



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2024 – 11:23 AM EST

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)

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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

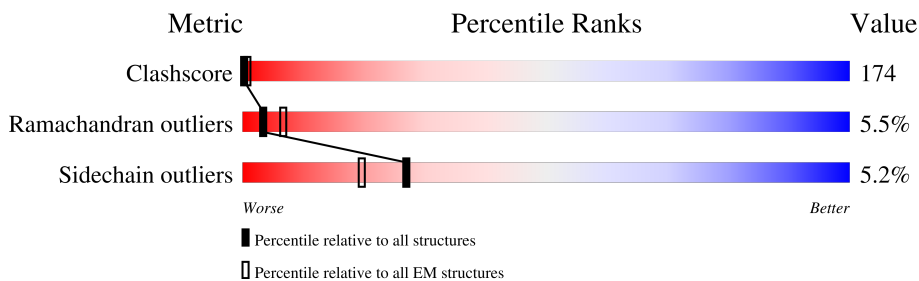
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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

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
			Total	C	N	O	P		
1	1	112	2302	1102	425	663	112	0	0

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

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

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

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

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
			Total	C	N	O	S		
4	B	1217	9292	5802	1639	1823	28	0	0

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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		

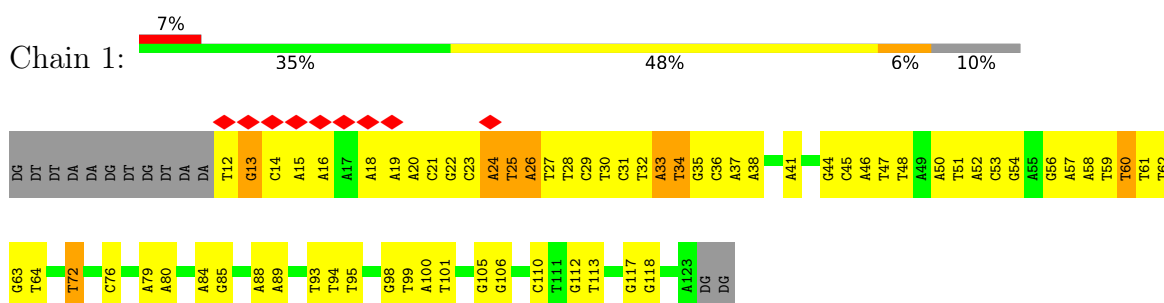
- Molecule 10 is a protein called NtcA.

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

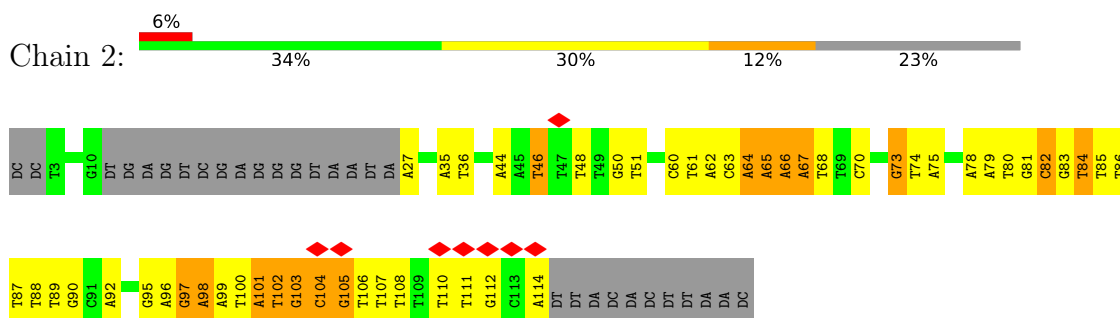
3 Residue-property plots [i](#)

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

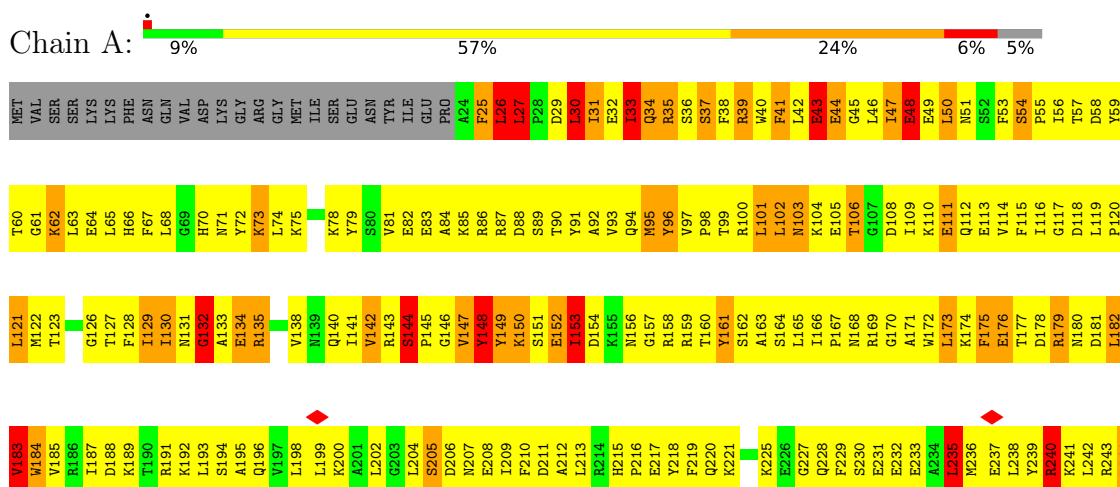
- Molecule 1: DNA (125-MER)



- Molecule 2: DNA (125-MER)

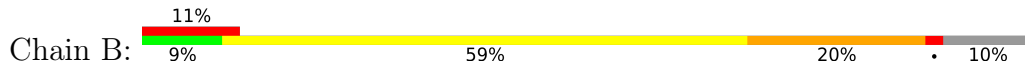


- Molecule 3: DNA-directed RNA polymerase subunit beta

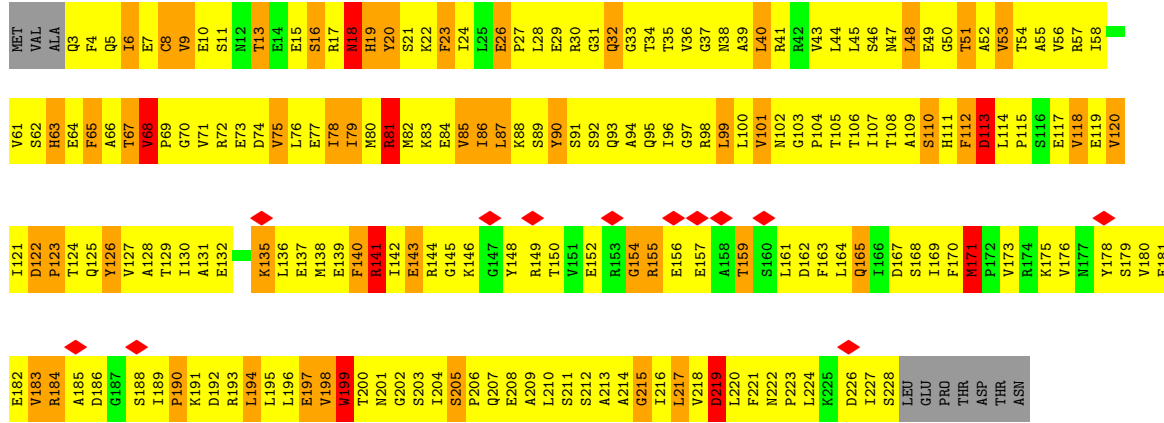


S1097	I1096	V976	K795	E735	T675	G612	N551	V490	R429	P369	I305	G245
D1098	V1100	A977	A796	I736	E676	Q613	R552	A491	I430	L370	N306	E246
V1100	GLU	P978	R797	T737	G677	L614	A553	P492	C431	V371	E308	P247
VAL	ASP	N979	D798	R738	G678	R615	L554	G493	A372	A373	E307	P248
ASP	LEU	L980	V799	E679	R680	T616	M555	I494	I434	D310	D310	T249
LEU	LEU	K981	R800	I740	L680	A617	G556	I495	G544	K375	L251	V250
LEU	LEU	L982	R802	P741	A681	S618	S557	P496	T435	E376	G252	L251
LEU	LEU	N983	S803	N742	L682	G619	M558	V497	P436	F377	G253	G252
LEU	LEU	H984	L804	G743	G683	K620	M559	F378	E437	D315	Q254	Q255
ALA	ALA	L985	R805	G744	Q684	T622	Q560	G379	F378	D315	Q255	Q255
ASP	ASP	R986	V806	E745	Q685	R621	R561	F379	F378	D318	L256	L256
ASP	GLN	P987	P807	G746	I686	G623	R562	G380	G379	H319	L257	L257
GLN	LEU	L988	R808	L747	V687	A563	A441	S381	S381	H319	L257	L257
LEU	ALA	E989	M808	L748	V688	V664	G442	Q382	Q382	L320	D258	D258
ALA	ALA	D990	G809	R749	A689	P665	L443	L383	L383	R323	S259	S259
ARG	ARG	R991	E810	Q750	Y690	T628	I444	S384	S384	R323	R260	R260
ARG	ARG	L992	R811	L566	S629	S629	L566	Q385	Q385	R323	R261	R261
THR	THR	R993	G812	D752	M691	Q630	L567	Q385	Q385	R323	R261	R261
PRO	PRO	A994	R813	R692	P692	K631	K568	Q507	S446	V325	V325	F262
PRO	PRO	T995	V814	G754	M693	G632	L447	V508	L447	M387	D263	D263
ARG	ARG	V996	V815	G755	E694	R633	A448	P509	A448	D388	P264	P264
PRO	PRO	F997	D816	I756	Y696	E634	T449	V510	T449	Q389	K265	K265
THR	THR	Y998	V817	I757	M697	L573	H450	R390	H450	T390	R266	R266
TYR	TYR	R999	R818	R758	Y698	V574	A451	E330	A451	E330	Y267	Y267
GLU	GLU	L1000	L819	I759	Y699	G575	R452	L331	R452	L331	D268	D268
SER	SER	V1001	F820	G760	D700	T576	V453	L332	L332	L332	L269	L269
LEU	LEU	L1002	T821	A761	A701	S640	Y456	A394	A394	A394	G270	G270
SER	SER	Q1003	R822	R762	I702	G641	G457	E395	E395	N334	R271	R271
ARG	ARG	Q1004	E823	L763	L703	Y642	F458	L396	L396	Q335	V272	V272
GLU	GLU	P1005	R824	G764	A580	Q643	L459	T397	T397	Q336	G273	G273
SER	SER	L1006	G825	A765	S705	R644	E460	H398	H398	R337	R274	R274
LEU	LEU	W947	D826	G766	E706	S645	T461	K399	K399	P521	Y275	Y275
ASP	ASP	V948	E827	D767	R707	G646	P462	R400	R400	L340	K276	K276
ASP	ASP	Y949	R828	L768	L708	D648	F463	R401	R401	R342	L277	L277
ASP	ASP	N950	R829	R769	V709	T649	R464	L402	L402	R343	N278	N278
GLU	GLU	P951	P830	V770	Q710	C650	A465	S403	S403	E344	K280	K280
GLU	GLU	D952	G831	G771	D711	L651	V466	A404	A404	R405	K281	K281
ALA	ALA	D953	A832	K772	L713	M652	E467	L405	L405	R345	E282	E282
ALA	ALA	P954	M834	V773	I713	Q653	M468	G406	G406	I346	E282	E282
ALA	ALA	G955	V835	P774	T714	I590	G469	P407	P407	I347	L283	L283
LEU	LEU	K956	V836	P775	T715	K654	R470	G408	G408	R348	S284	S284
LEU	LEU	L957	R837	G776	S716	P655	R471	G409	G409	E349	V285	V285
LEU	LEU	M958	R838	G777	I717	G657	R472	L410	L410	R350	P286	P286
LEU	LEU	E959	Y839	V778	H718	R658	F473	T411	T411	M351	D287	D287
PRO	PRO	M1020	R840	G779	I719	V529	G474	R412	R412	T352	T288	T288
PRO	PRO	Y960	V841	L774	E659	I590	Q475	E413	E413	V353	V289	V289
PRO	PRO	D961	R842	G781	D721	E661	Q475	R414	R414	S354	R290	R290
PRO	PRO	G962	K843	P782	K721	R662	A476	G416	G416	D355	V291	V291
PRO	PRO	T964	R844	R783	E723	V663	A477	A356	A356	L292	L292	L292
PRO	PRO	G965	K845	E784	E724	V664	A478	F417	F417	E357	T293	T293
PRO	PRO	E966	L846	R785	E725	A665	Y479	A418	A418	V358	S284	S284
PRO	PRO	E967	R847	K786	A666	M541	T481	L359	L359	L358	G295	G295
PRO	PRO	F968	Q847	L787	G666	I542	T481	T360	T360	T360	D296	D296
PRO	PRO	G969	R848	R788	Q667	P543	A482	P361	P361	P361	I297	I297
PRO	PRO	R970	D850	L789	V668	F544	D483	I422	I422	A362	L298	L298
PRO	PRO	R971	L910	R789	L669	L545	E484	H293	H293	A299	A300	A300
PRO	PRO	P972	K851	A790	A670	E546	E485	P424	P424	L364	A300	A300
PRO	PRO	V973	M852	I791	L731	H547	D486	S425	S425	V365	V301	V301
PRO	PRO	T974	R853	G792	G672	D548	D487	H426	H426	N366	B302	B302
PRO	PRO	I975	G854	G793	S673	V610	L488	Y427	Y427	Y303	Y303	Y303
PRO	PRO	G975	R855	E794	S674	S611	R489	G428	G428	K368	L304	L304

