



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 10:01 AM UTC

PDB ID : 6C9Y / pdb_00006c9y
EMDB ID : EMD-7438
Title : Cryo-EM structure of E. coli RNAP sigma70 holoenzyme
Authors : Narayanan, A.; Vago, F.; Li, K.; Qayyum, M.Z.; Yenool, D.; Jiang, W.; Murakami, K.S.
Deposited on : 2018-01-29
Resolution : 4.25 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

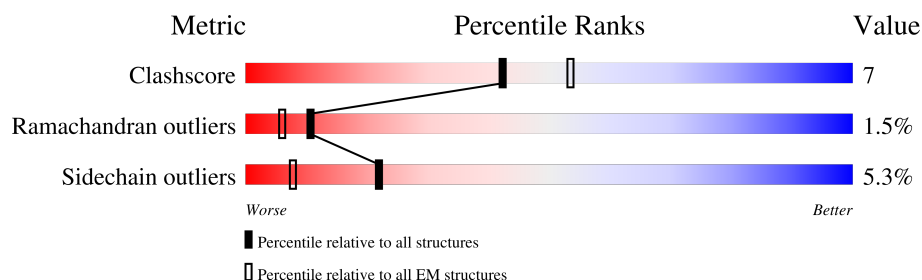
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.25 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	329	37% 52% 17% 30%
1	B	329	34% 52% 13% 33%
2	C	1342	65% 80% 18%
3	D	1407	63% 72% 22%
4	E	91	75% 74% 8% 16%
5	F	613	70% 61% 15% 24%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28920 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1787	1112	317	352	6		
1	B	221	Total	C	N	O	S	0	0
			1708	1067	302	333	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1350	Total	C	N	O	S	0	0
			10434	6553	1856	1976	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	468	Total	C	N	O	S	0	0
			3813	2389	678	723	23		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total 1	Mg 1	0

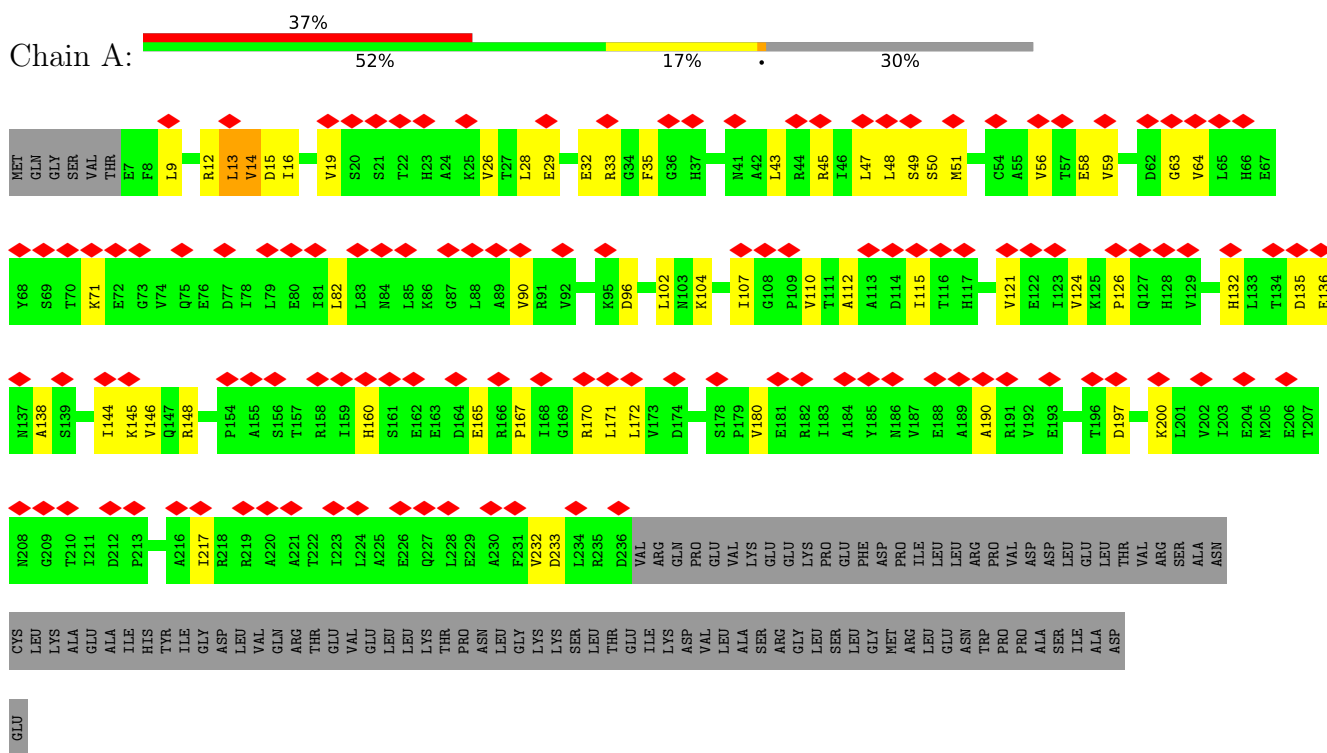
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total 2	Zn 2	0

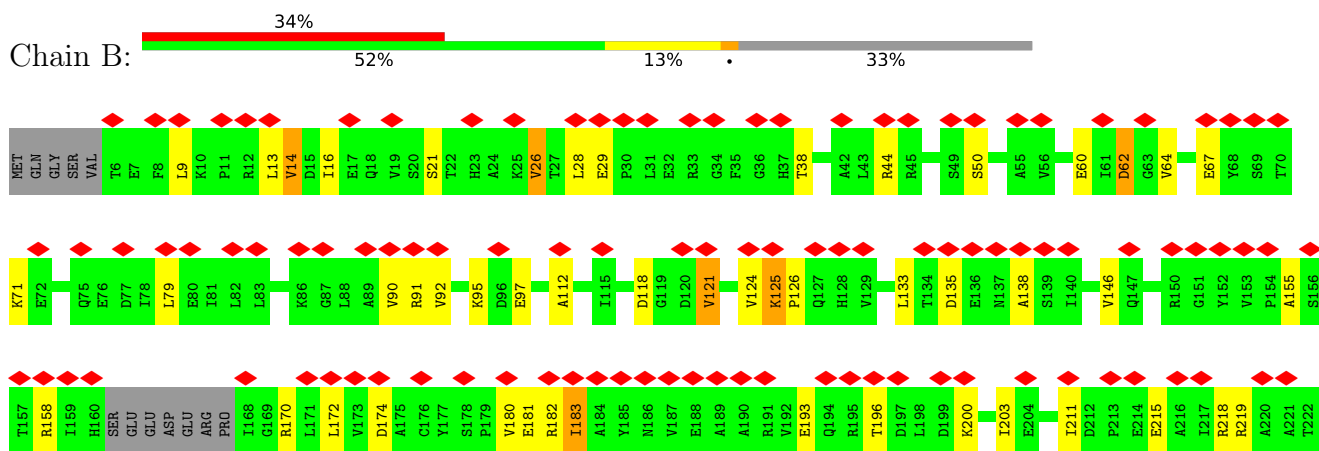
3 Residue-property plots

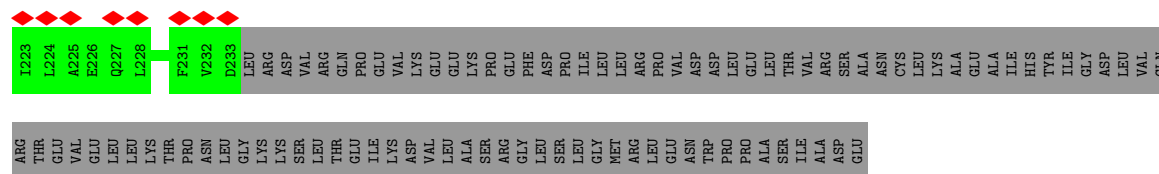
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

