A85	F86	L87	P88	E89	D90	T91	S92	L93	S94	D95	V96	F97	I98	P99	P100	N101	E102	L103	N104	A105	T106	M107	N108	G109	D110	L111	V112	M113	V114	R115	L116	N117	S118	Q119	S120	
S121	G122	S123	R124	Q125	E126	G127	T128	V129	I130	R131	I132	K133	E134	R135	A136	S137	Q138	R139	V140	V141	G142	F143	Y144	I145	E146	T147	R148	N149	I150	G151	F152	V153	I154	P155	D156	D157	K158	K159	I160	L161	S162	D163	I164	F165	T166	P167	K168	L169	G170	K171	N172	G173	A174	A175	E176	G177	H178	K179	V180	
V181	V182	K183	L184	T185	S186	Y187	P188	E189	G190	R191	M192	N193	A194	E195	G196	E197	V198	E199	T200	I201	L202	G203	H204	K205	N206	D207	R208	G209	I210	D211	T212	L213	S214	V215	I216	H217	K218	H219	L220	L221	P222	G223	E224	F225	P226	A227	D228	A229	M230	E231	Q232	A233	S234	S235	T236	P237	D238	T239	I240	
D241	E242	K243	D244	L245	K246	R247	R248	R249	D250	L251	R252	D253	Q254	V255	L256	V257	T258	I259	D260	G261	A262	D263	A264	K265	D266	L267	D268	D269	A270	V271	T272	V273	K274	K275	L276	D277	D278	G279	S280	Y281	K282	L283	G284	H285	V286	I287	A288	D289	V290	S291	H292	Y293	V294	T295	E296	N297	S298	P299	I300	
D301	K302	E303	A304	L305	R306	R307	G308	T309	S310	V311	Y312	L313	V314	D315	R316	V317	L318	P319	M320	I321	P322	H323	R324	L325	N326	G327	K328	I329	C330	S331	L332	M333	P334	K335	V336	D337	R338	L339	T340	L341	S342	C343	E344	M345	L346	I347	D348	K349	S349	Q350	G351	Q352	V353	T354	E355	H356	E357	L358	F359	Q360
S361	V362	I363	K364	T365	T366	E367	R368	K369	T370	Y371	S372	D373	V374	N375	K376	L377	L378	V379	D380	D381	S382	E383	E384	L385	K386	Q387	K388	Y389	E390	P391	L392	V393	P394	M395	F396	K397	D398	M399	E400	R401	L402	A403	Q404	L405	L406	R407	D408	K409	S449	R410	M411	D412	R413	G414	A415	V416	D417	F418	D419	F420
K421	E422	A423	K424	V425	L426	V427	D428	D429	E430	G431	A432	V433	K434	D435	V436	V437	L438	R439	E440	R441	S442	V443	A444	E445	K446	L447	L448	E449	E450	F451	M452	L453	V454	A455	N456	E457	T458	V459	A460	E461	H462	F463	H464	W465	N466	N467	P468	P469	F470	L471	V472	R473	L474	H475	E476	E477	N478	A480		
E481	K482	L483	Q484	K485	F486	L487	E488	F489	V490	T491	T492	F493	G494	Y495	V496	V497	K498	G499	T500	A501	G502	N503	I504	H505	P506	R507	L508	L509	Q510	S511	L512	L513	D514	A515	V516	R517	D518	R519	P520	E521	E522	T523	V524	L525	S526	T527	V528	H529	L530	R531	S532	M533	K534	Q535	A536	K537	D538	P540		
Q541	S542	L543	G544	H545	F546	G547	L548	S549	T550	E551	F552	Y553	T554	H555	F556	T557	S558	P559	I560	R561	E562	Y563	P564	D565	L566	I567	V568	H569	R570	S571	L572	R573	T574	Y575	L576	L577	N578	G579	K580	V581	E582	E583	A584	L585	O586	E587	K588	W589	A590	E591	R592	L593	P594	D595	I596	A597	E598	H599	T600	
S601	S602	M603	E604	R605	R606	G607	V608	D609	A610	E611	R612	E613	T614	D615	D616	L617	K618	G619	A620	E621	Y622	M623	L624	D625	K626	I627	G628	E629	E630	F631	L632	G633	M634	L635	S636	S637	L638	T639	M640	F641	G642	M643	F644	V645	E646	L647	P648	M649	T650	I651	F652	G653	L654	V655	H656	V657	S658	F659	M660	



• Molecule 4: 30S ribosomal protein S2

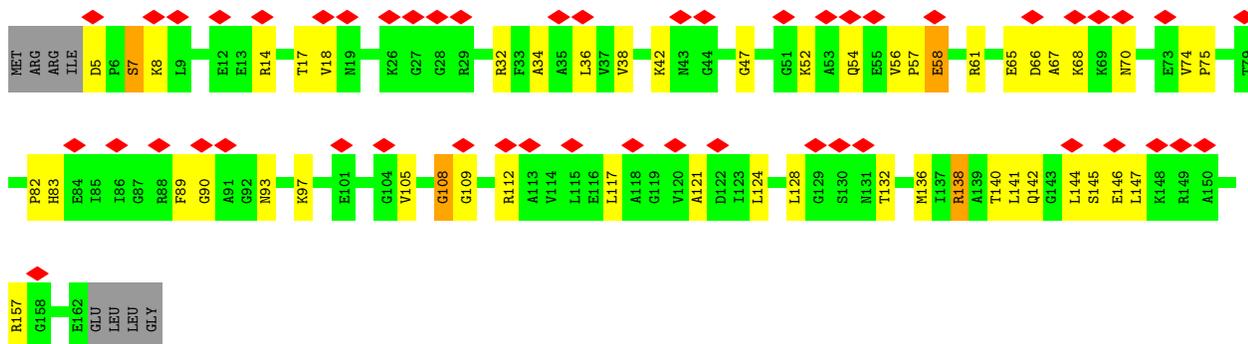


• Molecule 5: 30S ribosomal protein S4

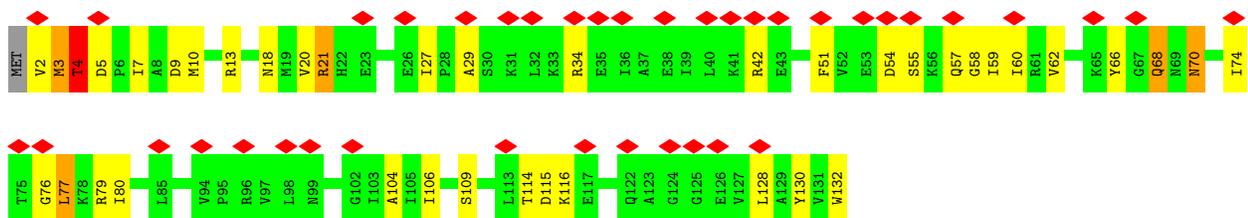


• Molecule 6: 30S ribosomal protein S5

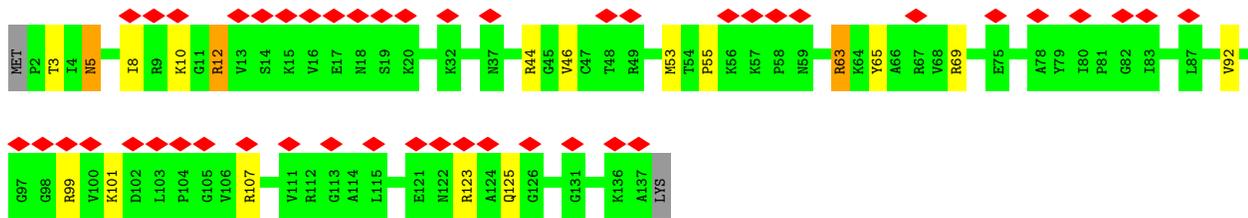
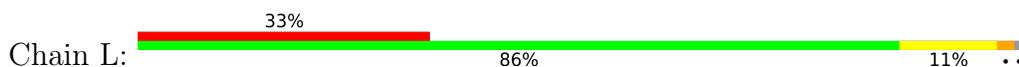




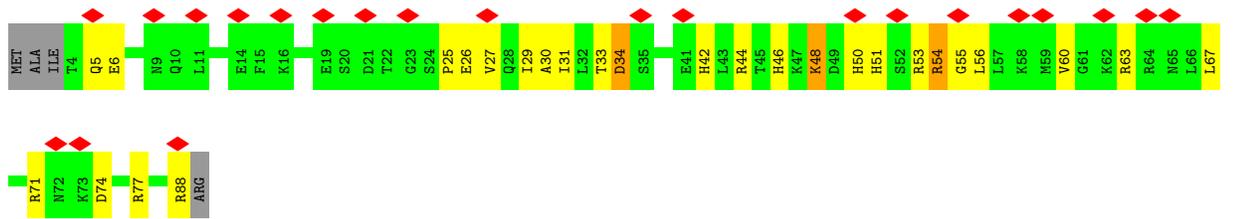
• Molecule 7: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S12