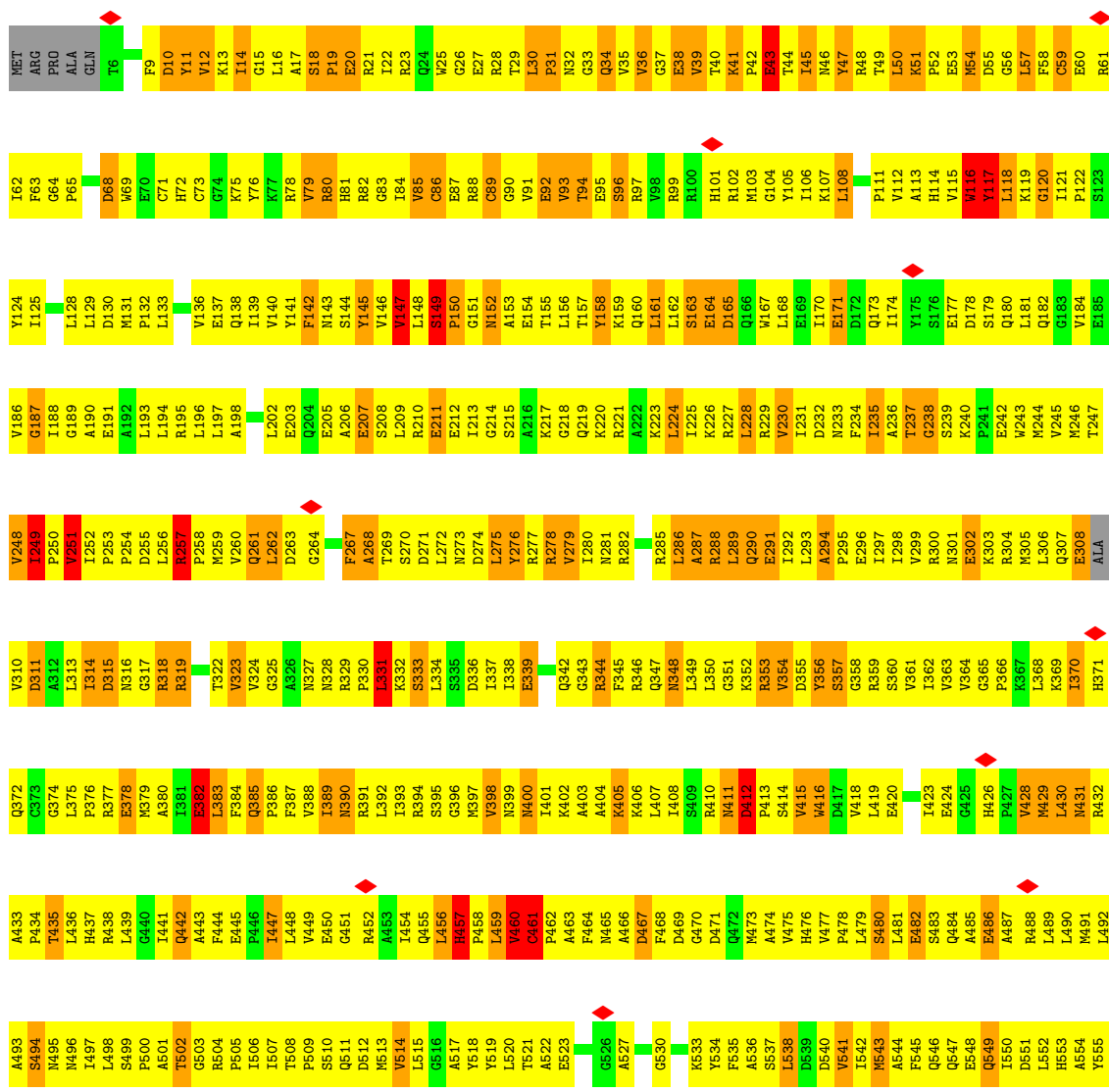
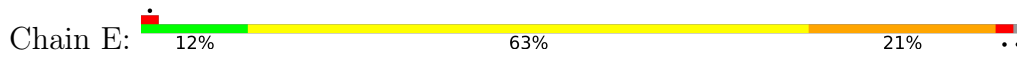
● Molecule 4: DNA-directed RNA polymerase subunit beta'

