



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 09:29 PM EDT

PDB ID : 8H3V
EMDB ID : EMD-34475
Title : Cryo-EM structure of the full transcription activation complex NtcA-NtcB-TAC
Authors : Han, S.J.; Jiang, Y.L.; You, L.L.; Shen, L.Q.; Wu, X.X.; Yang, F.; Kong, W.W.; Chen, Z.P.; Zhang, Y.; Zhou, C.Z.
Deposited on : 2022-10-09
Resolution : 4.50 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

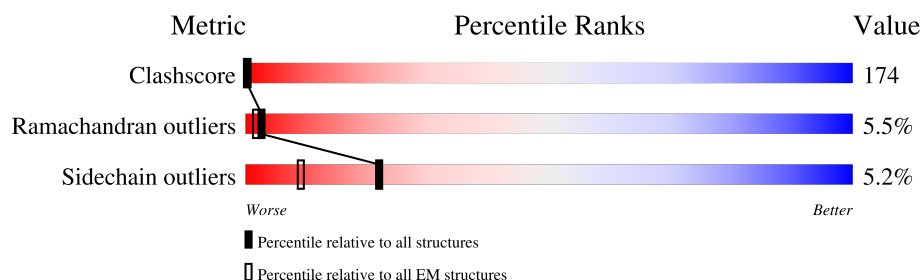
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	125	
2	2	125	
3	A	1132	
4	B	1350	
5	C	236	
5	D	236	
6	E	625	
7	F	78	

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Mol	Chain	Length	Quality of chain
8	G	390	
9	S	312	
9	T	312	
9	U	312	
9	V	312	
10	X	223	
10	Y	223	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 46048 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 DNA chain called DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	112	Total	C	N	O	P	0	0
			2302	1102	425	663	112		

- Molecule 2 is a DNA chain called DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	96	Total	C	N	O	P	0	0
			1967	946	341	584	96		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1077	Total	C	N	O	S	0	0
			8473	5326	1505	1618	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P22703
A	1	VAL	-	expression tag	UNP P22703

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1217	Total	C	N	O	S	0	0
			9292	5802	1639	1823	28		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	226	Total	C	N	O	S	0	0
			1762	1106	305	346	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	226	Total	C	N	O	S	0	0
			1762	1106	305	346	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q8YPK3
C	1	VAL	-	expression tag	UNP Q8YPK3
D	0	MET	-	initiating methionine	UNP Q8YPK3
D	1	VAL	-	expression tag	UNP Q8YPK3

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	619	Total	C	N	O	S	0	0
			4918	3104	884	909	21		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	58	Total	C	N	O	S	0	0
			474	290	90	90	4		

- Molecule 8 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	314	Total	C	N	O	S	0	0
			2600	1628	482	484	6		

- Molecule 9 is a protein called NtcB.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	304	Total	C	N	O	S	0	0
			2389	1518	423	438	10		
9	T	294	Total	C	N	O	S	0	0
			2320	1477	411	422	10		
9	U	294	Total	C	N	O	S	0	0
			2320	1477	411	422	10		
9	V	304	Total	C	N	O	S	0	0
			2389	1518	423	438	10		

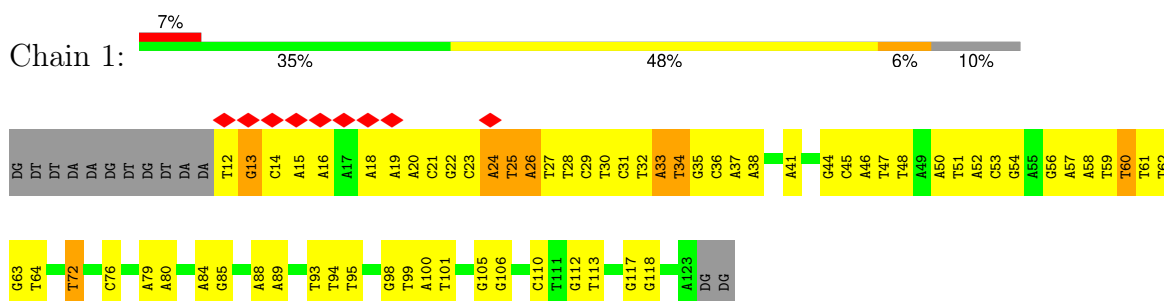
- Molecule 10 is a protein called NtcA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	0	0
			1540	984	268	280	8		
10	Y	196	Total	C	N	O	S	0	0
			1540	984	268	280	8		

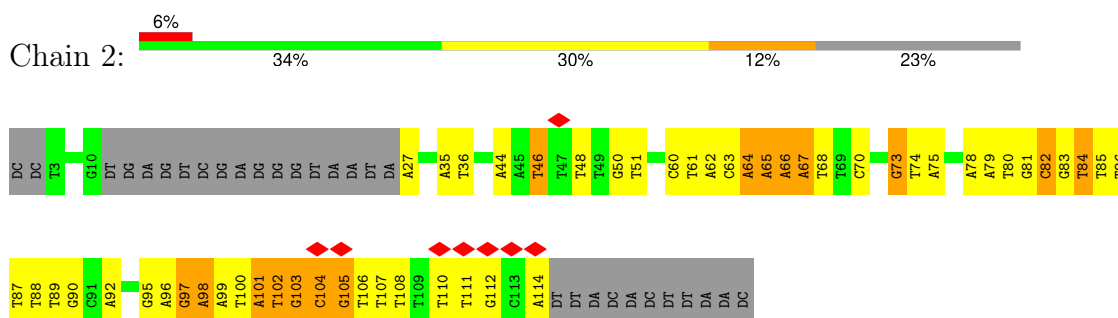
3 Residue-property plots

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.

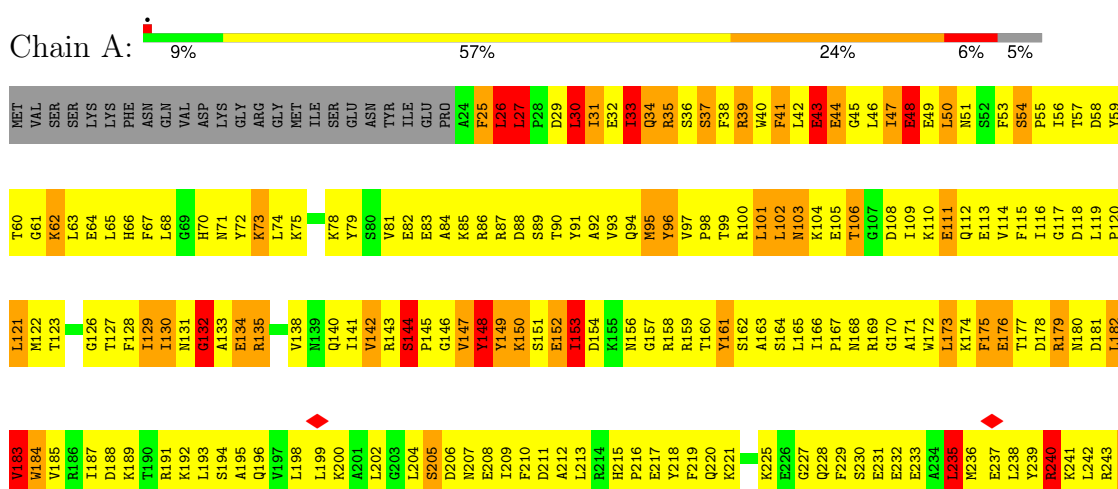
• Molecule 1: DNA (125-MER)



• Molecule 2: DNA (125-MER)

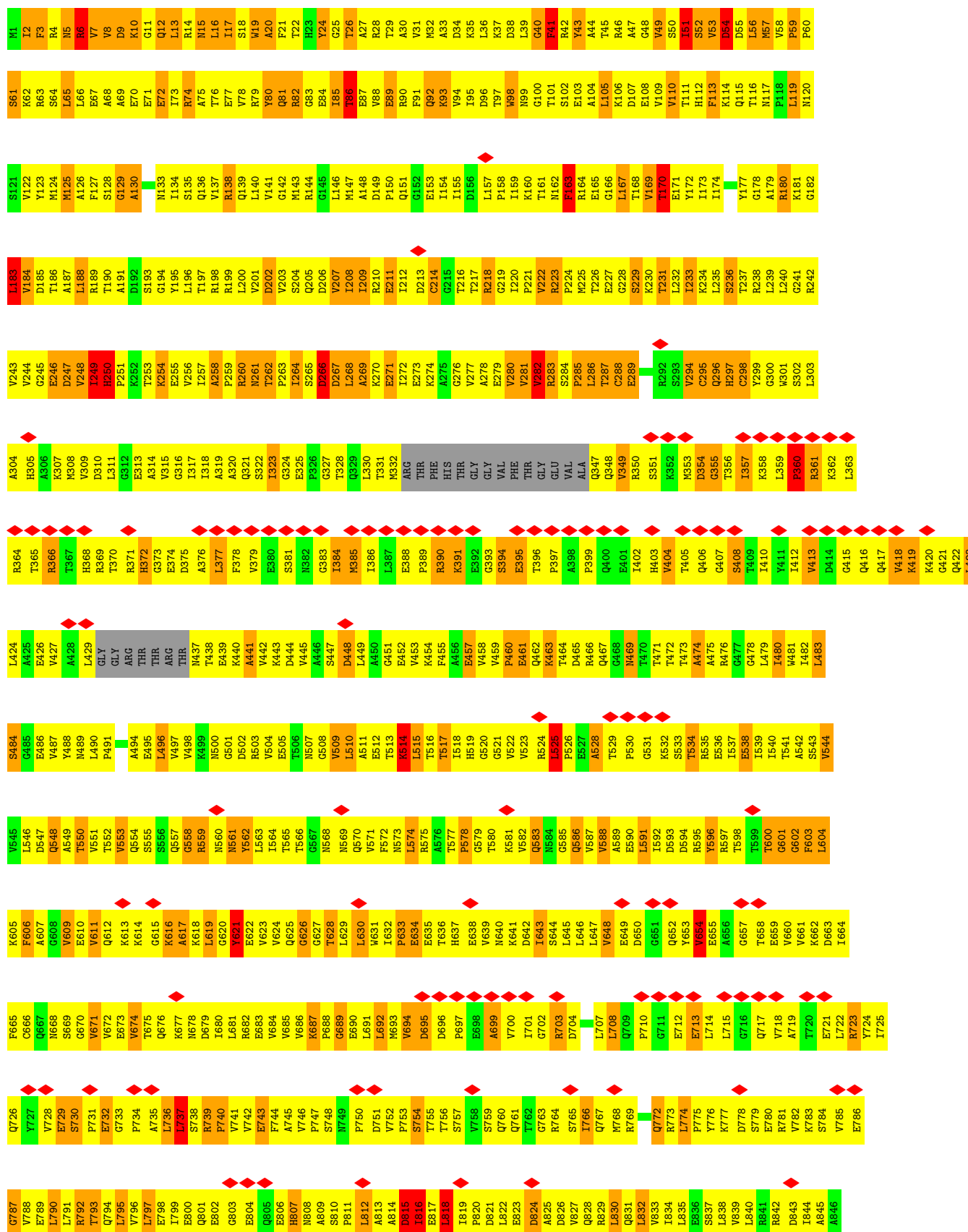
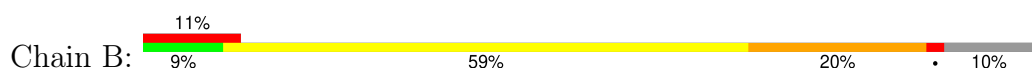