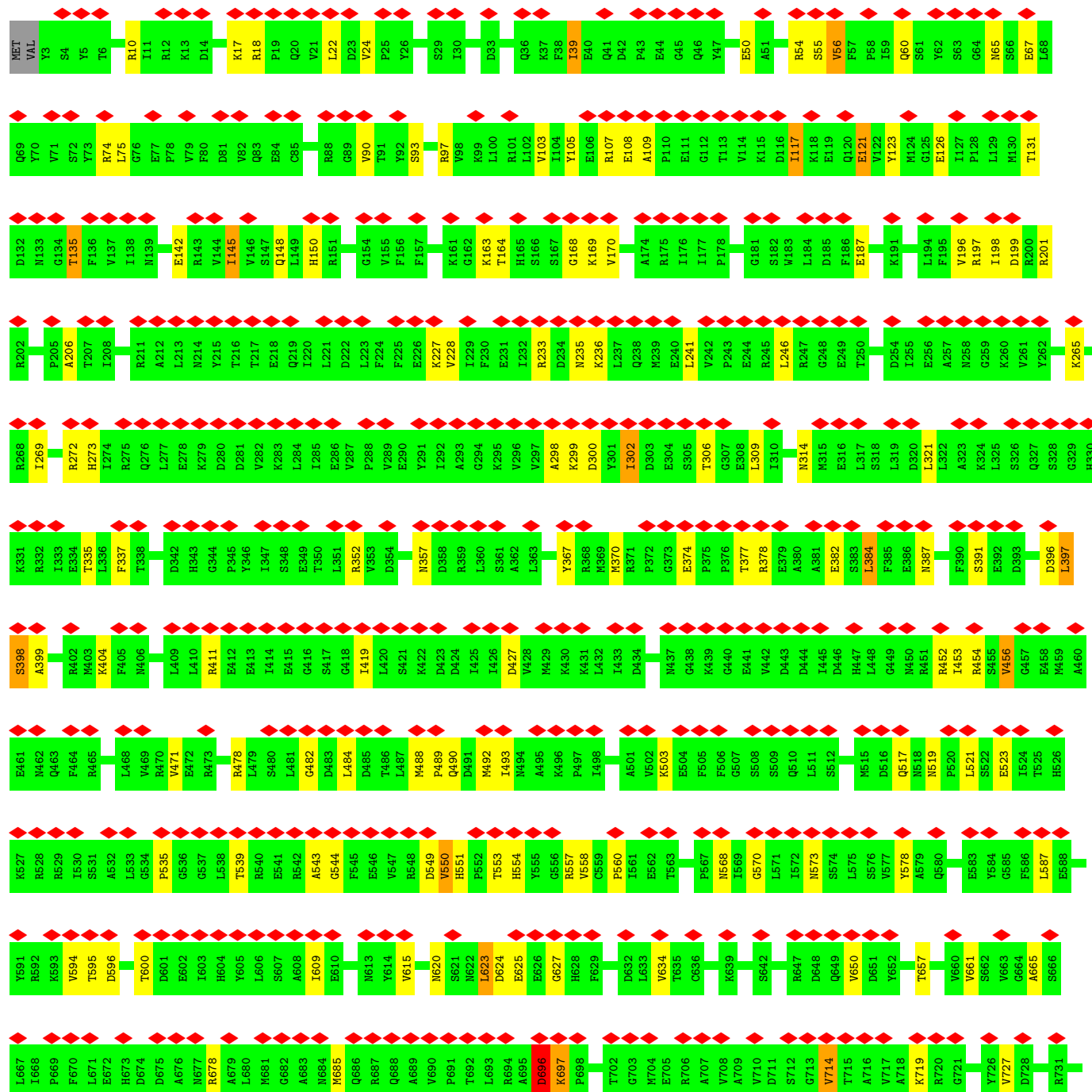
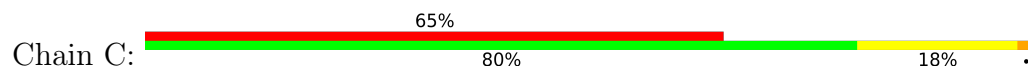


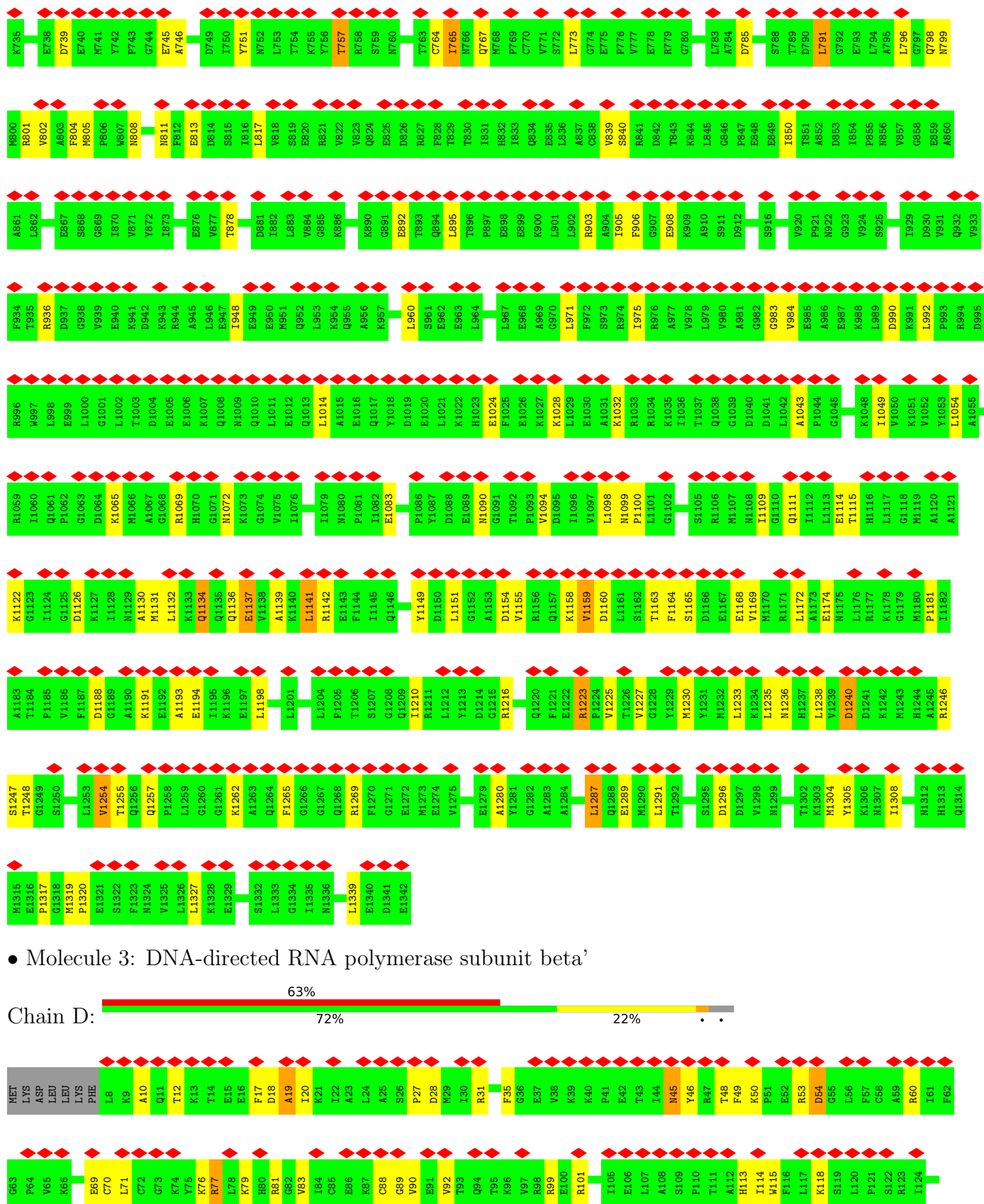
• Molecule 1: DNA-directed RNA polymerase subunit alpha