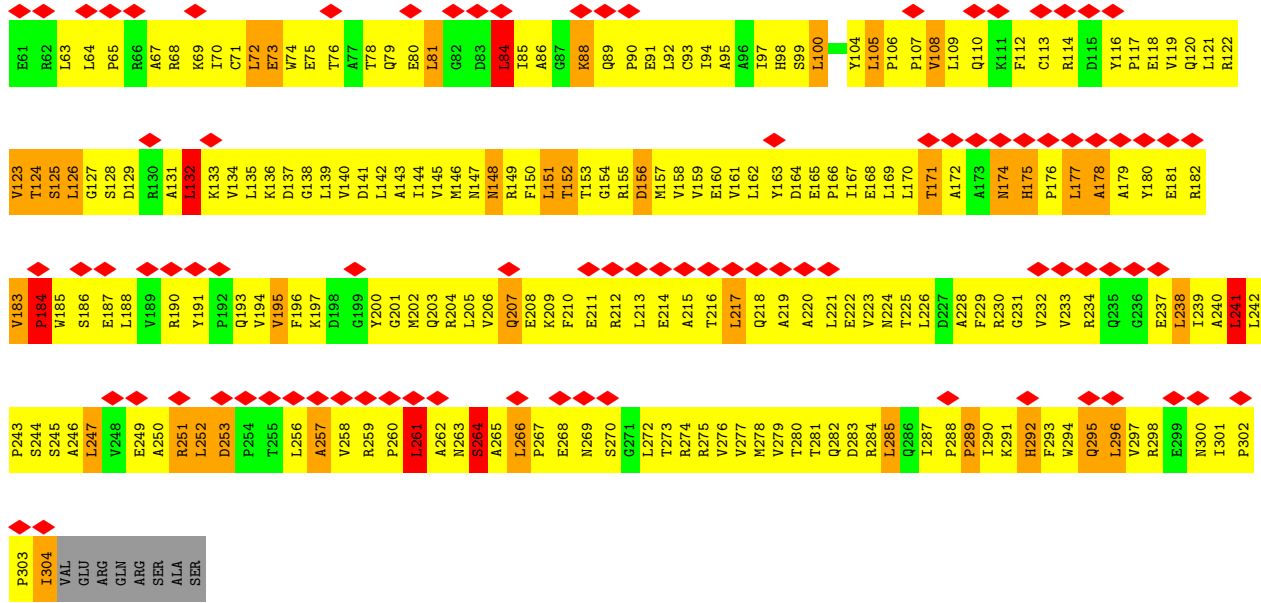


M1	S81	S121	L183	V243	A304	R364	L424	S484	V545	K605	F665	Q726	G787
I2	K62	V122	V184	V244	H905	T365	A425	G485	L546	F606	C666	Y727	V788
F3	R63	Y123	V186	G245	A306	R366	E426	E486	O547	A607	G667	W728	E789
R4	S64	M124	T186	E246	K307	R367	V427	V487	O548	V609	N668	E729	L790
N5	L65	M125	A187	D247	K308	T367	A428	Y488	A549	V609	S669	S730	L791
R6	L66	A126	L188	V248	V309	H368	L429	N489	T550	E610	G670	W731	R792
V7	E67	F127	R189	T249	D310	H369	L429	L490	V551	V611	V671	W732	T793
V8	A68	F128	T190	H250	L311	T370	GLY	L491	V552	Q612	W672	E733	Q794
D9	A69	G129	A191	H251	G312	H371	ARG	P491	V553	Q612	W673	G734	L795
G10	E70	A130	D192	K252	E313	R372	THR	A494	O554	K613	W674	P734	V796
G11	E71	G130	G194	R253	A314	H373	THR	E495	S555	K614	T675	A735	L797
Q12	E72	M133	G194	K254	V315	G374	ARG	L496	S556	G615	Q676	L736	E798
Q13	E73	L134	L196	E255	G316	D375	THR	V497	S557	G616	K677	L737	L799
R14	N74	S135	L196	V256	I317	A376	A437	V498	S558	R599	K678	S738	E800
N15	A75	Q136	T197	I257	I318	L377	T438	A499	R599	L618	N679	R739	Q801
L16	T76	Q137	R198	A258	A319	F378	E439	N500	N560	L619	L680	P740	Q802
L17	E77	Q138	R199	P259	A320	V379	E440	O501	N561	L620	L681	W741	Q803
S18	V78	Q139	L200	R260	Q321	V379	K440	D502	V562	L621	R682	W742	E804
S19	V78	Q140	L200	R260	Q322	V379	K440	D503	L563	E622	R683	W743	E805
A20	R80	V141	V201	N261	Q323	E380	V442	R504	L564	E623	R684	W744	E806
F21	Q81	G142	V203	P263	I323	S381	K443	E505	T565	V624	V685	A745	E807
R22	R82	M143	S204	I264	E324	E382	D444	E506	T566	V625	V686	W746	E808
T22	G83	R144	Q205	S265	E325	N382	V445	N507	G567	G626	K687	W747	E809
H23	G83	R144	Q205	S265	E325	N382	V445	N507	G567	G627	K688	W748	E810
Y24	E84	G145	D206	D267	P326	G383	A446	O508	N568	T628	P689	W749	P811
G25	E85	L146	V207	D267	G327	I384	S447	V509	N569	L629	L690	W750	P812
T26	T86	M147	L208	L268	T328	I385	D448	L510	O570	L630	L691	W751	A813
A27	E87	M148	L208	A269	Q329	K385	L449	L511	V571	L631	L692	W752	A814
R28	V88	A149	I209	R270	T330	I386	A450	E512	V572	L632	W753	W753	A815
T29	E89	P150	R210	K270	T331	L387	K451	T513	N573	P633	W754	W754	B816
R30	R90	Q151	E89	E271	M332	E388	E452	K514	L574	P634	W755	W755	B817
A30	R90	Q151	E89	E271	M332	E388	E453	L515	R575	E634	W756	W756	B818
V31	F91	G152	I212	L272	Q322	P389	K454	L516	T576	E635	W757	W757	B819
M32	F91	G152	I212	L272	Q322	P389	K454	L516	T577	E636	W758	W758	P820
K33	Q92	E153	D213	K274	Q322	P389	K455	L517	R578	E637	W759	W759	D821
A34	Q92	E154	D213	K274	Q322	P389	K455	L517	R579	E638	W760	W760	L822
M35	K93	E155	D216	K275	Q322	P389	K456	L518	T579	E639	W761	W761	E823
D34	I95	I155	T217	V277	Q322	P389	K457	L519	R580	E640	W762	W762	D824
K35	I95	I155	T217	V277	Q322	P389	K457	L519	R581	E641	W763	W763	A825
L36	D96	L156	T217	A278	Q322	P389	K458	L520	R582	E642	W764	W764	D826
L37	D96	L156	T217	A278	Q322	P389	K458	L520	R583	E643	W765	W765	R827
D38	K98	L157	R219	E279	Q322	P389	K459	L521	R584	E644	W766	W766	Q828
L39	M99	P158	I220	V280	Q322	P389	K460	L522	R585	E645	W767	W767	R829
L39	M99	P158	I220	V280	Q322	P389	K460	L522	R586	E646	W768	W768	L830
G40	G100	K160	P221	V281	Q322	P389	K461	L523	R587	E647	W769	W769	Q831
F41	T101	M161	V222	V282	Q322	P389	K462	L524	R588	E648	W770	W770	L832
R42	S102	M162	V222	V282	Q322	P389	K463	L525	R589	E649	W771	W771	R833
Y43	E103	E163	R223	R283	Q322	P389	K464	L526	R590	E650	W772	W772	L834
A44	A104	R164	R224	R284	Q322	P389	K465	L527	R591	E651	W773	W773	L835
T45	L105	E165	R224	R284	Q322	P389	K466	L528	R592	E652	W774	W774	F836
R46	K106	E166	R224	R284	Q322	P389	K467	L529	R593	E653	W775	W775	S837
D107	D107	L167	R224	R284	Q322	P389	K468	L530	R594	E654	W776	W776	L838
E108	E108	T168	R224	R284	Q322	P389	K469	L531	R595	E655	W777	W777	R839
C48	C48	V169	R224	R284	Q322	P389	K470	L532	R596	E656	W778	W778	L840
V49	V109	V169	R224	R284	Q322	P389	K471	L533	R597	E657	W779	W779	R841
S50	V110	T170	R224	R284	Q322	P389	K472	L534	R598	E658	W780	W780	R842
S51	V111	E171	R224	R284	Q322	P389	K473	L535	R599	E659	W781	W781	D843
S52	H112	I172	R224	R284	Q322	P389	K474	L536	R600	E660	W782	W782	R844
S53	H113	I173	R224	R284	Q322	P389	K475	L537	R601	E661	W783	W783	A845
S54	H114	I174	R224	R284	Q322	P389	K476	L538	R602	E662	W784	W784	A846
D55	K114	D84	R224	R284	Q322	P389	K477	L539	R603	E663	W785	W785	A846
D55	K114	D84	R224	R284	Q322	P389	K477	L539	R603	E663	W785	W785	A846
L56	Q115	Y177	R224	R284	Q322	P389	K478	L540	R604	E664	W786	W786	A846
L56	Q115	Y177	R224	R284	Q322	P389	K478	L540	R604	E664	W786	W786	A846
M57	M117	G178	R224	R284	Q322	P389	K479	L541	R605	E665	W787	W787	A846
P58	P118	A179	R224	R284	Q322	P389	K480	L542	R606	E666	W788	W788	A846
P59	P118	A179	R224	R284	Q322	P389	K481	L543	R607	E667	W789	W789	A846
P60	P118	A179	R224	R284	Q322	P389	K482	L544	R608	E668	W790	W790	A846
P60	P118	A179	R224	R284	Q322	P389	K483	L545	R609	E669	W791	W791	A846
P60	P118	A179	R224	R284	Q322	P389	K484	L546	R610	E670	W792	W792	A846
P60	P118	A179	R224	R284	Q322	P389	K485	L547	R611	E671	W793	W793	A846
P60	P118	A179	R224	R284	Q322	P389	K486	L548	R612	E672	W794	W794	A846
P60	P118	A179	R224	R284	Q322	P389	K487	L549	R613	E673	W795	W795	A846
P60	P118	A179	R224	R284	Q322	P389	K488	L550	R614	E674	W796	W796	A846
P60	P118	A179	R224	R284	Q322	P389	K489	L551	R615	E675	W797	W797	A846
P60	P118	A179	R224	R284	Q322	P389	K490	L552	R616	E676	W798	W798	A846
P60	P118	A179	R224	R284	Q322	P389	K491	L553	R617	E677	W799	W799	A846
P60	P118	A179	R224	R284	Q322	P389	K492	L554	R618	E678	W800	W800	A846
P60	P118	A179	R224	R284	Q322	P389	K493	L555	R619	E679	W801	W801	A846
P60	P118	A179	R224	R284	Q322	P389	K494	L556	R620	E680	W802	W802	A846
P60	P118	A179	R224	R284	Q322	P389	K495	L557	R621	E681	W803	W803	A846
P60	P118	A179	R224	R284	Q322	P389	K496	L558	R622	E682	W804	W804	A846
P60	P118	A179	R224	R284	Q322	P389	K497	L559	R623	E683	W805	W805	A846
P60	P118	A179	R224	R284	Q322	P389	K498	L560	R624	E684	W806	W806	A846
P60	P118	A179	R224	R284	Q322	P389	K499	L561	R625	E685	W807	W807	A846
P60	P118	A179	R224	R284	Q322	P389	K500	L562	R626	E686	W808	W808	A846
P60	P118	A179	R224	R284	Q322	P389	K501	L563	R627	E687	W809	W809	A846
P60	P118	A179	R224	R284	Q322	P389	K502	L564	R628	E688	W810	W810	A846
P60	P118	A179	R224	R284	Q322	P389	K503	L565	R629	E689	W811	W811	A846
P60	P118	A179	R224	R284	Q322	P389	K504	L566	R630	E690	W812	W812	A846
P60	P118	A179	R224	R284	Q322	P389	K505	L567	R631	E691	W813	W813	A846
P60	P118	A179	R224	R284	Q322	P389	K506	L568	R632	E692	W814	W814	A846
P60	P118	A179	R224	R284	Q322	P389	K507	L569	R633	E693	W815	W815	A846
P60	P118	A179	R224	R284	Q322	P389	K508	L570	R634	E694	W816	W816	A846
P60	P118	A179	R224	R284	Q322	P389	K509	L571	R635	E695	W817	W817	A846
P60	P118	A179	R224	R284	Q322	P389	K510	L572	R636	E696	W818	W818	A846
P60	P118	A179	R224	R284	Q322	P389	K511	L573	R637	E697	W819	W819	A846
P60	P118	A179	R224	R284	Q322	P389	K512	L574	R638	E698	W820	W820	A846
P60	P118	A179	R224	R284	Q322	P389	K513	L575	R639	E699	W821	W821	A846
P60	P118	A179	R224	R284	Q322	P389	K514	L576	R640	E700	W822	W822	A846
P60	P118	A179	R224	R284	Q322	P389	K515	L577	R641	E701	W823	W823	A846
P60	P118	A179	R224	R284	Q322	P389	K516	L578	R642	E702	W824	W824	A846
P60	P118	A179	R224	R284	Q322	P389	K517	L579	R643	E703	W82		