• Molecule 9: 30S ribosomal protein S15

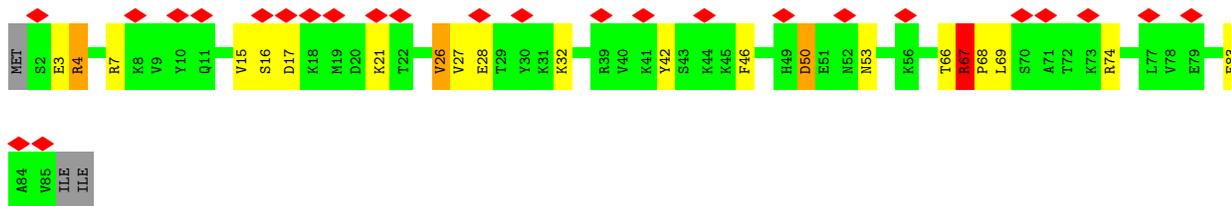


• Molecule 10: 30S ribosomal protein S16

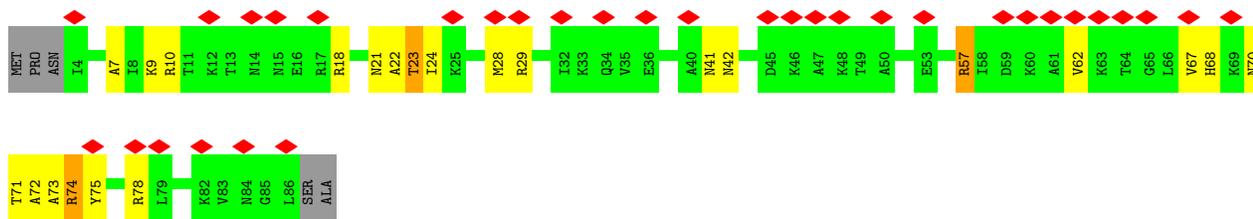




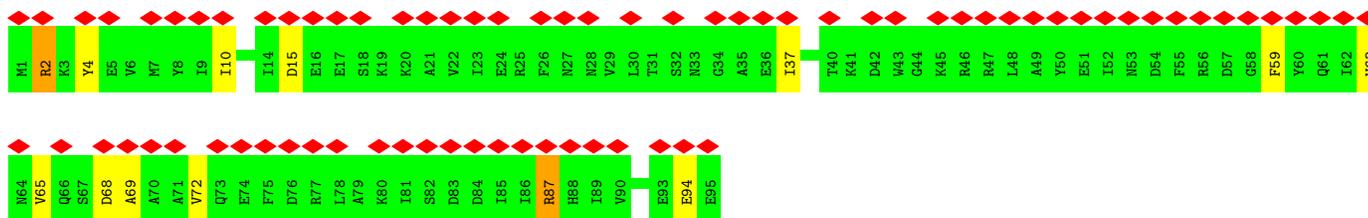
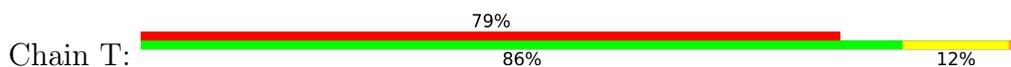
• Molecule 11: 30S ribosomal protein S17



• Molecule 12: 30S ribosomal protein S20



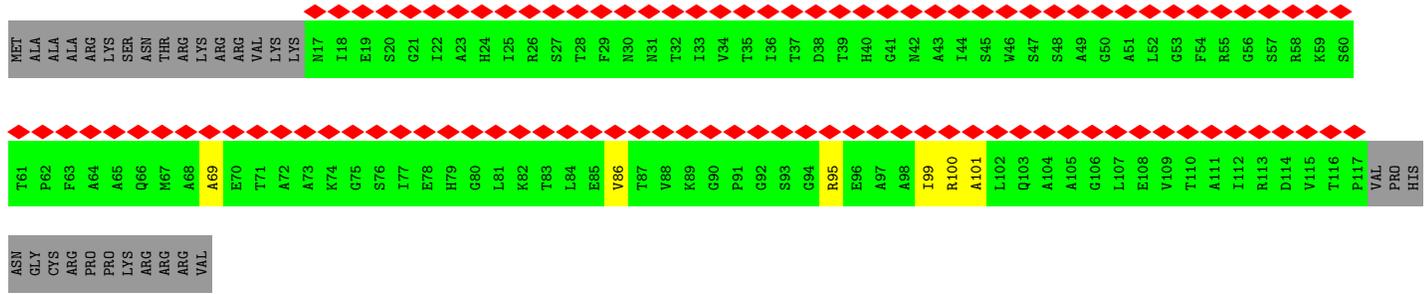
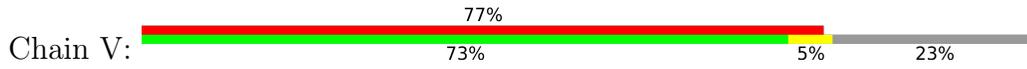
• Molecule 13: 30S ribosomal protein S6



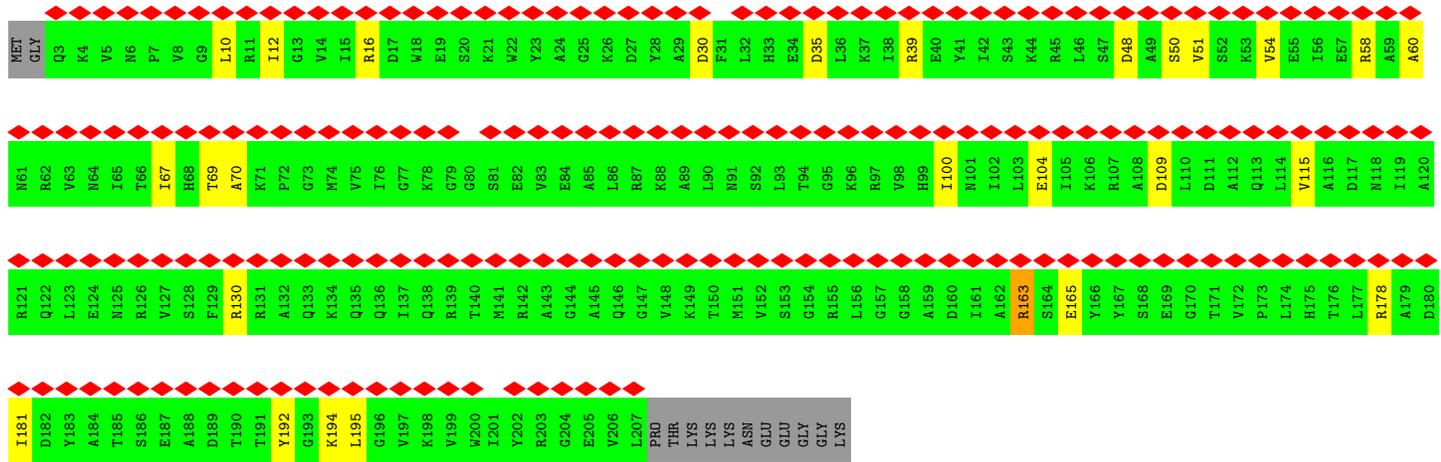
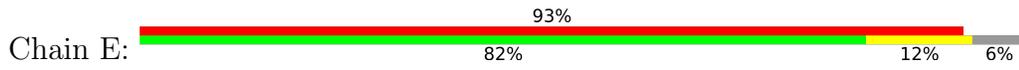
• Molecule 14: 30S ribosomal protein S18



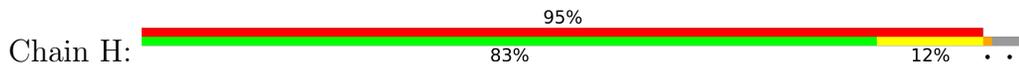
• Molecule 15: 30S ribosomal protein S11