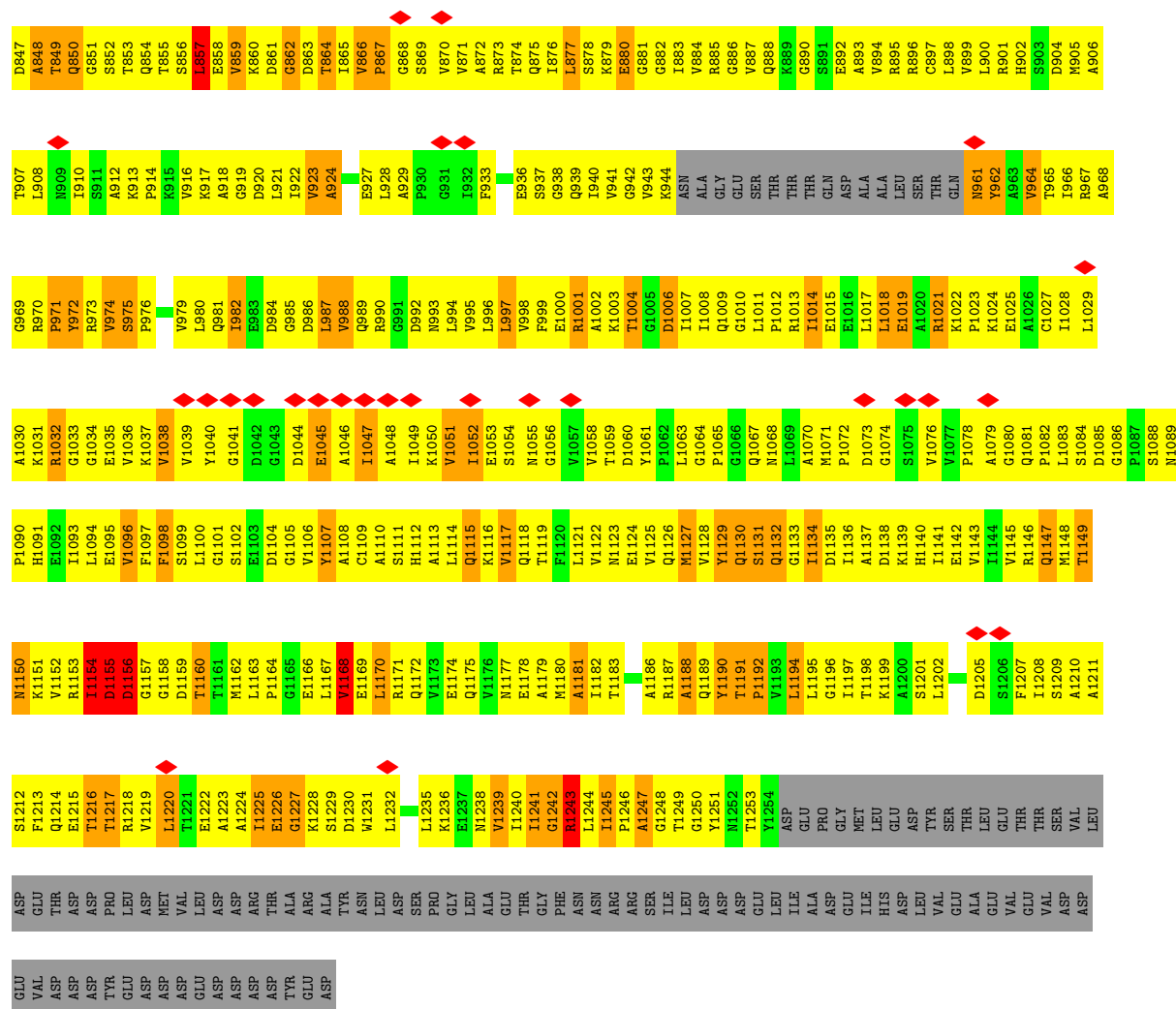
• Molecule 3: DNA-directed RNA polymerase subunit beta



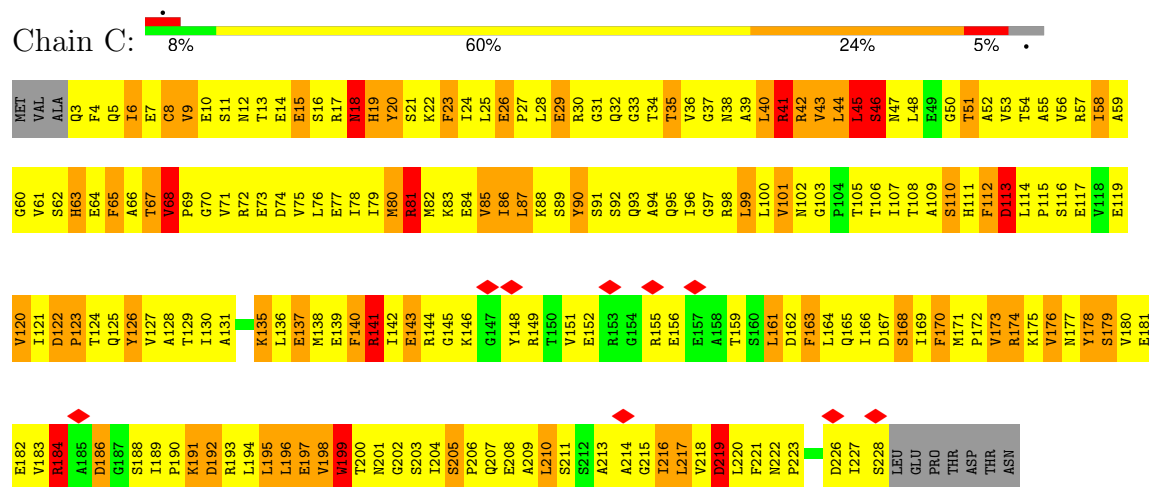
S1096	E1036	Y976	I916	H856	K795	E735	T675	G612	N551	V490	R429	P369	I305	G245
S1097	L1037	A977	T917	G857	A796	I736	E676	Q613	R552	A491	I430	L370	N306	E246
D1098	L1038	Y978	P918	N858	R797	T737	G677	L614	A553	P492	P432	V371	E308	P247
D1099	T1039	Y979	F919	K859	D798	R738	G678	P615	L554	G493	P433	A372	E307	P248
V1100	V1040	L980	D920	I861	R799	E739	E679	T616	M555	D494	I434	A373	I310	T249
GLU	K1041	K981	E921	G860	R800	I740	L680	A617	G556	P496	I435	K375	L251	V250
VAL	S1042	L982	M922	I862	D801	P741	A681	A618	S557	V497	T436	E376	I311	L251
ASP	D1043	Y983	Y923	S863	I802	T742	L682	G619	N558	E498	P436	E377	I314	G252
LEU	D1044	H984	G924	R864	S803	G744	G683	K620	M559	E499	E437	F377	D315	G253
MET	M1045	L985	E925	L865	L804	E745	Q684	S621	G560	E499	P438	F378	Q255	Q255
ALA	Q1046	V986	E926	L866	R805	E746	Q685	T622	R561	N500	G439	G379	Q256	Q256
ASP	G1047	D987	S927	P867	V806	D746	I866	D623	G562	G501	N440	G379	L257	L257
GLN	R1048	T988	S928	I868	P807	A747	V687	D624	A563	Y502	N441	G381	H319	L258
LEU	N1049	K989	S929	E869	N808	L748	V688	L627	V664	I503	G442	Q382	L320	D258
ALA	E1050	R929	R929	D870	G809	R749	A689	T628	P665	I504	I443	L383	L320	S259
ARG	A1051	R931	I931	M871	E810	Q750	Y690	S629	L566	G504	I444	S384	R323	R260
ARG	L1052	H931	R932	P872	K811	L751	M691	Q830	G445	F386	G446	Q385	R324	F261
THR	N1053	H933	H933	Y873	G812	D752	P692	K631	K568	Q507	S446	F386	V325	F262
PRO	A1054	G934	R933	L874	R813	E753	M693	G632	P569	V508	L447	M387	R376	D263
PRO	T1055	P935	K935	P875	V814	Q754	E694	Q633	E570	P509	A448	D388	S327	P264
ARG	V1056	G996	L936	D876	V815	G755	G695	E634	R571	V510	T449	Q389	V328	K265
PRO	K1057	Y997	Q937	G877	D816	I756	Y696	R635	P572	R511	H450	T390	G329	R266
THR	G1058	Y998	E938	S878	V817	I757	M697	R636	L573	Y512	A451	N391	E330	Y267
TYR	K1059	A939	A939	P879	R818	R758	Y698	Y637	G574	R513	R452	P392	L331	D268
GLU	A1060	V880	R940	V880	L819	I759	E699	G575	G574	Q514	V453	L393	L332	L269
SER	I1061	D881	R940	D881	F820	G760	D700	S640	T576	E515	Y456	A394	Q333	G270
LEU	P1062	I882	E942	I882	T821	A761	A701	K641	G577	F516	G456	E395	N334	R271
SER	K1063	V883	T943	V883	R822	G762	I702	Y642	L578	L396	G457	L396	Q335	V272
ARG	Q1064	L884	G944	L884	E823	P763	L703	Q643	E579	T397	F458	T397	V336	G273
GLU	G1065	N885	K945	N885	Q824	E764	L704	R644	A580	H398	L459	H398	R337	R274
SER	T1066	P886	D946	P886	G825	A765	S705	S645	Q681	P521	E460	K399	Y275	Y275
LEU	P1067	L887	D947	L887	D826	G766	E706	N646	G582	R400	T461	R400	L340	K276
ASP	E1068	G888	V948	G888	E827	D767	R707	Q647	A583	R401	P462	R401	H341	L277
ASP	S1069	V889	V949	V889	P829	L768	L708	T649	R584	L402	F463	L402	R342	N278
ASP	F1070	S891	N950	S891	P830	V770	V709	C650	P586	S403	R464	S403	L343	K279
GLU	K1071	R892	P951	R892	G831	G771	Q710	C650	S586	Y526	P465	A404	E344	K280
V1072	L1073	D952	D952	K831	L651	K772	D711	L651	G587	V527	V466	L405	R345	L281
L1073	H1074	D953	D953	A832	N652	K773	D712	N652	M588	A528	E467	L406	I346	R282
R1075	E1076	P954	P954	M833	Q653	T773	I713	Q653	V529	V529	N468	P407	I347	L283
E1076	L1016	G955	G955	M834	K654	T774	Y714	K654	I590	S530	G469	G408	R348	S284
L1077	L1017	K956	K956	V835	P655	P775	T715	P655	V591	P531	R470	G409	E349	V285
Q1078	G1018	Y957	Y957	Q897	V836	K776	S716	L656	S692	V532	V471	L410	R350	P286
S1079	E1019	M958	M958	V898	R837	G777	I717	V657	R593	Q533	R472	T411	M351	D287
L1080	M1020	V959	V959	E900	V838	E778	H718	R658	T594	I534	F473	R412	T352	T288
G1081	E1021	Y960	Y960	C901	V840	S779	I719	I659	D595	V535	D474	E413	V353	V289
L1082	E1022	D961	D961	L902	Q842	Q781	E720	G660	G596	S536	Q475	R414	S354	R290
D1083	V1023	G962	G962	L903	Q842	P782	K721	E661	D597	V537	P476	A415	D355	V291
I1084	A1024	R963	R963	G904	K843	P783	E723	R662	V598	A538	G416	A415	D355	L292
A1085	L1025	T964	T964	I905	R844	E784	E723	V663	V599	T539	A477	F417	E357	T293
V1086	E1026	G965	G965	A906	K845	E785	E725	V664	Y600	S540	A478	A418	V358	S284
H1087	E1027	E966	E966	A907	K846	E786	E726	A665	M541	M541	Y479	A419	L359	G295
K1088	F1028	H967	H967	H908	I846	K786	A726	G666	D602	I542	M480	R420	T360	D296
V1089	G1029	P968	P968	T909	Q847	L787	R727	Q667	L781	P543	T481	D421	T361	I297
E1090	R969	L910	L910	T909	L788	Q728	F544	V668	A482	I422	A362	I298	A362	L298
A1030	R970	G911	G911	D850	R789	L669	T729	L669	D483	F544	D483	H423	S363	A299
A1031	P971	K851	K851	R850	A790	L669	T729	L669	E484	L545	L545	H423	S363	A300
Q1092	Y1032	P971	P971	M852	A670	D670	K730	A670	E485	E546	P424	P424	L364	A300
A1093	T1033	Y972	Y972	R912	D671	L731	L731	D671	V608	H547	S425	S425	V365	V301
D1094	L1034	T973	T973	R913	A853	G792	G732	G672	R609	D548	H426	H426	N366	D302
G1095	Q1035	G975	G975	K915	G854	G793	P733	S673	R610	D549	Y427	Y427	Y303	Y303

