



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 03:29 am BST

PDB ID : 8P4E
EMDB ID : EMD-17407
Title : Structural insights into human co-transcriptional capping - structure 5
Authors : Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on : 2023-05-20
Resolution : 3.90 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.37.1

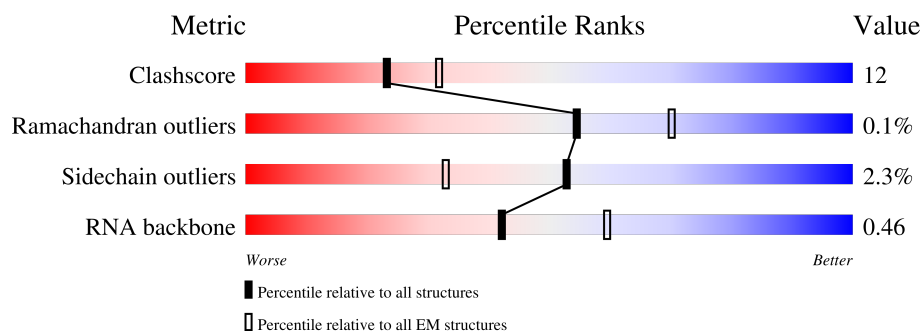
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	Z	1087	
2	M	597	
3	A	1970	
4	B	1174	
5	C	275	
6	E	210	
7	F	127	

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	D	142	
14	G	172	
15	O	835	
16	P	21	
17	N	26	
18	T	35	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 41213 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 Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	52	Total	C	N	O	S	0	0
			397	243	73	80	1		

- Molecule 2 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	329	Total	C	N	O	S	0	0
			2649	1689	456	483	21		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1407	Total	C	N	O	S	0	0
			11142	7014	1997	2063	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1116	Total	C	N	O	S	0	0
			8928	5652	1568	1644	64		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	258	Total	C	N	O	S	0	0
			2071	1301	353	411	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	82	Total	C	N	O	S	0	0
			658	418	113	122	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 13 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	129	Total	C	N	O	S	0	1
			998	629	170	195	4		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	171	Total	C	N	O	S	0	0
			1305	852	205	240	8		

- Molecule 15 is a protein called Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	695	Total	C	N	O	S	0	0
			5643	3606	962	1040	35		

- Molecule 16 is a RNA chain called RNA (5'-D(*(MGT))-R(P*GP*AP*CP*AP*UP*AP*C P*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	21	Total	C	N	O	P	0	0
			462	204	89	146	23		

- Molecule 17 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	26	Total	C	N	O	P	0	0
			538	257	100	155	26		

- Molecule 18 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	35	Total	C	N	O	P	0	0
			714	342	126	211	35		

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

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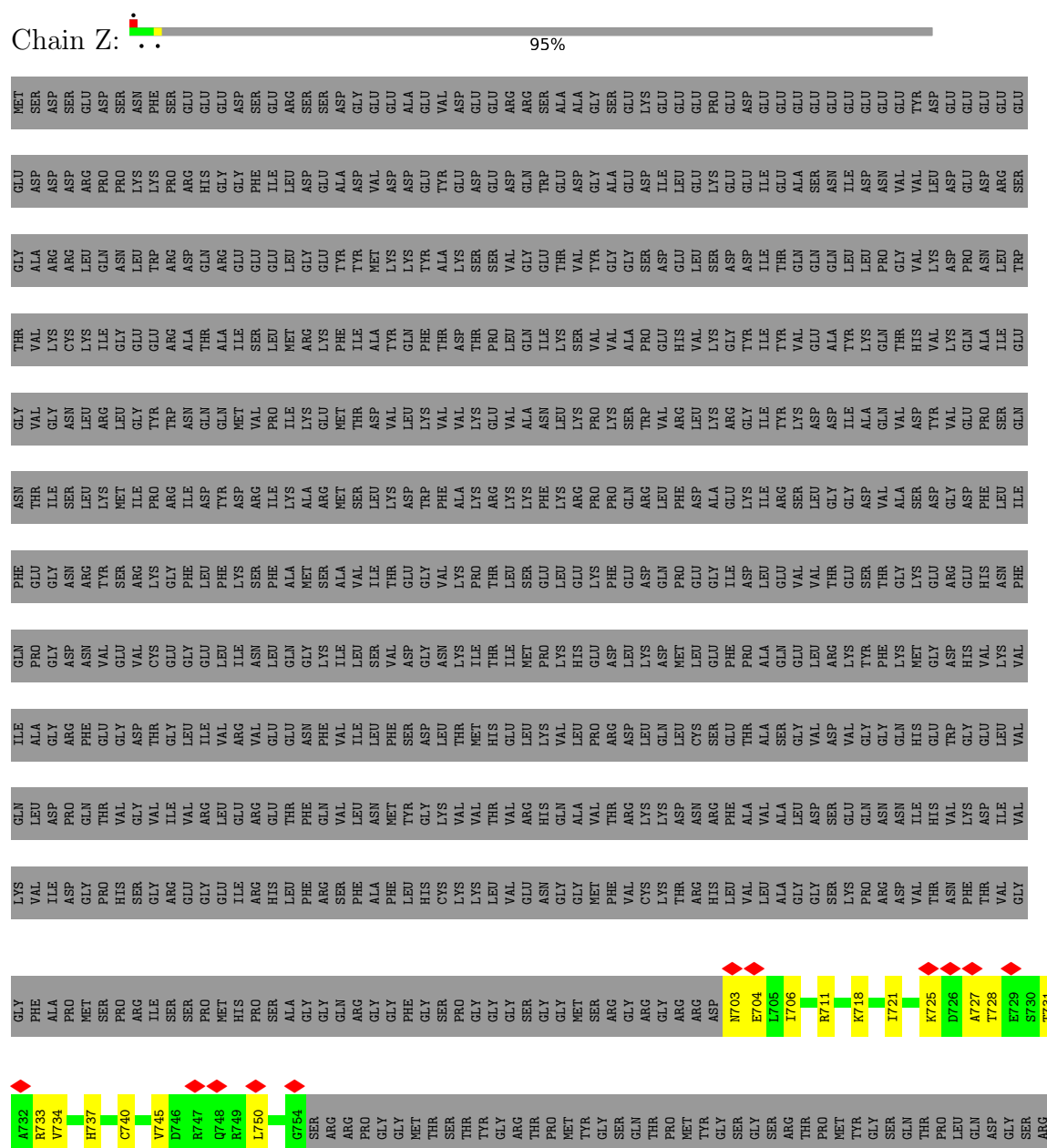
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Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total 1	Zn 1	0
20	I	2	Total 2	Zn 2	0
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

3 Residue-property plots

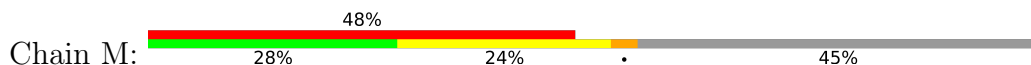
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transcription elongation factor SPT5