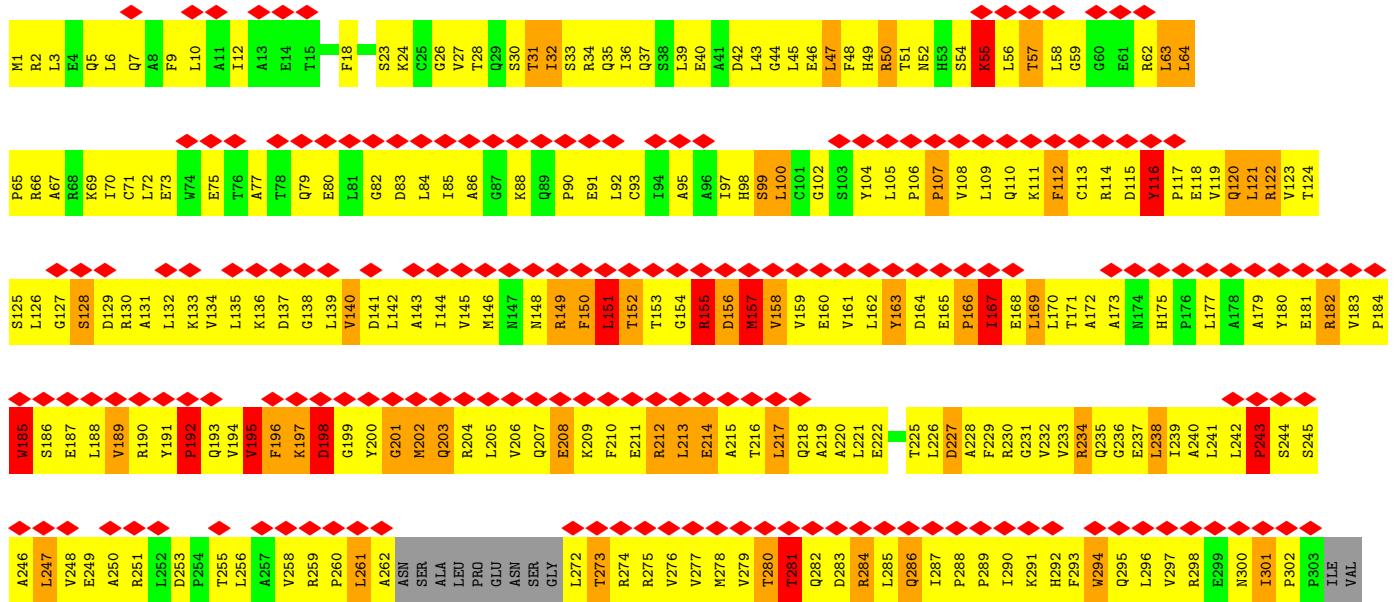
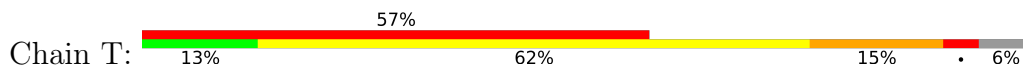


● Molecule 6: DNA-directed RNA polymerase subunit gamma

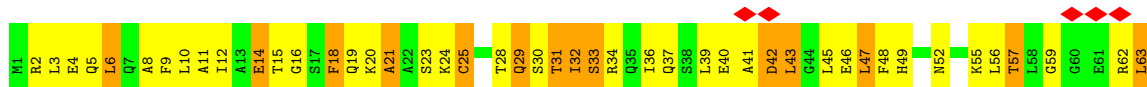
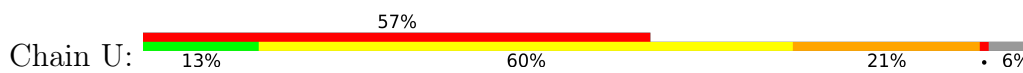


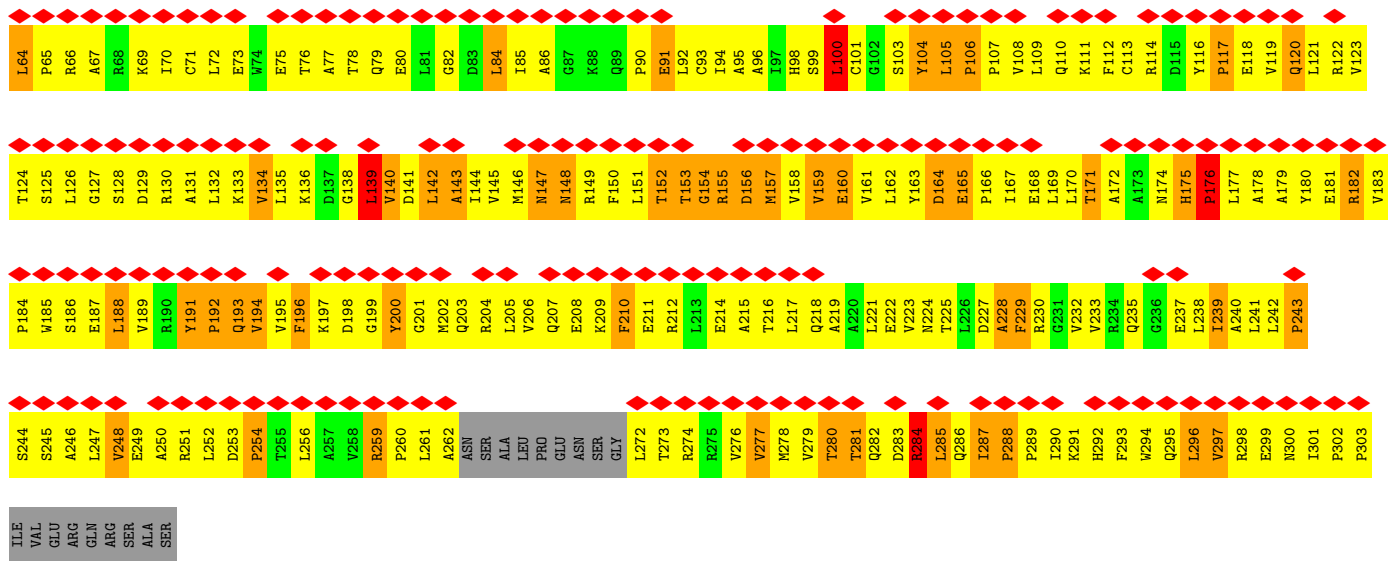


• Molecule 9: NtcB

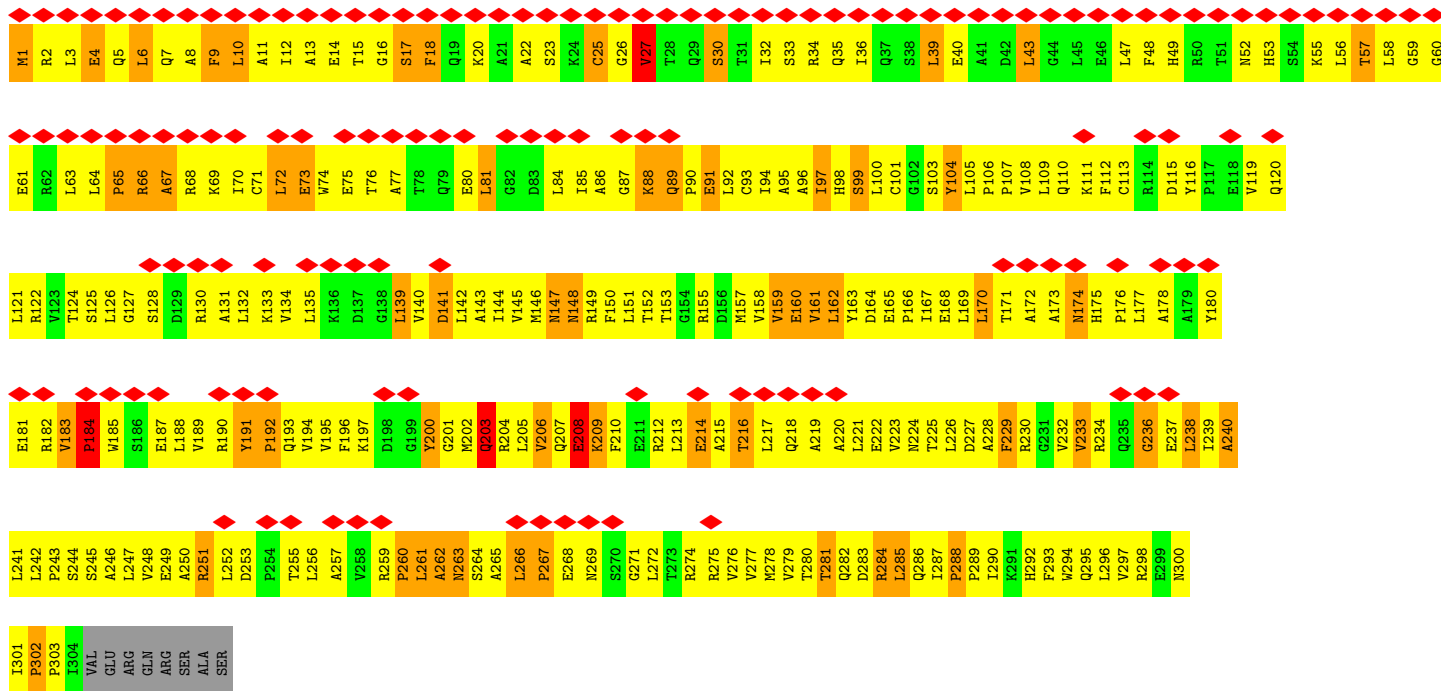
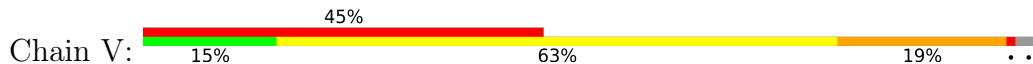