● Molecule 4: DNA-directed RNA polymerase subunit beta'

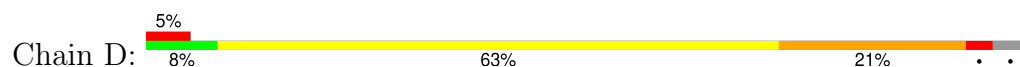


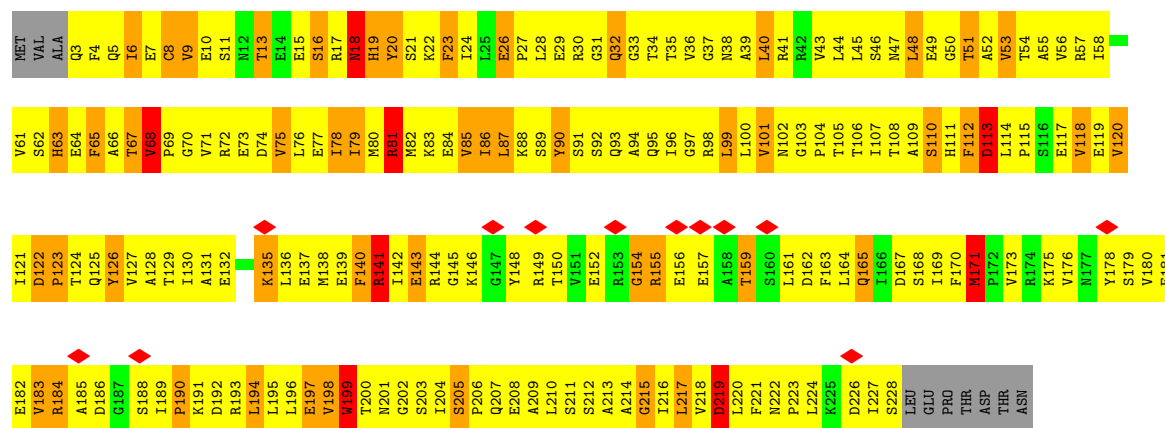


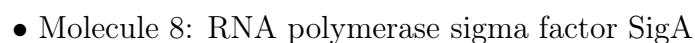
• Molecule 5: DNA-directed RNA polymerase subunit alpha