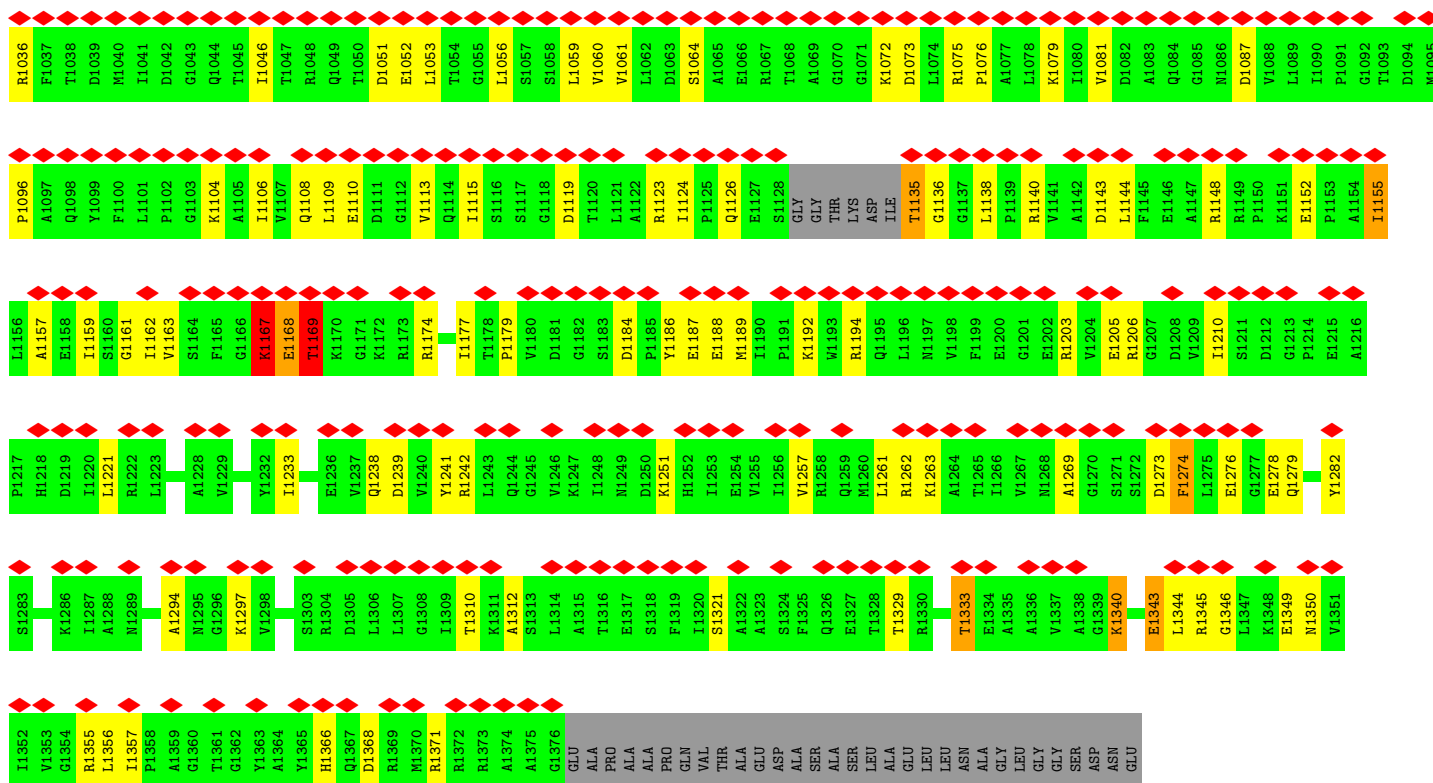


• Molecule 2: DNA-directed RNA polymerase subunit beta

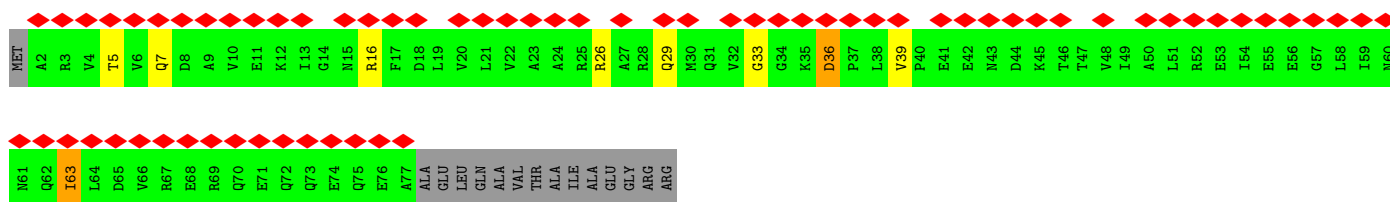
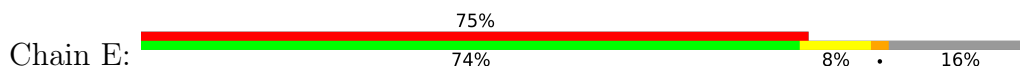