• Molecule 16: 30S ribosomal protein S3

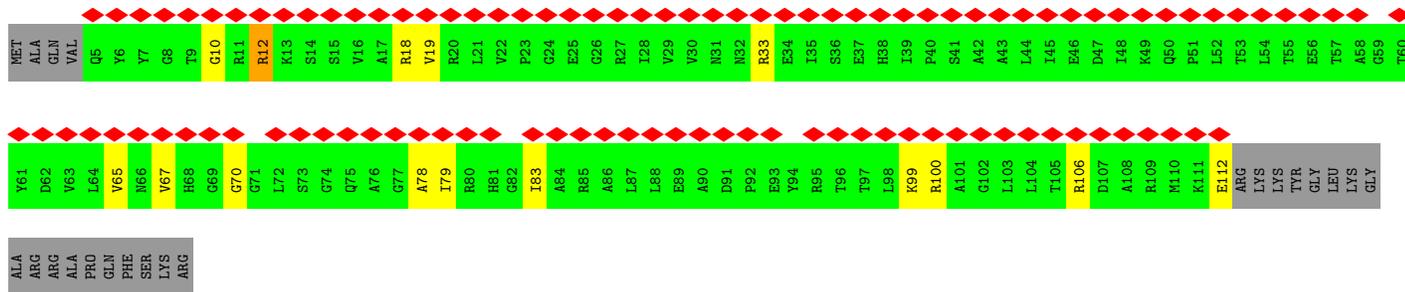


• Molecule 17: 30S ribosomal protein S7

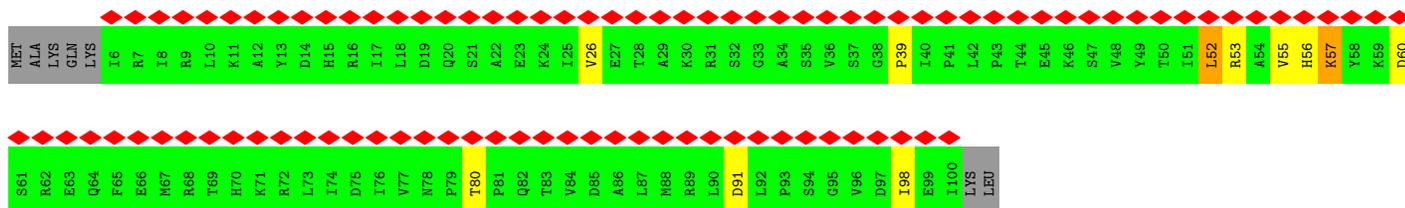


• Molecule 18: 30S ribosomal protein S9





• Molecule 19: 30S ribosomal protein S10

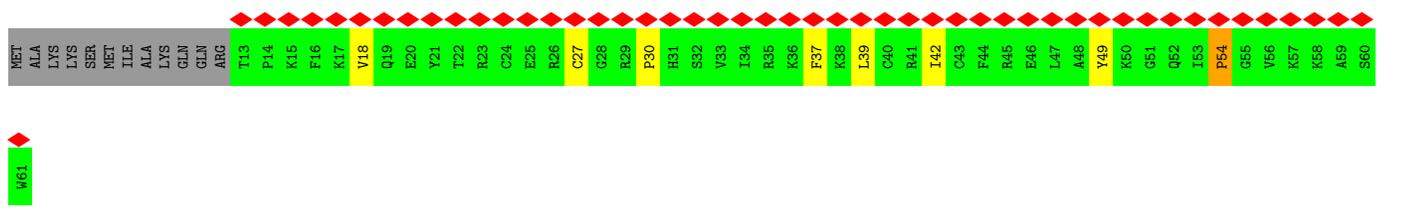


• Molecule 20: 30S ribosomal protein S13

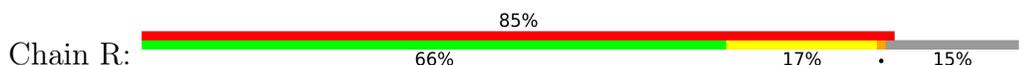


LYS

• Molecule 21: 30S ribosomal protein S14



• Molecule 22: 30S ribosomal protein S19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6540	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)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0103	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.58	1/32015 (0.0%)	0.97	17/49936 (0.0%)
2	B	0.69	0/174	1.89	8/269 (3.0%)
3	C	0.32	0/5748	0.68	1/7760 (0.0%)
4	D	0.36	0/1782	0.85	2/2392 (0.1%)
5	F	0.47	0/1517	1.00	0/2036
6	G	0.50	0/1182	1.08	4/1591 (0.3%)
7	I	0.55	0/1048	1.10	1/1407 (0.1%)
8	L	0.52	0/1069	1.08	2/1435 (0.1%)
9	O	0.48	0/718	1.09	2/960 (0.2%)
10	P	0.57	0/708	1.21	0/950
11	Q	0.52	0/699	1.20	3/933 (0.3%)
12	S	0.50	0/639	1.02	2/852 (0.2%)
13	T	0.39	0/795	0.93	3/1067 (0.3%)
14	U	0.43	0/526	0.99	3/705 (0.4%)
15	V	0.35	0/740	0.65	0/1002
16	E	0.35	0/1637	0.75	0/2203
17	H	0.34	0/1196	0.74	0/1604
18	J	0.36	0/836	0.75	0/1128
19	K	0.35	0/773	0.77	0/1044
20	M	0.34	0/873	0.74	0/1166
21	N	0.36	0/419	0.98	1/558 (0.2%)
22	R	0.33	0/649	0.75	0/872
All	All	0.51	1/55743 (0.0%)	0.94	49/81870 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	6
4	D	0	4
5	F	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	4
7	I	0	2
8	L	0	1
9	O	0	1
10	P	0	4
11	Q	0	2
12	S	0	3
16	E	0	5
18	J	0	2
20	M	0	1
All	All	0	39

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	946	C	O3'-P	6.11	1.68	1.61

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9002	A	N1-C6-N6	-9.28	113.03	118.60
2	B	9002	A	O3'-P-O5'	-8.64	87.58	104.00
13	T	87	ARG	NE-CZ-NH1	8.02	124.31	120.30
2	B	9005	A	P-O3'-C3'	-7.79	110.35	119.70
2	B	9002	A	C5-C6-N6	7.62	129.79	123.70

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	441	ARG	Sidechain
3	C	573	ARG	Sidechain
3	C	612	ARG	Sidechain
3	C	69	MET	Peptide,Mainchain
3	C	70	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28597	0	14401	647	0
2	B	154	0	78	27	0
3	C	5650	0	5618	71	0
4	D	1757	0	1830	32	0
5	F	1490	0	1518	32	0
6	G	1170	0	1245	29	0
7	I	1036	0	1095	25	0
8	L	1052	0	1112	12	0
9	O	710	0	735	13	0
10	P	695	0	721	11	0
11	Q	691	0	728	12	0
12	S	637	0	696	16	0
13	T	784	0	777	7	0
14	U	518	0	555	10	0
15	V	730	0	735	3	0
16	E	1615	0	1655	7	0
17	H	1181	0	1235	20	0
18	J	826	0	849	6	0
19	K	761	0	795	4	0
20	M	868	0	925	5	0
21	N	409	0	427	4	0
22	R	633	0	649	9	0
All	All	51964	0	38379	914	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 10.

The worst 5 of 914 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:1002:U:H2'	1:A:1053:G:H1	1.08	1.09
3:C:119:GLN:OE1	17:H:150:ALA:C	1.86	1.07
3:C:119:GLN:OE1	17:H:149:LYS:O	1.73	1.07
1:A:1002:U:H2'	1:A:1053:G:N1	1.69	1.05
1:A:1140:A:OP2	1:A:1140:A:H3'	1.59	1.02

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	
3	C	706/779 (91%)	694 (98%)	11 (2%)	1 (0%)	51	85
4	D	216/246 (88%)	199 (92%)	16 (7%)	1 (0%)	29	68
5	F	179/200 (90%)	156 (87%)	19 (11%)	4 (2%)	6	38
6	G	156/166 (94%)	140 (90%)	14 (9%)	2 (1%)	12	48
7	I	129/132 (98%)	114 (88%)	11 (8%)	4 (3%)	4	32
8	L	134/138 (97%)	126 (94%)	8 (6%)	0	100	100
9	O	83/89 (93%)	71 (86%)	12 (14%)	0	100	100
10	P	86/90 (96%)	80 (93%)	6 (7%)	0	100	100
11	Q	82/87 (94%)	76 (93%)	4 (5%)	2 (2%)	6	36
12	S	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
13	T	93/95 (98%)	86 (92%)	6 (6%)	1 (1%)	14	52
14	U	62/79 (78%)	60 (97%)	2 (3%)	0	100	100
15	V	99/131 (76%)	93 (94%)	6 (6%)	0	100	100
16	E	203/218 (93%)	169 (83%)	33 (16%)	1 (0%)	29	68
17	H	147/156 (94%)	138 (94%)	7 (5%)	2 (1%)	11	47
18	J	106/130 (82%)	100 (94%)	6 (6%)	0	100	100
19	K	93/102 (91%)	88 (95%)	5 (5%)	0	100	100
20	M	106/121 (88%)	102 (96%)	4 (4%)	0	100	100
21	N	47/61 (77%)	43 (92%)	3 (6%)	1 (2%)	7	39
22	R	76/92 (83%)	72 (95%)	2 (3%)	2 (3%)	5	35
All	All	2884/3200 (90%)	2679 (93%)	184 (6%)	21 (1%)	26	62