• Molecule 9: NtcB

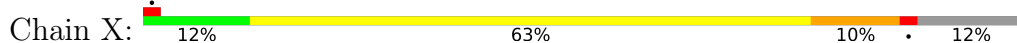


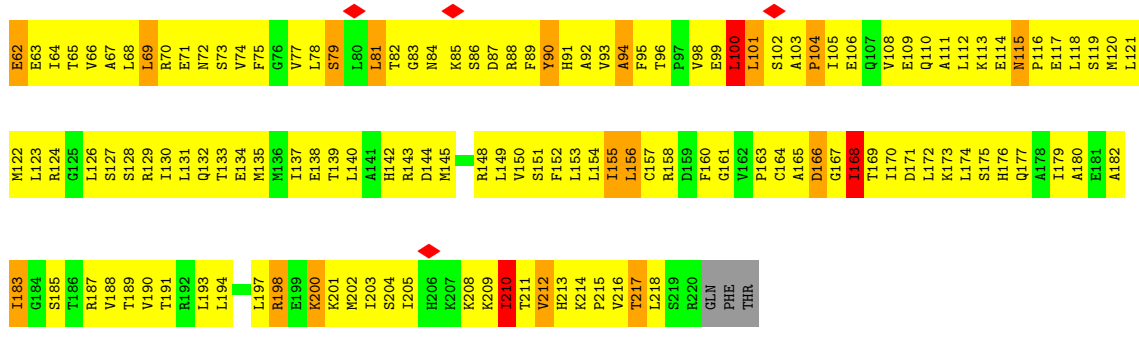


• Molecule 9: NtcB

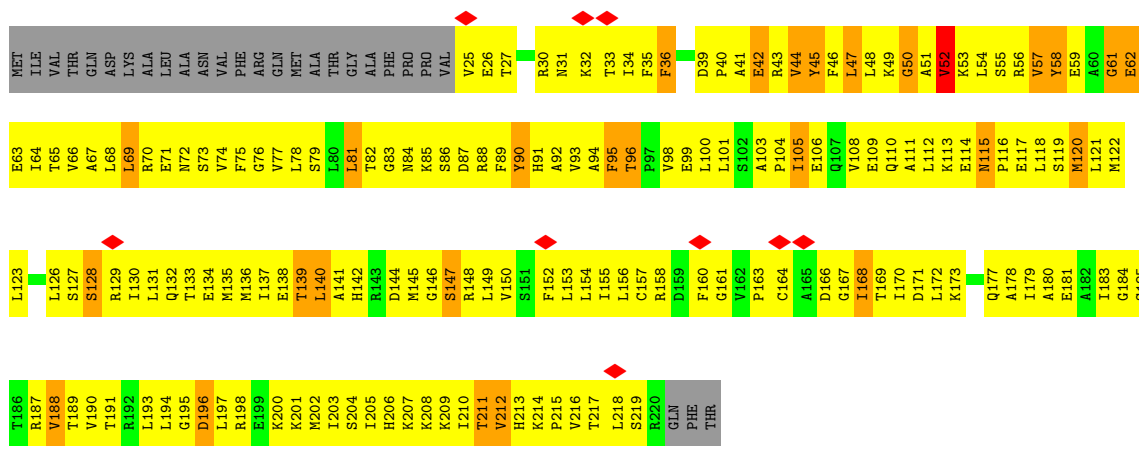
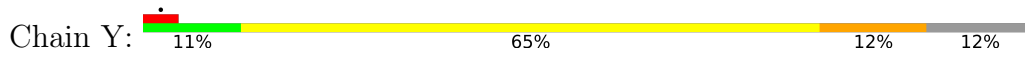


• Molecule 10: NtcA





• 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 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	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 [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	A	1075/1132 (95%)	613 (57%)	417 (39%)	45 (4%)	3	25
4	B	1209/1350 (90%)	693 (57%)	451 (37%)	65 (5%)	2	22
5	C	224/236 (95%)	131 (58%)	79 (35%)	14 (6%)	1	19
5	D	224/236 (95%)	131 (58%)	79 (35%)	14 (6%)	1	19
6	E	617/625 (99%)	395 (64%)	193 (31%)	29 (5%)	2	24
7	F	56/78 (72%)	38 (68%)	17 (30%)	1 (2%)	8	42
8	G	312/390 (80%)	204 (65%)	94 (30%)	14 (4%)	2	24
9	S	302/312 (97%)	207 (68%)	83 (28%)	12 (4%)	3	26
9	T	290/312 (93%)	196 (68%)	74 (26%)	20 (7%)	1	17
9	U	290/312 (93%)	175 (60%)	87 (30%)	28 (10%)	0	11
9	V	302/312 (97%)	193 (64%)	80 (26%)	29 (10%)	0	11
10	X	194/223 (87%)	121 (62%)	61 (31%)	12 (6%)	1	19
10	Y	194/223 (87%)	113 (58%)	73 (38%)	8 (4%)	3	25
All	All	5289/5741 (92%)	3210 (61%)	1788 (34%)	291 (6%)	3	21

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 [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	A	918/969 (95%)	887 (97%)	31 (3%)	37	61
4	B	1017/1132 (90%)	975 (96%)	42 (4%)	30	56
5	C	196/205 (96%)	187 (95%)	9 (5%)	27	53
5	D	196/205 (96%)	184 (94%)	12 (6%)	18	46
6	E	534/538 (99%)	500 (94%)	34 (6%)	17	44
7	F	50/69 (72%)	49 (98%)	1 (2%)	55	73
8	G	282/351 (80%)	267 (95%)	15 (5%)	22	49
9	S	261/268 (97%)	237 (91%)	24 (9%)	9	31
9	T	253/268 (94%)	233 (92%)	20 (8%)	12	38
9	U	253/268 (94%)	231 (91%)	22 (9%)	10	34
9	V	261/268 (97%)	245 (94%)	16 (6%)	18	46
10	X	172/194 (89%)	164 (95%)	8 (5%)	26	52
10	Y	172/194 (89%)	167 (97%)	5 (3%)	42	64
All	All	4565/4929 (93%)	4326 (95%)	239 (5%)	27	50

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 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](#)

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

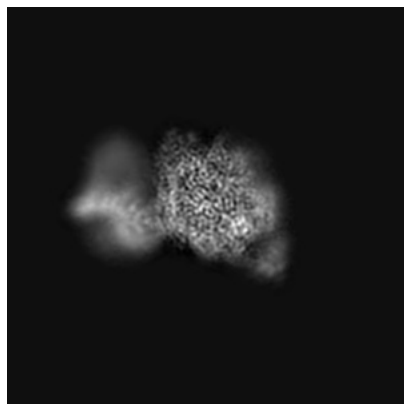
6 Map visualisation [i](#)

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.

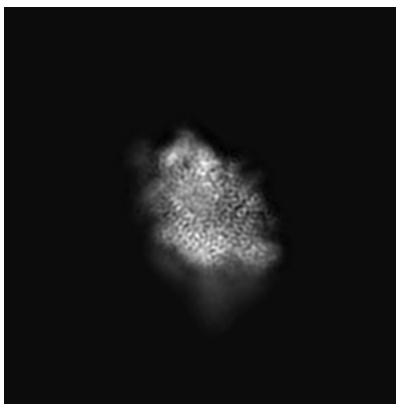
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

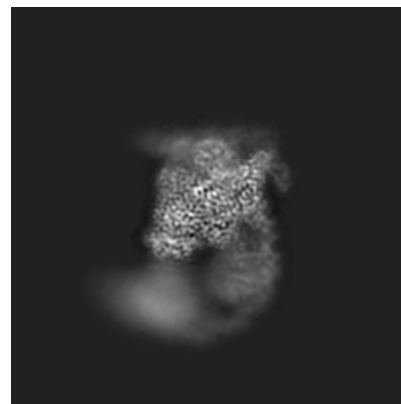
6.1.1 Primary map



X

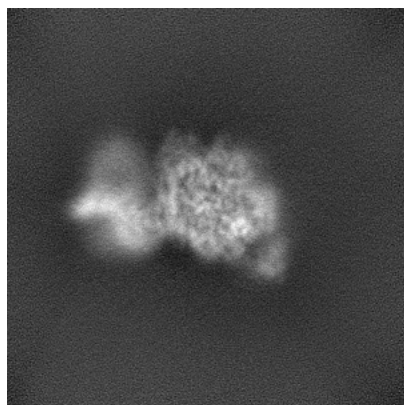


Y

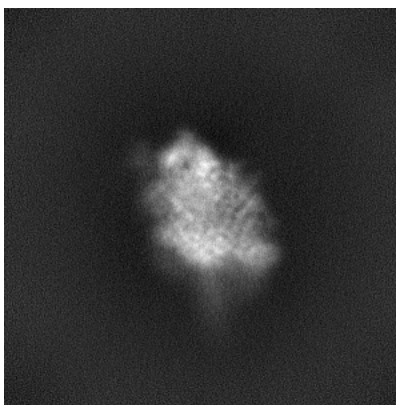


Z

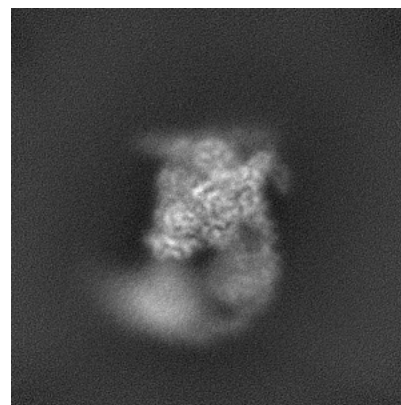
6.1.2 Raw map



X



Y

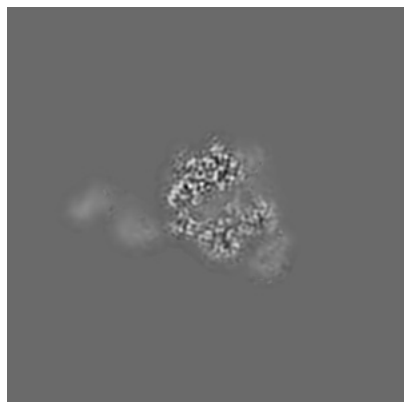


Z

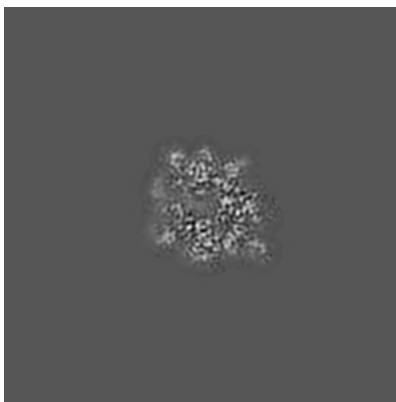
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

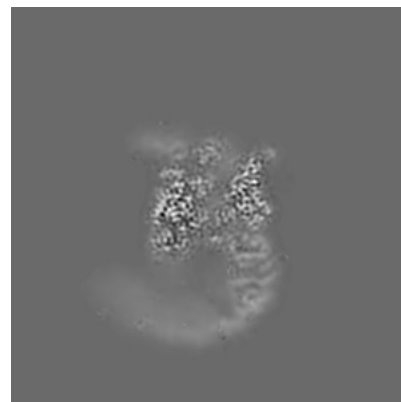
6.2.1 Primary map



X Index: 175

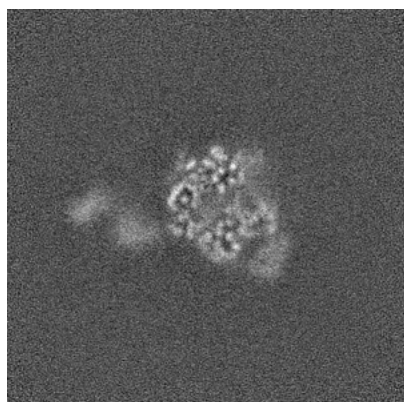


Y Index: 175

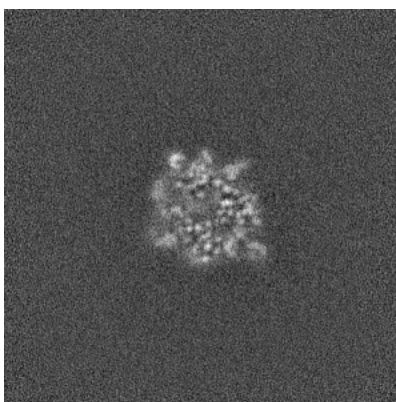


Z Index: 175

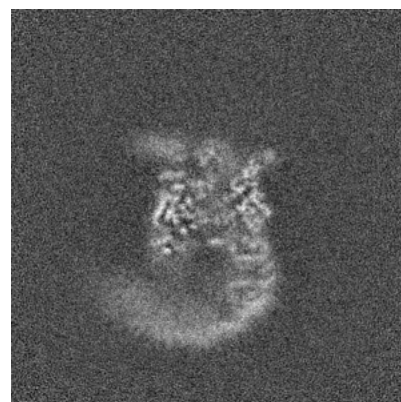
6.2.2 Raw map



X Index: 175



Y Index: 175

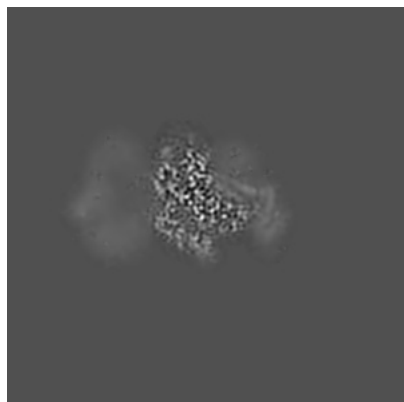


Z Index: 175

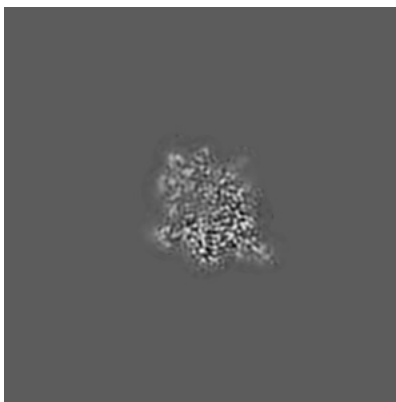
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