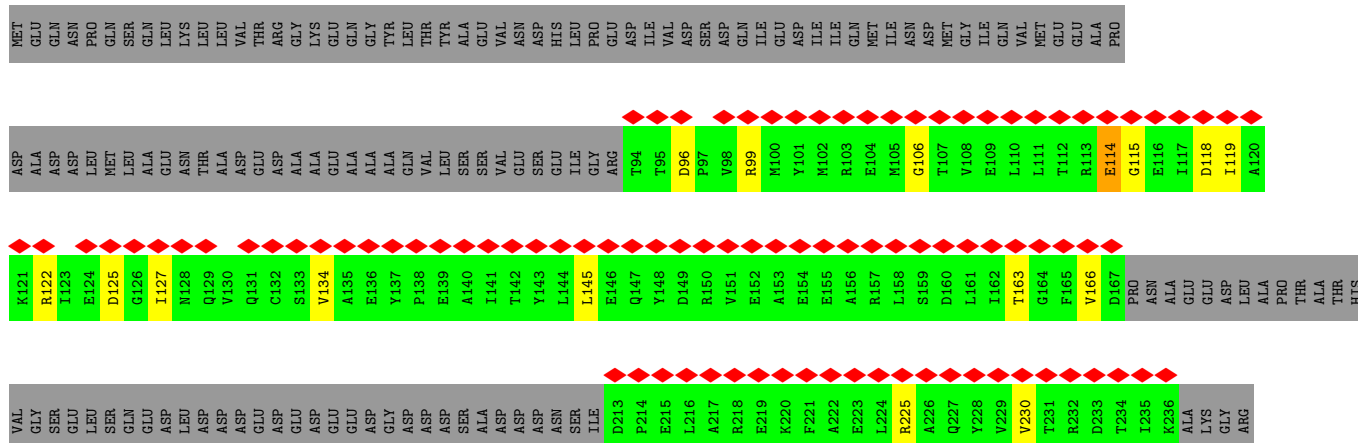
V974	A914	L849	L783	P647	H581	G512	L449	L385	G319	L255	L189	L128
V975	I915	K850	A784	H651	I582	H513	H450	E386	S319	L255	K190	D129
V976	G916	P851	D785	E652	V583	T614	P451	L387	N320	G257	S191	M130
S977	V917	G852	T786	E653	P584	R515	L452	R388	K321	G258	M192	P131
S978	I918	T853	A787	T654	G586	D516	L453	G389	R322	G259	D193	L132
S979	A919	L854	L788	T723	L587	V518	C454	L390	R323	R259	L194	R133
T980	A920	V855	K789	M724	P588	N519	A456	A391	L324	F260	E195	D134
E981	Q921	P859	T790	M725	V589	A520	Y457	T392	K325	A261	Q196	I135
L982	S922	R860	A791	A657	S590	K521	N458	I394	T262	E197	E136	E137
K983	I923	L863	N792	A659	I591	L527	D460	K398	D329	S263	C198	R137
L984	G924	L864	S793	E660	V592	T528	F461	K399	M330	D264	E199	V138
E985	E925	H865	G794	V661	N593	G529	D462	M400	I331	L265	Q200	L139
F986	F926	E866	L795	A662	Q594	P530	D463	V401	K332	N266	E202	Y140
G989	Q927	Q867	T797	E663	A595	K531	G463	E402	G333	D267	E203	F141
R990	T928	W868	R798	E664	L596	E532	D464	R403	K334	Y269	E204	E142
Q929	Q929	C869	R799	Q665	G597	A533	Q465	A467	Q335	R270	E207	S143
K992	L930	D870	L800	Q667	K598	E534	M466	V468	G336	R271	E208	Y144
E993	T931	L871	W801	Q668	K599	R535	A467	V469	R337	N274	T209	V146
S994	ME1	L872	D802	F668	A600	L536	N468	H469	F338	R275	N210	I147
Y995	ARG	L873	W803	Q669	I601	Y537	H470	W409	E148	E211	E211	E148
K996	THR	E873	R803	S670	S602	R538	P471	D410	G149	R278	E211	G149
V997	PHE	E874	Q805	G671	M604	S539	L472	I411	L342	L279	T212	G150
P998	HIS	S876	D806	L672	L605	G540	L473	L412	L343	K213	K213	M151
Y999	ILE	V877	T810	G745	L606	L541	L474	D413	G344	R281	R214	T152
G1000	GLY	L746	D813	L747	A542	S543	E475	E414	K345	L282	K215	M153
A1001	ALA	M747	E814	T674	A544	H545	A476	I416	R346	K216	K216	L154
V1002	ALA	M748	E815	G676	L544	H546	Q477	R417	V347	L217	L217	E155
L1003	ARG	K749	E816	E877	H546	R547	L478	E418	D284	E156	R156	R156
A1004	ALA	P750	E817	R678	L614	R548	L479	E419	L285	K219	K219	Q157
K1005	A945	D751	G819	G679	K615	V548	E479	H419	A286	R220	R220	Q158
G1006	A946	G752	I820	N680	P616	G752	A480	L422	A287	I221	I221	I159
D1007	E947	S753	M821	G685	T617	K549	L483	L423	P288	K222	K222	L160
S948	V886	T754	M822	G686	V618	V550	M484	N424	D289	L223	L223	E162
Q1008	S887	T755	R823	A689	L619	E554	M485	R425	I290	L224	L224	E163
G1009	S888	E756	P824	N690	F620	Y555	S486	A426	I291	E225	E225	E164
Q1010	D889	T757	W825	G690	A621	E556	N489	P427	R293	F227	F227	Y165
V1011	F892	T758	I826	N691	D622	K557	L489	T428	N294	V228	V228	L166
A1012	G893	P759	G828	V693	Q623	D558	S492	L429	R297	Q229	Q229	D167
G1013	V894	T760	S894	G695	L624	A559	P493	H430	M298	S230	S230	A168
E1014	C895	A761	K695	N697	H625	N560	A494	R431	E301	E301	E301	E171
L1015	A896	M762	G696	G697	V626	G561	N495	L432	V303	A302	A302	E171
T1016	H897	F763	W697	G700	T627	E562	G496	G433	D304	L239	L239	G173
V1017	C898	R764	L701	V705	G628	K566	E497	L434	A305	T240	T240	D174
A1018	G899	E765	Q702	T706	F629	T567	P498	Q435	L306	L242	L242	E175
N1019	N900	H768	A632	V707	A632	S568	P499	A436	F176	P243	P243	F176
V1020	P834	V769	A633	E704	L634	S569	I500	F377	D308	V244	V244	D177
D1021	N962	L770	E704	T705	R634	L569	V501	P439	N309	L245	L245	A178
P1022	G963	Q771	G638	V706	S638	K570	S502	V440	R311	P246	P246	K179
H1023	K964	T772	A639	T707	V639	D571	S503	L441	G310	L247	L247	M180
T1024	A904	V773	R708	W708	G640	T572	Q504	L442	E375	E375	E375	E183
M1025	R905	T774	R709	G711	I641	F673	G505	I443	F377	R312	R312	A184
P1026	G906	T775	D710	G711	D643	R576	V507	G444	L376	G313	G313	I185
V1027	H907	T776	T844	G712	P643	A577	S507	K445	R314	A315	A315	Q186
E1030	N968	H777	T844	Q712	V645	L579	G508	I446	Y382	I316	I316	A187
N1031	N910	R780	E713	E714	L646	W580	L510	Q448	E382	T317	T317	L188
V1032	K911	K781	E714	G782								
G1033	Q912											
F1034	L973											
V1035												



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size ($\text{\AA}$)	315.84, 315.84, 315.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.316, 1.316, 1.316	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/1809	1.15	11/2451 (0.4%)
1	B	0.36	0/1728	1.00	3/2341 (0.1%)
2	C	0.37	0/10739	0.92	23/14489 (0.2%)
3	D	0.36	0/10591	0.95	17/14307 (0.1%)
4	E	0.34	0/607	0.91	0/817
5	F	0.34	0/3864	1.02	9/5194 (0.2%)
All	All	0.36	0/29338	0.96	63/39599 (0.2%)

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
2	C	0	4
3	D	0	2
5	F	0	3
All	All	0	9

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LEU	CA-C-N	8.92	130.84	119.78
1	A	28	LEU	C-N-CA	8.92	130.84	119.78
3	D	1343	GLU	CA-C-N	8.79	138.34	121.54
3	D	1343	GLU	C-N-CA	8.79	138.34	121.54
1	A	160	HIS	N-CA-C	-7.70	105.85	114.62

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	198	ILE	Peptide
2	C	236	LYS	Peptide
2	C	397	LEU	Peptide
3	D	901	ARG	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	1787	0	1810	33	0
1	B	1708	0	1741	28	0
2	C	10570	0	10582	125	0
3	D	10434	0	10599	181	0
4	E	605	0	612	6	0
5	F	3813	0	3880	52	0
6	D	1	0	0	0	0
7	D	2	0	0	0	0
All	All	28920	0	29224	392	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 7.