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

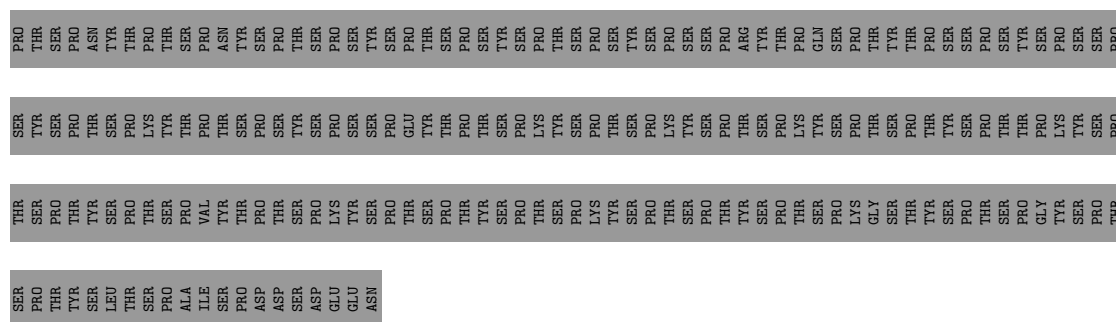
- Molecule 2: mRNA-capping enzyme



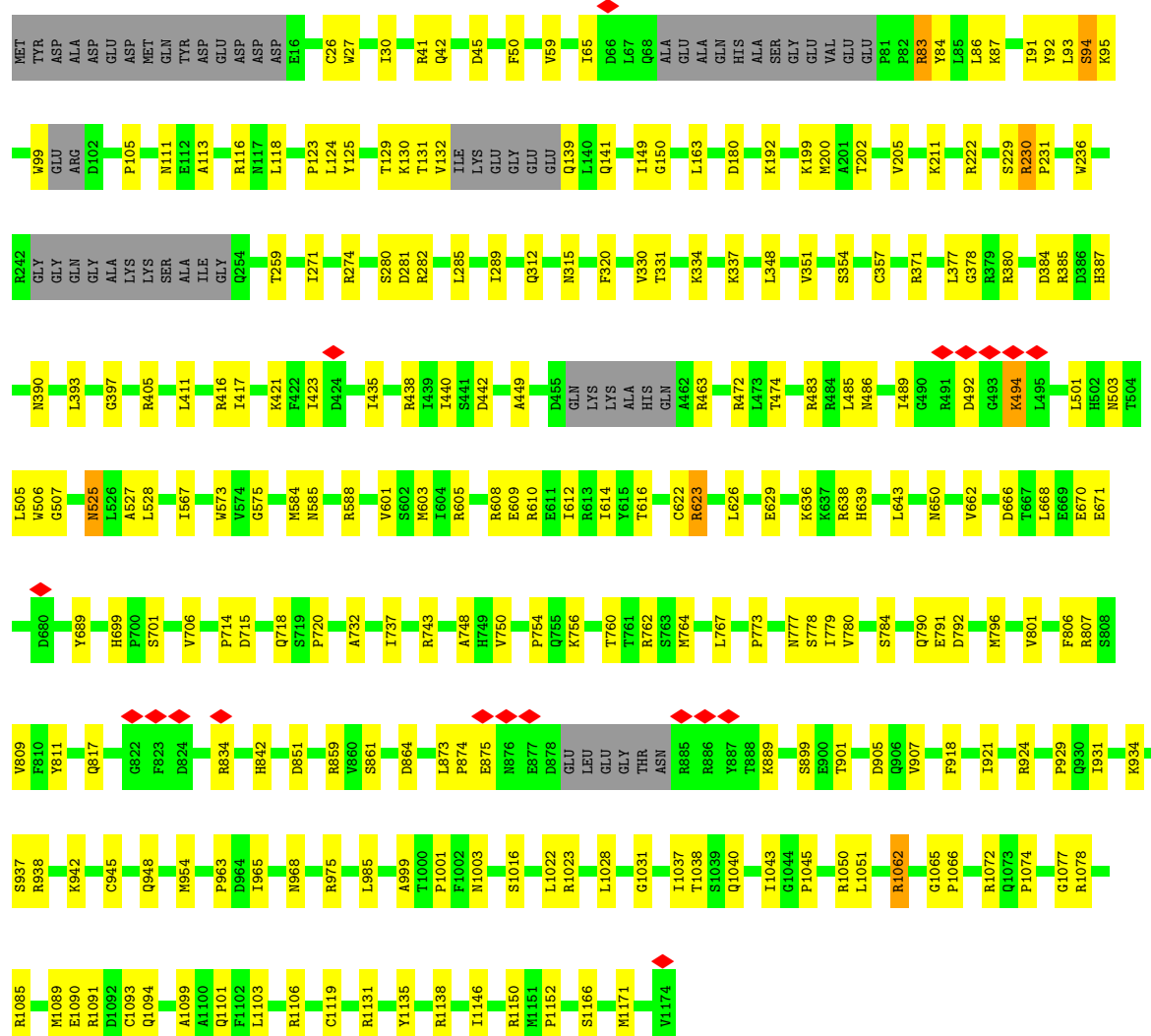
N547	L481	S421	I361	M301	V241	LEU	NET
S548	L482	R422	Y362	M302	T242	ILE	GLY
I549	P483	R423	D363	L303	Q243	LEU	LEU
S550	N485	L424	I364	I304	V244	VAL	VAL
N551	V486	L425	I365	D305	T245	CYS	ASP
P552	L489	GLY	K366	G306	T246	THR	LEU
V553	V490	ASN	F367	T307	Q247	THR	THR
T554	V491	PHE	N368	N308	P248	GLY	ASN
K555	Q492	ALA	S369	E309	K249	THR	THR
E556	G493	LYS	Q370	V310	L250	ARG	ASN
M557	V494	GLU	F371	F311	G251	THR	CYS
L558	E495	VAL	V372	M312	E252	GLY	THR
F559	R496	SER	G373	I313	V253	PHE	ASP
S560	F497	HIS	D374	D314	Q254	ASN	ARG
F561	F498	E436	C375	R315	Q255	CYS	ASP
I562	I501	M437	D376	D316	K256	ALA	ILE
D563	K502	G439	F377	N317	C257	PHE	GLU
S564	V503	L440	N378	S318	H258	VAL	GLY
C565	K508	I441	V379	V319	Q259	GLY	GLY
T566	F509	F442	R380	F320	P260	LYS	ILE
A567	Q443	Q443	L381	H321	C261	MET	LYS
ALA	P444	P444	Q382	V322	G262	THR	ASP
SER	N512	T445	C383	S323	W263	LEU	LYS
GLN	I514	G446	I384	N324	E264	ILE	GLN
GLY	I515	K447	E385	L325	G265	GLU	CYS
GLN	E516	Y448	R386	E326	S266	ALA	LYS
LYS	C517	Y448	E387	F327	G267	VAL	GLY
ARG	K518	K449	I388	P328	P268	ALA	HIS
LYS	F519	P450	I389	F329	P269	SER	THR
HIS	E520	G451	S390	R330	G270	PHE	GLY
LEU	N521	R452	P391	K331	A271	ALA	ASP
LEU	N522	C453	R392	D332	Q272	THR	GLN
ASP	S523	A523	H393	L333	P273	VAL	PRO
PRO	W524	D455	E394	R334	T274	GLY	ALA
THR	V525	I456	K395	M335	S275	ARG	GLU
GLU	F526	L457	M396	H336	M276	ILE	ASN
LEU	M527	K458	K397	L337	D277	THR	GLY
MET	R528	W459	T398	S338	K278	ASP	ILE
PRO	K460	P461	G399	N339	Q279	ARG	SER
PRO	T531	P462	L400	T340	N280	LEU	NET
PRO	F532	K463	I401	L341	I281	CYS	LEU
ARG	K533	S463	D402	L342	K282	GLU	ASN
ARG	S534	L464	K403	D343	L283	PHE	THR
PRO	F535	N465	G343	R343	E284	ARG	LEU
PRO	V536	S466	T404	G344	L284	GLY	GLY
THR	N537	V467	Q405	E345	D285	THR	ASN
	A538	D468	E406	M346	L286	PRO	LYS
		F469				ASP	VAL

- Molecule 3: DNA-directed RNA polymerase II subunit RPB1

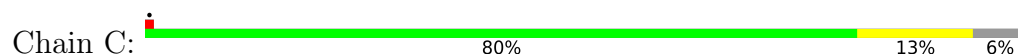


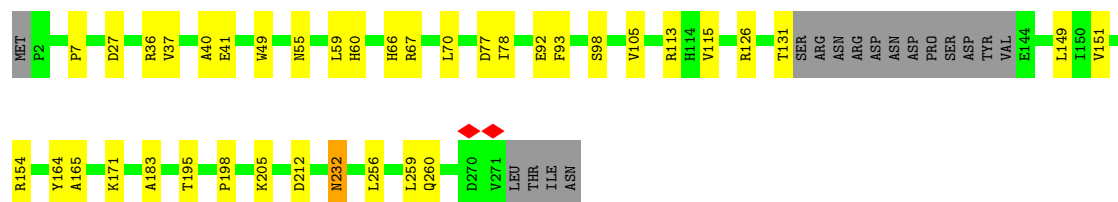


- Molecule 4: DNA-directed RNA polymerase subunit beta

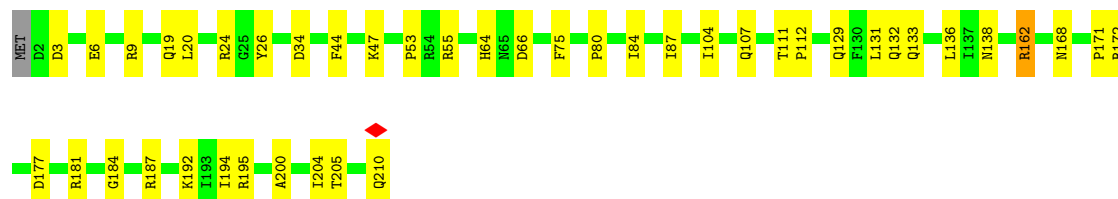
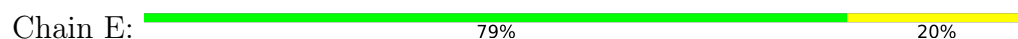


- Molecule 5: DNA-directed RNA polymerase II subunit RPB3

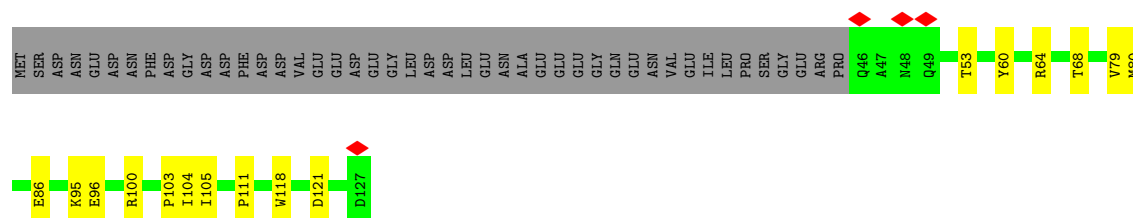




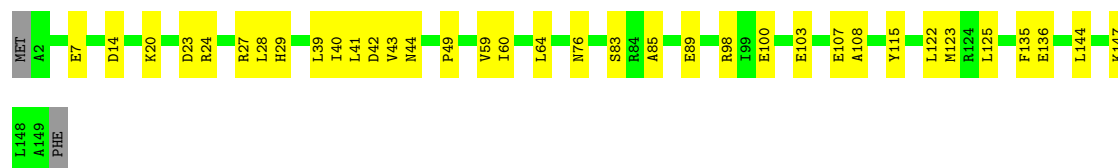
- Molecule 6: DNA-directed RNA polymerase II subunit E



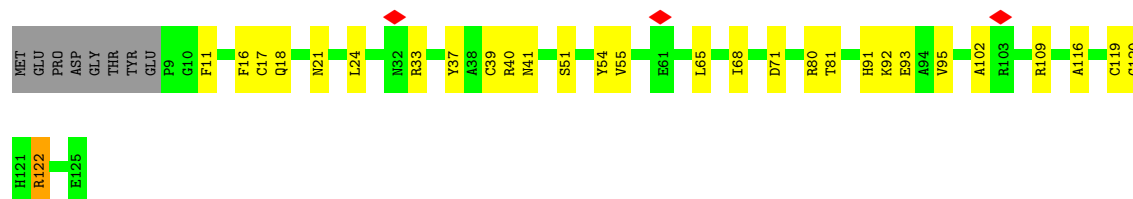
- Molecule 7: DNA-directed RNA polymerase II subunit F



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

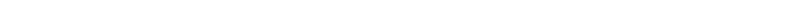
Category	Count
M1	100
R6	100
C10	100
I13	100
N16	100
R42	100
R47	100
P64	100
L65	100
E66	100
K67	100

- Chain K: 82% 15% .