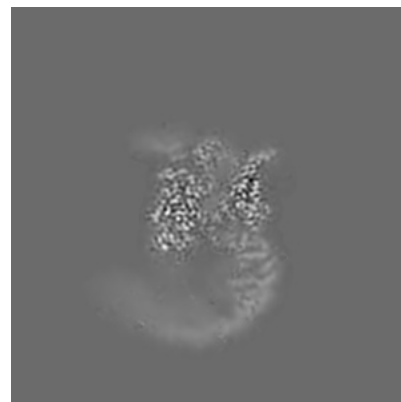
6.3.1 Primary map



X Index: 145

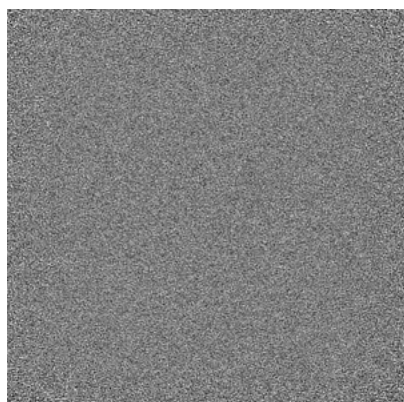


Y Index: 169

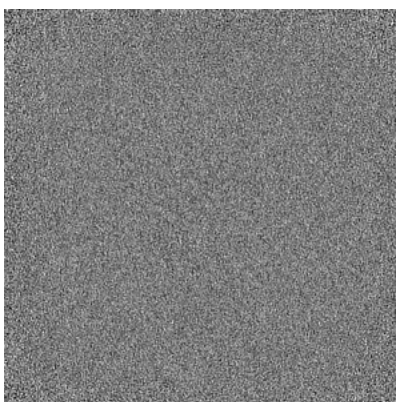


Z Index: 173

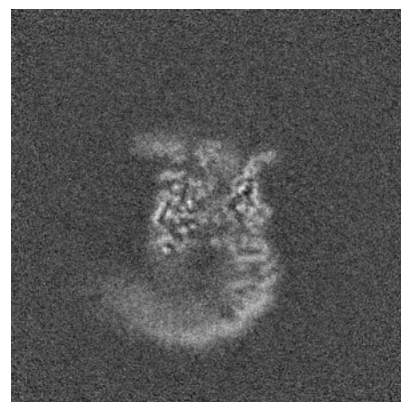
6.3.2 Raw map



X Index: 0



Y Index: 0

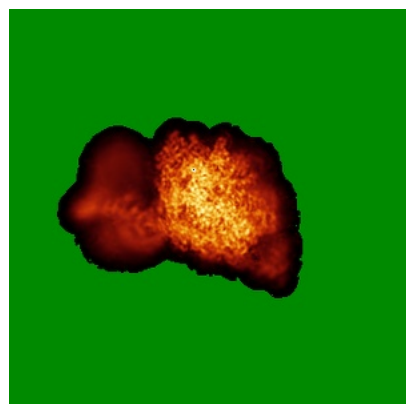


Z Index: 174

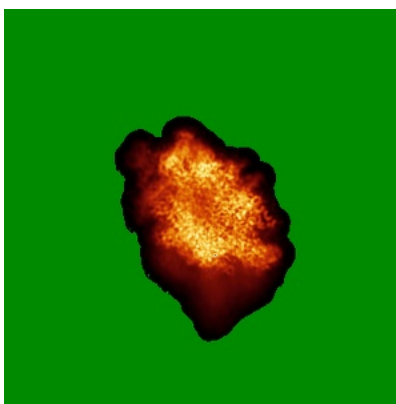
The images above show the largest variance slices of the map in three orthogonal directions.

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

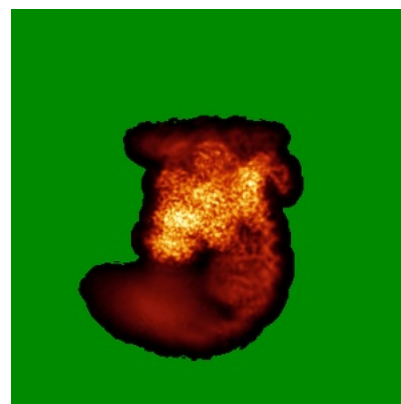
6.4.1 Primary map



X

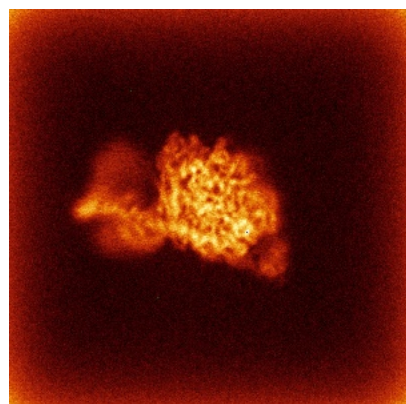


Y

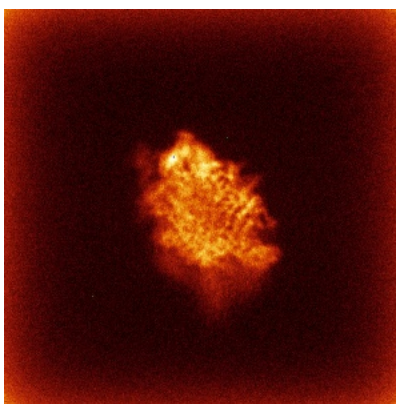


Z

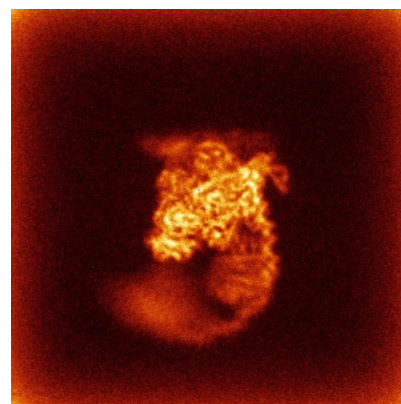
6.4.2 Raw map



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.

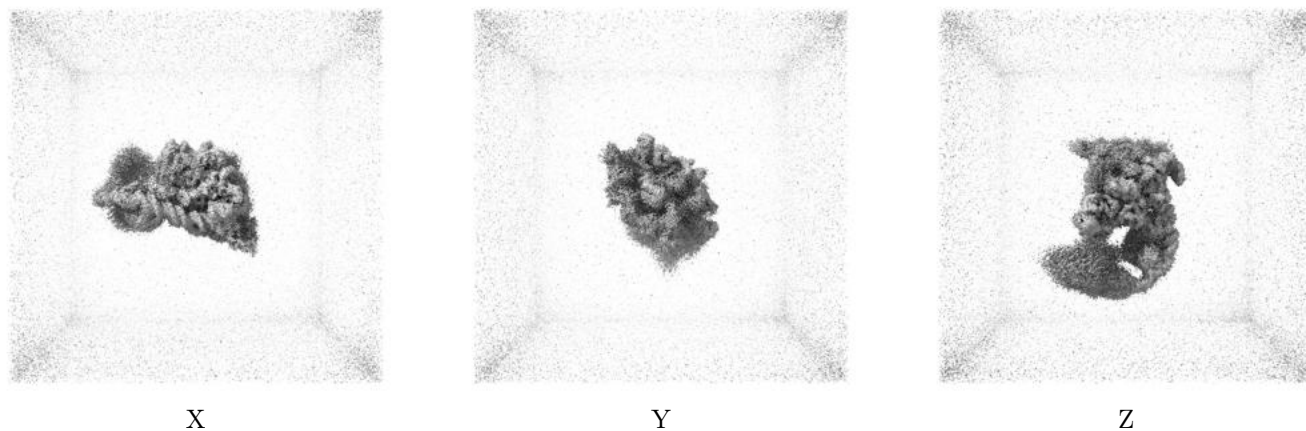
6.5 Orthogonal surface views [i](#)

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.