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	130	PRO

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Mol	Chain	Res	Type
5	F	181	GLU
5	F	182	ARG
7	I	4	THR
22	R	27	LYS

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	
3	C	628/692 (91%)	624 (99%)	4 (1%)	86	92
4	D	189/212 (89%)	186 (98%)	3 (2%)	62	79
5	F	159/173 (92%)	153 (96%)	6 (4%)	33	58
6	G	123/130 (95%)	119 (97%)	4 (3%)	38	61
7	I	111/112 (99%)	104 (94%)	7 (6%)	18	45
8	L	114/116 (98%)	112 (98%)	2 (2%)	59	76
9	O	80/83 (96%)	75 (94%)	5 (6%)	18	45
10	P	74/76 (97%)	73 (99%)	1 (1%)	67	80
11	Q	77/80 (96%)	73 (95%)	4 (5%)	23	50
12	S	66/70 (94%)	64 (97%)	2 (3%)	41	63
13	T	84/84 (100%)	81 (96%)	3 (4%)	35	60
14	U	56/64 (88%)	53 (95%)	3 (5%)	22	49
15	V	74/100 (74%)	73 (99%)	1 (1%)	67	80
16	E	168/178 (94%)	157 (94%)	11 (6%)	17	44
17	H	125/132 (95%)	118 (94%)	7 (6%)	21	48
18	J	85/102 (83%)	80 (94%)	5 (6%)	19	47
19	K	86/92 (94%)	78 (91%)	8 (9%)	9	30
20	M	94/104 (90%)	92 (98%)	2 (2%)	53	71
21	N	44/54 (82%)	41 (93%)	3 (7%)	16	43
22	R	70/81 (86%)	65 (93%)	5 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2507/2735 (92%)	2421 (97%)	86 (3%)	40 60

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	H	9	LYS
19	K	57	LYS
17	H	30	MET
18	J	100	ARG
19	K	98	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
14	U	21	ASN
20	M	104	ASN
15	V	42	ASN
22	R	14	HIS
18	J	75	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1329/1554 (85%)	391 (29%)	113 (8%)
2	B	6/7 (85%)	3 (50%)	0
All	All	1335/1561 (85%)	394 (29%)	113 (8%)

5 of 394 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	11	G
1	A	15	U
1	A	24	G
1	A	32	C

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	827	G

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Mol	Chain	Res	Type
1	A	1306	U
1	A	980	C
1	A	1294	A
1	A	1177	C

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 [i](#)

There are no chain breaks in this entry.

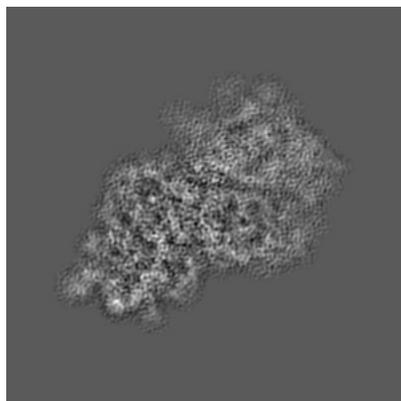
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16606. These allow visual inspection of the internal detail of the map and identification of artifacts.

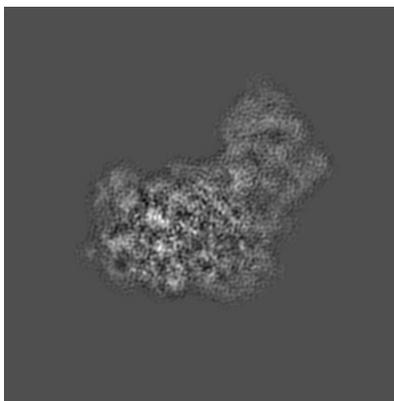
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

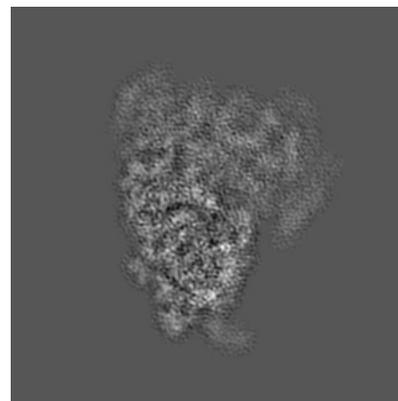
6.1.1 Primary map



X

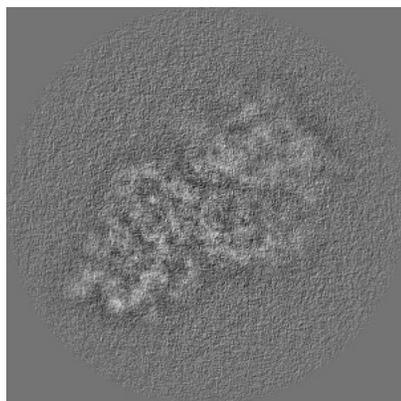


Y

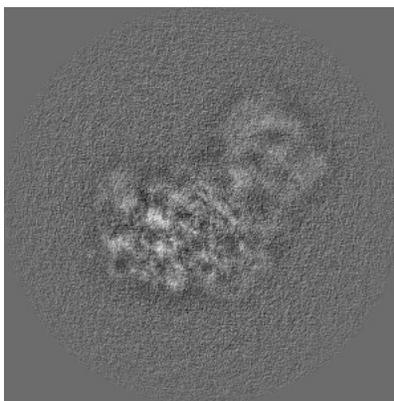


Z

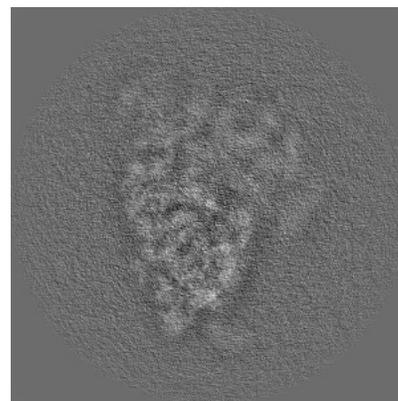
6.1.2 Raw map



X



Y

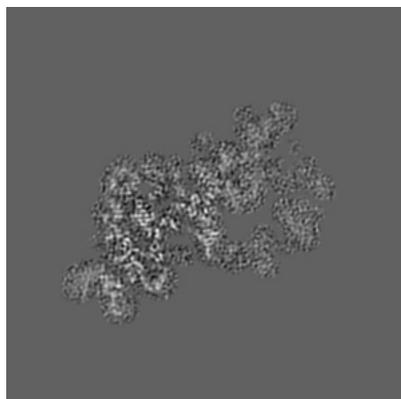


Z

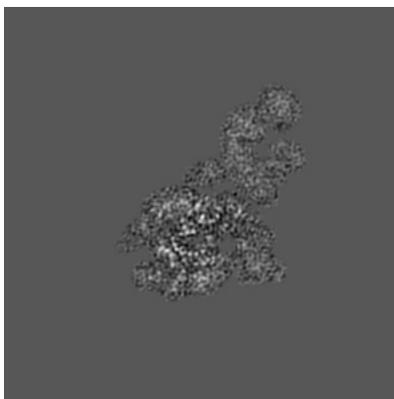
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