N1	N2	F7	L11	I35	L42	K47	K52	V56	Y61	G62	V63	F64	H65	I71	I72	T77	T78	P79	D80	T91	L94	R104	G115	I1E	GLU
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- Chain L:  67% 12% 21%


MET	ASP	THR	GLN	ASP	VAL	GLN	PRO	PRO	LYS	GLN	Q13	Y17	R31	R37	M44	V53	V54	F55	D56	A57	R58
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- Chain D:  11% 80% 11% 9%

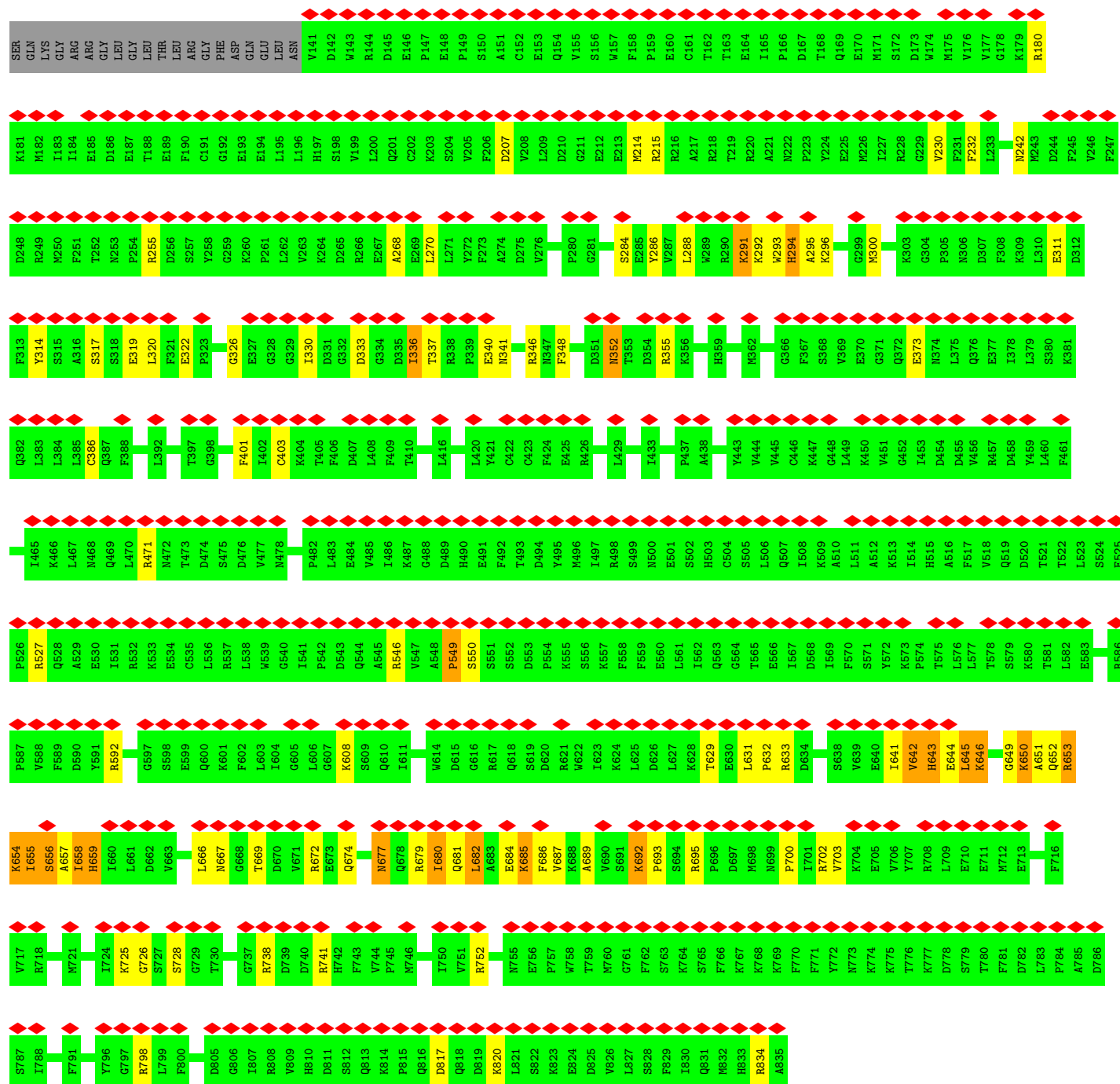
Met	ALA	ALA	GLY	GLY	SER	ASP	PRO	ARG	ALA	ALA	GLY	ASP	VAL	E14	E15	D16	A17	S18	T31	L32	E42	E49	S50	A51	E52	D53	E56	V60	L65	N66	Y67	L88	E96	L100	C104	K112	A113	L114	E119	G120	R121	Q135	R138	Q141	R142	E143	E144	E145	E146	E147	E148	E149	E150	E151	E152	E153	E154	E155	E156	E157	E158	E159	E160	E161	E162	E163	E164	E165	E166	E167	E168	E169	E170	E171	E172	E173	E174	E175	E176	E177	E178	E179	E180	E181	E182	E183	E184	E185	E186	E187	E188	E189	E190	E191	E192	E193	E194	E195	E196	E197	E198	E199	E200	E201	E202	E203	E204	E205	E206	E207	E208	E209	E210	E211	E212	E213	E214	E215	E216	E217	E218	E219	E220	E221	E222	E223	E224	E225	E226	E227	E228	E229	E230	E231	E232	E233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245	E246	E247	E248	E249	E250	E251	E252	E253	E254	E255	E256	E257	E258	E259	E260	E261	E262	E263	E264	E265	E266	E267	E268	E269	E270	E271	E272	E273	E274	E275	E276	E277	E278	E279	E280	E281	E282	E283	E284	E285	E286	E287	E288	E289	E290	E291	E292	E293	E294	E295	E296	E297	E298	E299	E300	E301	E302	E303	E304	E305	E306	E307	E308	E309	E310	E311	E312	E313	E314	E315	E316	E317	E318	E319	E320	E321	E322	E323	E324	E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612
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- Chain G:  8% 70% 29%

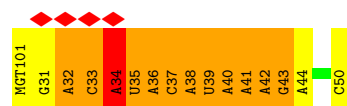
H1	F2	Y3	L13	H14	Y17	K29	V45	T49	D62	G57	V58	P61	G62	R63	K73	V76	F77	R78	P79	F80	H84	V85	D86	A87	H88	V89	T90	Q91	L97	F98	T99	E100	P103	I108	D120	P121	N122	S123	M124	P125	P126	C127	V131
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- Chain O:  62% 9% 17%

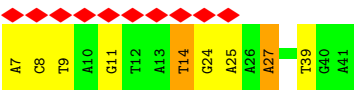
MET	LVS	ARG	THR	ASP	PRO	GLU	CYS	THR	ALA	PRO	LVS	ILE	LVS	LYS	GLN	LYS	LYS	ARG	VAL	ALA	GLU	LEU	ALA	LEU	SER	THR	SER	ASP	GLU	GLY	PRO	PRO	SER	SER	SER	VAL	SER	HIS	GLY	ALA	LYS	ALA	SER	THR	SER	LEU	SER	GLY	SER	ASP	GLU	THR	GLU	GLY			
GLN	HIS	SER	SER	ASP	PHE	ASP	ASP	ALA	PHE	LYS	ALA	ASP	SER	SER	LEU	VAL	GLU	THR	SER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



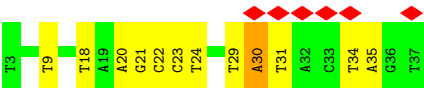
- Molecule 16: RNA (5'-D*(MGT))-R(P*GP*AP*CP*AP*UP*AP*CP*AP*UP*AP*AP*AP*G P*AP*CP*CP*AP*GP*GP*C)-3')



- Molecule 17: DNA (26-MER)



• Molecule 18: DNA (35-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48148	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0221	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, MGT