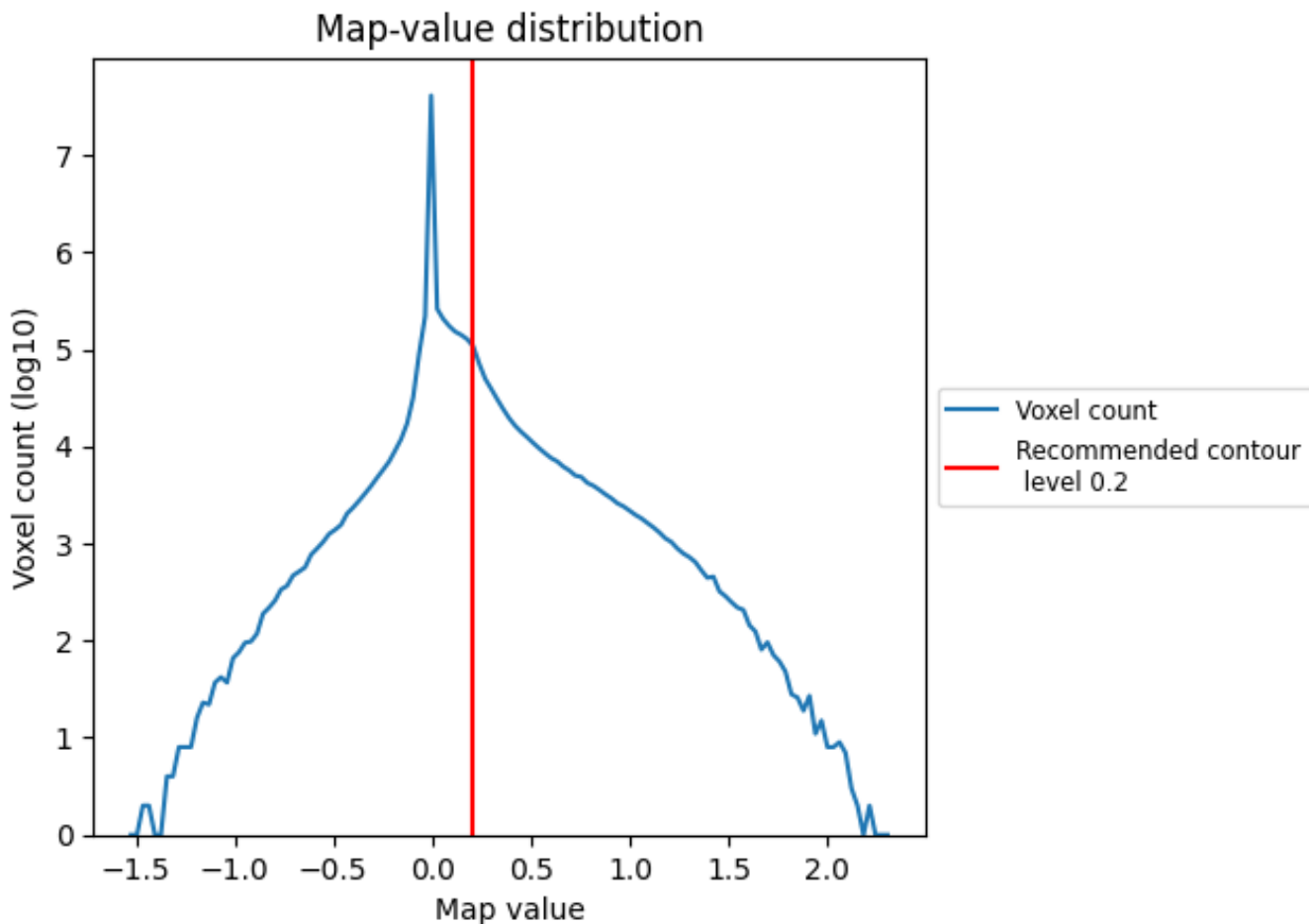
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

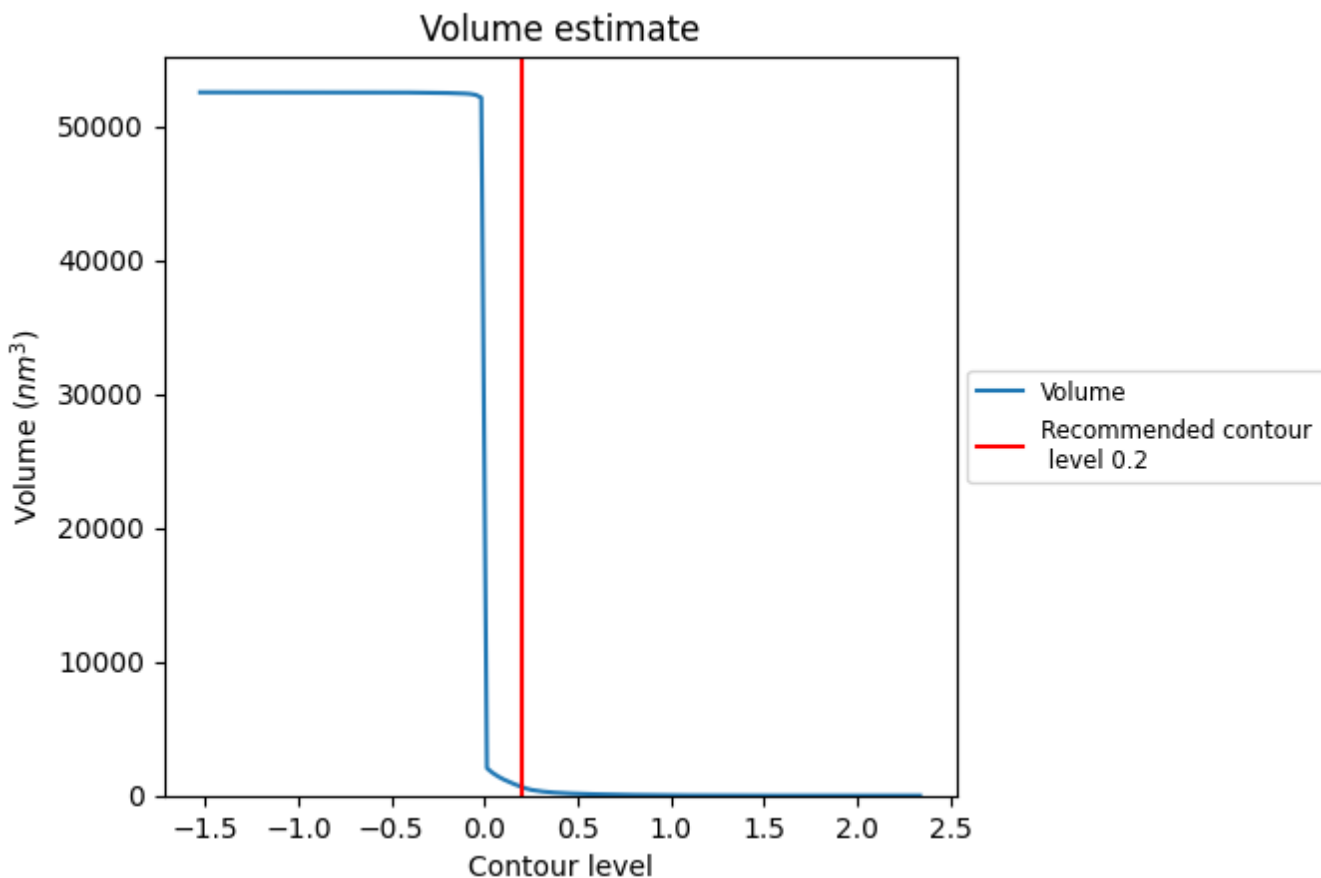
This section contains the results of statistical analysis of the map.

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.

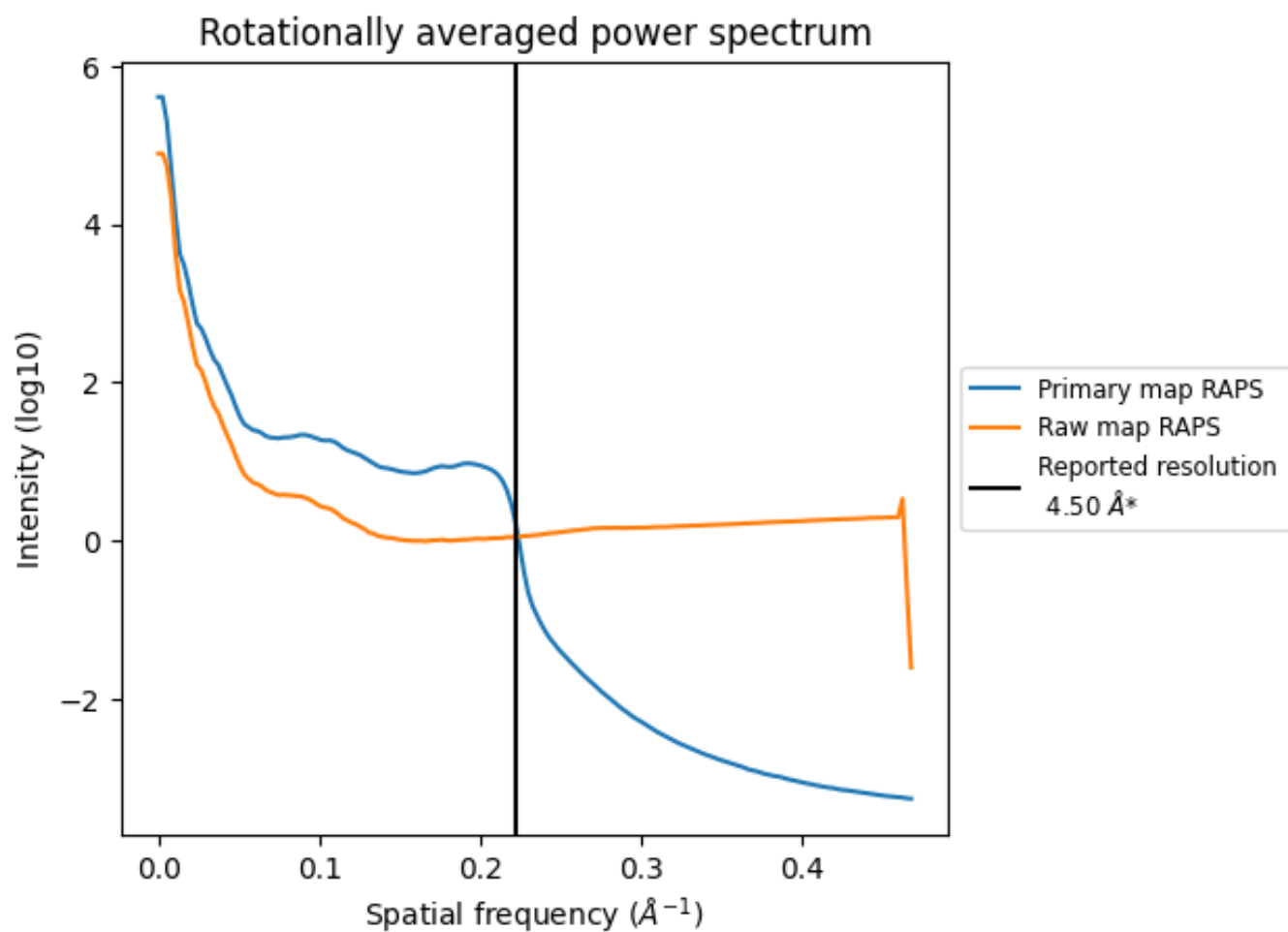
7.2 Volume estimate [i](#)