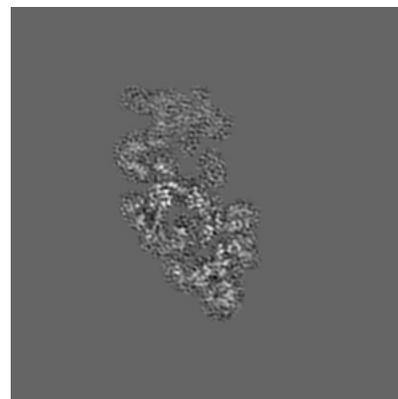
6.2.1 Primary map



X Index: 192

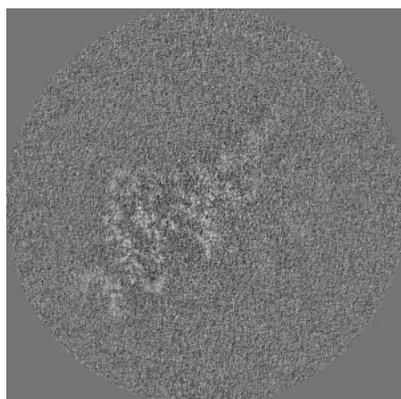


Y Index: 192

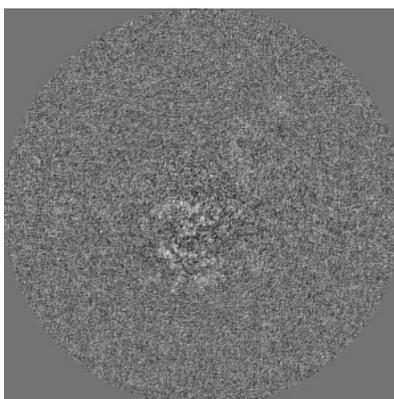


Z Index: 192

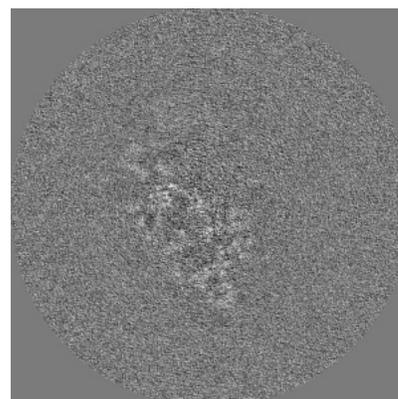
6.2.2 Raw map



X Index: 192



Y Index: 192

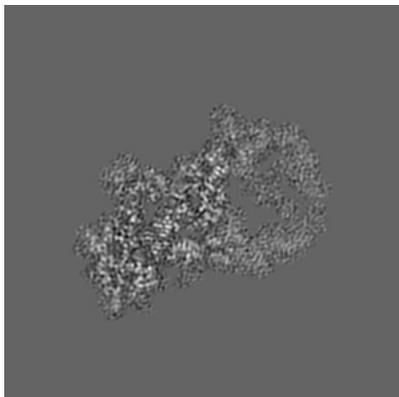


Z Index: 192

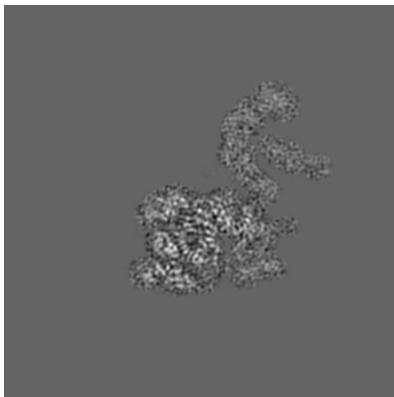
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

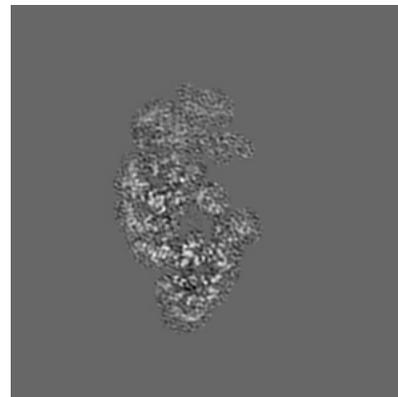
6.3.1 Primary map



X Index: 176

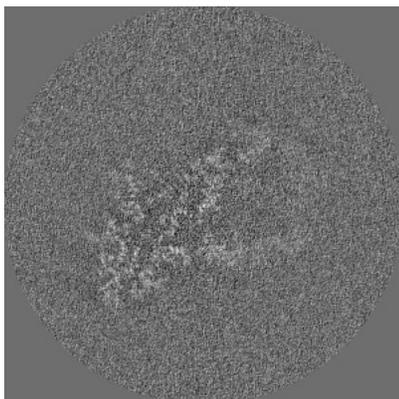


Y Index: 199

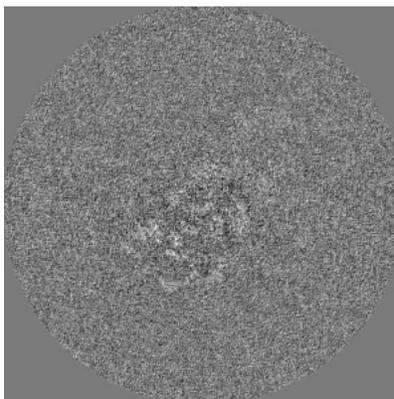


Z Index: 162

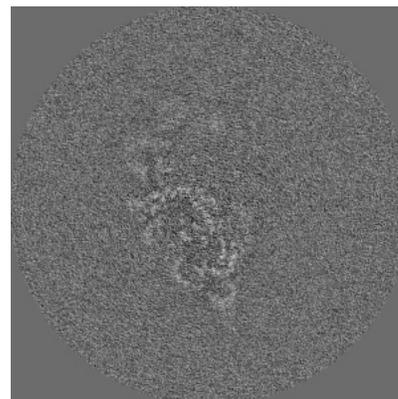
6.3.2 Raw map



X Index: 181



Y Index: 184

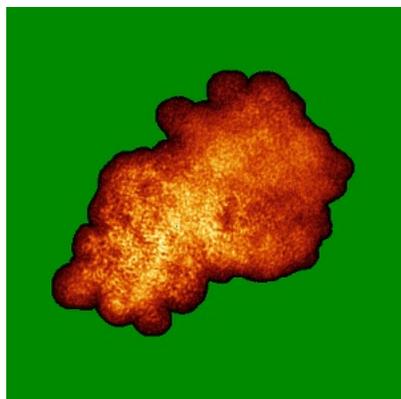


Z Index: 189

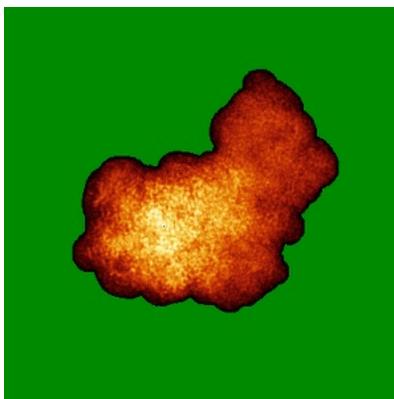
The images above show the largest variance slices of the map in three orthogonal directions.

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

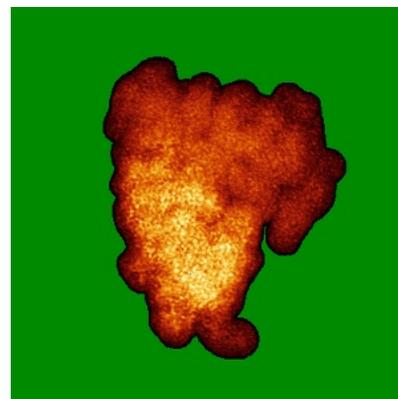
6.4.1 Primary map



X

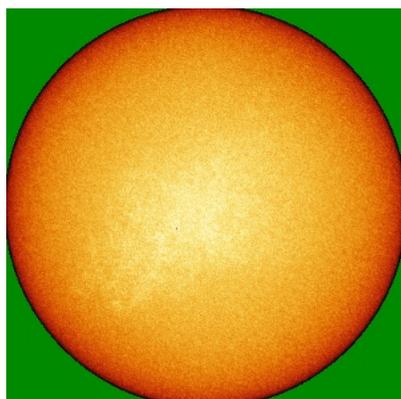


Y

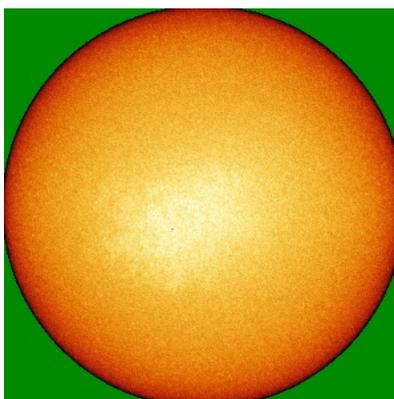


Z

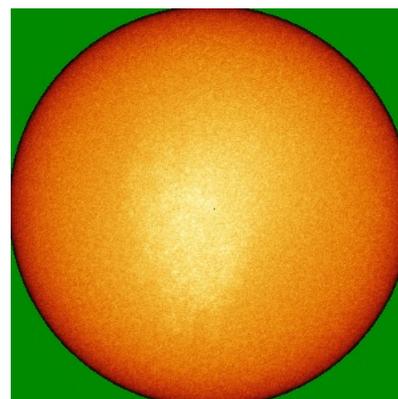
6.4.2 Raw map



X



Y

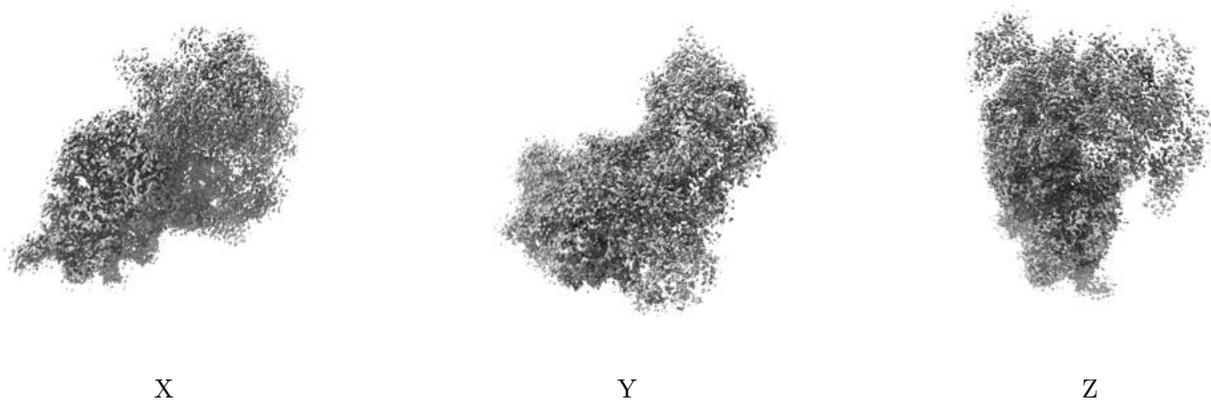


Z

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.