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	Z	0.40	0/400	0.52	0/541
2	M	0.56	0/2706	0.74	0/3646
3	A	0.41	0/11345	0.62	2/15315 (0.0%)
4	B	0.45	1/9105 (0.0%)	0.61	2/12290 (0.0%)
5	C	0.48	0/2114	0.61	0/2873
6	E	0.40	0/1752	0.60	0/2366
7	F	0.40	0/668	0.56	0/901
8	H	0.45	0/1207	0.64	1/1628 (0.1%)
9	I	0.38	0/973	0.53	0/1316
10	J	0.46	0/542	0.56	0/730
11	K	0.43	0/939	0.64	2/1271 (0.2%)
12	L	0.46	0/395	0.59	0/524
13	D	0.27	0/1012	0.47	0/1366
14	G	0.32	0/1336	0.53	0/1820
15	O	1.17	4/5775 (0.1%)	1.09	21/7785 (0.3%)
16	P	0.69	0/482	2.27	2/749 (0.3%)
17	N	0.72	0/603	1.19	4/927 (0.4%)
18	T	0.93	1/799 (0.1%)	1.11	0/1230
All	All	0.61	6/42153 (0.0%)	0.76	34/57278 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	5
4	B	0	1
14	G	0	1
15	O	0	1
16	P	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	1	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	659	HIS	CE1-NE2	52.37	2.53	1.32
15	O	659	HIS	CD2-NE2	34.64	2.14	1.42
15	O	659	HIS	ND1-CE1	32.45	2.15	1.34
15	O	549	PRO	C-N	14.10	1.66	1.34
18	T	30	DA	O3'-P	-5.98	1.53	1.61

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	34	A	O5'-P-OP1	-43.84	58.09	110.70
16	P	34	A	O5'-P-OP2	-37.32	65.92	110.70
15	O	549	PRO	O-C-N	26.84	165.65	122.70
15	O	549	PRO	CA-C-N	-23.65	65.18	117.20
15	O	549	PRO	C-N-CA	-18.26	76.05	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	P	40	A	C4'

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1108	HIS	Peptide
3	A	1112	VAL	Peptide
3	A	1467	GLY	Peptide
3	A	412	GLN	Peptide
3	A	910	LYS	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	Z	397	0	403	31	0
2	M	2649	0	2658	187	0
3	A	11142	0	11286	222	0
4	B	8928	0	8945	214	0
5	C	2071	0	2016	42	0
6	E	1721	0	1737	42	0
7	F	658	0	684	17	0
8	H	1186	0	1147	28	0
9	I	950	0	880	20	0
10	J	533	0	553	7	0
11	K	920	0	942	14	0
12	L	389	0	395	9	0
13	D	998	0	953	13	0
14	G	1305	0	1264	150	0
15	O	5643	0	5592	220	0
16	P	462	0	234	39	0
17	N	538	0	296	33	0
18	T	714	0	397	47	0
19	A	1	0	0	0	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
All	All	41213	0	40382	1004	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 12.

The worst 5 of 1004 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)
14:G:125:PRO:HG3	15:O:655:ILE:CG1	1.18	1.60
14:G:170:LEU:CD2	15:O:650:LYS:HA	1.36	1.53
14:G:170:LEU:HD23	15:O:650:LYS:CA	1.32	1.53
6:E:112:PRO:CG	18:T:9:DT:H5''	1.47	1.45
14:G:137:ILE:HA	15:O:725:LYS:NZ	1.11	1.38

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	Z	50/1087 (5%)	48 (96%)	2 (4%)	0	100	100
2	M	325/597 (54%)	308 (95%)	17 (5%)	0	100	100
3	A	1395/1970 (71%)	1298 (93%)	96 (7%)	1 (0%)	51	84
4	B	1102/1174 (94%)	1030 (94%)	72 (6%)	0	100	100
5	C	254/275 (92%)	242 (95%)	12 (5%)	0	100	100
6	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
7	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
8	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
9	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	D	127/142 (89%)	120 (94%)	7 (6%)	0	100	100
14	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
15	O	693/835 (83%)	666 (96%)	25 (4%)	2 (0%)	41	75
All	All	4885/7106 (69%)	4611 (94%)	271 (6%)	3 (0%)	54	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	O	294	HIS
3	A	1108	HIS
15	O	230	VAL

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	Z	45/940 (5%)	45 (100%)	0	100	100
2	M	297/534 (56%)	268 (90%)	29 (10%)	8	31
3	A	1238/1749 (71%)	1222 (99%)	16 (1%)	69	82
4	B	979/1027 (95%)	963 (98%)	16 (2%)	62	79
5	C	235/252 (93%)	232 (99%)	3 (1%)	69	82
6	E	191/192 (100%)	189 (99%)	2 (1%)	76	86
7	F	71/111 (64%)	71 (100%)	0	100	100
8	H	129/131 (98%)	127 (98%)	2 (2%)	62	79
9	I	105/112 (94%)	102 (97%)	3 (3%)	42	65
10	J	56/56 (100%)	55 (98%)	1 (2%)	59	77
11	K	104/106 (98%)	103 (99%)	1 (1%)	76	86
12	L	43/55 (78%)	42 (98%)	1 (2%)	50	71
13	D	104/126 (82%)	104 (100%)	0	100	100
14	G	138/153 (90%)	138 (100%)	0	100	100
15	O	623/741 (84%)	598 (96%)	25 (4%)	31	58
All	All	4358/6285 (69%)	4259 (98%)	99 (2%)	53	71

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	650	ASN
10	J	47	ARG
4	B	1003	ASN
6	E	168	ASN
15	O	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	315	ASN
15	O	352	ASN
4	B	842	HIS
14	G	14	HIS
9	I	32	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	19/21 (90%)	12 (63%)	7 (36%)

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	32	A
16	P	33	C
16	P	34	A
16	P	35	U
16	P	36	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	37	C
16	P	39	U
16	P	42	A
16	P	40	A
16	P	36	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	P	1
17	N	1
15	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	101:MGT	O3'	31:G	P	51.64
1	N	14:DT	O3'	24:DG	P	27.51
1	O	549:PRO	C	550:SER	N	1.66

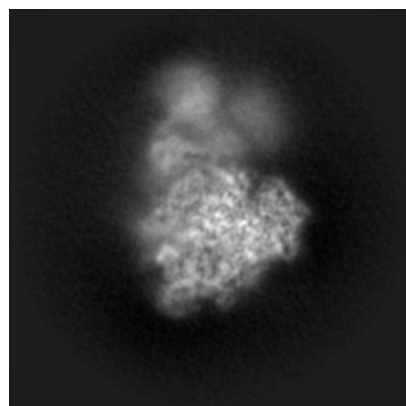
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17407. These allow visual inspection of the internal detail of the map and identification of artifacts.

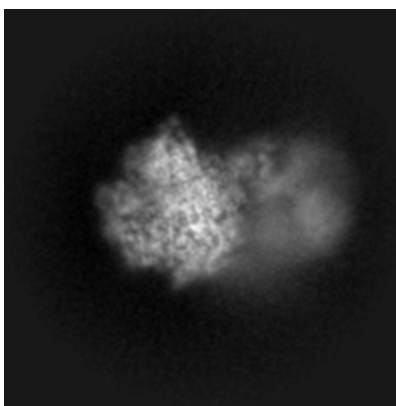
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

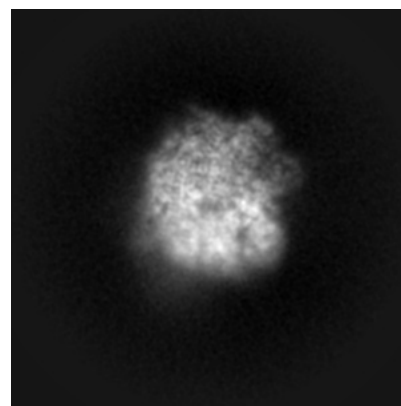
6.1.1 Primary map



X

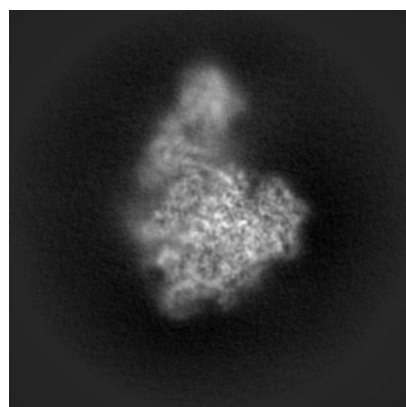


Y

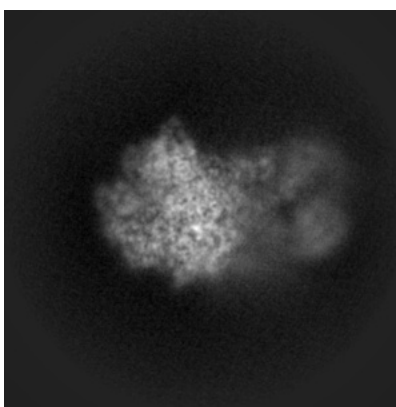


Z

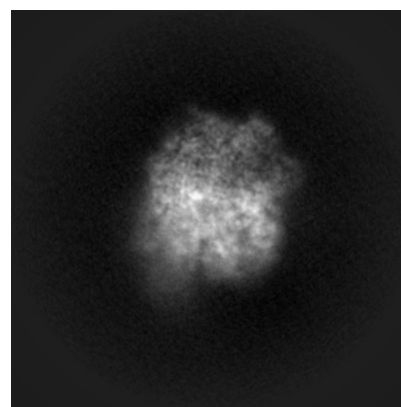
6.1.2 Raw map



X



Y

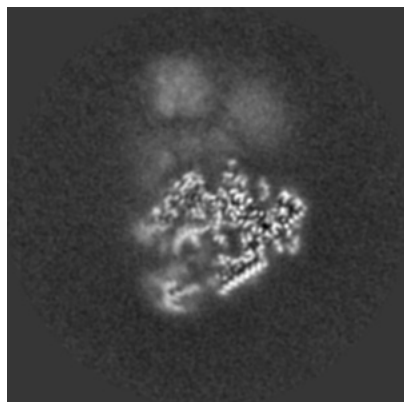


Z

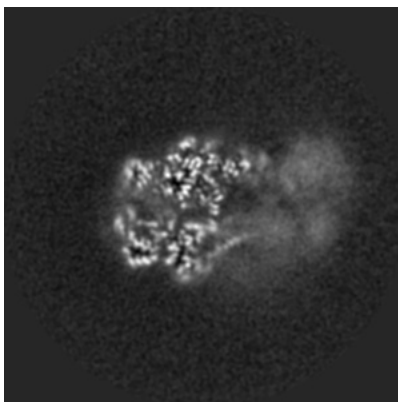
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