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 i

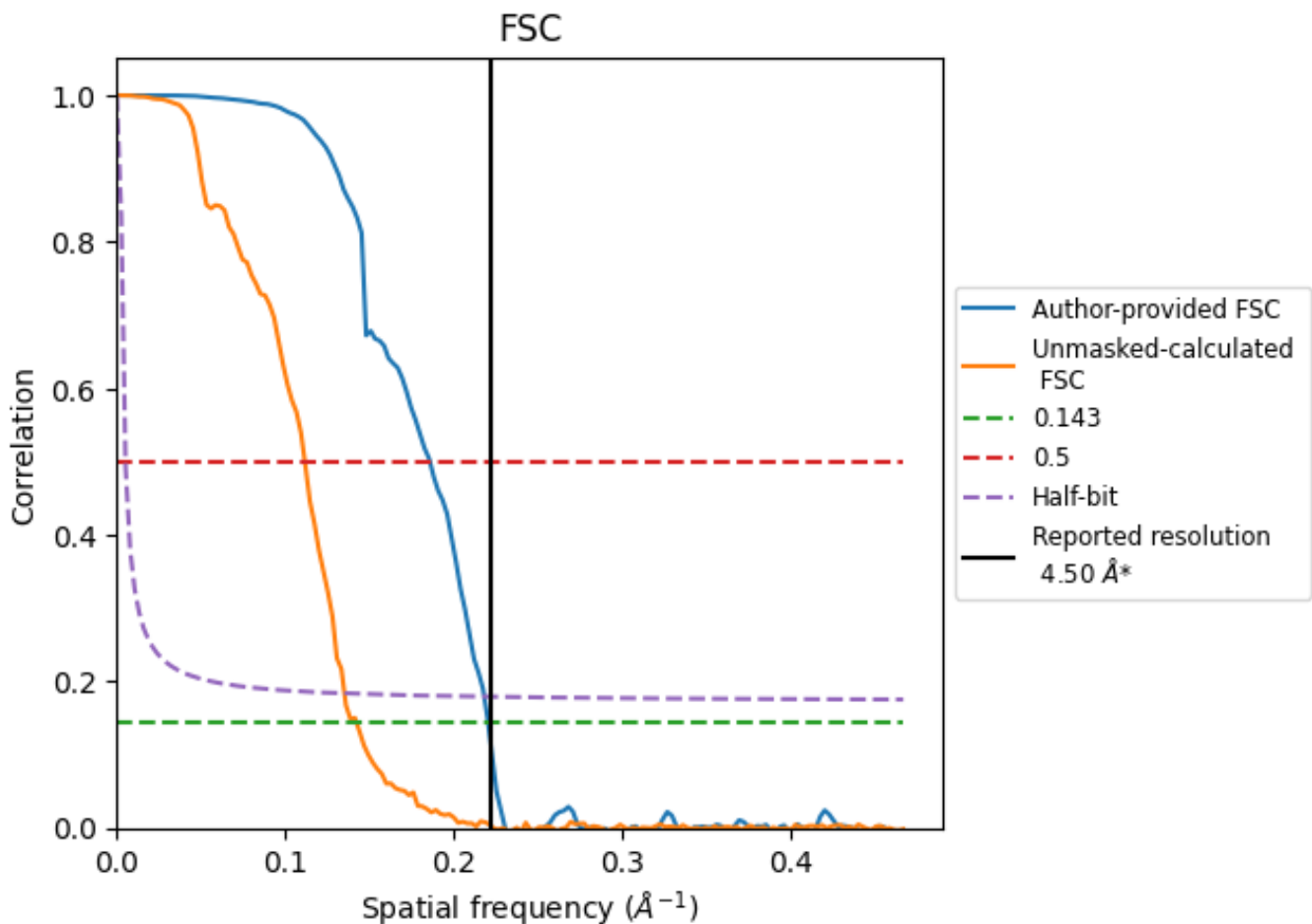


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

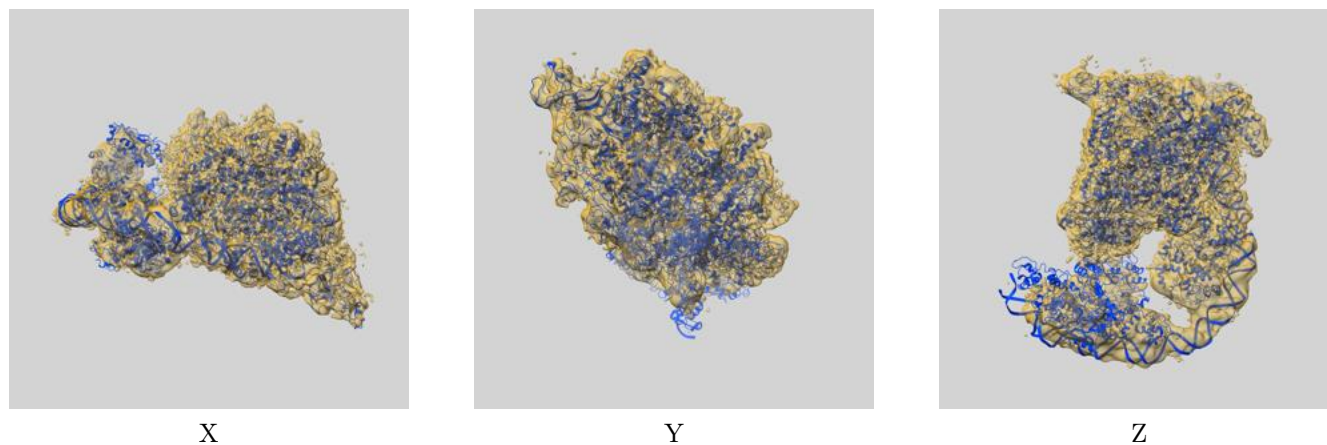
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.53	5.38	4.58
Unmasked-calculated*	7.02	8.94	7.39

*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](#)



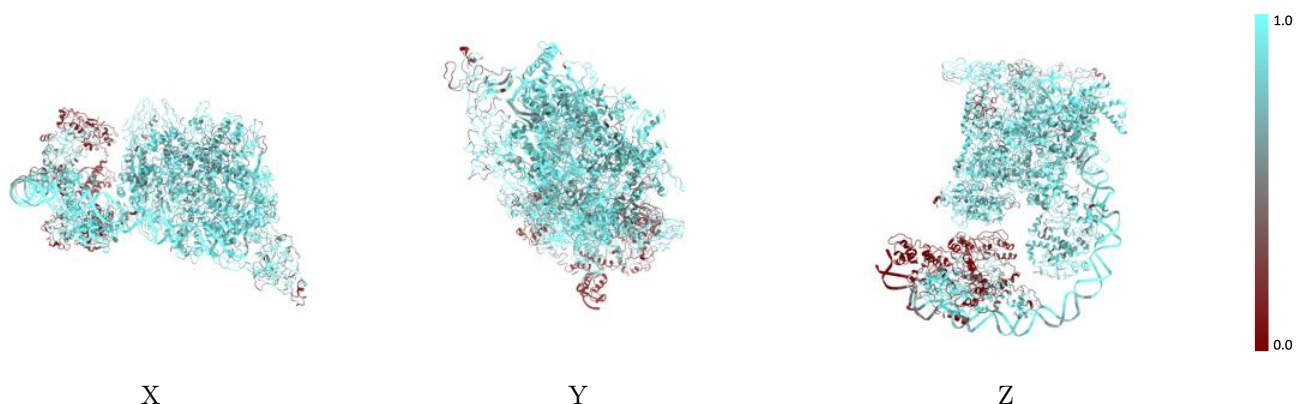
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



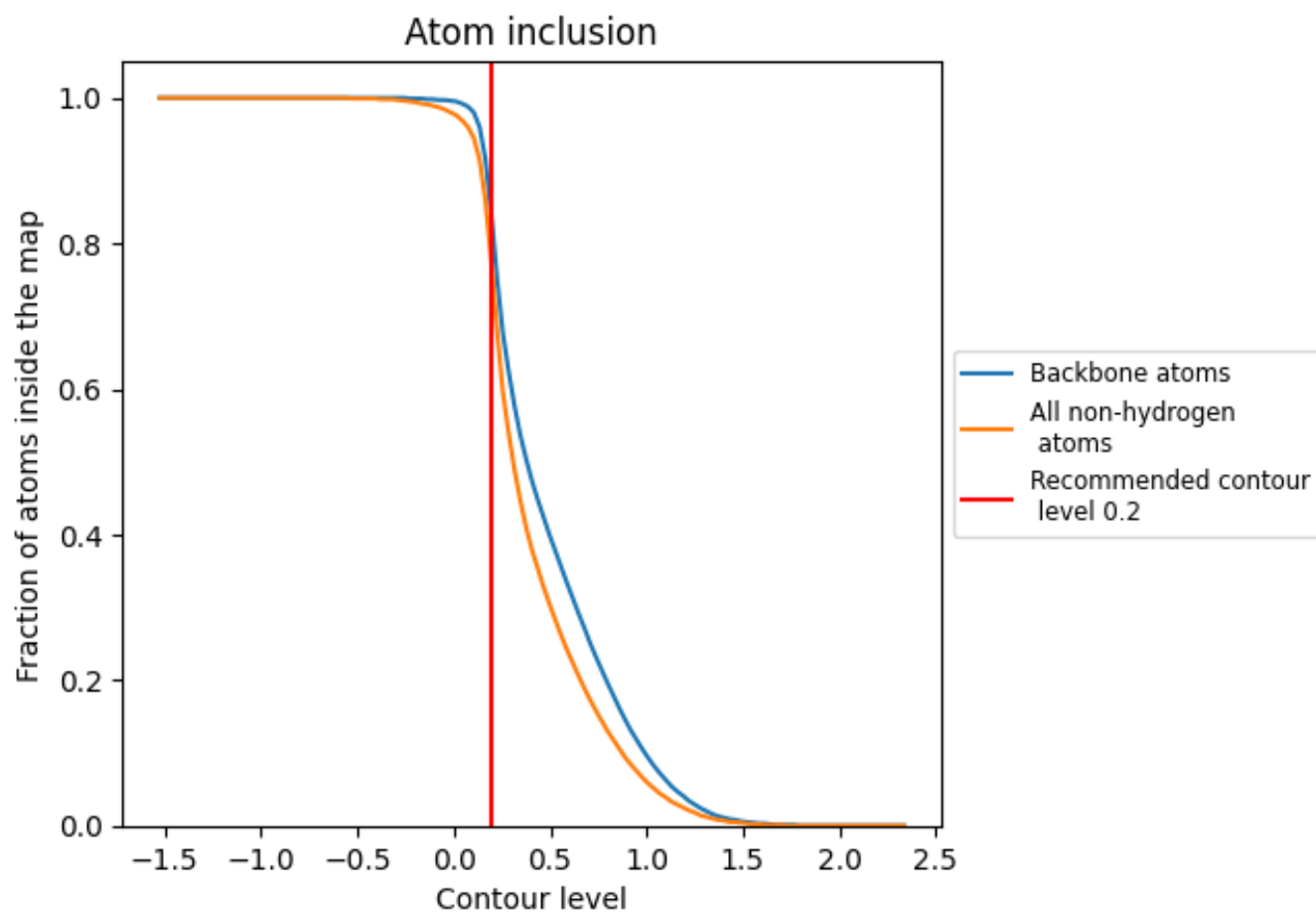
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