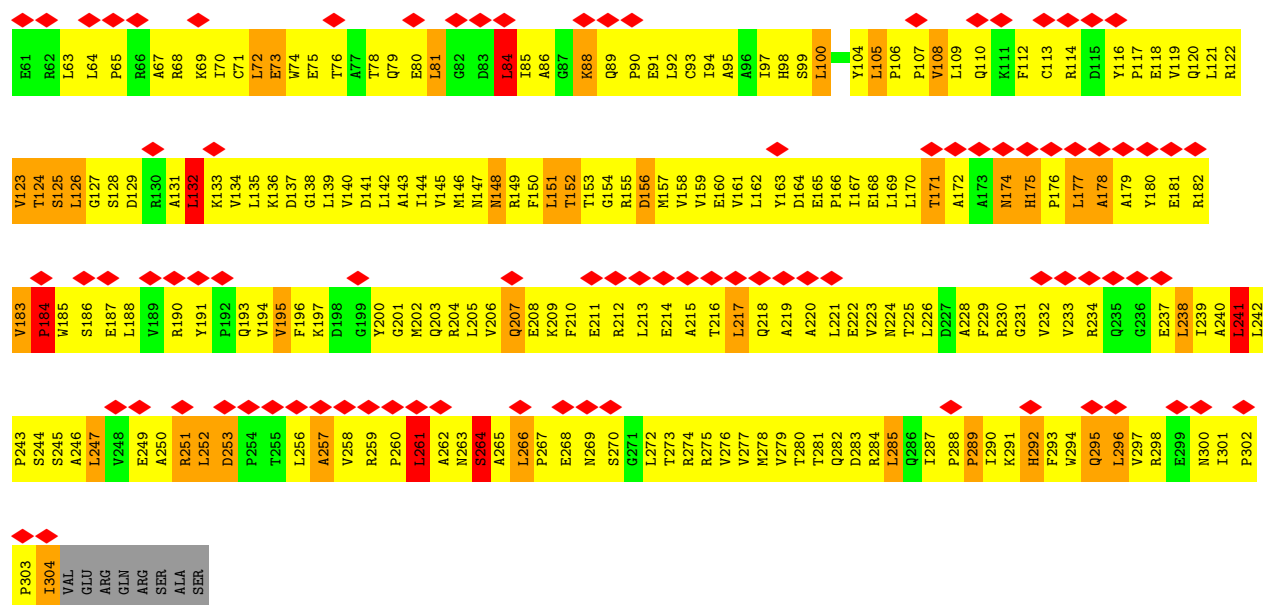


• Molecule 5: DNA-directed RNA polymerase subunit alpha



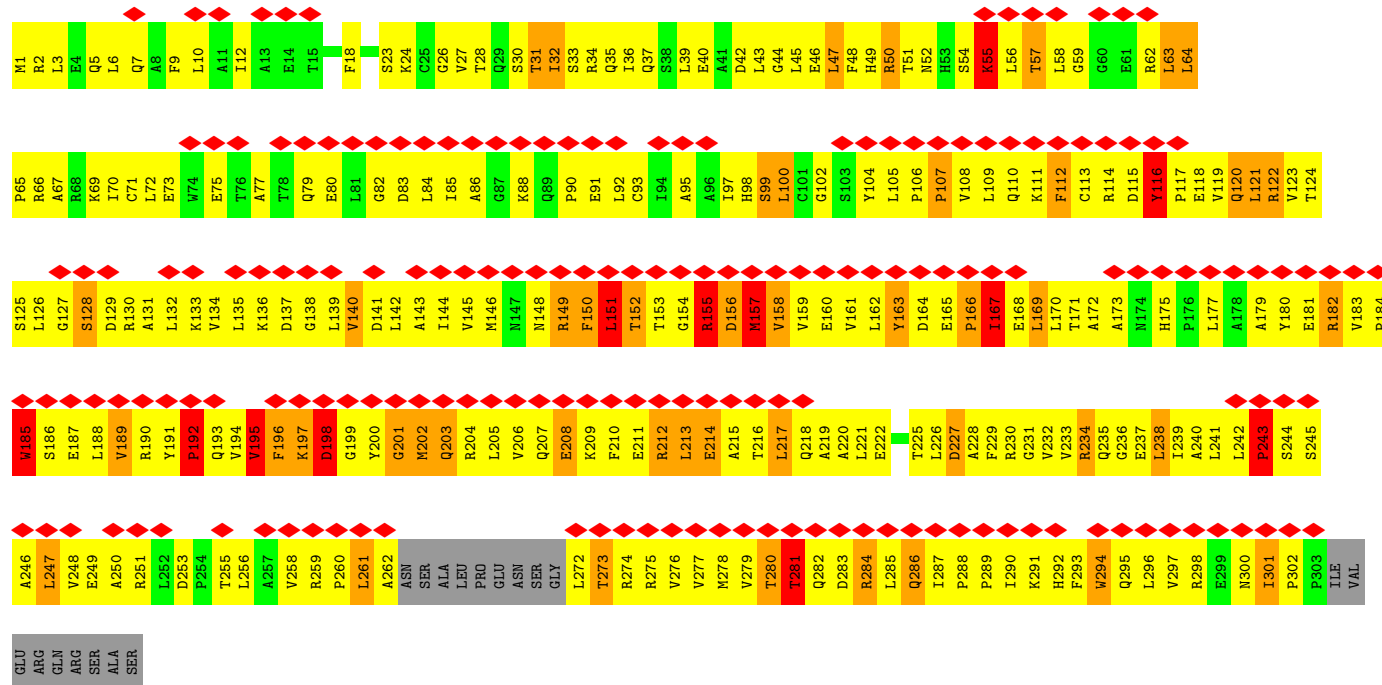






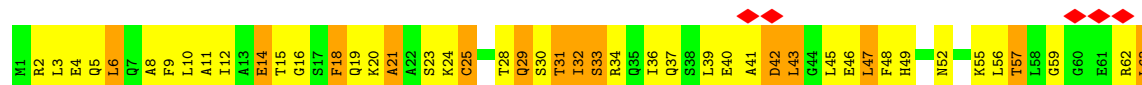
• Molecule 9: NtcB

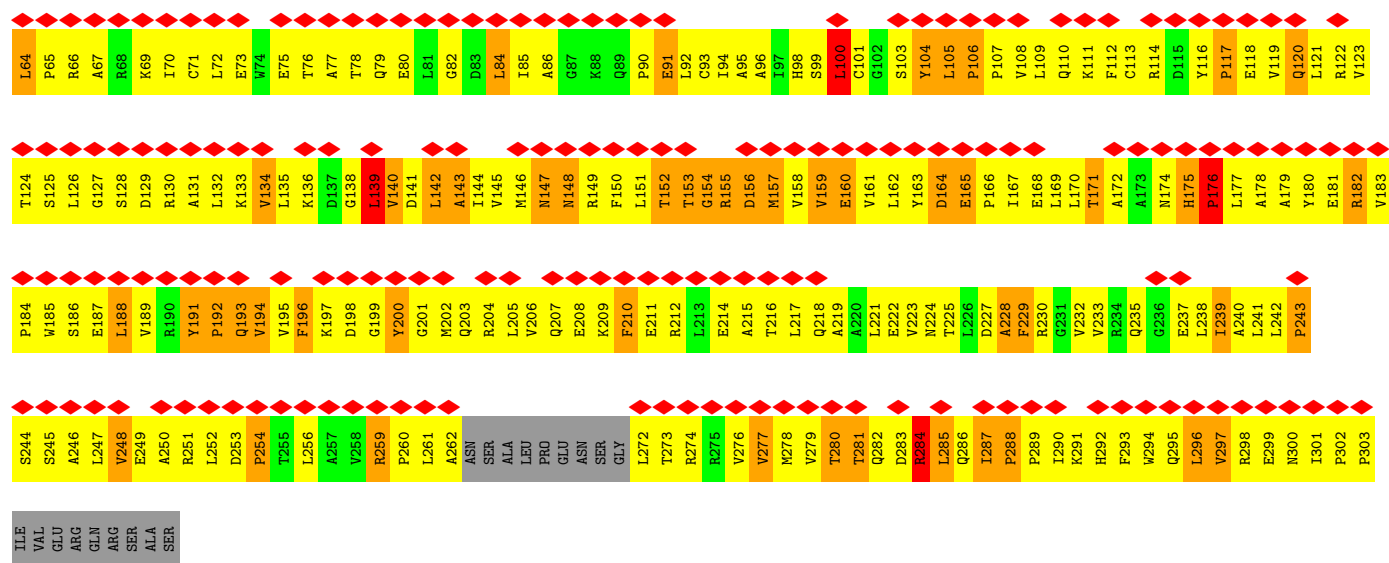
Chain T: 13% 57% 62% 15% 6%



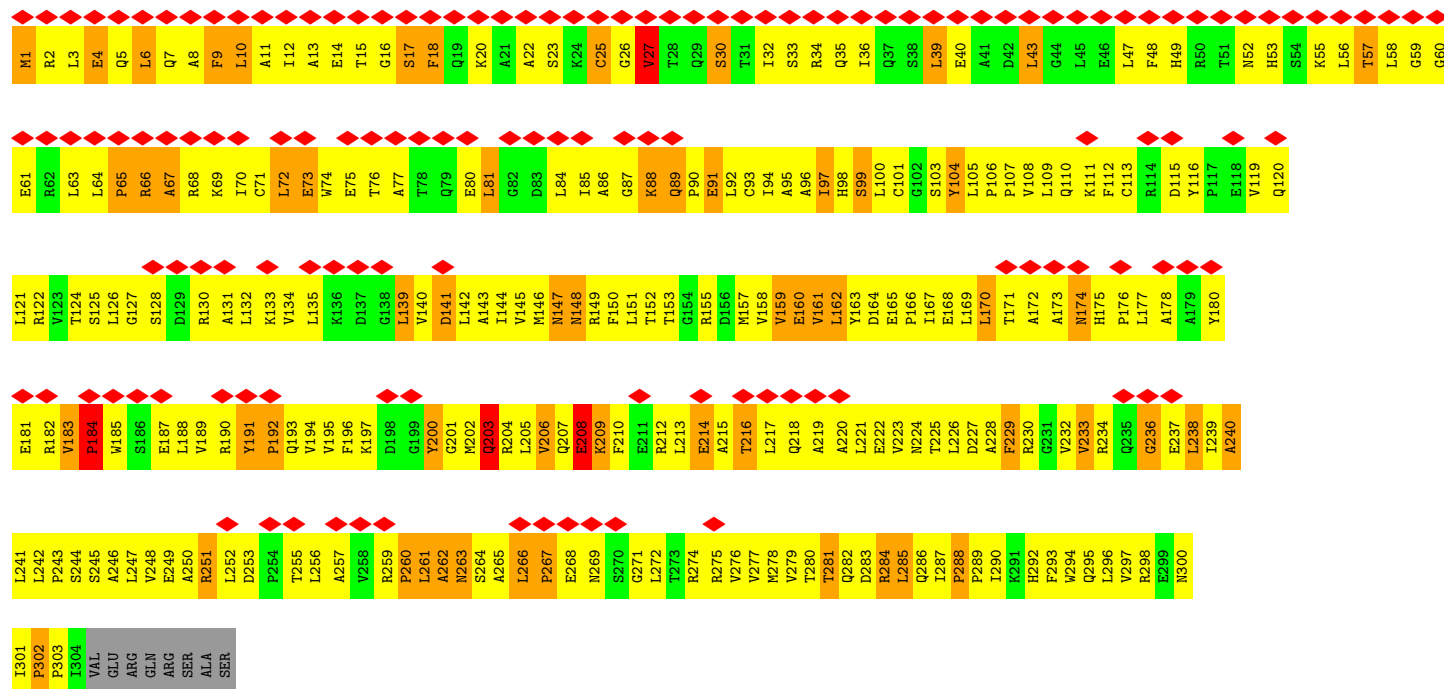
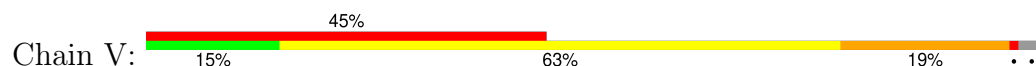
• Molecule 9: NtcB

Chain U: 13% 57% 60% 21% 6%

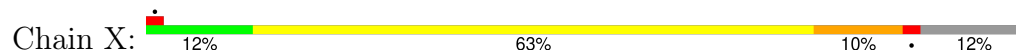




• Molecule 9: NtcB



• Molecule 10: NtcA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65446	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.337	Depositor
Minimum map value	-1.526	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	374.50003, 374.50003, 374.50003	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.78	4/2585 (0.2%)	1.15	11/3985 (0.3%)
2	2	0.84	7/2202 (0.3%)	1.16	14/3395 (0.4%)
3	A	1.90	254/8632 (2.9%)	1.58	195/11688 (1.7%)
4	B	1.38	119/9414 (1.3%)	1.35	118/12760 (0.9%)
5	C	1.60	33/1788 (1.8%)	1.54	33/2420 (1.4%)
5	D	1.42	24/1788 (1.3%)	1.25	16/2420 (0.7%)
6	E	1.66	105/5009 (2.1%)	1.35	65/6782 (1.0%)
7	F	1.85	10/478 (2.1%)	1.58	9/639 (1.4%)
8	G	1.45	41/2635 (1.6%)	1.33	39/3533 (1.1%)
9	S	0.91	9/2431 (0.4%)	1.14	27/3301 (0.8%)
9	T	0.94	8/2360 (0.3%)	1.25	28/3202 (0.9%)
9	U	1.07	5/2360 (0.2%)	1.17	15/3202 (0.5%)
9	V	0.87	6/2431 (0.2%)	1.08	18/3301 (0.5%)
10	X	0.89	1/1563 (0.1%)	1.03	7/2107 (0.3%)
10	Y	0.88	1/1563 (0.1%)	1.04	7/2107 (0.3%)
All	All	1.40	627/47239 (1.3%)	1.33	602/64842 (0.9%)

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
1	1	1	0
3	A	0	91
4	B	0	83
5	C	0	22
5	D	0	14
6	E	0	33
7	F	0	5
8	G	0	24
9	S	0	11
9	T	1	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	U	0	13
9	V	0	12
10	X	0	10
10	Y	0	11
All	All	2	337

The worst 5 of 627 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	150	PRO	N-CD	-23.30	1.15	1.47
9	U	176	PRO	N-CD	-23.25	1.15	1.47
6	E	116	TRP	CB-CG	-20.07	1.14	1.50
9	U	154	GLY	C-N	17.26	1.73	1.34
4	B	288	CYS	CB-SG	-17.22	1.52	1.82

The worst 5 of 602 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	149	SER	C-N-CD	-23.46	69.00	120.60
9	T	157	MET	CA-CB-CG	22.98	152.37	113.30
3	A	383	LEU	CA-CB-CG	-18.84	71.98	115.30
6	E	118	LEU	CA-CB-CG	-17.47	75.12	115.30
6	E	57	LEU	CA-CB-CG	-17.44	75.18	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	13	DG	C3'
9	T	157	MET	CA

5 of 337 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	26	LEU	Peptide
3	A	27	LEU	Peptide
3	A	30	LEU	Peptide
3	A	43	GLU	Peptide
3	A	44	GLU	Peptide

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	1	2302	0	1264	198	0
2	2	1967	0	1095	163	0
3	A	8473	0	8479	3435	0
4	B	9292	0	9454	3485	0
5	C	1762	0	1773	688	0
5	D	1762	0	1773	604	0
6	E	4918	0	4980	1843	0
7	F	474	0	477	192	0
8	G	2600	0	2686	938	0
9	S	2389	0	2464	922	0
9	T	2320	0	2397	1216	0
9	U	2320	0	2396	1060	0
9	V	2389	0	2459	1141	0
10	X	1540	0	1616	480	0
10	Y	1540	0	1616	498	0
All	All	46048	0	44929	15849	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 174.