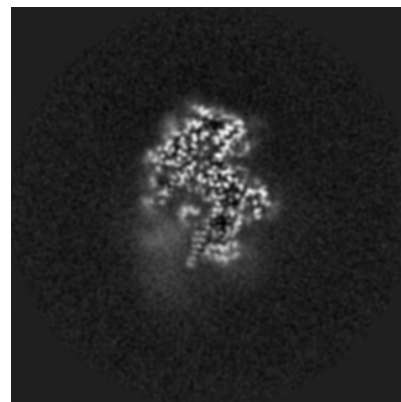
6.2.1 Primary map



X Index: 150

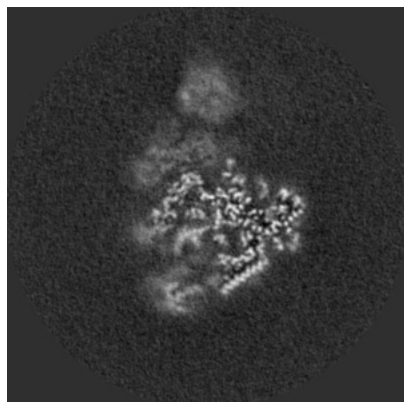


Y Index: 150

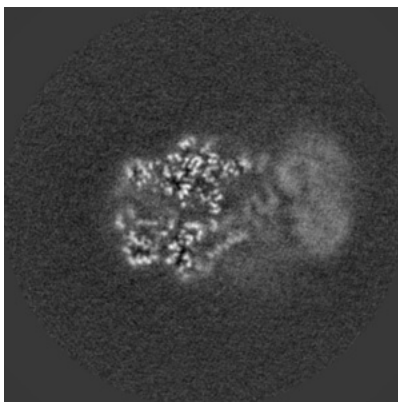


Z Index: 150

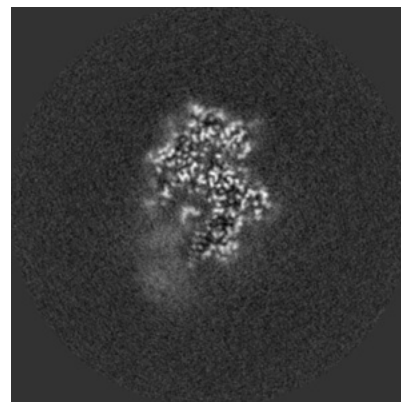
6.2.2 Raw map



X Index: 150



Y Index: 150

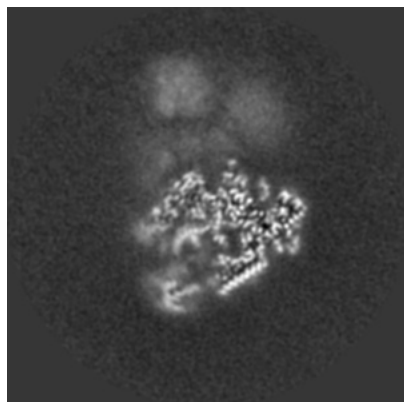


Z Index: 150

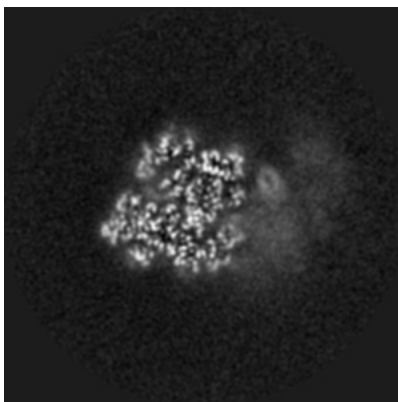
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

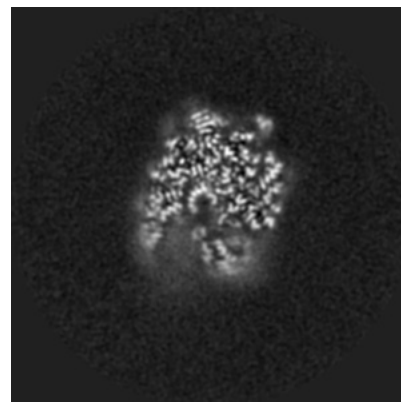
6.3.1 Primary map



X Index: 150

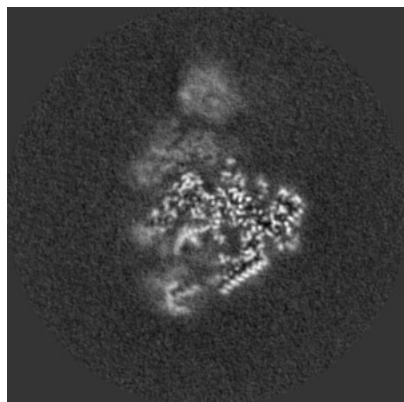


Y Index: 161

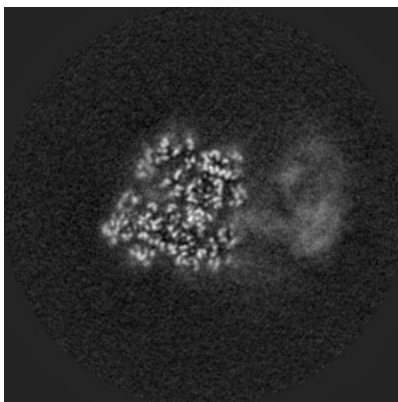


Z Index: 139

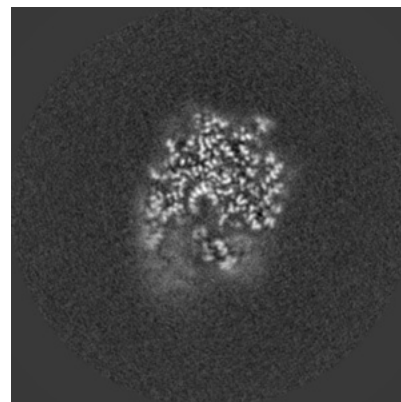
6.3.2 Raw map



X Index: 151



Y Index: 161

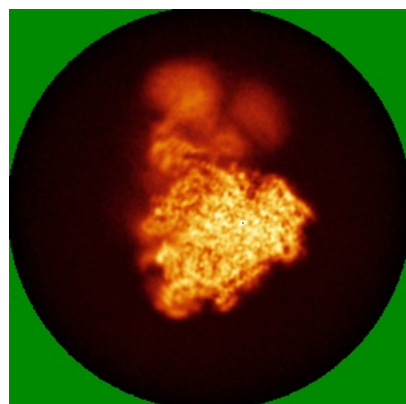


Z Index: 139

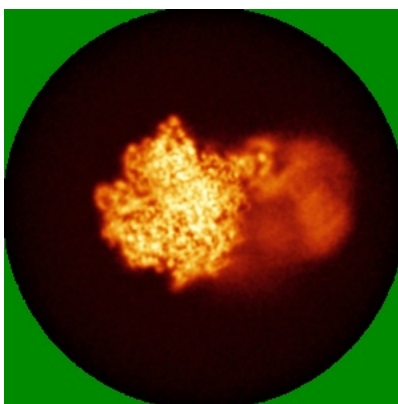
The images above show the largest variance slices of the map in three orthogonal directions.