The worst 5 of 392 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)
3:D:1140:ARG:HH12	3:D:1144:LEU:HG	1.32	0.94
1:A:233:ASP:HA	1:B:218:ARG:HH12	1.40	0.87
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.06	0.87
2:C:299:LYS:NZ	2:C:300:ASP:O	2.11	0.81
1:A:33:ARG:NH2	1:A:197:ASP:OD2	2.13	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/329 (69%)	204 (90%)	24 (10%)	0	100	100
1	B	217/329 (66%)	196 (90%)	18 (8%)	3 (1%)	9	39
2	C	1338/1342 (100%)	1209 (90%)	109 (8%)	20 (2%)	8	38
3	D	1344/1407 (96%)	1212 (90%)	105 (8%)	27 (2%)	6	31
4	E	74/91 (81%)	70 (95%)	3 (4%)	1 (1%)	9	39
5	F	462/613 (75%)	430 (93%)	27 (6%)	5 (1%)	11	45
All	All	3663/4111 (89%)	3321 (91%)	286 (8%)	56 (2%)	11	38

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
1	B	193	GLU
2	C	398	SER
2	C	484	LEU
2	C	697	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/286 (69%)	194 (98%)	4 (2%)	48	66
1	B	189/286 (66%)	177 (94%)	12 (6%)	16	38
2	C	1155/1157 (100%)	1087 (94%)	68 (6%)	18	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1115/1168 (96%)	1053 (94%)	62 (6%)	19	42
4	E	65/75 (87%)	61 (94%)	4 (6%)	16	39
5	F	417/540 (77%)	400 (96%)	17 (4%)	27	49
All	All	3139/3512 (89%)	2972 (95%)	167 (5%)	22	43

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	569	LEU
3	D	1333	THR
3	D	678	ARG
3	D	853	THR
5	F	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	865	HIS
4	E	31	GLN
3	D	907	HIS
3	D	1086	ASN
5	F	338	HIS

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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

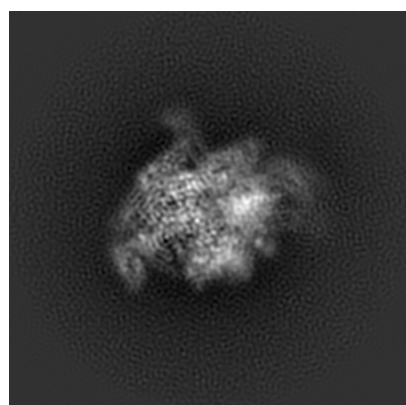
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7438. These allow visual inspection of the internal detail of the map and identification of artifacts.

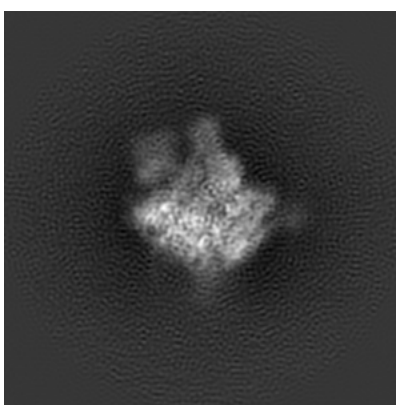
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

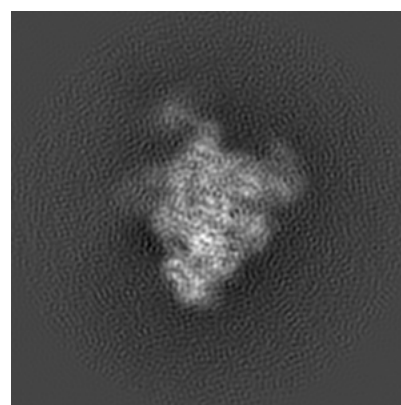
6.1.1 Primary map



X



Y

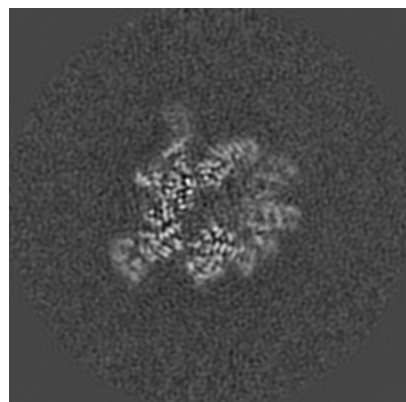


Z

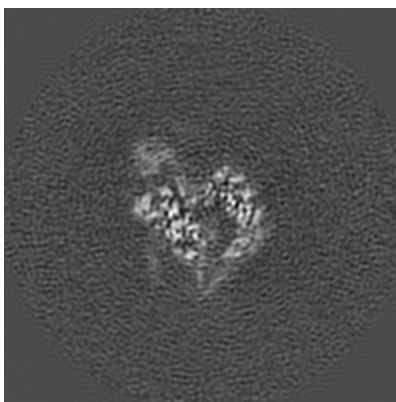
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

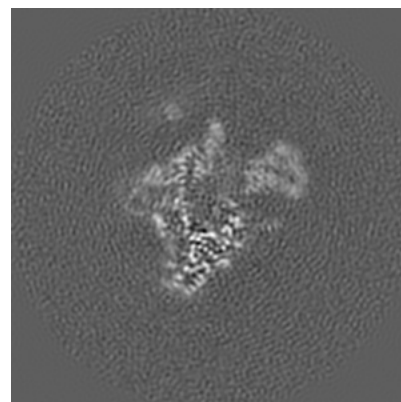
6.2.1 Primary map



X Index: 120



Y Index: 120

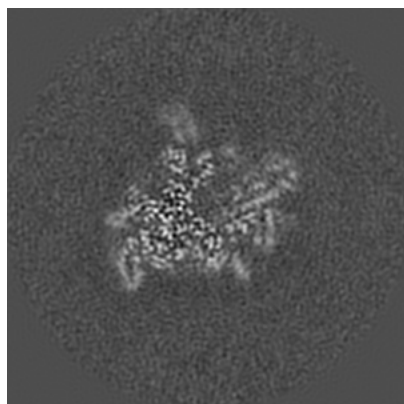


Z Index: 120

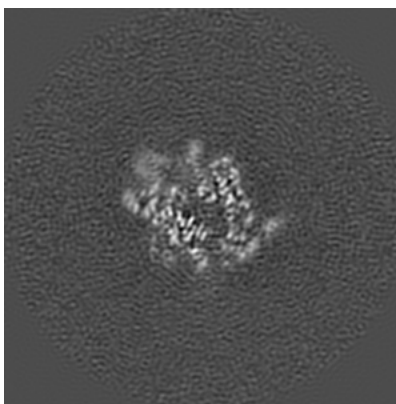
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

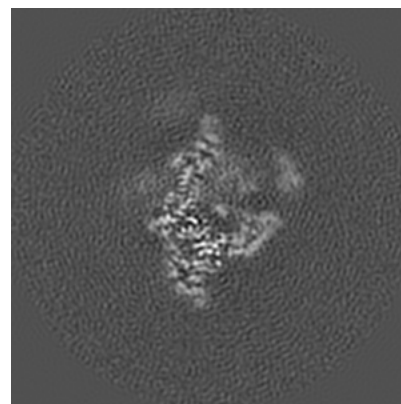
6.3.1 Primary map



X Index: 114



Y Index: 114

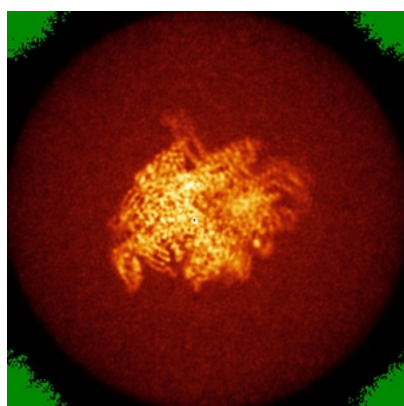


Z Index: 114

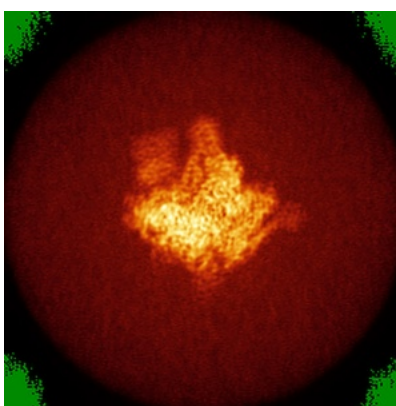
The images above show the largest variance slices of the map in three orthogonal directions.

