



Full wwPDB EM Validation Report ⓘ

Dec 22, 2024 – 06:22 am GMT

PDB ID : 9FD2
EMDB ID : EMD-50325
Title : Structure of Pol II-TC-NER-STK19 complex
Authors : Lee, S.-H.; Sixma, T.K.
Deposited on : 2024-05-16
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

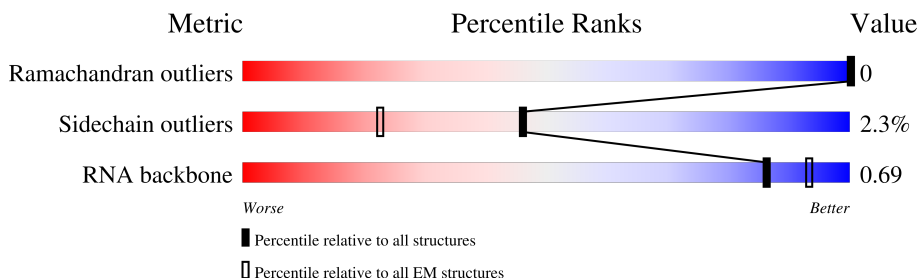
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.40 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1970	
2	B	1300	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	f	85	
14	N	60	
15	M	25	
16	T	60	
17	a	408	
18	b	1160	
19	c	152	
20	g	257	
21	e	1493	
22	d	729	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 51949 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1409	Total	C	N	O	S	0	0
			11161	7022	1998	2070	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1130	Total	C	N	O	S	0	0
			9048	5725	1591	1668	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	260	Total	C	N	O	S	0	0
			2089	1309	359	415	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- 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
			949	587	169	182	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, I and III subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	f	64	Total	C	N	O	S	0	0
			505	312	81	105	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-1	GLY	-	expression tag	UNP P60002
f	0	ALA	-	expression tag	UNP P60002

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	40	Total	C	N	O	P	0	0
			831	393	162	236	40		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	54	Total	C	N	O	P	0	0
			1091	521	187	329	54		

- Molecule 17 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	377	Total	C	N	O	S	0	0
			2951	1842	520	570	19		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	397	GLY	-	expression tag	UNP Q13216
a	398	THR	-	expression tag	UNP Q13216
a	399	SER	-	expression tag	UNP Q13216
a	400	ALA	-	expression tag	UNP Q13216
a	401	TRP	-	expression tag	UNP Q13216
a	402	SER	-	expression tag	UNP Q13216
a	403	HIS	-	expression tag	UNP Q13216
a	404	PRO	-	expression tag	UNP Q13216
a	405	GLN	-	expression tag	UNP Q13216
a	406	PHE	-	expression tag	UNP Q13216
a	407	GLU	-	expression tag	UNP Q13216
a	408	LYS	-	expression tag	UNP Q13216

- Molecule 18 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	814	Total	C	N	O	S	0	0
			6405	4059	1079	1231	36		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-19	MET	-	initiating methionine	UNP Q16531
b	-18	ALA	-	expression tag	UNP Q16531
b	-17	HIS	-	expression tag	UNP Q16531
b	-16	HIS	-	expression tag	UNP Q16531
b	-15	HIS	-	expression tag	UNP Q16531
b	-14	HIS	-	expression tag	UNP Q16531
b	-13	HIS	-	expression tag	UNP Q16531
b	-12	HIS	-	expression tag	UNP Q16531
b	-11	SER	-	expression tag	UNP Q16531
b	-10	ALA	-	expression tag	UNP Q16531
b	-9	ALA	-	expression tag	UNP Q16531
b	-8	LEU	-	expression tag	UNP Q16531
b	-7	GLU	-	expression tag	UNP Q16531
b	-6	VAL	-	expression tag	UNP Q16531
b	-5	LEU	-	expression tag	UNP Q16531
b	-4	PHE	-	expression tag	UNP Q16531
b	-3	GLN	-	expression tag	UNP Q16531
b	-2	GLY	-	expression tag	UNP Q16531
b	-1	PRO	-	expression tag	UNP Q16531
b	0	GLY	-	expression tag	UNP Q16531

- Molecule 19 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	c	36	Total	C	N	O	0	0
			302	199	49	54		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	103	ASP	-	expression tag	UNP Q9BW61
c	104	VAL	-	expression tag	UNP Q9BW61
c	105	LEU	-	expression tag	UNP Q9BW61
c	106	PHE	-	expression tag	UNP Q9BW61
c	107	GLN	-	expression tag	UNP Q9BW61

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Chain	Residue	Modelled	Actual	Comment	Reference
c	108	GLY	-	expression tag	UNP Q9BW61
c	109	PRO	-	expression tag	UNP Q9BW61
c	110	GLY	-	expression tag	UNP Q9BW61
c	111	ALA	-	expression tag	UNP Q9BW61
c	112	TRP	-	expression tag	UNP Q9BW61
c	113	SER	-	expression tag	UNP Q9BW61
c	114	HIS	-	expression tag	UNP Q9BW61
c	115	PRO	-	expression tag	UNP Q9BW61
c	116	GLN	-	expression tag	UNP Q9BW61
c	117	PHE	-	expression tag	UNP Q9BW61
c	118	GLU	-	expression tag	UNP Q9BW61
c	119	LYS	-	expression tag	UNP Q9BW61
c	120	GLY	-	expression tag	UNP Q9BW61
c	121	GLY	-	expression tag	UNP Q9BW61
c	122	GLY	-	expression tag	UNP Q9BW61
c	123	SER	-	expression tag	UNP Q9BW61
c	124	GLY	-	expression tag	UNP Q9BW61
c	125	GLY	-	expression tag	UNP Q9BW61
c	126	GLY	-	expression tag	UNP Q9BW61
c	127	SER	-	expression tag	UNP Q9BW61
c	128	GLY	-	expression tag	UNP Q9BW61
c	129	GLY	-	expression tag	UNP Q9BW61
c	130	GLY	-	expression tag	UNP Q9BW61
c	131	SER	-	expression tag	UNP Q9BW61
c	132	TRP	-	expression tag	UNP Q9BW61
c	133	SER	-	expression tag	UNP Q9BW61
c	134	HIS	-	expression tag	UNP Q9BW61
c	135	PRO	-	expression tag	UNP Q9BW61
c	136	GLN	-	expression tag	UNP Q9BW61
c	137	PHE	-	expression tag	UNP Q9BW61
c	138	GLU	-	expression tag	UNP Q9BW61
c	139	LYS	-	expression tag	UNP Q9BW61
c	140	GLY	-	expression tag	UNP Q9BW61
c	141	ALA	-	expression tag	UNP Q9BW61
c	142	SER	-	expression tag	UNP Q9BW61
c	143	GLY	-	expression tag	UNP Q9BW61
c	144	GLU	-	expression tag	UNP Q9BW61
c	145	ASP	-	expression tag	UNP Q9BW61
c	146	TYR	-	expression tag	UNP Q9BW61
c	147	LYS	-	expression tag	UNP Q9BW61
c	148	ASP	-	expression tag	UNP Q9BW61
c	149	ASP	-	expression tag	UNP Q9BW61