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

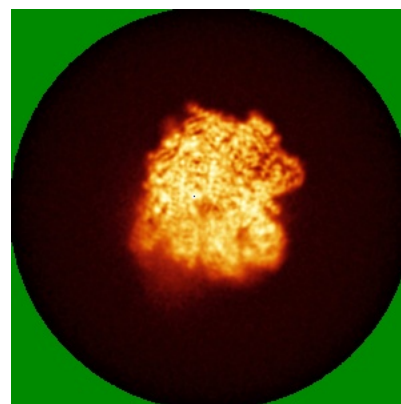
6.4.1 Primary map



X



Y

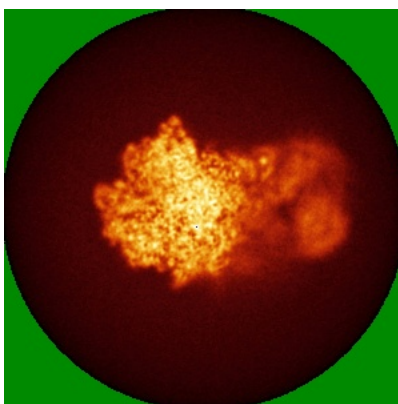


Z

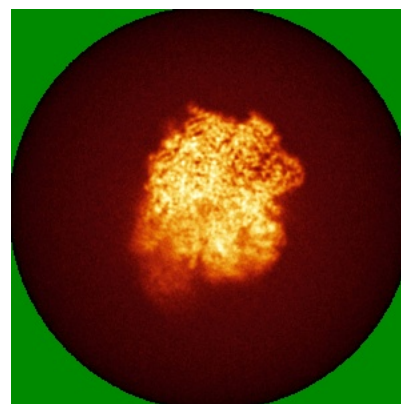
6.4.2 Raw map



X



Y

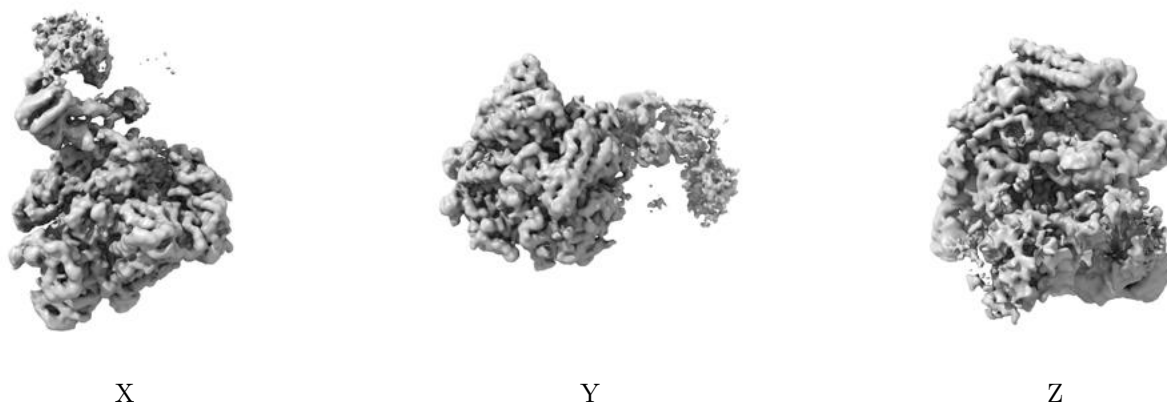


Z

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.

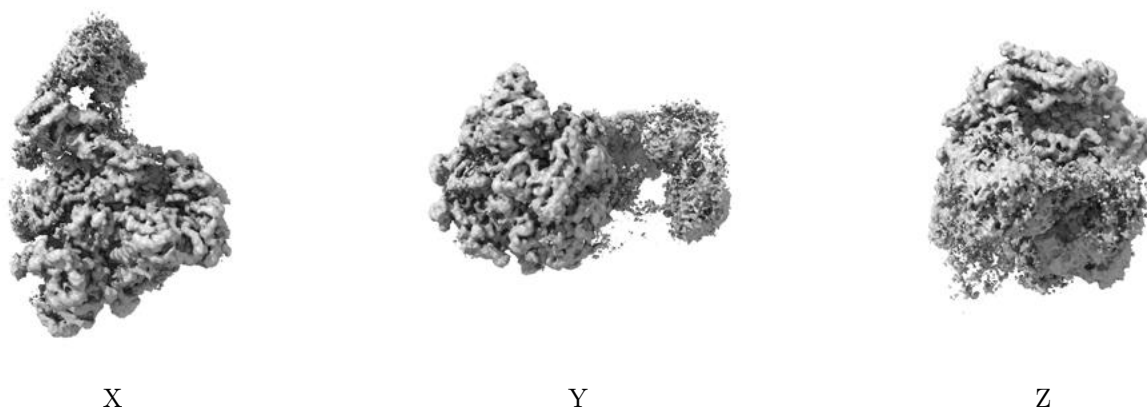
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0221. 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.

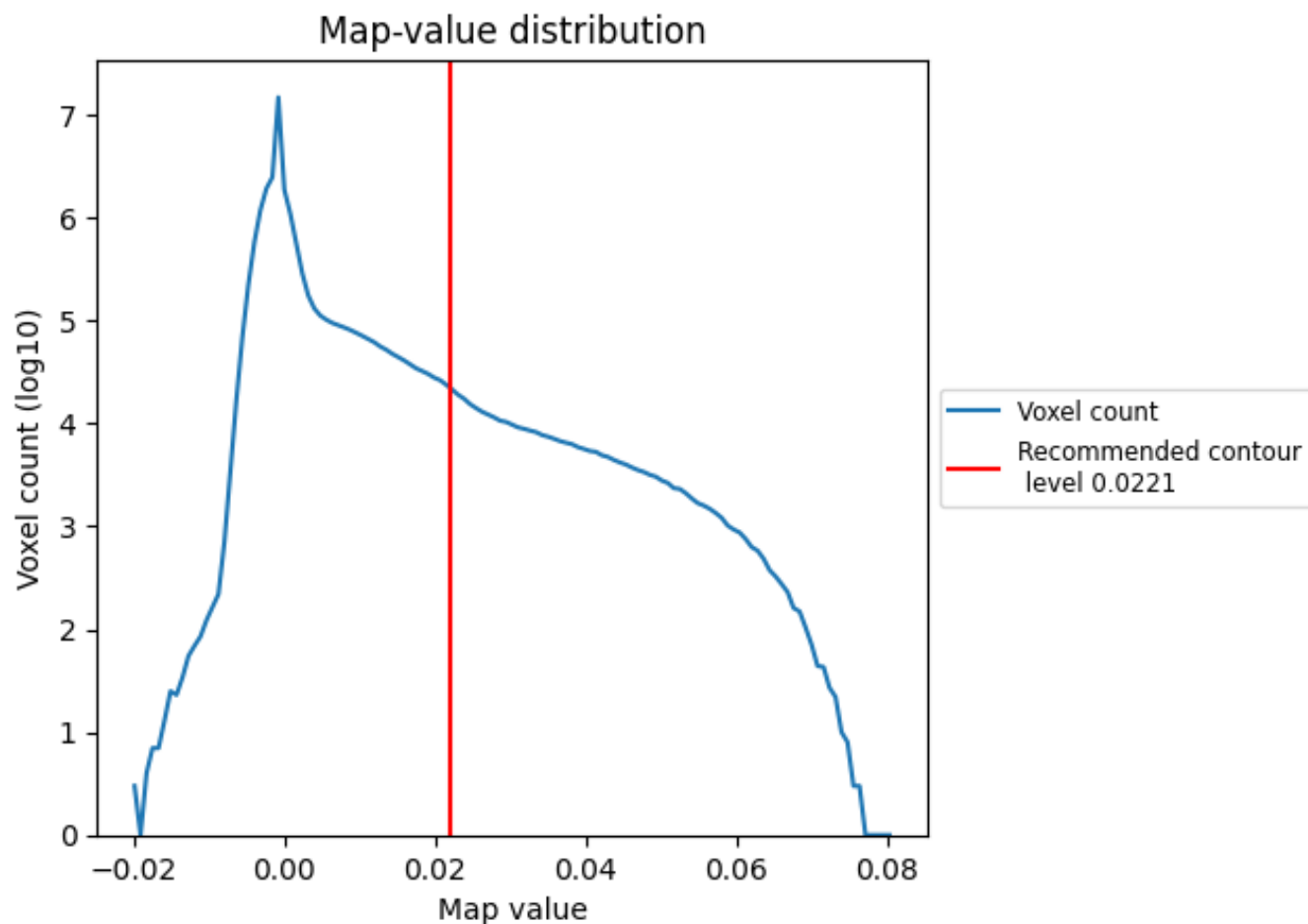
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

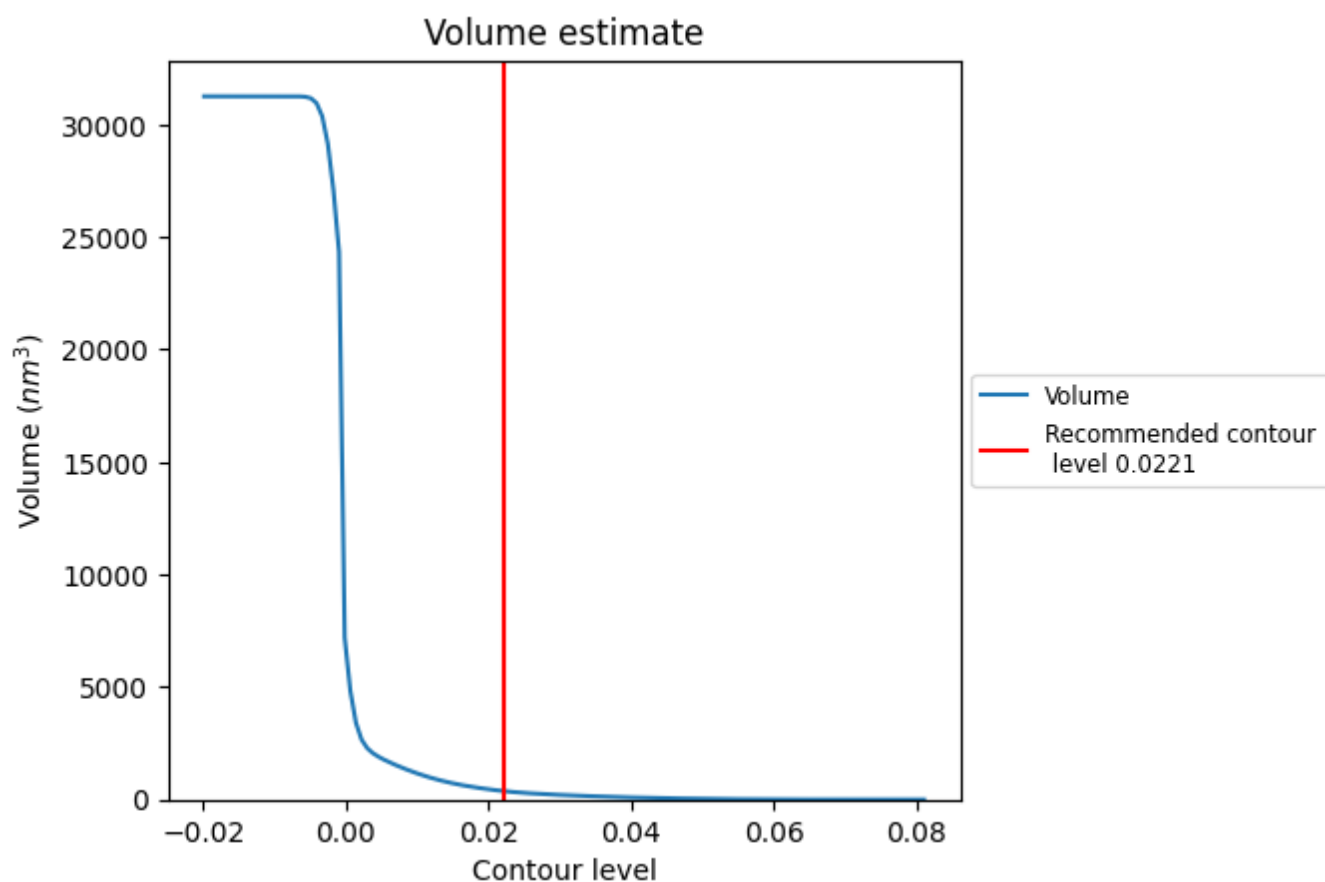
This section contains the results of statistical analysis of the map.