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

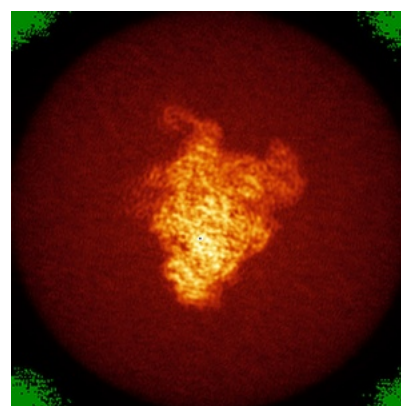
6.4.1 Primary map



X



Y

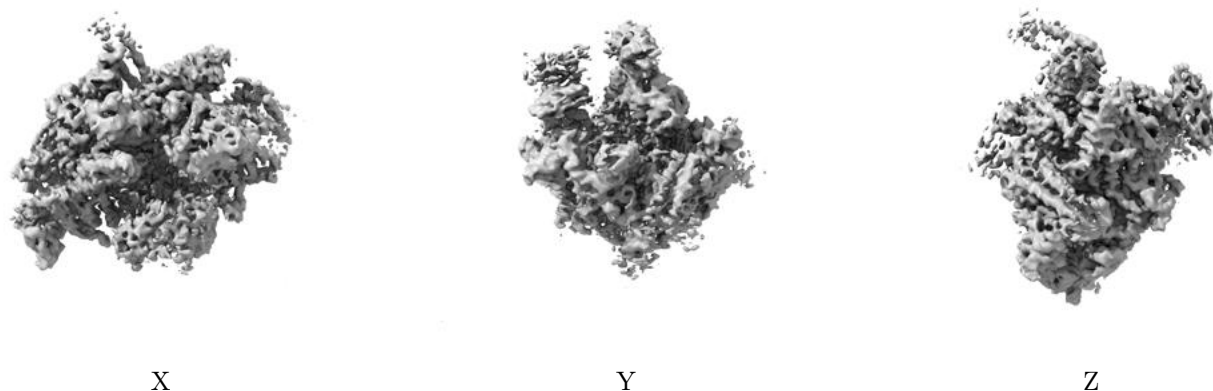


Z

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 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

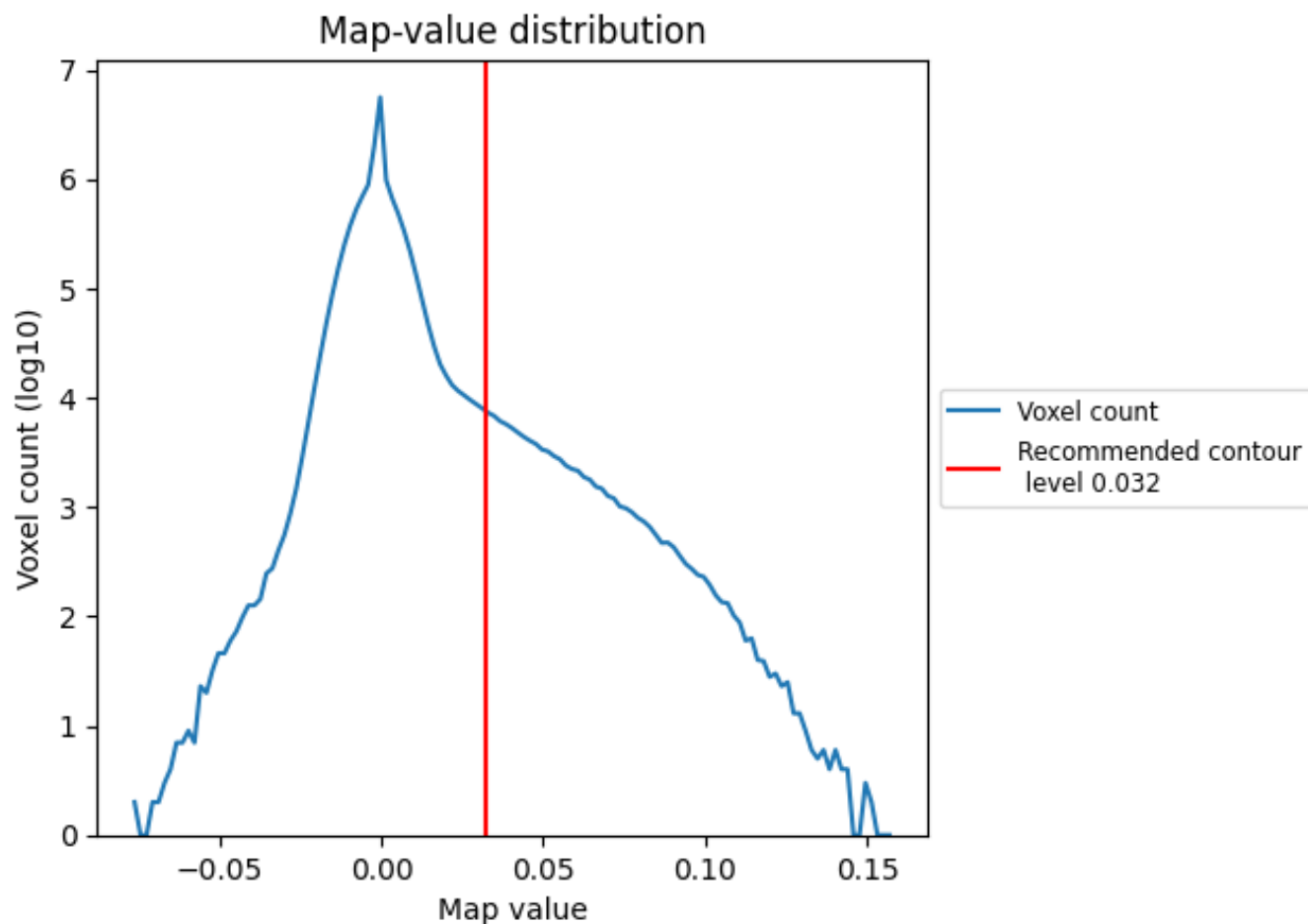
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