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Chain	Residue	Modelled	Actual	Comment	Reference
c	150	ASP	-	expression tag	UNP Q9BW61
c	151	ASP	-	expression tag	UNP Q9BW61
c	152	LYS	-	expression tag	UNP Q9BW61

- Molecule 20 is a protein called Inactive serine/threonine-protein kinase 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	g	220	Total	C	N	O	S	0	0
			1721	1098	308	309	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-2	GLY	-	expression tag	UNP P49842
g	-1	PRO	-	expression tag	UNP P49842
g	0	GLY	-	expression tag	UNP P49842

- Molecule 21 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	590	Total	C	N	O	S	0	0
			4820	3091	847	859	23		

- Molecule 22 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	249	Total	C	N	O	S	0	0
			2040	1274	397	361	8		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-19	MET	-	initiating methionine	UNP Q2YD98
d	-18	ALA	-	expression tag	UNP Q2YD98
d	-17	HIS	-	expression tag	UNP Q2YD98
d	-16	HIS	-	expression tag	UNP Q2YD98
d	-15	HIS	-	expression tag	UNP Q2YD98
d	-14	HIS	-	expression tag	UNP Q2YD98
d	-13	HIS	-	expression tag	UNP Q2YD98
d	-12	HIS	-	expression tag	UNP Q2YD98
d	-11	SER	-	expression tag	UNP Q2YD98

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Chain	Residue	Modelled	Actual	Comment	Reference
d	-10	ALA	-	expression tag	UNP Q2YD98
d	-9	ALA	-	expression tag	UNP Q2YD98
d	-8	LEU	-	expression tag	UNP Q2YD98
d	-7	GLU	-	expression tag	UNP Q2YD98
d	-6	VAL	-	expression tag	UNP Q2YD98
d	-5	LEU	-	expression tag	UNP Q2YD98
d	-4	PHE	-	expression tag	UNP Q2YD98
d	-3	GLN	-	expression tag	UNP Q2YD98
d	-2	GLY	-	expression tag	UNP Q2YD98
d	-1	PRO	-	expression tag	UNP Q2YD98
d	0	GLY	-	expression tag	UNP Q2YD98

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

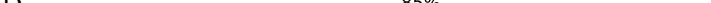
Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total 2	Zn 2	0
23	B	1	Total 1	Zn 1	0
23	C	1	Total 1	Zn 1	0
23	I	2	Total 2	Zn 2	0
23	J	1	Total 1	Zn 1	0
23	L	1	Total 1	Zn 1	0
23	f	1	Total 1	Zn 1	0
23	d	1	Total 1	Zn 1	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:  6% 85% 13%

[illegible]

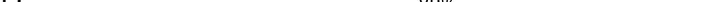
Protein	Residue	Category	Score
PR0	GLY	Non-Conserved	0.00
	SER	Non-Conserved	0.00
	CYS	Non-Conserved	0.00
	ALA	Non-Conserved	0.00
	ASN	Non-Conserved	0.00
	MET	Non-Conserved	0.00
	TYR	Non-Conserved	0.00
	ASP	Non-Conserved	0.00
	ALA	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
ASP	ASP	Non-Conserved	0.00
	MET	Non-Conserved	0.00
	GLN	Non-Conserved	0.00
	TYR	Non-Conserved	0.00
	ASP	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	ASP	Non-Conserved	0.00
	ASP	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
GLU	GLU	Non-Conserved	0.00
	VAL	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
	GLU	Non-Conserved	0.00
P81	P81	Conserved	0.99
	P82	Conserved	0.99
	P83	Conserved	0.99
	Y84	Conserved	0.99
	L85	Conserved	0.99
	E89	Conserved	0.99
	E100	Conserved	0.99
	R101	Conserved	0.99
	D102	Conserved	0.99
	G103	Conserved	0.99
V132	V132	Conserved	0.99
	D424	Conserved	0.99
	R425	Conserved	0.99
	G426	Conserved	0.99
	K421	Conserved	0.99
	A419	Conserved	0.99
	Q420	Conserved	0.99
	E414	Conserved	0.99
	D394	Conserved	0.99
	E333	Conserved	0.99
D306	D306	Conserved	0.99
	N319	Conserved	0.99
	F320	Conserved	0.99
	G325	Conserved	0.99
	A326	Conserved	0.99
	E293	Conserved	0.99
	E251	Conserved	0.99
	I252	Conserved	0.99
	G253	Conserved	0.99
	Q254	Conserved	0.99
R255	R255	Conserved	0.99
	E516	Conserved	0.99
	E503	Conserved	0.99
	L495	Conserved	0.99
	G493	Conserved	0.99
	G494	Conserved	0.99
	D492	Conserved	0.99
	R491	Conserved	0.99
	A462	Conserved	0.99
	Q461	Conserved	0.99
H460	Conserved	0.99	
K457	K457	Conserved	0.99
	K458	Conserved	0.99
	A459	Conserved	0.99
	H460	Conserved	0.99
	Q461	Conserved	0.99
	A462	Conserved	0.99
	S228	Conserved	0.99
	S229	Conserved	0.99
	R230	Conserved	0.99
	R242	Conserved	0.99
GLY	GLY	Non-Conserved	0.00
	GLN	Non-Conserved	0.00
	GLY	Non-Conserved	0.00
	ALA	Non-Conserved	0.00
	LYS	Non-Conserved	0.00
	LYS	Non-Conserved	0.00
	LYS	Non-Conserved	0.00
	SER	Non-Conserved	0.00
	A251	Conserved	0.99
	I252	Conserved	0.99
G253	Conserved	0.99	
Q254	Q254	Conserved	0.99
	E293	Conserved	0.99
	D306	Conserved	0.99
	N319	Conserved	0.99
	F320	Conserved	0.99
	G325	Conserved	0.99
	A326	Conserved	0.99
	E333	Conserved	0.99
	D394	Conserved	0.99
	E414	Conserved	0.99
A419	A419	Conserved	0.99
	Q420	Conserved	0.99
	K421	Conserved	0.99
	D424	Conserved	0.99
	R425	Conserved	0.99
	G426	Conserved	0.99
	H842	Conserved	0.99
	L873	Conserved	0.99
	P874	Conserved	0.99
	R834	R834	Conserved
Q838		Conserved	0.99
E826		Conserved	0.99
Q825		Conserved	0.99
D824		Conserved	0.99
F823		Conserved	0.99
G821		Conserved	0.99
K820		Conserved	0.99
S813		Conserved	0.99
C890		Conserved	0.99
E686	E686	Conserved	0.99
	K630	Conserved	0.99
	W548	Conserved	0.99
	K566	Conserved	0.99
	Q582	Conserved	0.99
	E516	Conserved	0.99
	E503	Conserved	0.99
	L495	Conserved	0.99
	G493	Conserved	0.99
	D492	Conserved	0.99
R491	Conserved	0.99	
A462	A462	Conserved	

- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 93% 5%

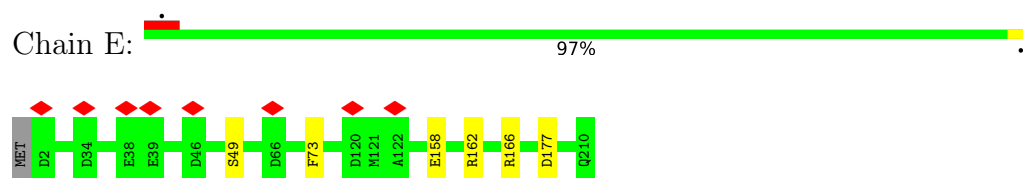
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P2	100
D61	100
E62	100
F63	100
E91	100
E92	100
R126	100
R133	100
M134	100
ARG	100
ASP	100
ASN	100
ASP	100
PRO	100
SER	100
ASP	100
TYR	100
VAL	100
E144	100
Q145	100
D214	100
R228	100
E234	100
S238	100
D270	100
VAL	100
LEU	100
THR	100
ILE	100
ASN	100

- Molecule 4: RNA polymerase II subunit D

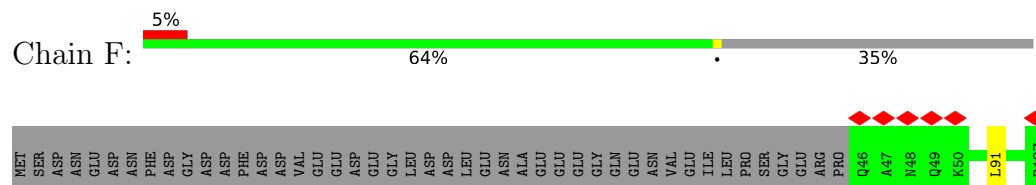
Chain D:  80% 89% 10%

[illegible]

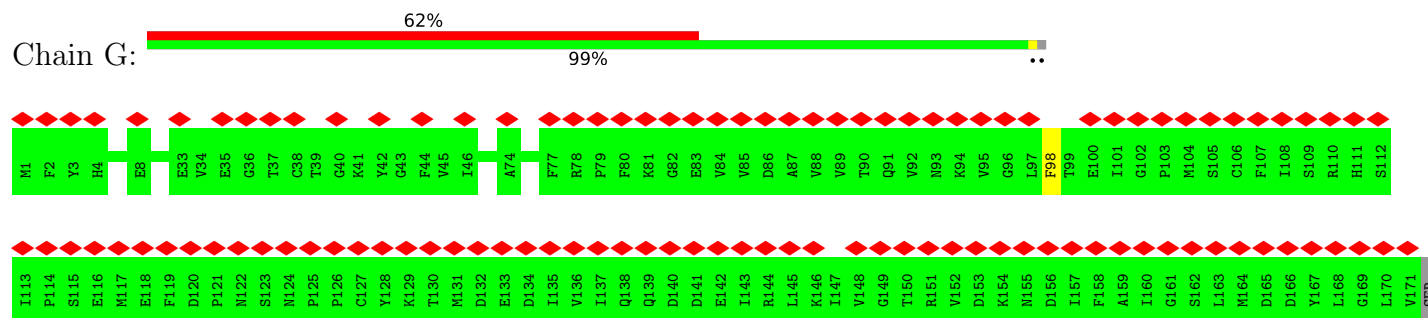
- Molecule 5: DNA-directed RNA polymerase II subunit E



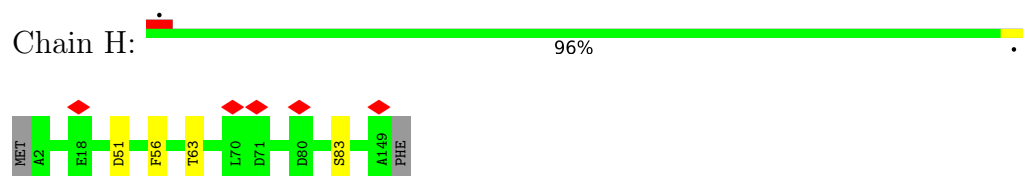
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



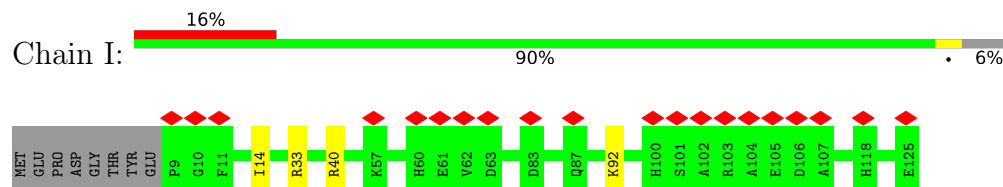
- Molecule 7: DNA-directed RNA polymerase subunit



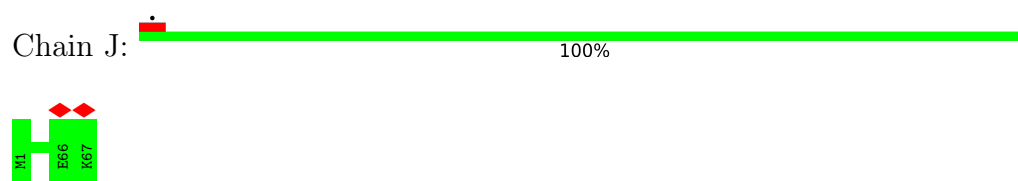
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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

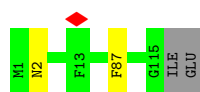


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5




- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  97%



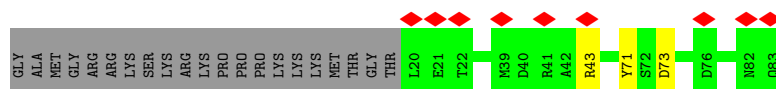
- Molecule 12: RNA polymerase II, I and III subunit K

Chain L:  9% 76% 21%



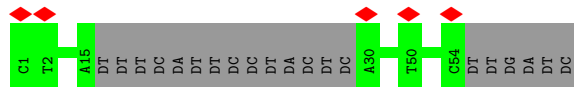
- Molecule 13: Transcription elongation factor 1 homolog