The worst 5 of 15849 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)
9:T:196:PHE:CE2	9:T:200:TYR:CD1	1.77	1.73
4:B:481:TRP:CD1	4:B:971:PRO:HB3	1.26	1.68
9:T:202:MET:CA	9:T:205:LEU:CD2	1.75	1.65
10:Y:150:VAL:CG1	10:Y:218:LEU:HD13	1.27	1.64
9:T:175:HIS:CE1	9:T:177:LEU:CB	1.80	1.64

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	
3	A	1075/1132 (95%)	613 (57%)	417 (39%)	45 (4%)	2	18
4	B	1209/1350 (90%)	693 (57%)	451 (37%)	65 (5%)	1	16
5	C	224/236 (95%)	131 (58%)	79 (35%)	14 (6%)	1	14
5	D	224/236 (95%)	131 (58%)	79 (35%)	14 (6%)	1	14
6	E	617/625 (99%)	395 (64%)	193 (31%)	29 (5%)	2	17
7	F	56/78 (72%)	38 (68%)	17 (30%)	1 (2%)	7	34
8	G	312/390 (80%)	204 (65%)	94 (30%)	14 (4%)	2	17
9	S	302/312 (97%)	207 (68%)	83 (28%)	12 (4%)	2	18
9	T	290/312 (93%)	196 (68%)	74 (26%)	20 (7%)	1	12
9	U	290/312 (93%)	175 (60%)	87 (30%)	28 (10%)	0	8
9	V	302/312 (97%)	193 (64%)	80 (26%)	29 (10%)	0	8
10	X	194/223 (87%)	121 (62%)	61 (31%)	12 (6%)	1	14
10	Y	194/223 (87%)	113 (58%)	73 (38%)	8 (4%)	2	18
All	All	5289/5741 (92%)	3210 (61%)	1788 (34%)	291 (6%)	2	16

5 of 291 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	48	GLU
3	A	129	ILE
3	A	700	ASP
3	A	889	VAL
3	A	961	ASP

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	
3	A	918/969 (95%)	887 (97%)	31 (3%)	32	53
4	B	1017/1132 (90%)	975 (96%)	42 (4%)	26	48
5	C	196/205 (96%)	187 (95%)	9 (5%)	23	45
5	D	196/205 (96%)	184 (94%)	12 (6%)	15	37
6	E	534/538 (99%)	500 (94%)	34 (6%)	14	36
7	F	50/69 (72%)	49 (98%)	1 (2%)	50	68
8	G	282/351 (80%)	267 (95%)	15 (5%)	19	41
9	S	261/268 (97%)	237 (91%)	24 (9%)	7	24
9	T	253/268 (94%)	233 (92%)	20 (8%)	10	29
9	U	253/268 (94%)	231 (91%)	22 (9%)	8	26
9	V	261/268 (97%)	245 (94%)	16 (6%)	15	37
10	X	172/194 (89%)	164 (95%)	8 (5%)	22	44
10	Y	172/194 (89%)	167 (97%)	5 (3%)	37	58
All	All	4565/4929 (93%)	4326 (95%)	239 (5%)	22	41

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	E	442	GLN
9	V	229	PHE
8	G	385	LEU
9	V	200	TYR
10	Y	120	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
8	G	138	GLN
9	T	52	ASN
9	V	292	HIS
8	G	200	HIS
9	S	193	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	13
6	E	8
4	B	3
1	1	1
9	U	1
8	G	1

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	45:DC	O3'	46:DA	P	2.95
1	U	154:GLY	C	155:ARG	N	1.73
1	G	231:LEU	C	232:PRO	N	1.20
1	A	263:ASP	C	264:PRO	N	1.19
1	A	829:PRO	C	830:PRO	N	1.19

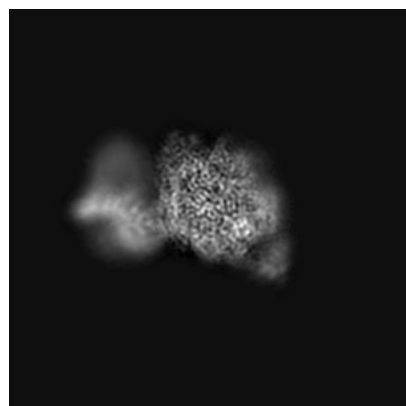
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34475. These allow visual inspection of the internal detail of the map and identification of artifacts.

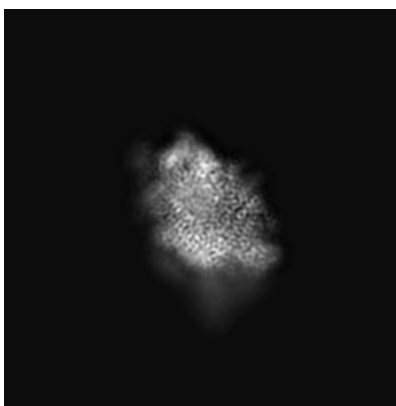
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

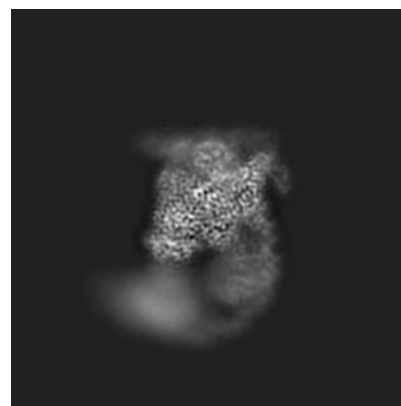
6.1.1 Primary map



X

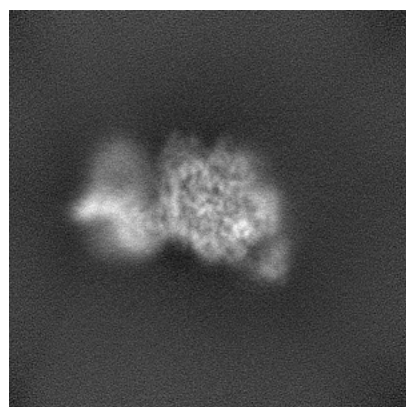


Y

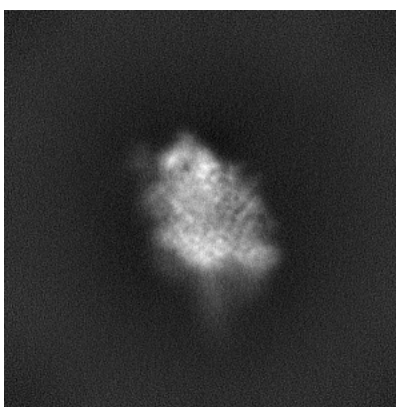


Z

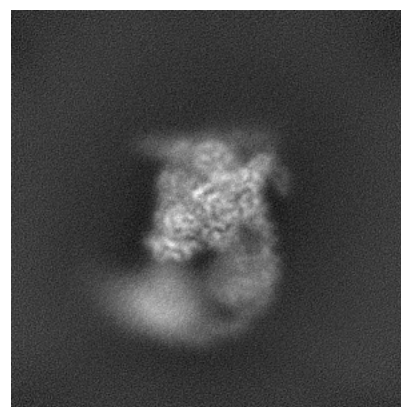
6.1.2 Raw map



X



Y

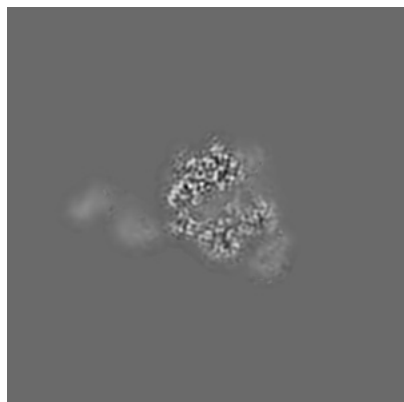


Z

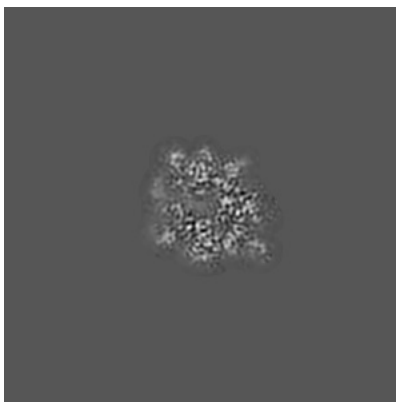
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

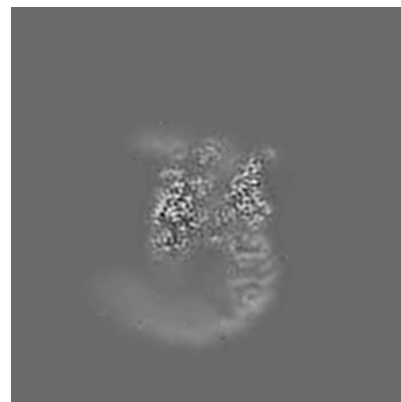
6.2.1 Primary map



X Index: 175

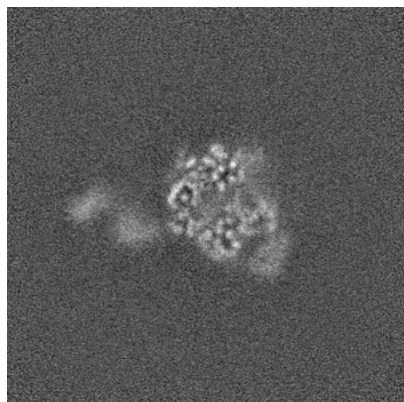


Y Index: 175

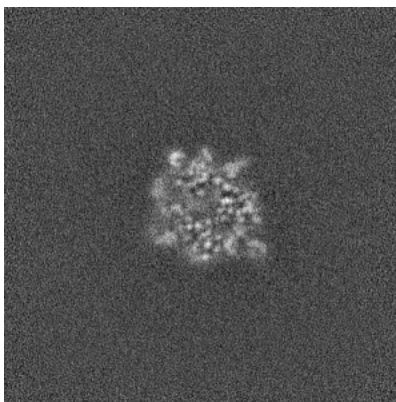


Z Index: 175

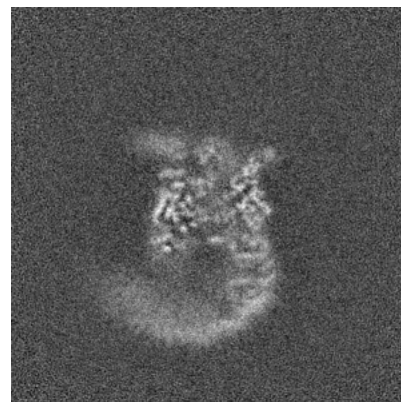
6.2.2 Raw map



X Index: 175



Y Index: 175

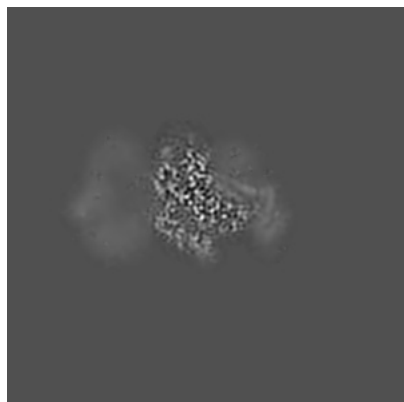


Z Index: 175

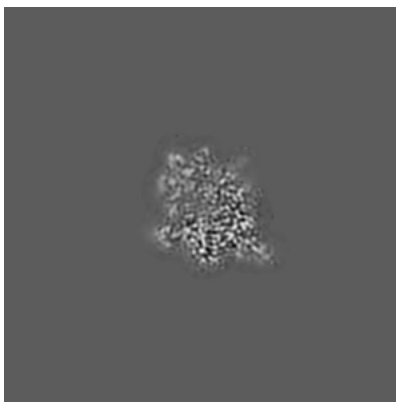
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