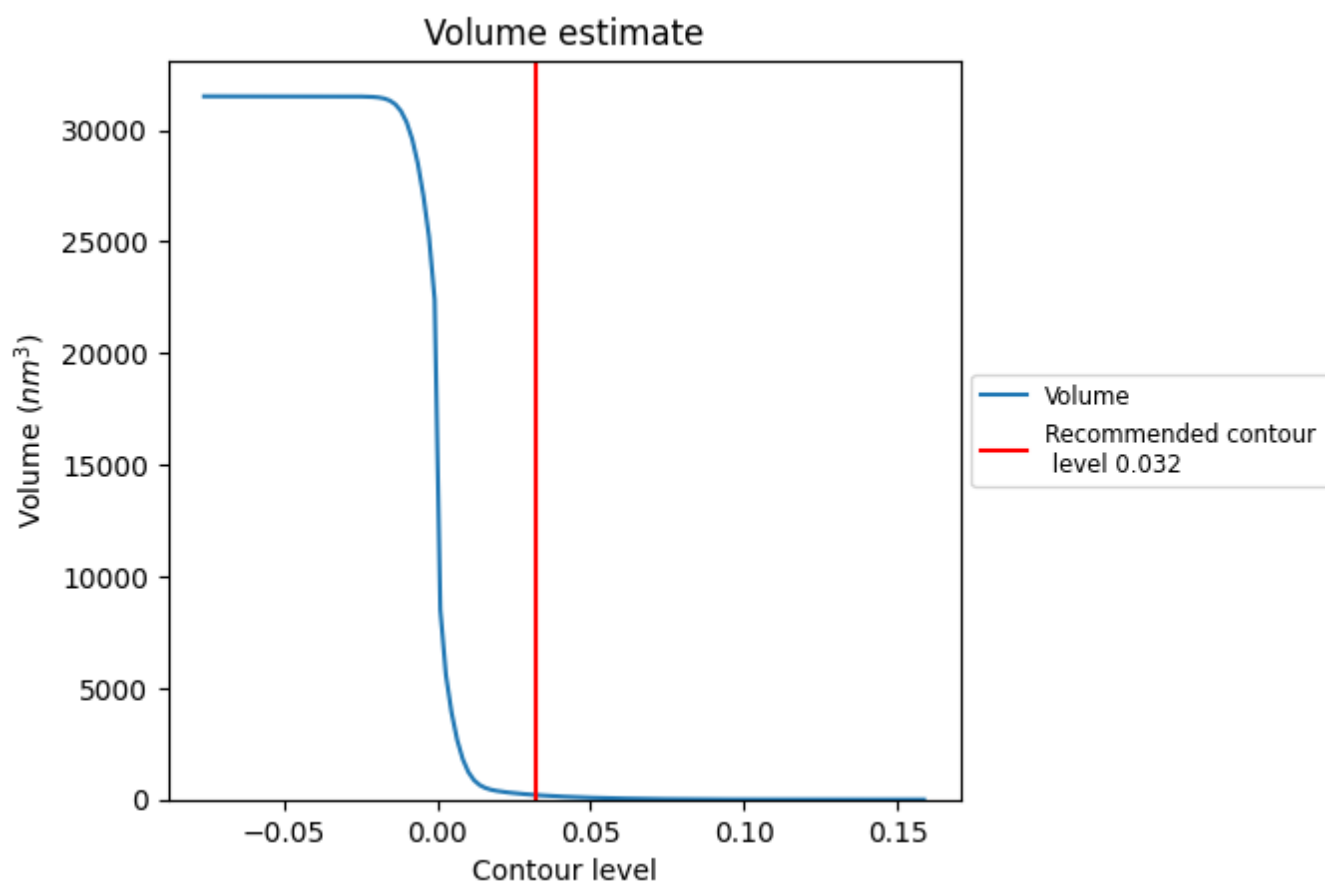
This section contains the results of statistical analysis of the map.

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.

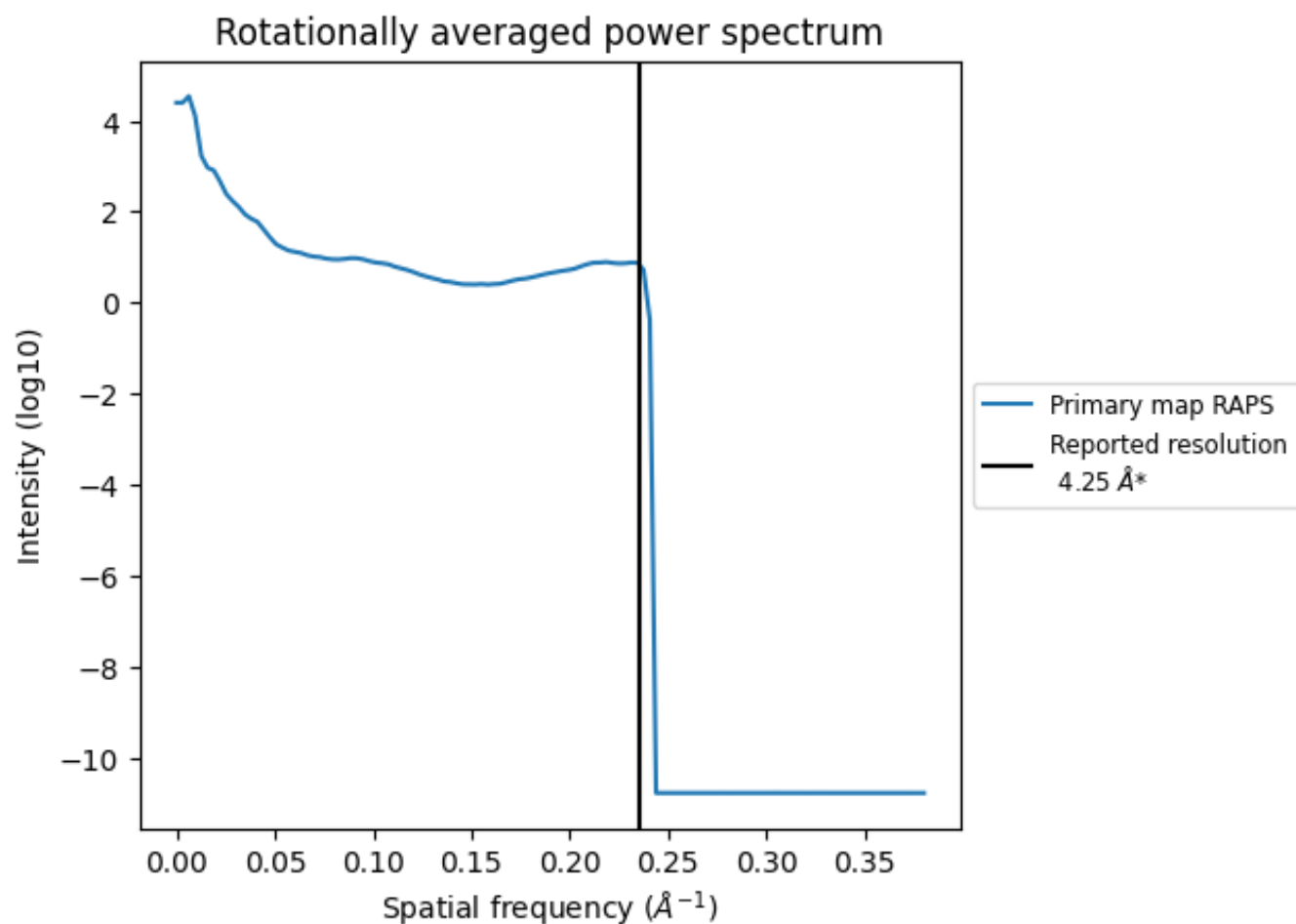
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 186 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 0.235 Å⁻¹

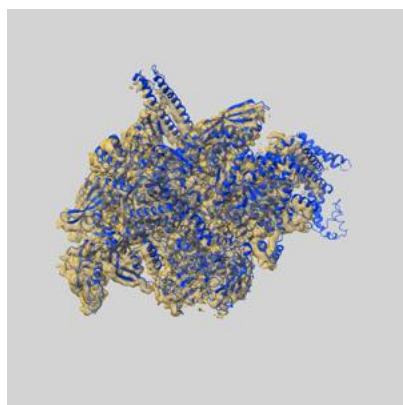
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

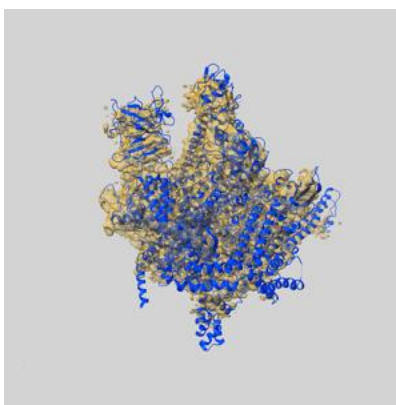
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7438 and PDB model 6C9Y. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

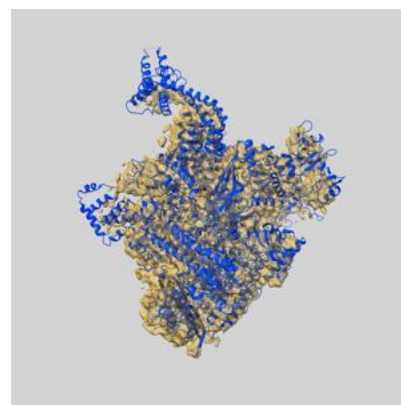
9.1 Map-model overlay [i](#)