Chain f:  11% 72% 25%



- Molecule 14: Non-template DNA

Chain N:  8% 67% 33%

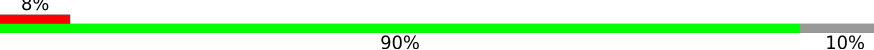


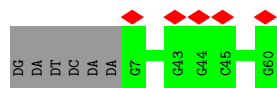
- Molecule 15: RNA

Chain M:  36% 60%




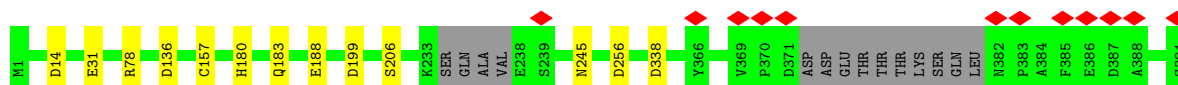
- Molecule 16: Template DNA

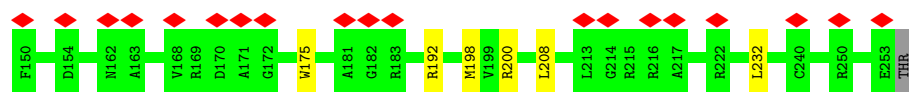
Chain T:  8% 90% 10%



- Molecule 17: DNA excision repair protein ERCC-8

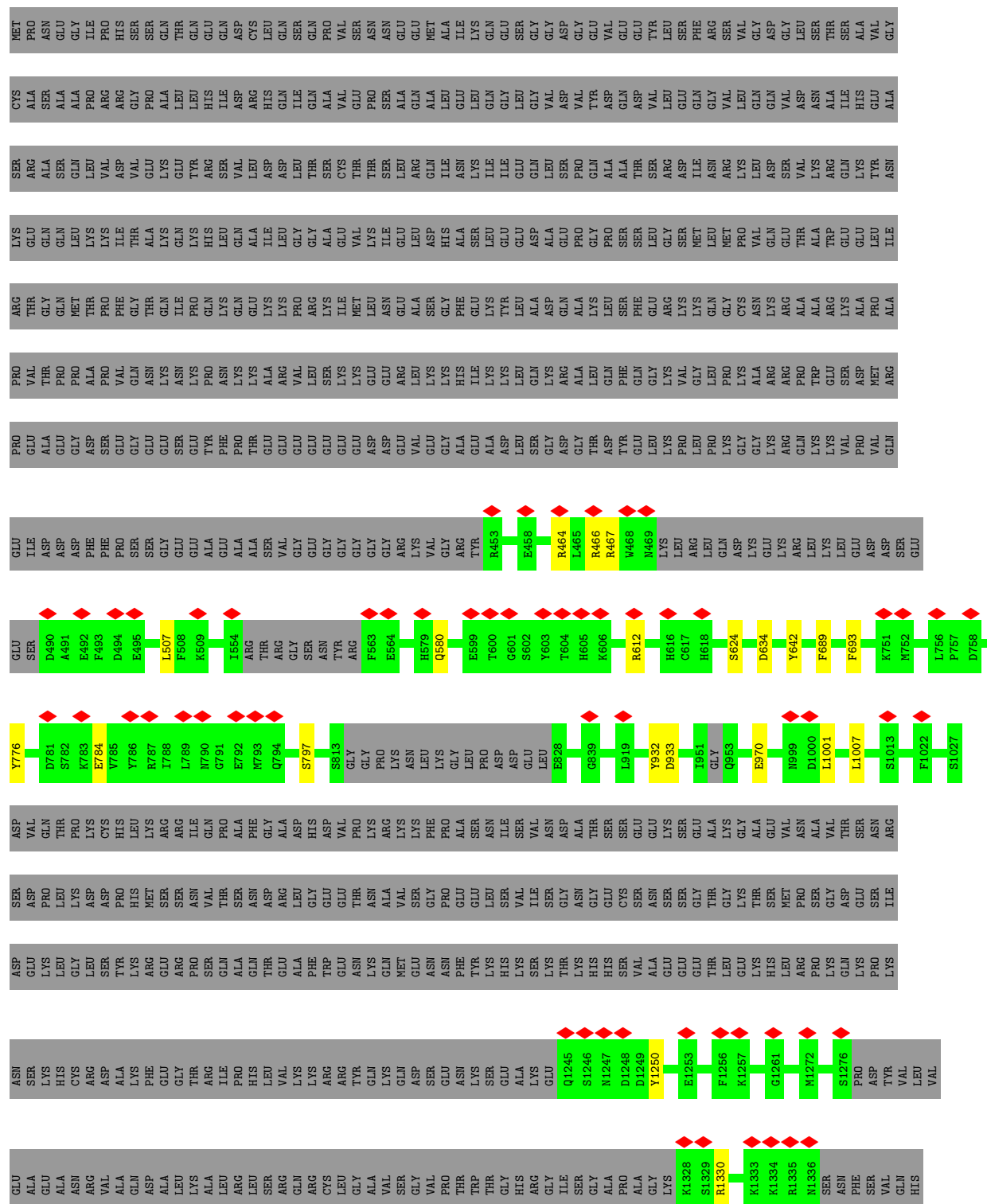
Chain a:  89% 8%



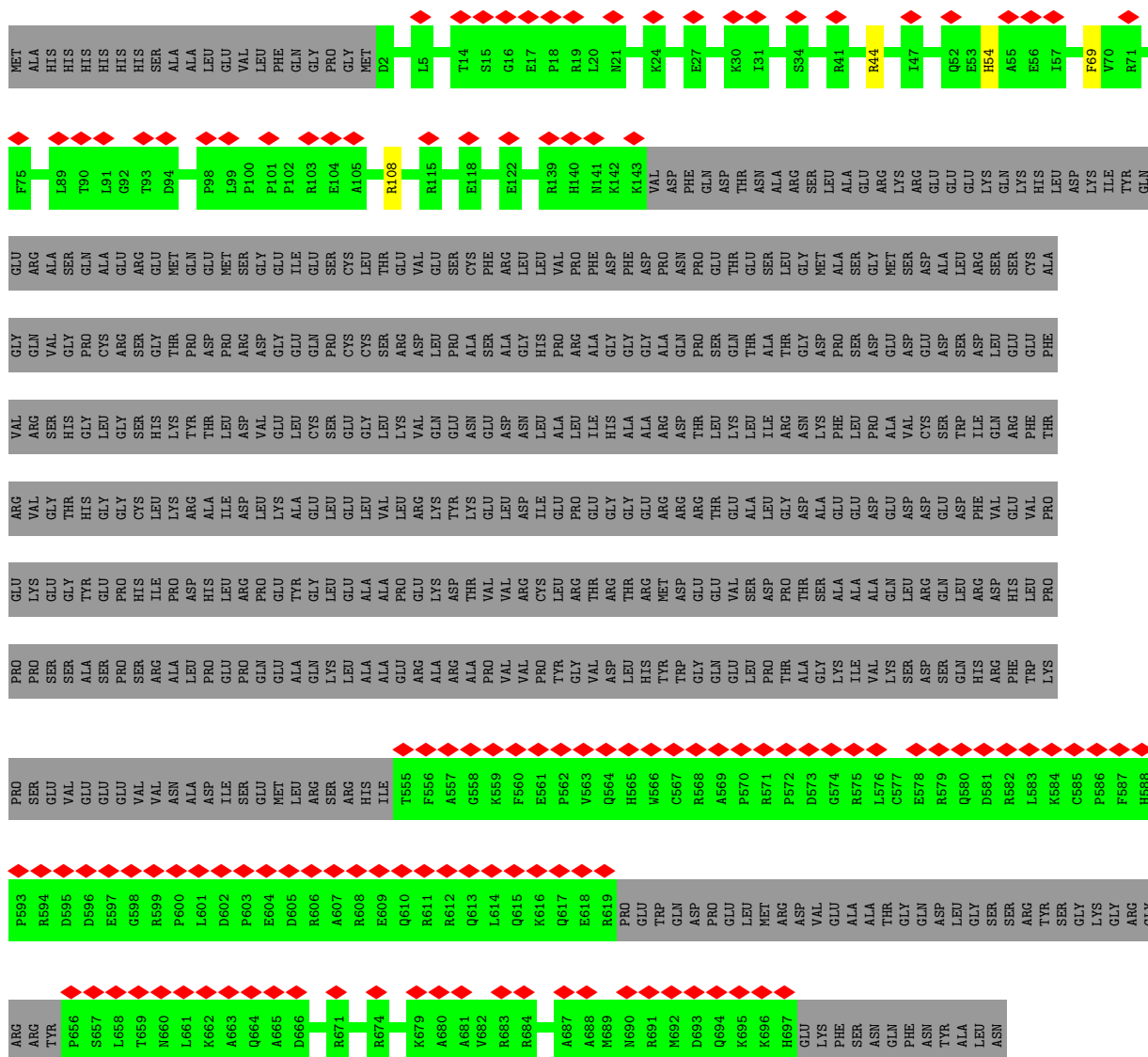


• Molecule 21: DNA excision repair protein ERCC-6

Chain e: 38% 60%



- Molecule 22: UV-stimulated scaffold protein A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	257539	Depositor
Resolution determination method	OTHER	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)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	114.502	Depositor
Minimum map value	-1.609	Depositor
Average map value	0.029	Depositor
Map value standard deviation	1.373	Depositor
Recommended contour level	4.4	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.25	0/11364	0.50	0/15342
2	B	0.26	0/9229	0.50	0/12458
3	C	0.26	0/2132	0.48	0/2896
4	D	0.24	0/1064	0.44	0/1428
5	E	0.26	0/1751	0.52	0/2366
6	F	0.26	0/667	0.50	0/901
7	G	0.25	0/1382	0.48	0/1874
8	H	0.26	0/1207	0.51	0/1628
9	I	0.24	0/972	0.48	0/1316
10	J	0.27	0/542	0.48	0/730
11	K	0.26	0/939	0.43	0/1271
12	L	0.26	0/394	0.58	0/524
13	f	0.24	0/515	0.46	0/700
14	N	0.54	0/934	0.89	0/1439
15	M	0.29	0/247	0.77	0/384
16	T	0.53	0/1218	0.96	0/1874
17	a	0.28	0/3015	0.53	0/4086
18	b	0.28	0/6518	0.51	0/8810
19	c	0.25	0/311	0.45	0/420
20	g	0.24	0/1753	0.55	0/2374
21	e	0.25	0/4929	0.50	0/6642
22	d	0.24	0/2077	0.51	0/2783
All	All	0.28	0/53160	0.53	0/72246

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	A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
5	E	0	2
9	I	0	1
12	L	0	1
13	f	0	1
17	a	0	1
18	b	0	3
20	g	0	3
21	e	0	4
22	d	0	1
All	All	0	21

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1160	ARG	Sidechain
1	A	20	ARG	Sidechain
1	A	532	ARG	Sidechain
2	B	975	ARG	Sidechain
5	E	162	ARG	Sidechain
5	E	166	ARG	Sidechain
9	I	33	ARG	Sidechain
12	L	51	ARG	Sidechain
17	a	78	ARG	Sidechain
18	b	753	ARG	Sidechain
18	b	847	ARG	Sidechain
18	b	889	ARG	Sidechain
22	d	44	ARG	Sidechain
21	e	464	ARG	Sidechain
21	e	466	ARG	Sidechain
21	e	467	ARG	Sidechain
21	e	612	ARG	Sidechain
13	f	43	ARG	Sidechain
20	g	192	ARG	Sidechain
20	g	200	ARG	Sidechain
20	g	72	ARG	Sidechain

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1399/1970 (71%)	1349 (96%)	50 (4%)	0	100	100
2	B	1122/1300 (86%)	1078 (96%)	44 (4%)	0	100	100
3	C	256/275 (93%)	250 (98%)	6 (2%)	0	100	100