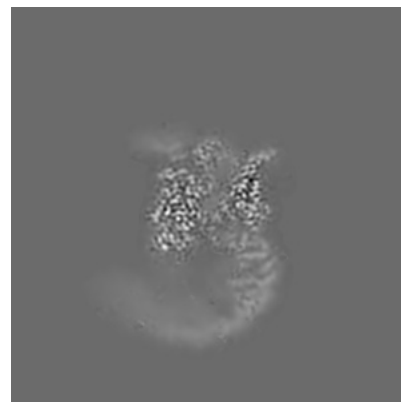
6.3.1 Primary map



X Index: 145

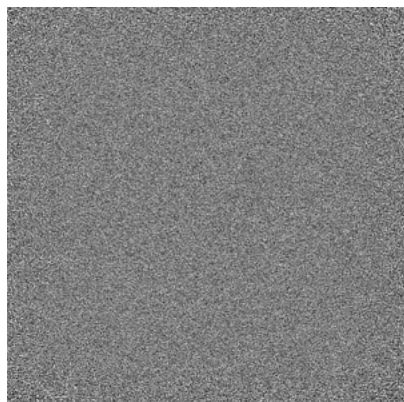


Y Index: 169

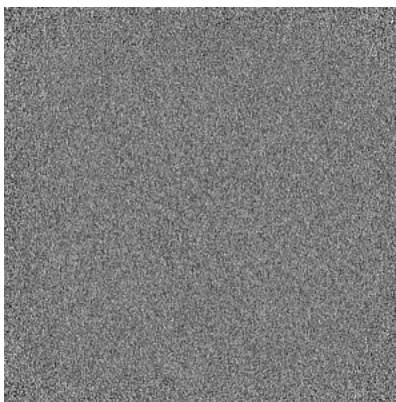


Z Index: 173

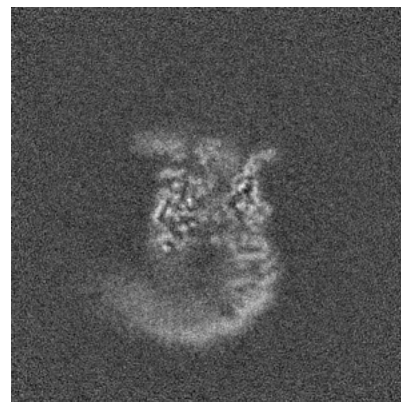
6.3.2 Raw map



X Index: 0



Y Index: 0

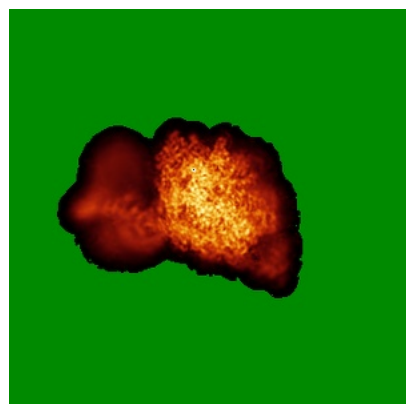


Z Index: 174

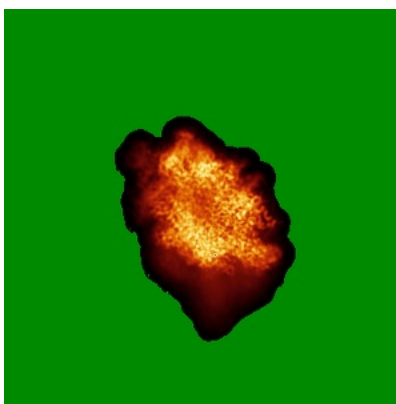
The images above show the largest variance slices of the map in three orthogonal directions.

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

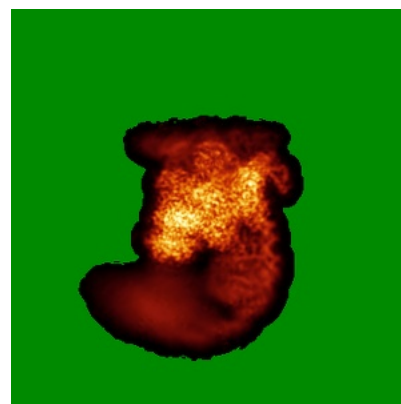
6.4.1 Primary map



X

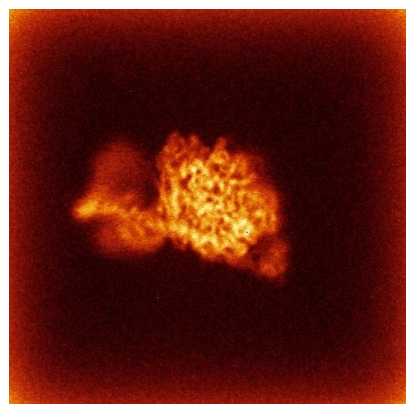


Y

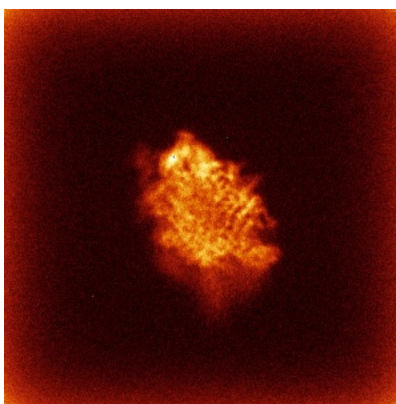


Z

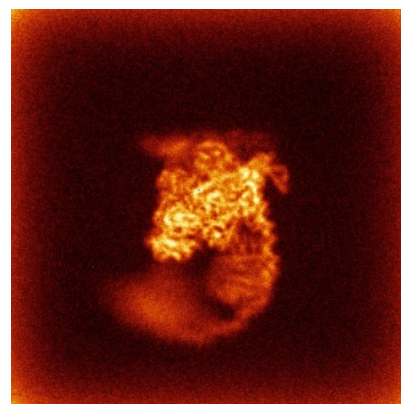
6.4.2 Raw map



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.

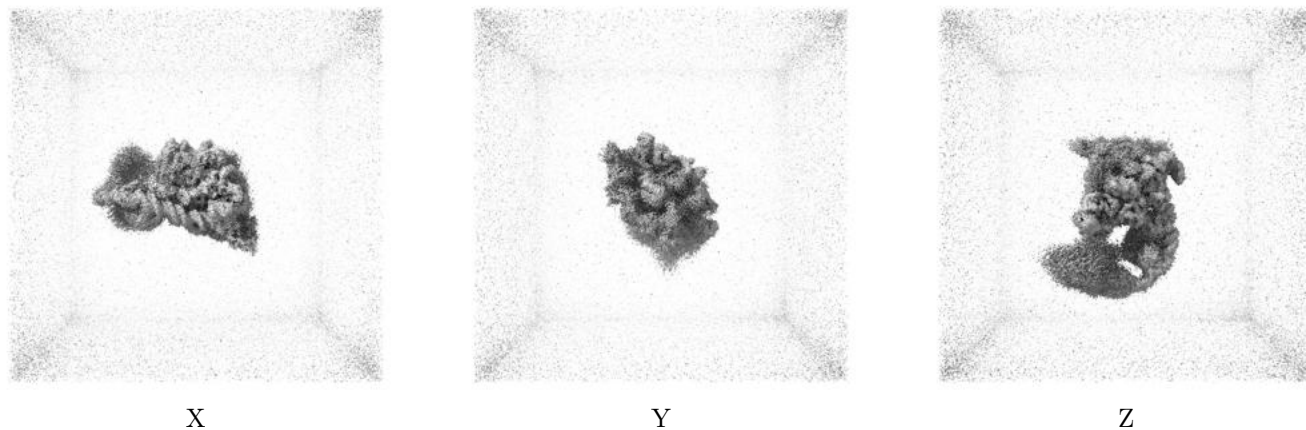
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

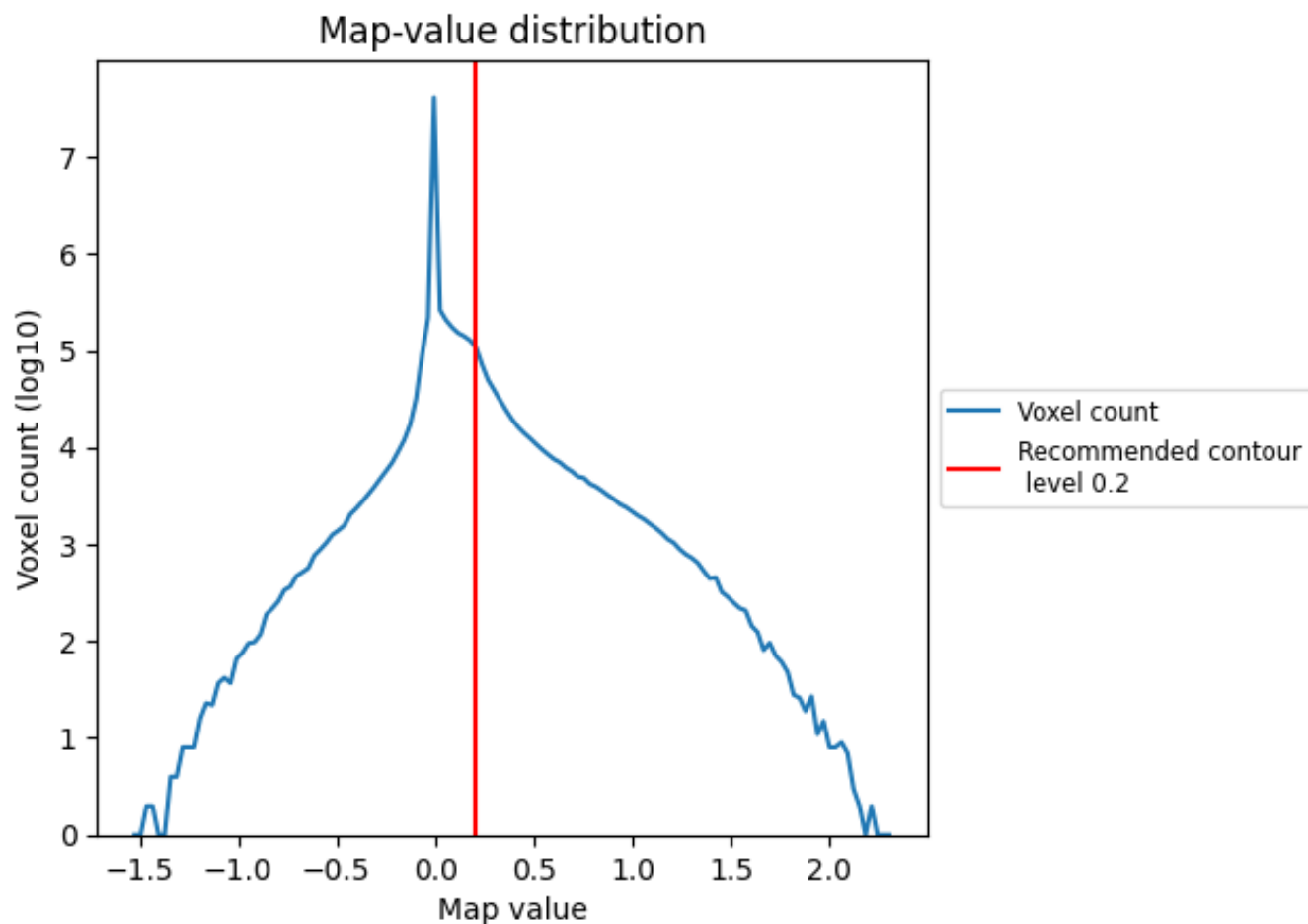
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