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.

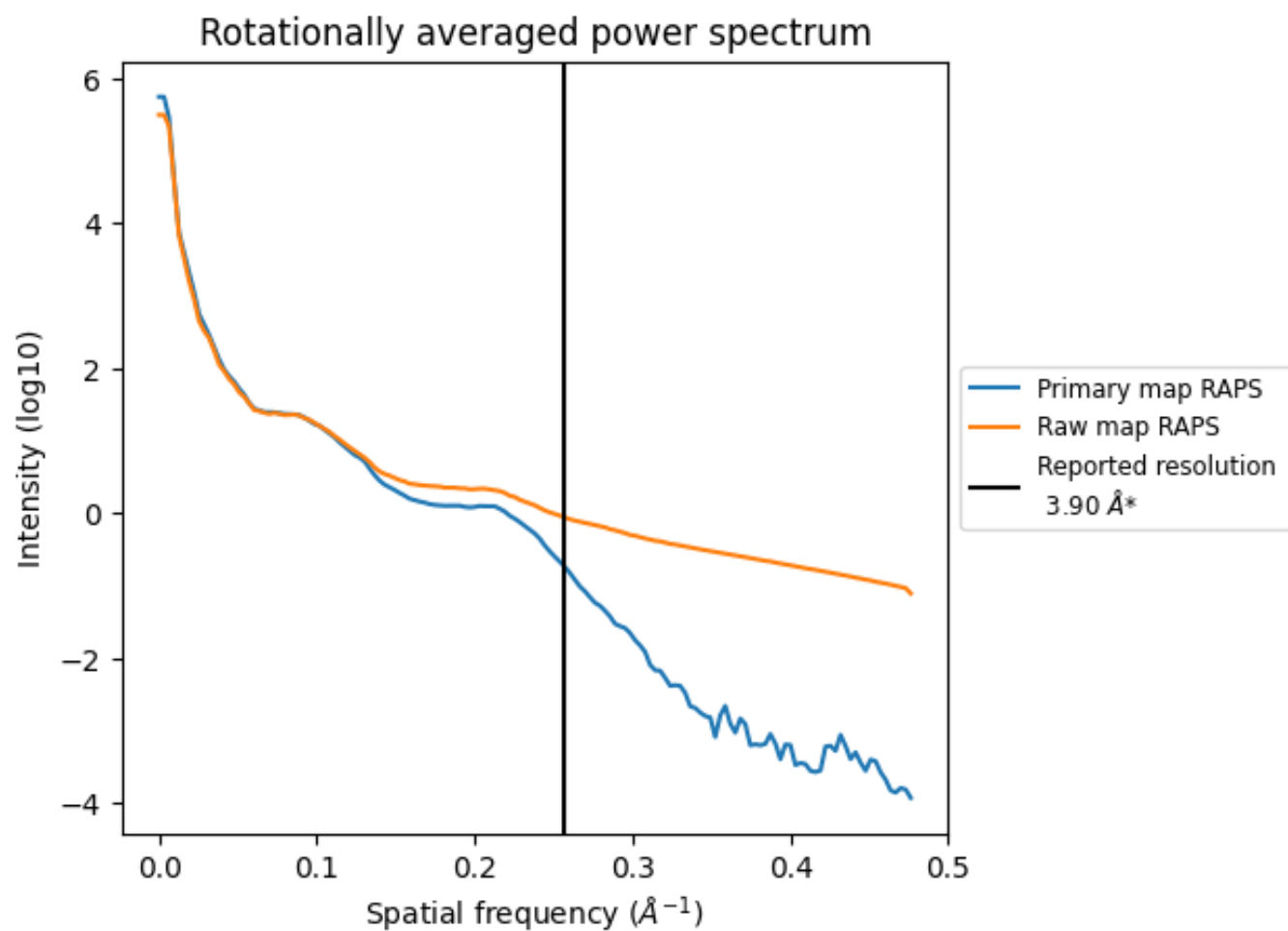
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 379 nm³; this corresponds to an approximate mass of 342 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 ⓘ