4	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
9	I	115/125 (92%)	104 (90%)	11 (10%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	f	62/85 (73%)	60 (97%)	2 (3%)	0	100	100
17	a	371/408 (91%)	345 (93%)	26 (7%)	0	100	100
18	b	806/1160 (70%)	766 (95%)	40 (5%)	0	100	100
19	c	32/152 (21%)	32 (100%)	0	0	100	100
20	g	218/257 (85%)	210 (96%)	8 (4%)	0	100	100
21	e	574/1493 (38%)	546 (95%)	28 (5%)	0	100	100
22	d	243/729 (33%)	234 (96%)	9 (4%)	0	100	100
All	All	6148/8997 (68%)	5900 (96%)	248 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1241/1749 (71%)	1211 (98%)	30 (2%)	44	66
2	B	992/1127 (88%)	974 (98%)	18 (2%)	54	73
3	C	237/252 (94%)	232 (98%)	5 (2%)	48	69
4	D	118/126 (94%)	116 (98%)	2 (2%)	56	74
5	E	191/192 (100%)	187 (98%)	4 (2%)	48	69
6	F	71/111 (64%)	70 (99%)	1 (1%)	62	77
7	G	152/153 (99%)	151 (99%)	1 (1%)	81	88
8	H	129/131 (98%)	125 (97%)	4 (3%)	35	60
9	I	105/112 (94%)	102 (97%)	3 (3%)	37	61
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	102 (98%)	2 (2%)	52	71
12	L	43/55 (78%)	42 (98%)	1 (2%)	45	67
13	f	59/76 (78%)	57 (97%)	2 (3%)	32	57
17	a	331/358 (92%)	319 (96%)	12 (4%)	30	56
18	b	712/1014 (70%)	700 (98%)	12 (2%)	56	74
19	c	35/128 (27%)	35 (100%)	0	100	100
20	g	183/215 (85%)	175 (96%)	8 (4%)	24	50
21	e	527/1297 (41%)	509 (97%)	18 (3%)	32	57
22	d	216/623 (35%)	213 (99%)	3 (1%)	62	77
All	All	5502/7881 (70%)	5376 (98%)	126 (2%)	46	67

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	85	PHE
1	A	114	CYS
1	A	233	CYS

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Mol	Chain	Res	Type
1	A	236	LEU
1	A	241	ARG
1	A	275	ASP
1	A	294	GLU
1	A	407	ARG
1	A	422	ASP
1	A	431	PHE
1	A	458	PHE
1	A	495	ASP
1	A	531	ASN
1	A	532	ARG
1	A	546	ARG
1	A	644	SER
1	A	701	ASP
1	A	715	GLU
1	A	778	LYS
1	A	910	LYS
1	A	923	ASP
1	A	924	TYR
1	A	943	LEU
1	A	1149	ARG
1	A	1220	HIS
1	A	1244	ASN
1	A	1430	CYS
1	A	1437	ASP
1	A	1472	ASP
2	B	16	GLU
2	B	24	GLU
2	B	26	CYS
2	B	179	LEU
2	B	255	ARG
2	B	319	ASN
2	B	320	PHE
2	B	394	ASP
2	B	503	ASN
2	B	548	TRP
2	B	566	LYS
2	B	582	GLN
2	B	690	CYS
2	B	813	SER
2	B	889	LYS
2	B	1017	ASP

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Mol	Chain	Res	Type
2	B	1048	TYR
2	B	1093	CYS
3	C	61	ASP
3	C	63	PHE
3	C	228	ARG
3	C	234	GLU
3	C	238	SER
4	D	86	LEU
4	D	89	GLN
5	E	49	SER
5	E	73	PHE
5	E	158	GLU
5	E	177	ASP
6	F	91	LEU
7	G	98	PHE
8	H	51	ASP
8	H	56	PHE
8	H	63	THR
8	H	83	SER
9	I	14	ILE
9	I	40	ARG
9	I	92	LYS
11	K	2	ASN
11	K	87	PHE
12	L	25	GLU
13	f	71	TYR
13	f	73	ASP
17	a	14	ASP
17	a	31	GLU
17	a	136	ASP
17	a	157	CYS
17	a	180	HIS
17	a	183	GLN
17	a	188	GLU
17	a	199	ASP
17	a	206	SER
17	a	245	ASN
17	a	256	ASP
17	a	338	ASP
18	b	25	SER
18	b	128	CYS
18	b	151	GLU