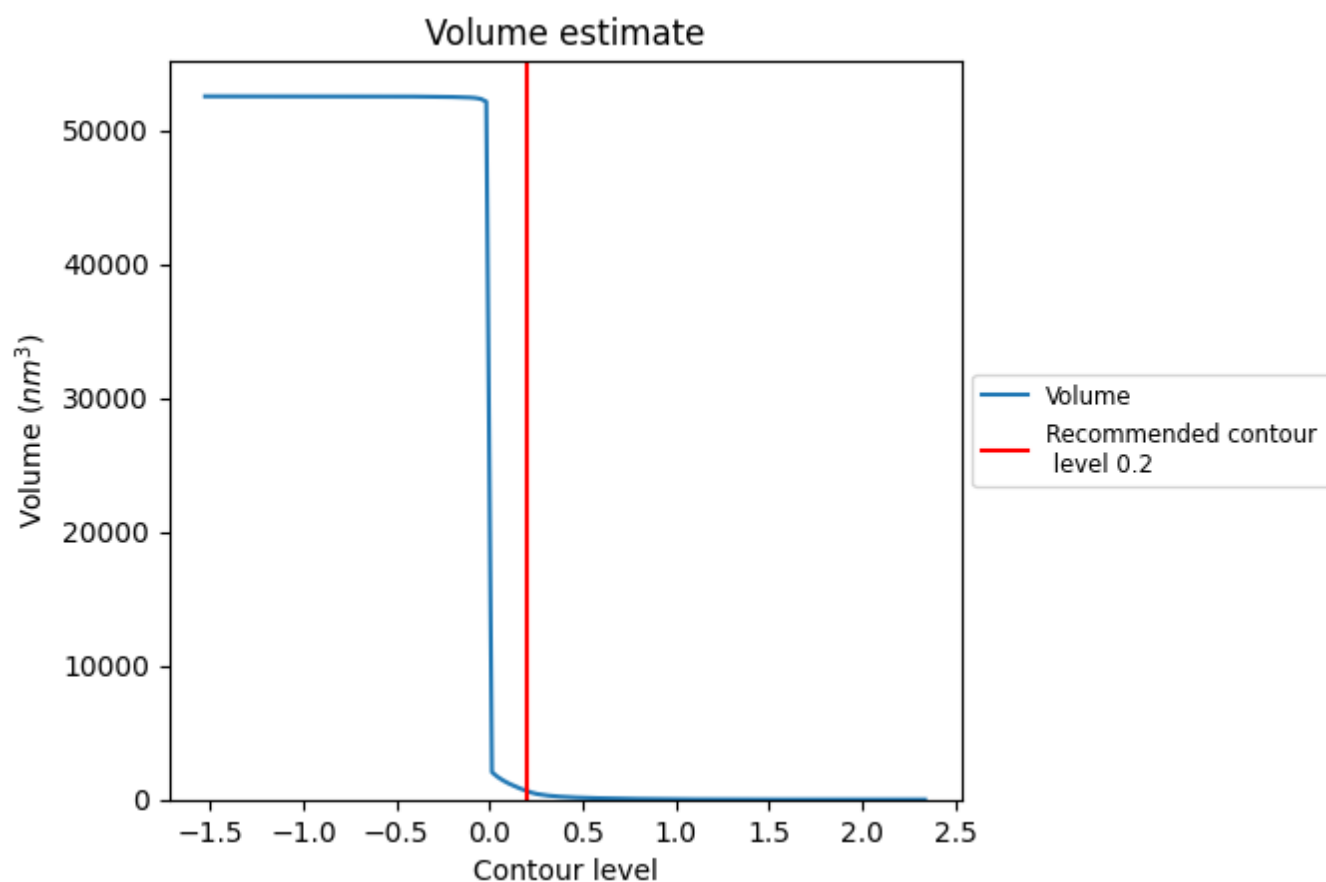
This section contains the results of statistical analysis of the map.

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.

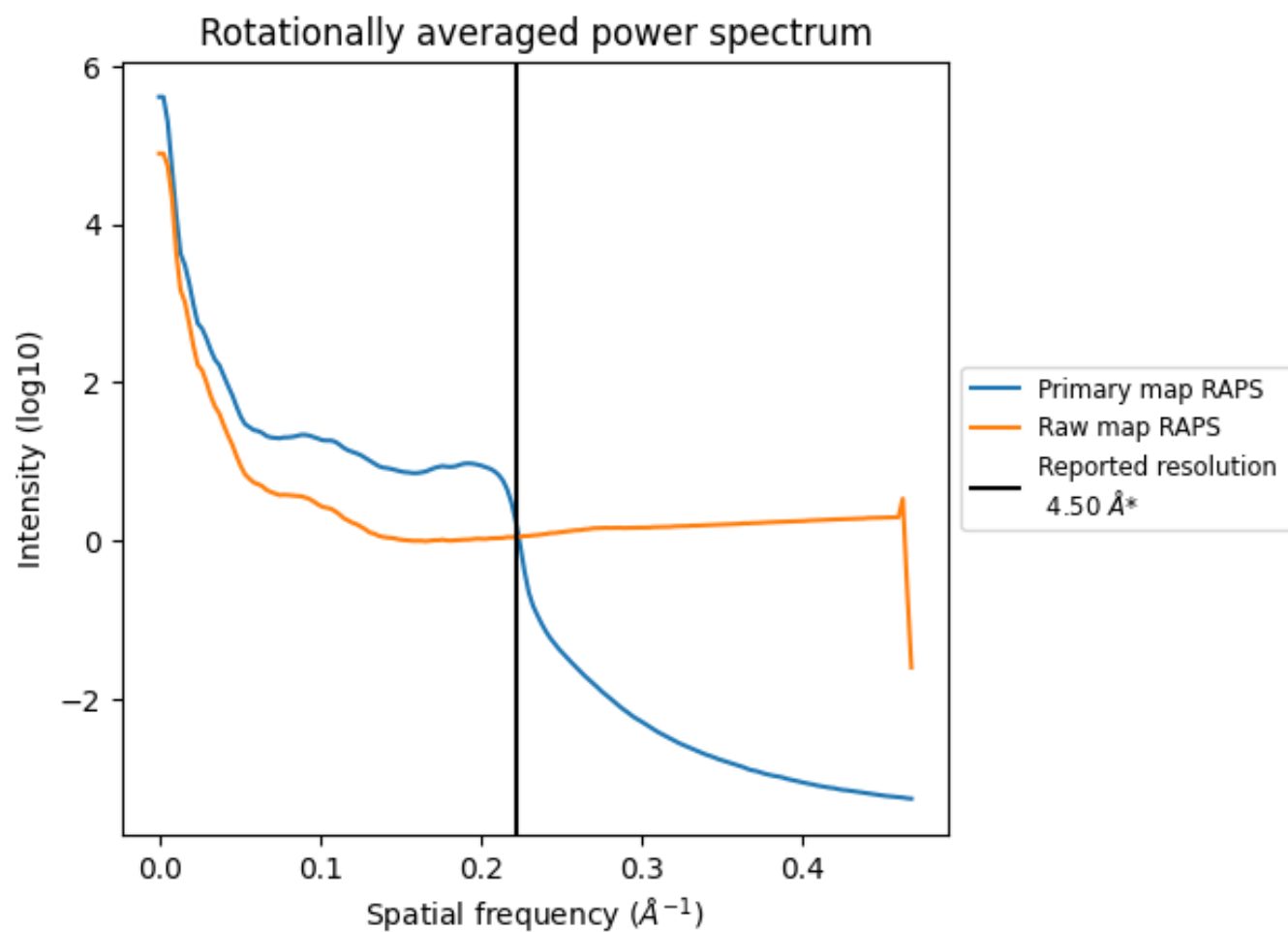
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 641 nm³; this corresponds to an approximate mass of 579 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 ⓘ