X



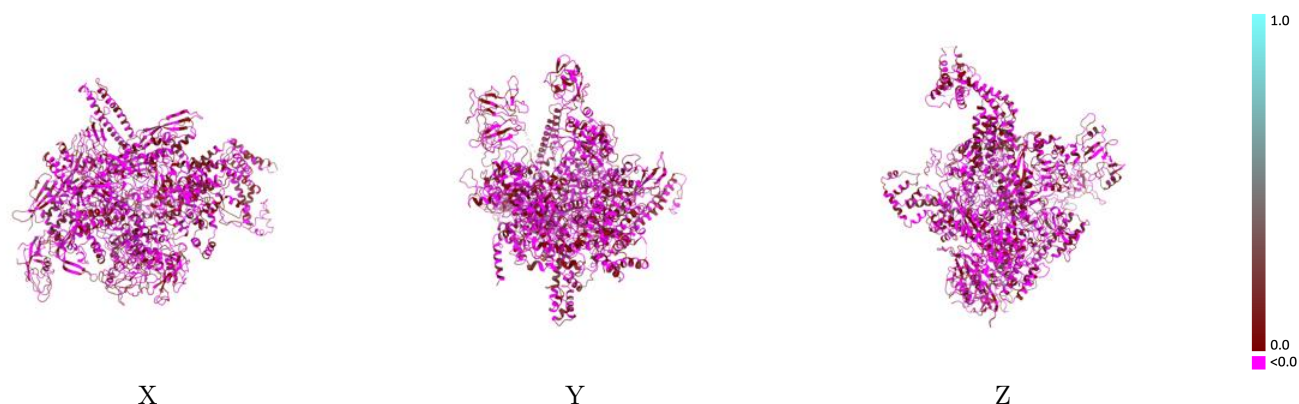
Y



Z

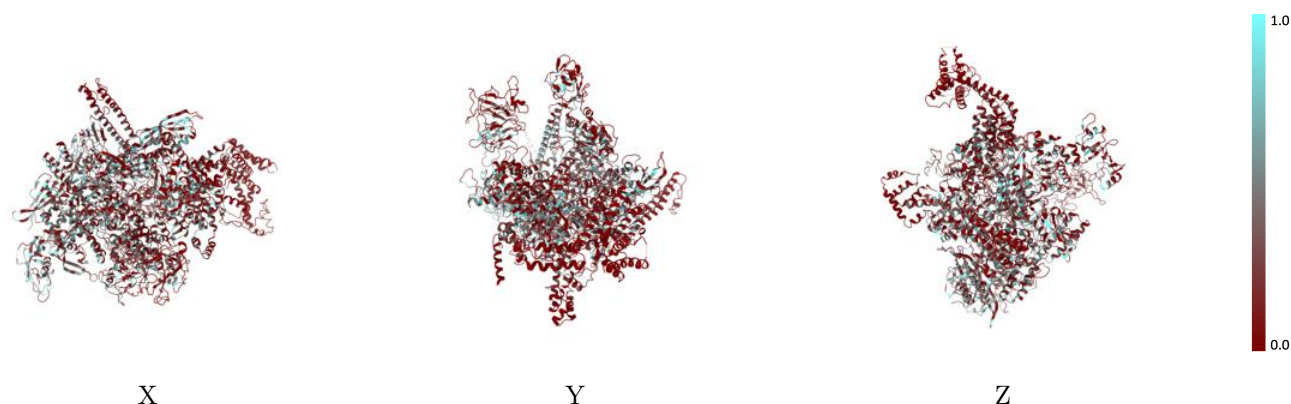
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



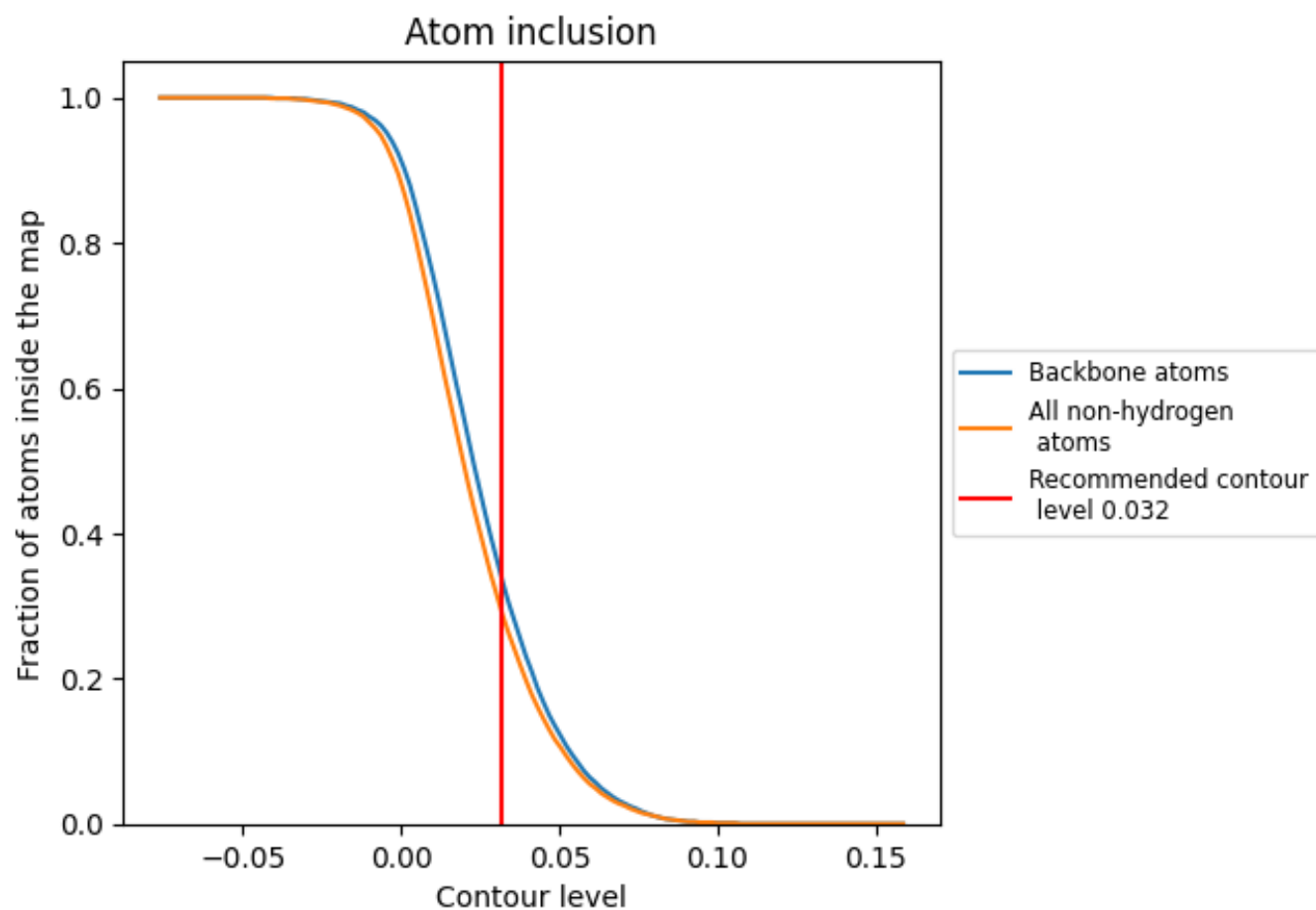
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2900	-0.0170
A	0.4000	-0.0020
B	0.4190	-0.0130
C	0.3110	-0.0300
D	0.3100	-0.0120
E	0.1140	-0.0490
F	0.0920	0.0030

1.0
0.0
-0.0