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Mol	Chain	Res	Type
18	b	173	CYS
18	b	245	TYR
18	b	265	ASP
18	b	291	MET
18	b	722	ARG
18	b	737	SER
18	b	826	ASN
18	b	928	ARG
18	b	1047	TRP
20	g	37	ARG
20	g	71	ASP
20	g	83	GLN
20	g	146	MET
20	g	175	TRP
20	g	198	MET
20	g	208	LEU
20	g	232	LEU
21	e	507	LEU
21	e	580	GLN
21	e	624	SER
21	e	634	ASP
21	e	642	TYR
21	e	689	PHE
21	e	693	PHE
21	e	776	TYR
21	e	784	GLU
21	e	797	SER
21	e	932	TYR
21	e	933	ASP
21	e	970	GLU
21	e	1001	LEU
21	e	1007	LEU
21	e	1250	TYR
21	e	1330	ARG
21	e	1387	SER
22	d	54	HIS
22	d	69	PHE
22	d	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	ASN
1	A	539	GLN
1	A	704	ASN
2	B	23	GLN
2	B	410	ASN
2	B	570	ASN
2	B	968	ASN
2	B	1003	ASN
2	B	1049	GLN
2	B	1068	GLN
2	B	1094	GLN
2	B	1097	HIS
5	E	132	GLN
7	G	24	ASN
17	a	228	GLN
20	g	159	HIS
21	e	641	HIS
21	e	772	GLN
21	e	773	HIS
21	e	778	ASN
21	e	854	GLN
22	d	38	GLN
22	d	74	GLN
22	d	580	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	M	9/25 (36%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	M	8	G

There are no RNA pucker outliers to report.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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](#)

There are no chain breaks in this entry.

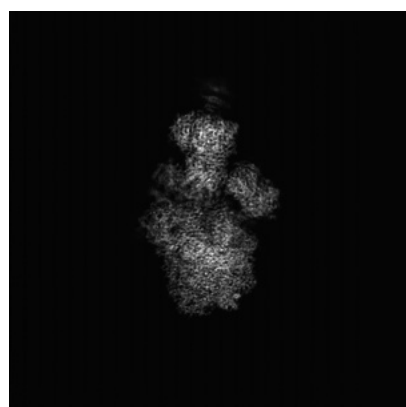
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50325. These allow visual inspection of the internal detail of the map and identification of artifacts.

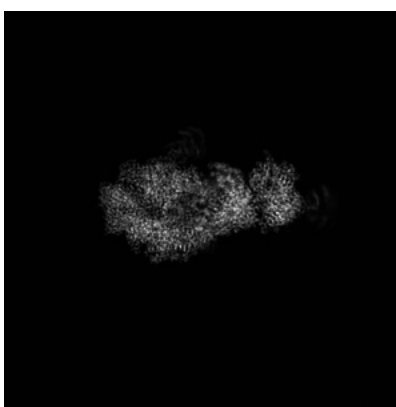
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

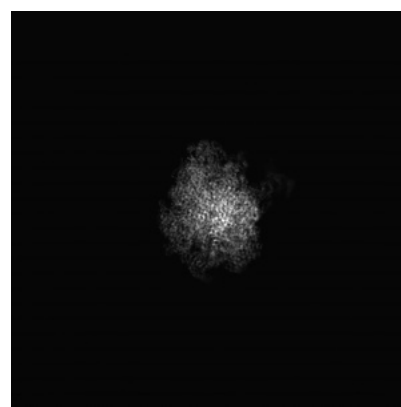
6.1.1 Primary map



X



Y



Z

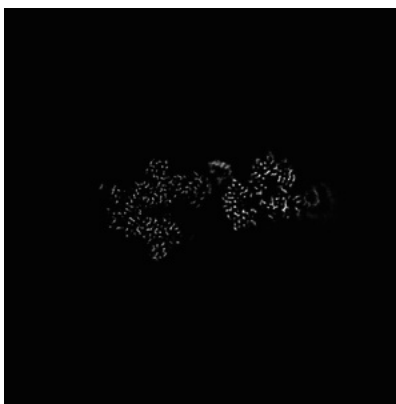
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

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: 214



Y Index: 191

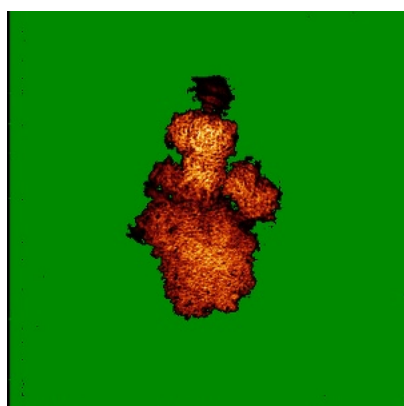


Z Index: 160

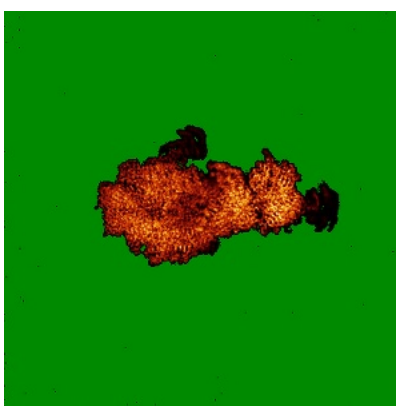
The images above show the largest variance slices of the map in three orthogonal directions.