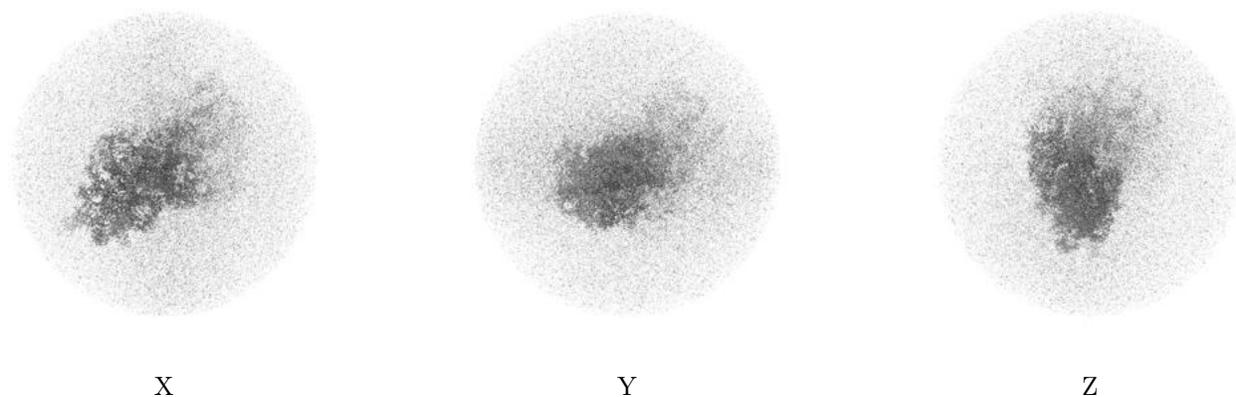
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0103. 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.

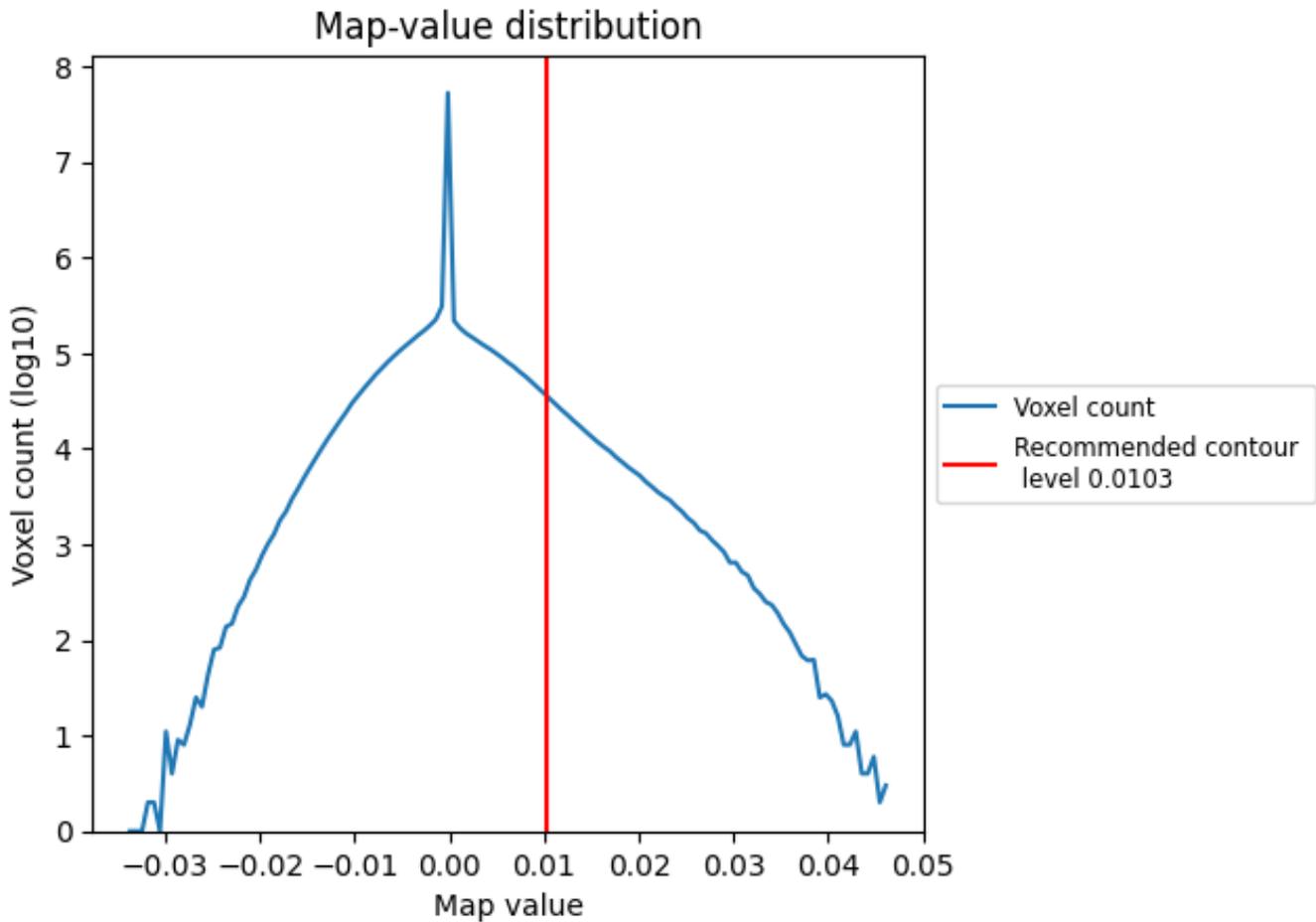
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

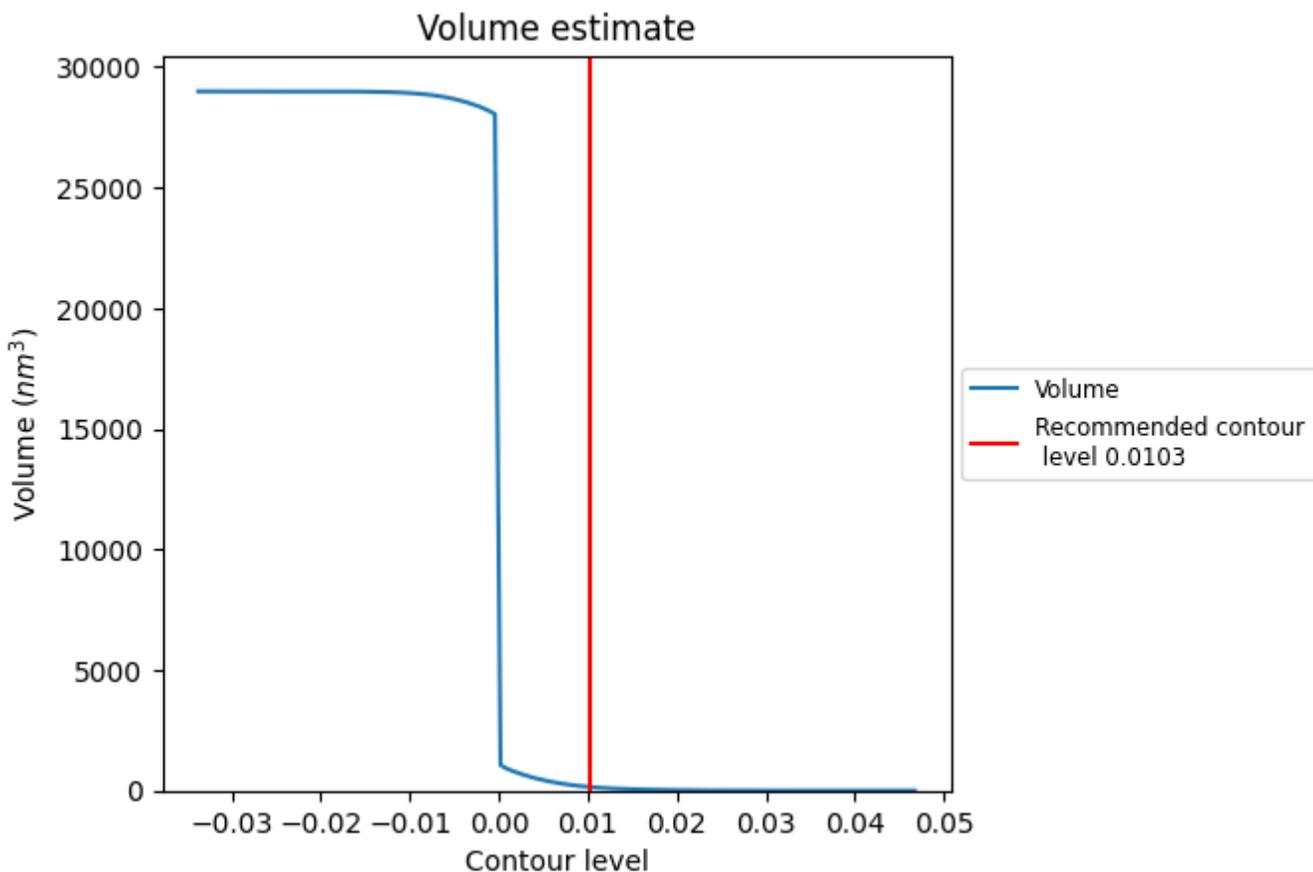
This section contains the results of statistical analysis of the map.