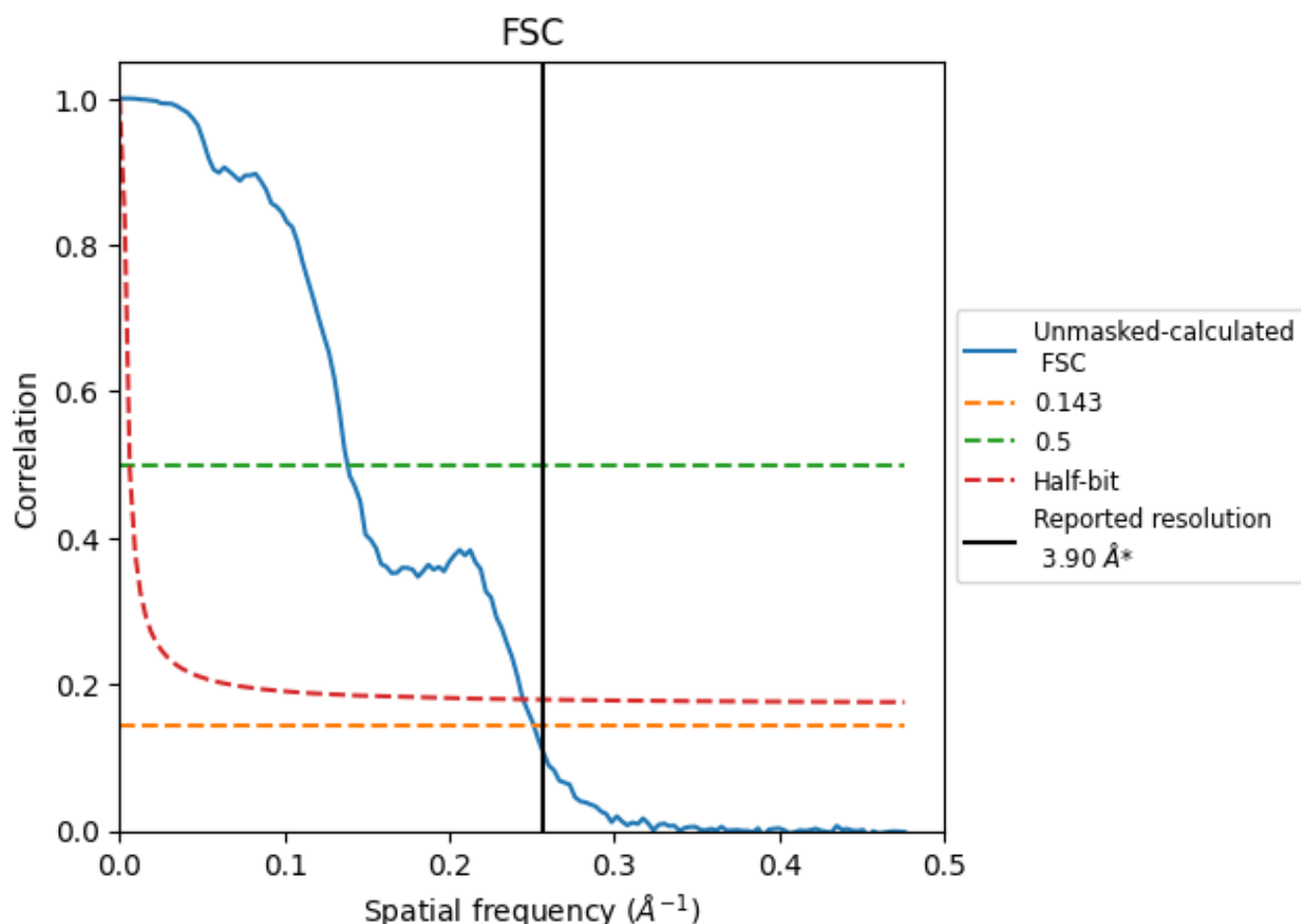


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

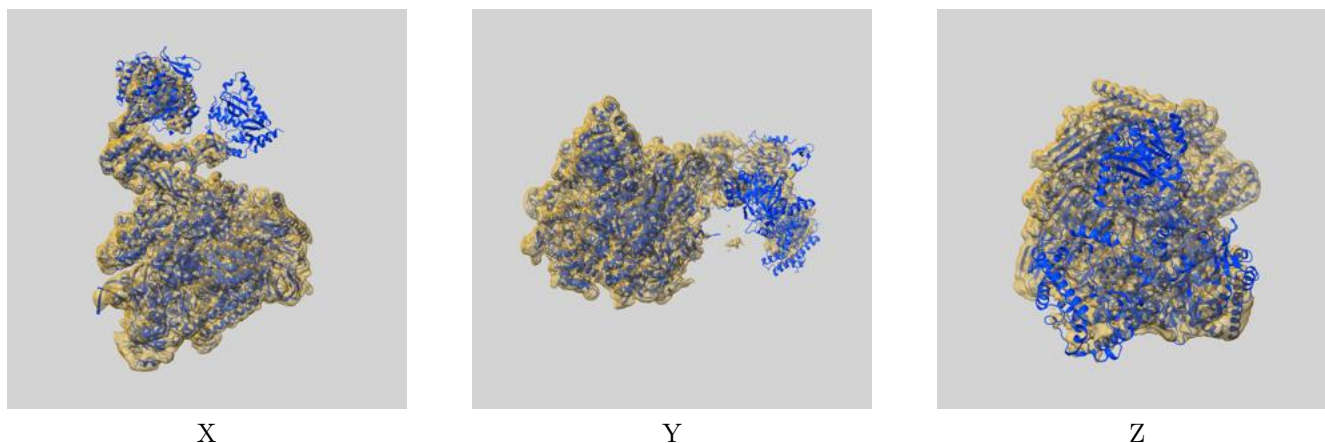
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	7.23	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

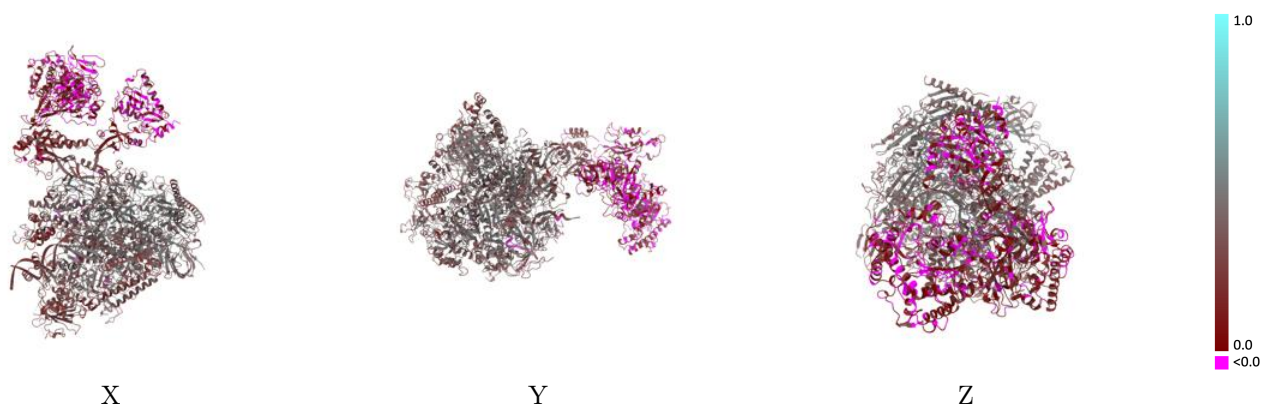
This section contains information regarding the fit between EMDB map EMD-17407 and PDB model 8P4E. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



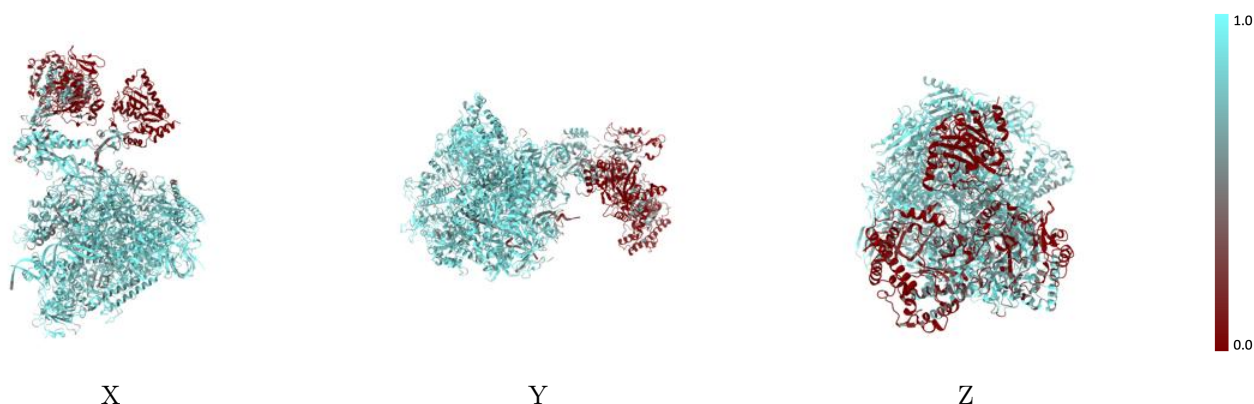
The images above show the 3D surface view of the map at the recommended contour level 0.0221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



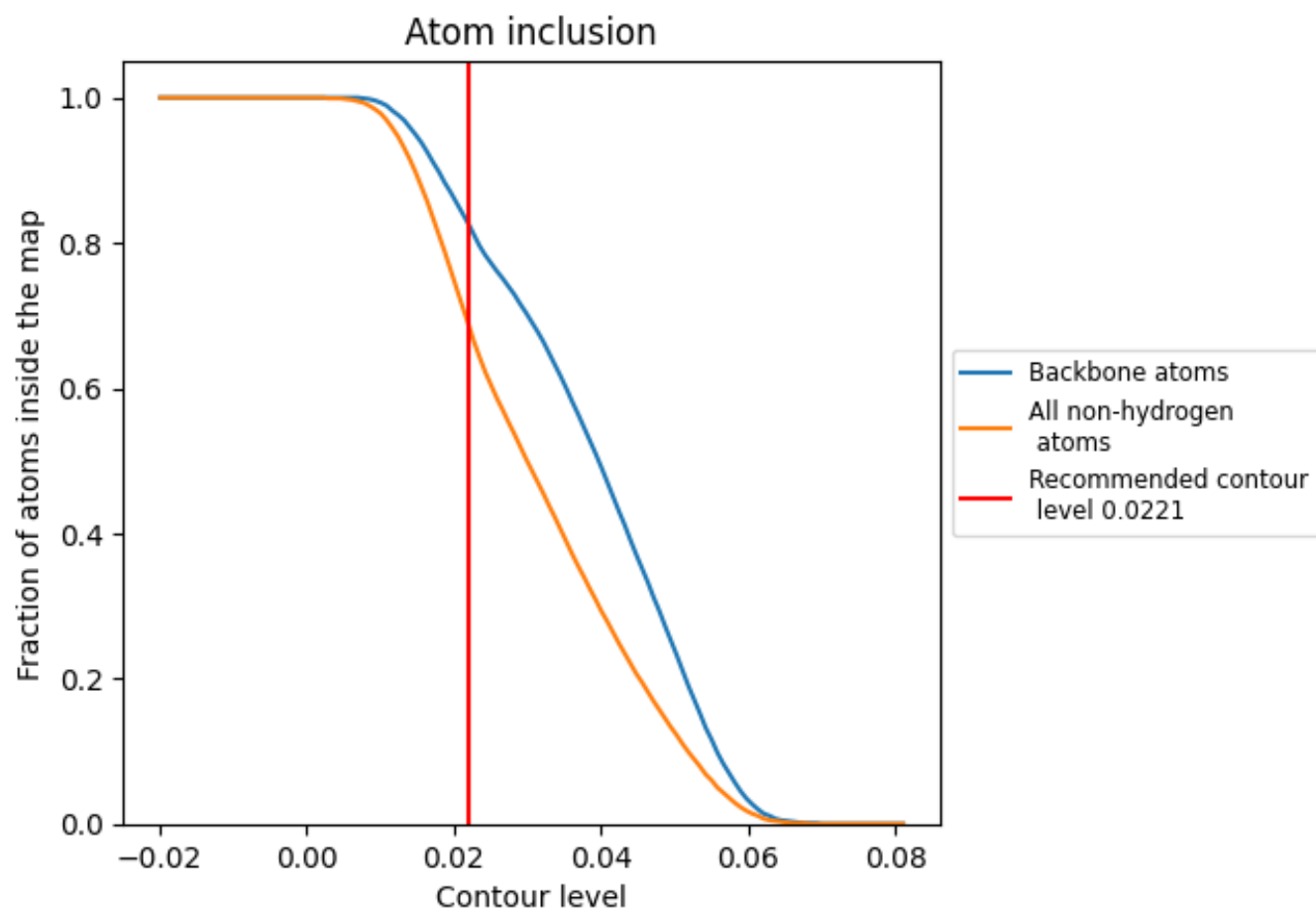
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0221).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.0221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6860	 0.2970
A	 0.8160	 0.3630
B	 0.8340	 0.3820
C	 0.8530	 0.4020
D	 0.7220	 0.1970
E	 0.8360	 0.3340
F	 0.8190	 0.3890
G	 0.7440	 0.2530
H	 0.8340	 0.3920
I	 0.8280	 0.3200
J	 0.8580	 0.4020
K	 0.8490	 0.4020
L	 0.8100	 0.3500
M	 0.1100	 0.0650
N	 0.6130	 0.2020
O	 0.2200	 0.0600
P	 0.7040	 0.2650
T	 0.7590	 0.2700
Z	 0.5740	 0.4180