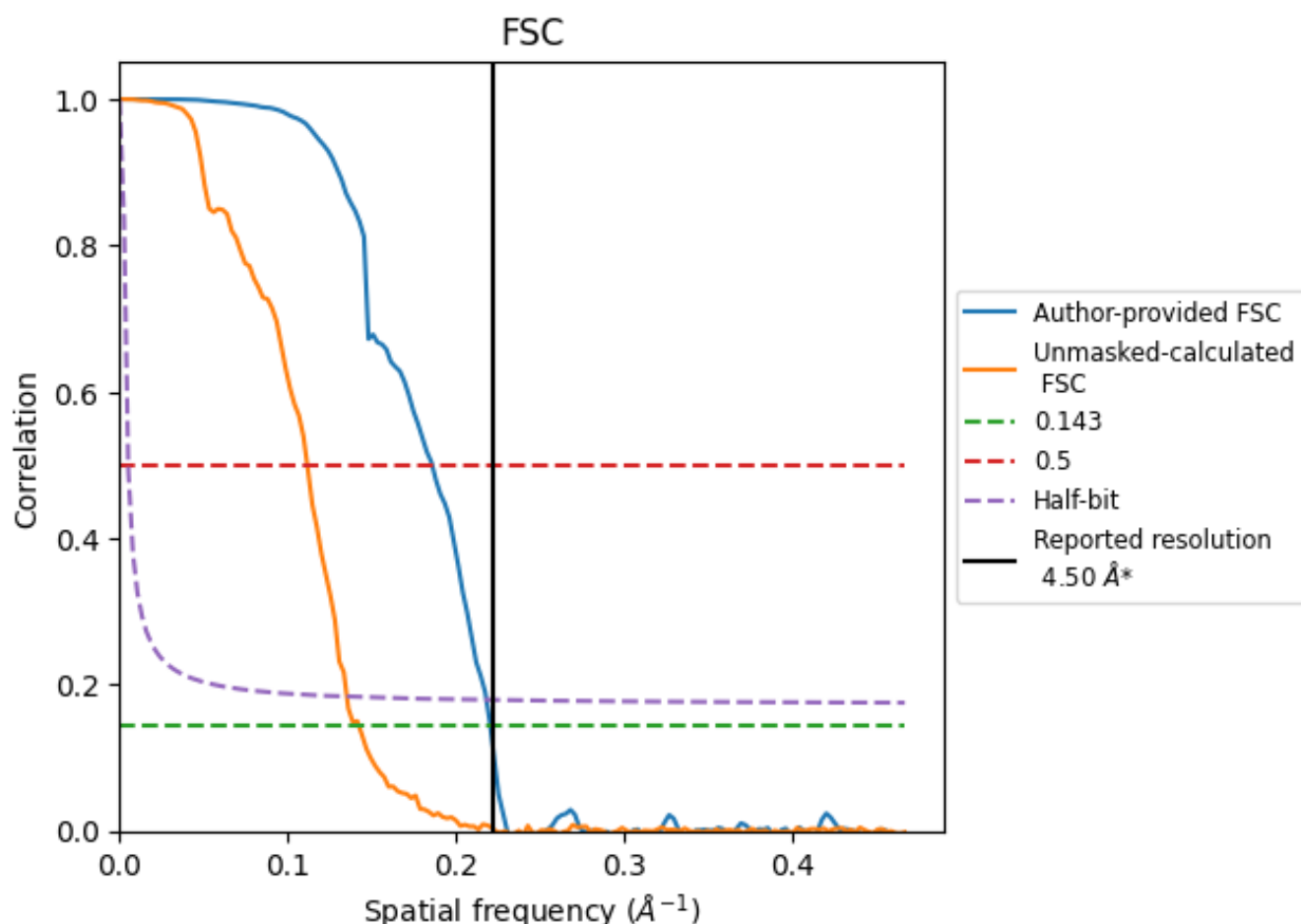


*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

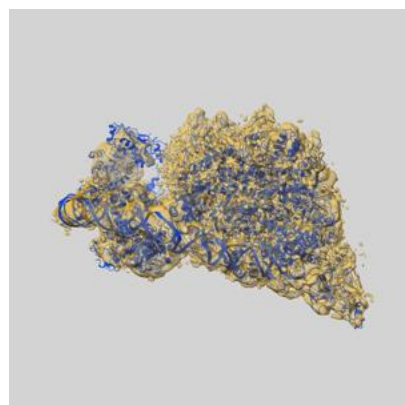
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.53	5.38	4.58
Unmasked-calculated*	7.02	8.94	7.39

*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 7.02 differs from the reported value 4.5 by more than 10 %

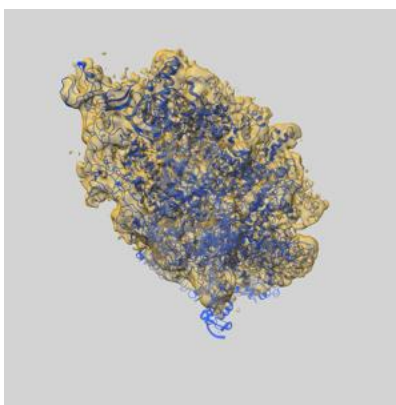
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34475 and PDB model 8H3V. Per-residue inclusion information can be found in section [3](#) on page [7](#).

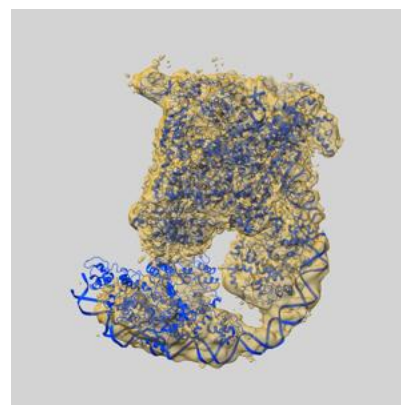
9.1 Map-model overlay [i](#)



X



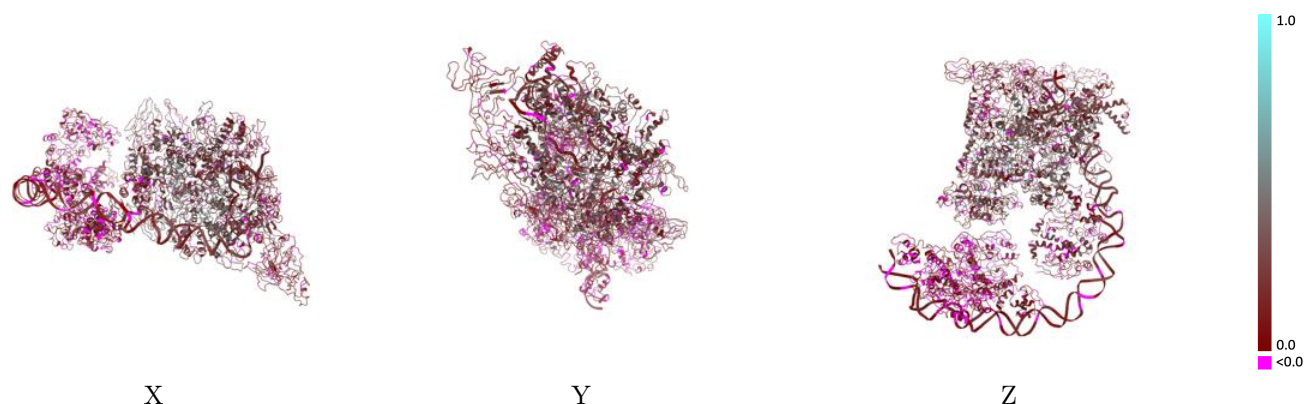
Y



Z

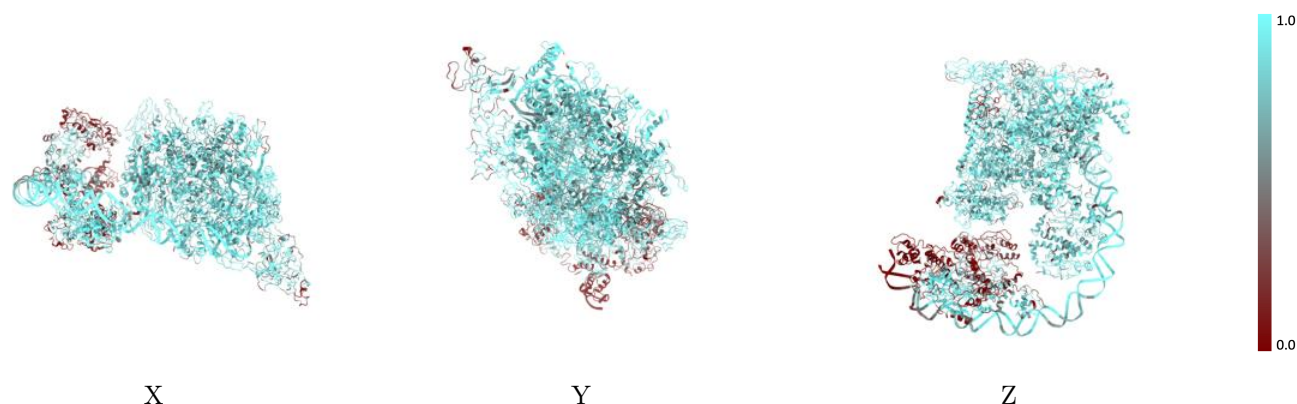
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



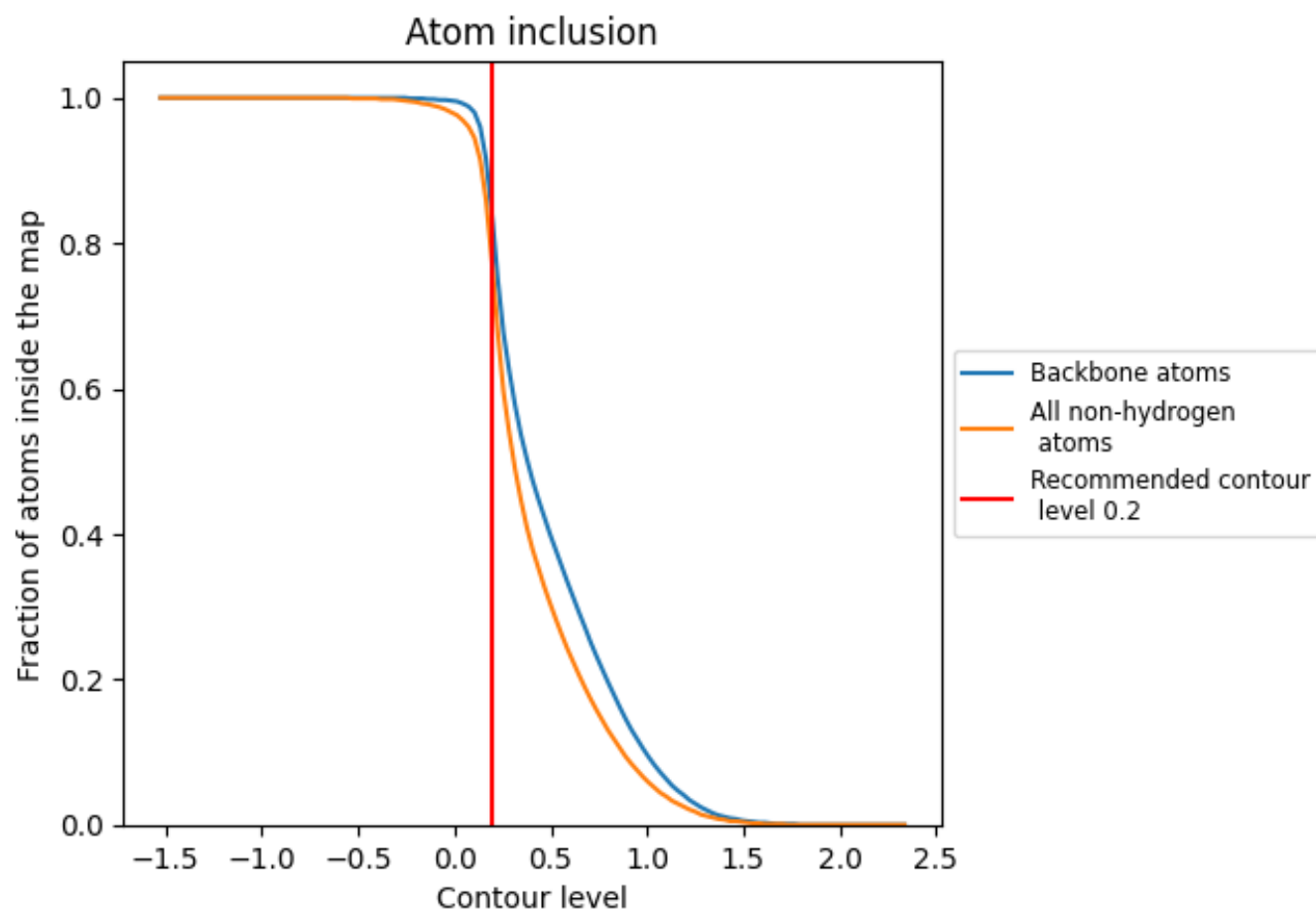
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.1910
1	 0.8030	 0.1340
2	 0.8250	 0.1340
A	 0.8860	 0.2980
B	 0.7750	 0.2000
C	 0.8500	 0.2680
D	 0.8140	 0.2280
E	 0.8430	 0.2770
F	 0.8900	 0.2890
G	 0.8680	 0.2280
S	 0.6310	 0.0590
T	 0.3480	 0.0470
U	 0.3660	 0.0520
V	 0.4850	 0.0670
X	 0.8740	 0.1290
Y	 0.8860	 0.1110