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.

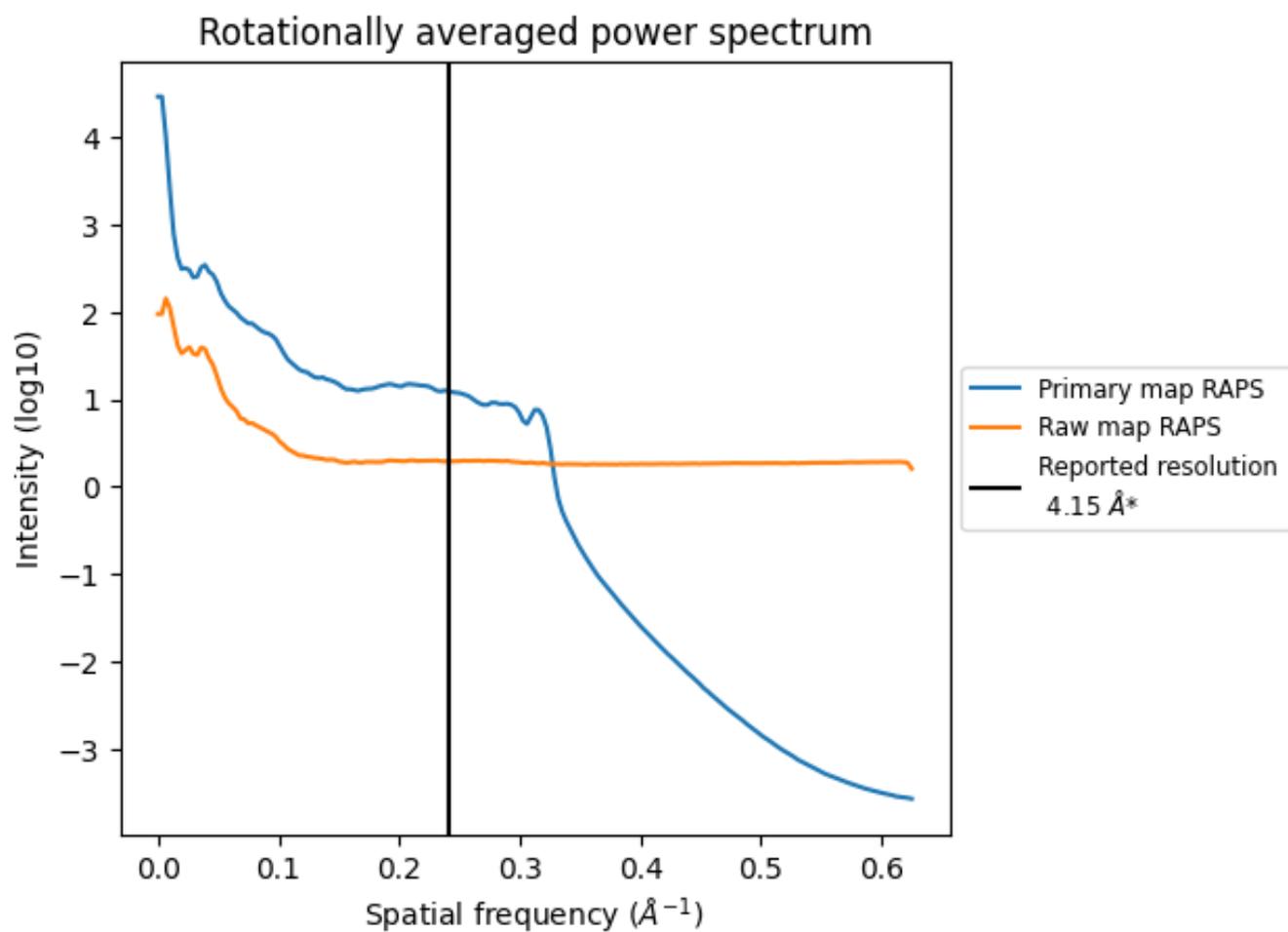
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 136 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