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

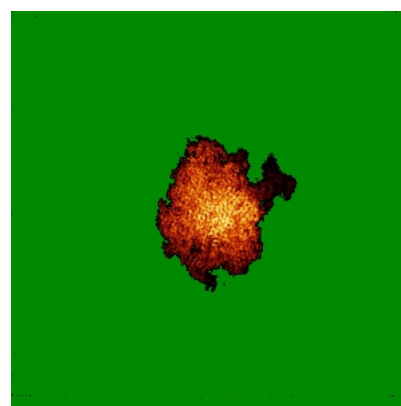
6.4.1 Primary map



X



Y

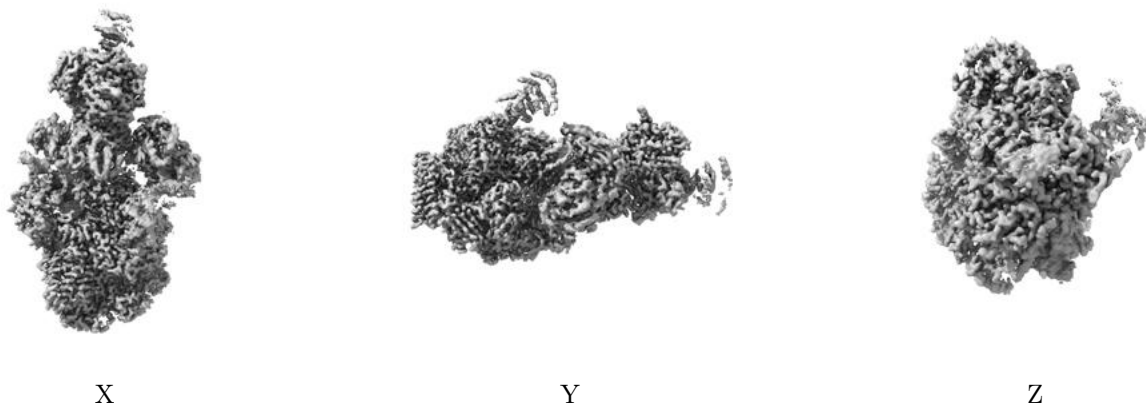


Z

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

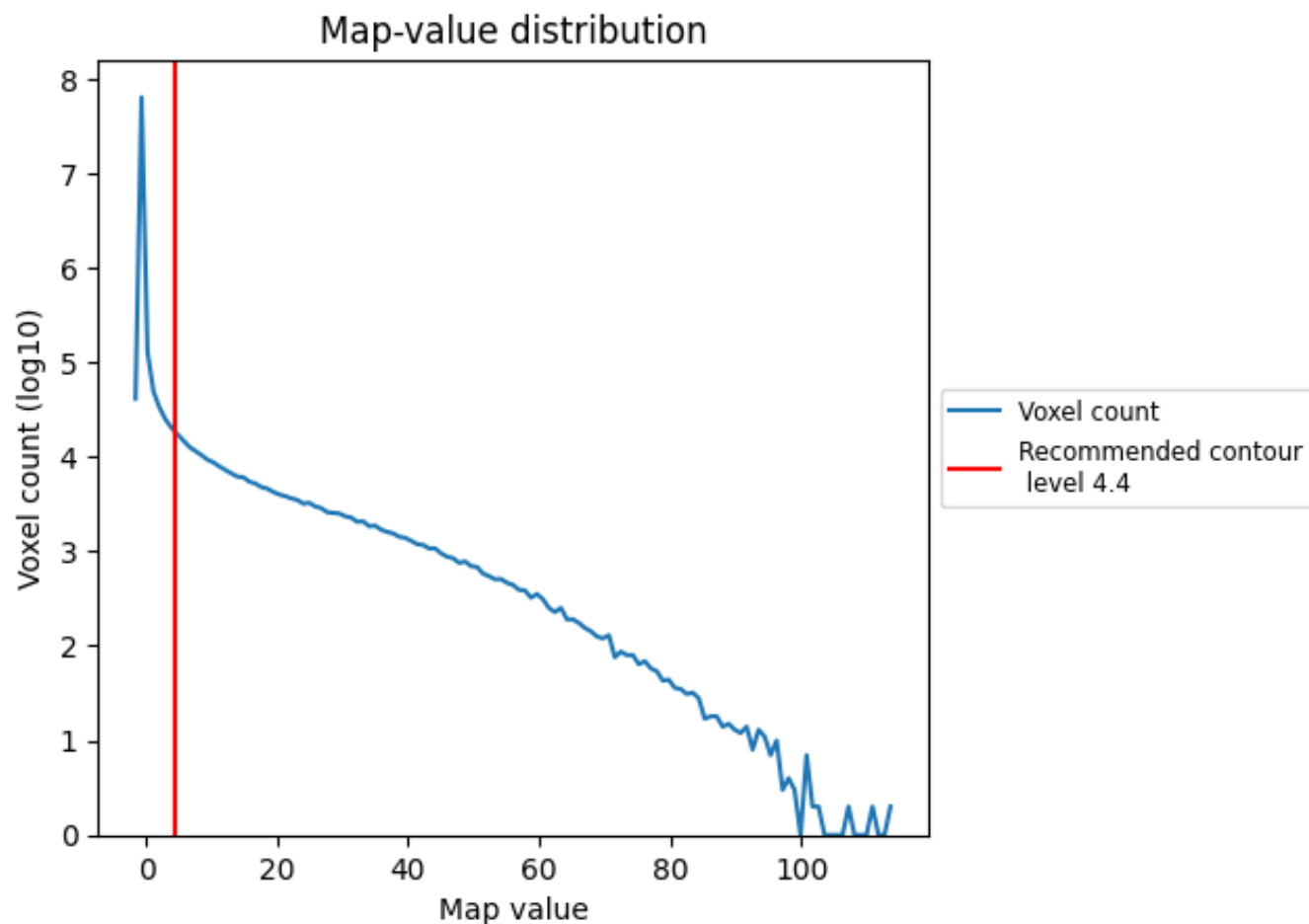
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

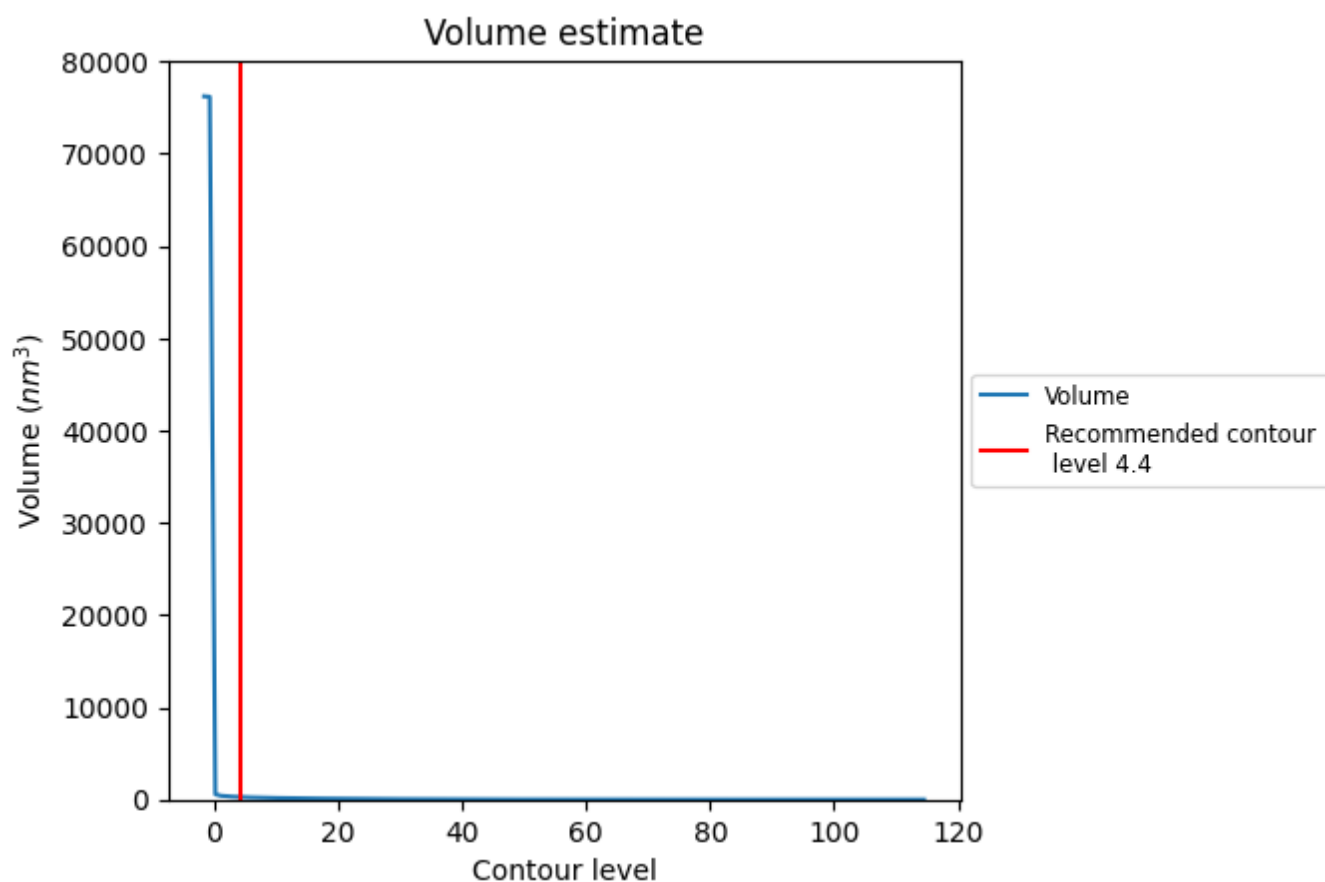
This section contains the results of statistical analysis of the map.