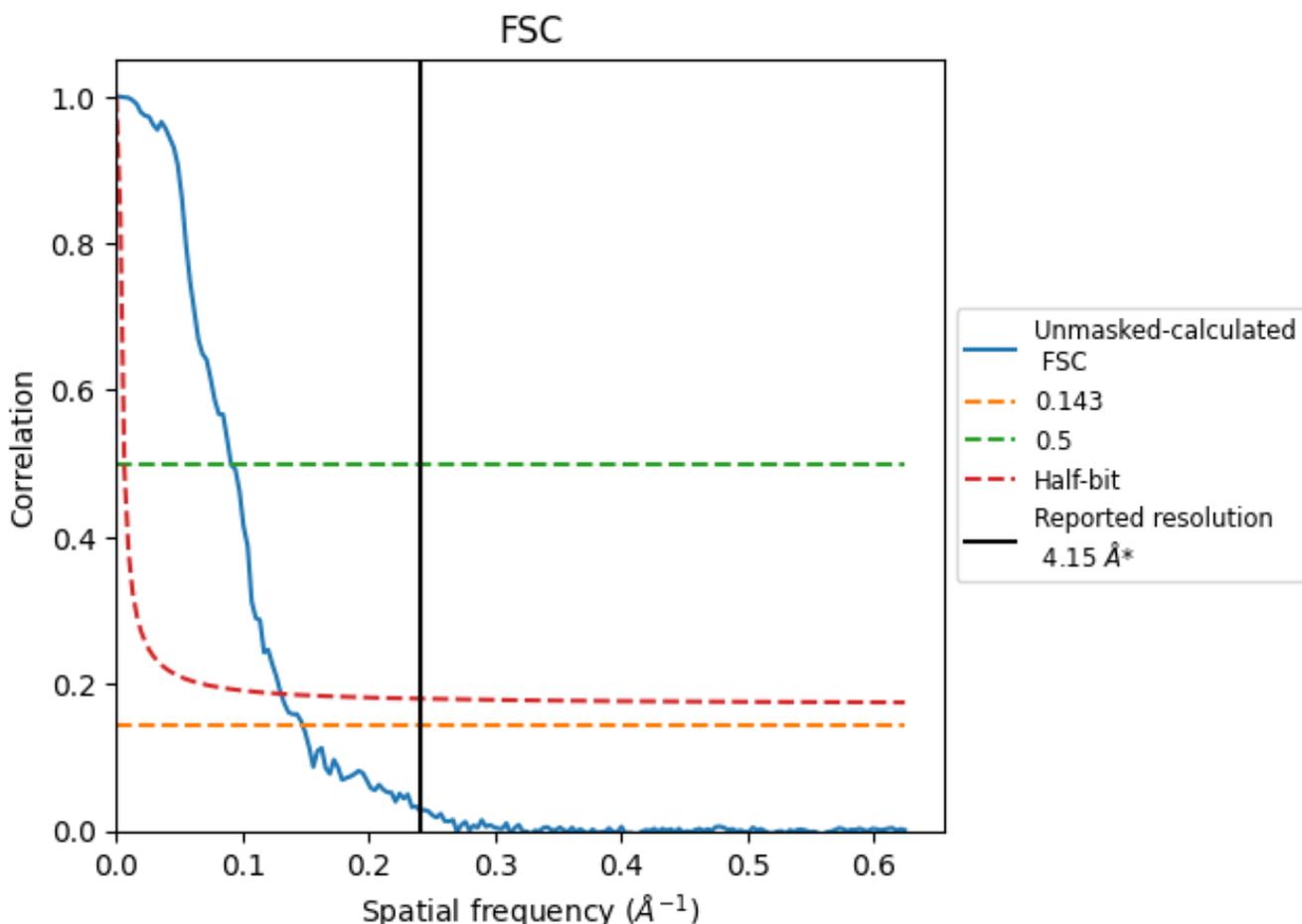


*Reported resolution corresponds to spatial frequency of 0.241 Å⁻¹

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 0.241 Å⁻¹

8.2 Resolution estimates [i](#)

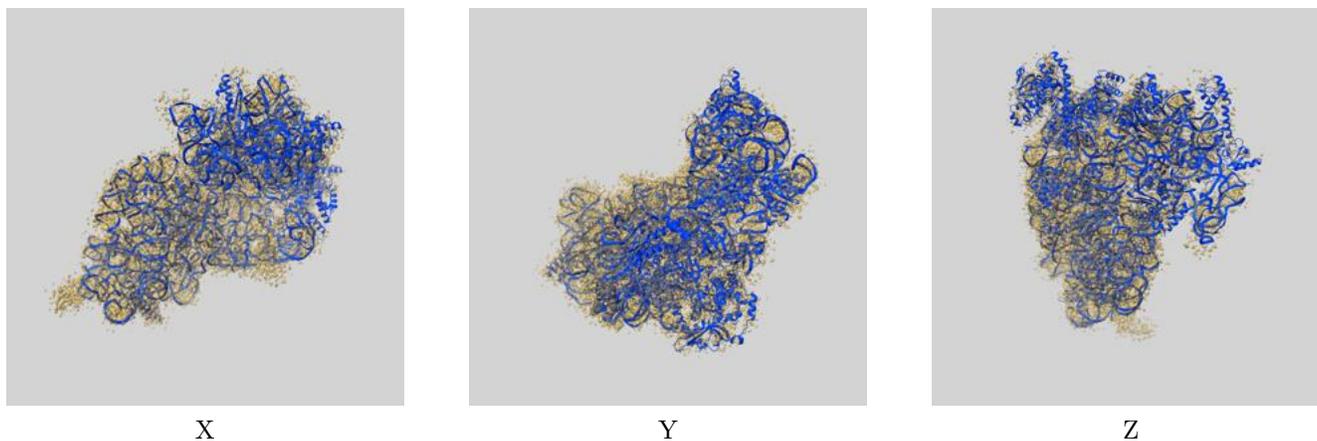
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.77	11.00	7.66

*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 6.77 differs from the reported value 4.15 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16606 and PDB model 8CED. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



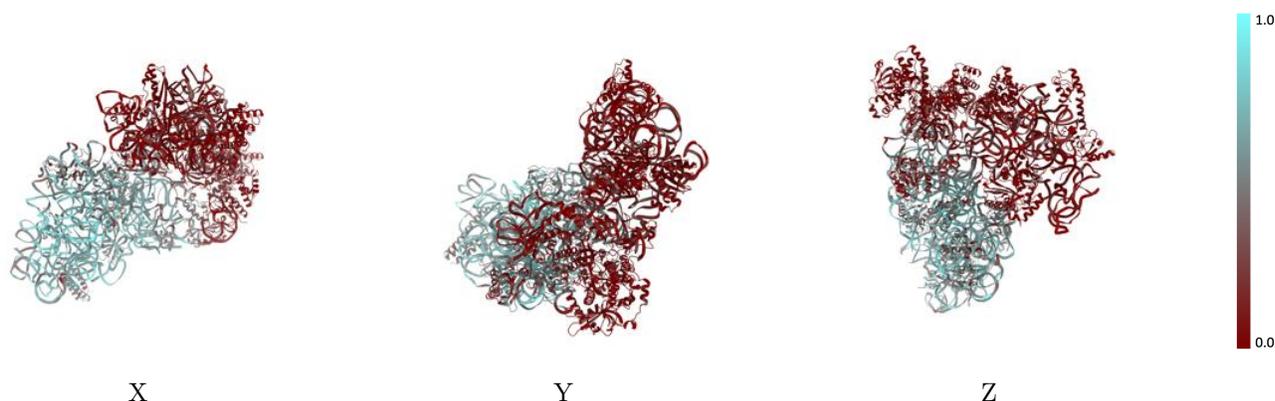
The images above show the 3D surface view of the map at the recommended contour level 0.0103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



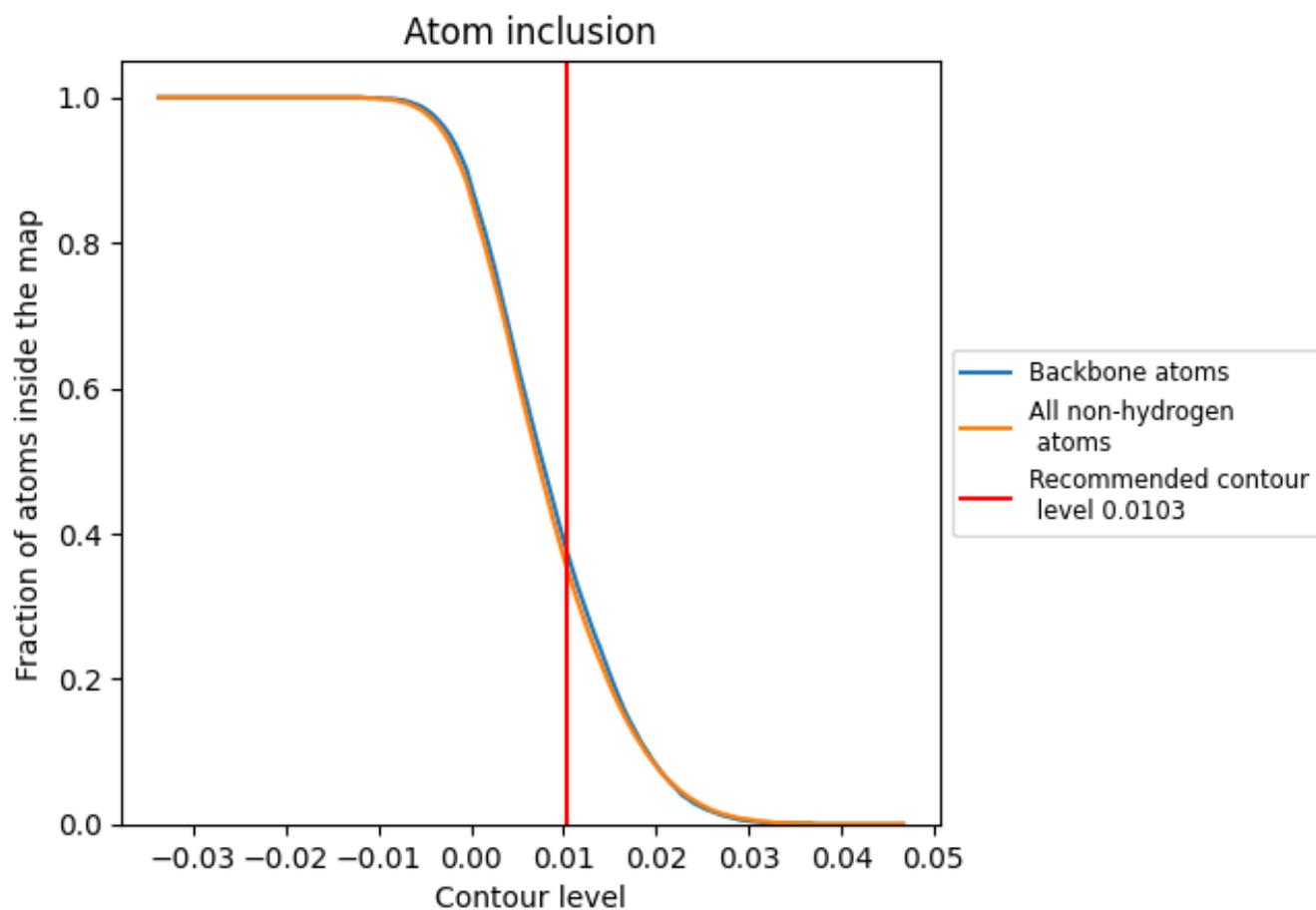
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0103).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 36% 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 (0.0103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3550	 0.2650
A	 0.4740	 0.3270
B	 0.0520	 0.0890
C	 0.0440	 0.0570
D	 0.1900	 0.2050
E	 0.0560	 0.0770
F	 0.4000	 0.3750
G	 0.4890	 0.3940
H	 0.0470	 0.0390
I	 0.5210	 0.4230
J	 0.0750	 0.0940
K	 0.0310	 0.0380
L	 0.4870	 0.3960
M	 0.0200	 0.0340
N	 0.0510	 0.0960
O	 0.5260	 0.3770
P	 0.5720	 0.4680
Q	 0.4980	 0.4160
R	 0.0150	 0.0280
S	 0.4520	 0.3540
T	 0.2310	 0.2120
U	 0.2630	 0.2570
V	 0.0260	 0.0980