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.

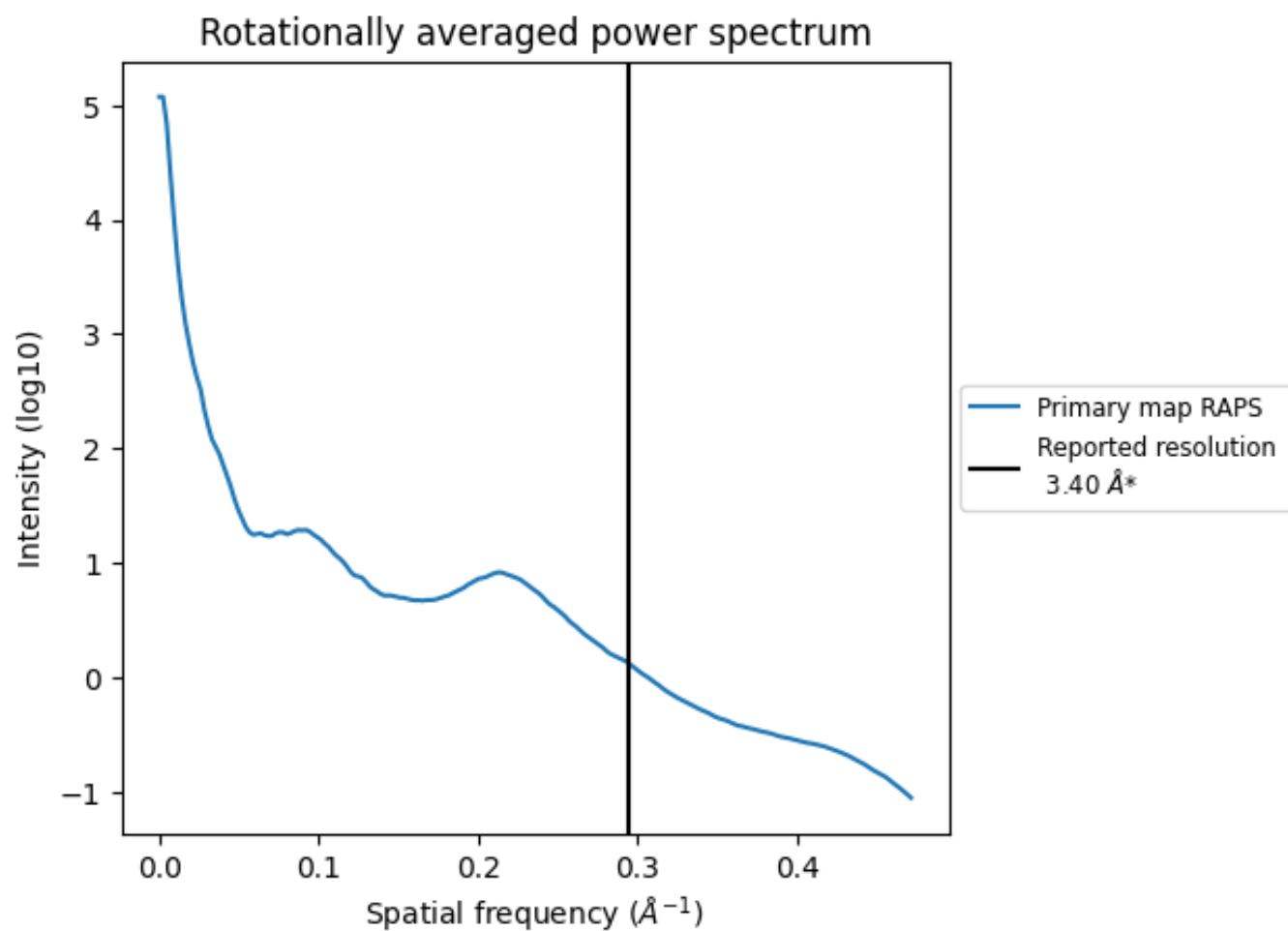
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm^3 ; this corresponds to an approximate mass of 243 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 0.294 Å⁻¹

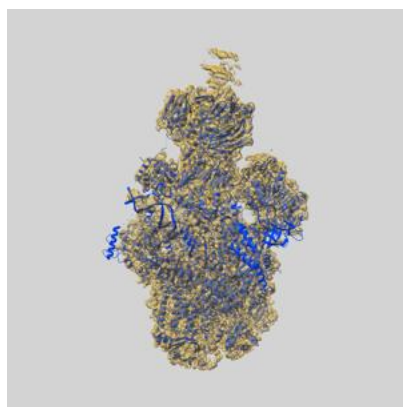
8 Fourier-Shell correlation ⓘ

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

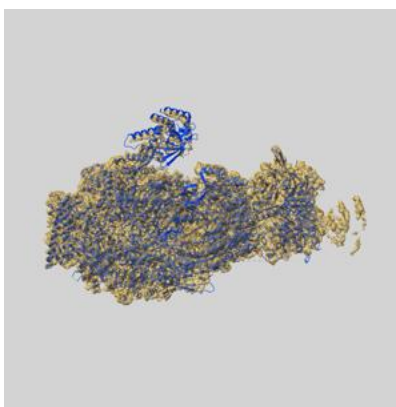
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50325 and PDB model 9FD2. Per-residue inclusion information can be found in section [3](#) on page [11](#).

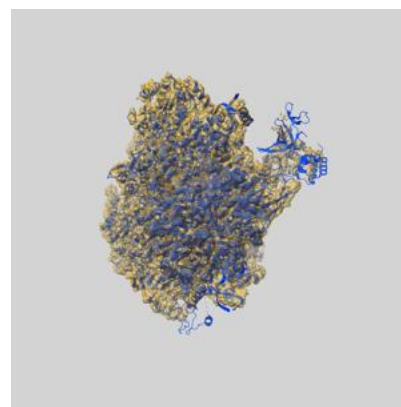
9.1 Map-model overlay [i](#)



X



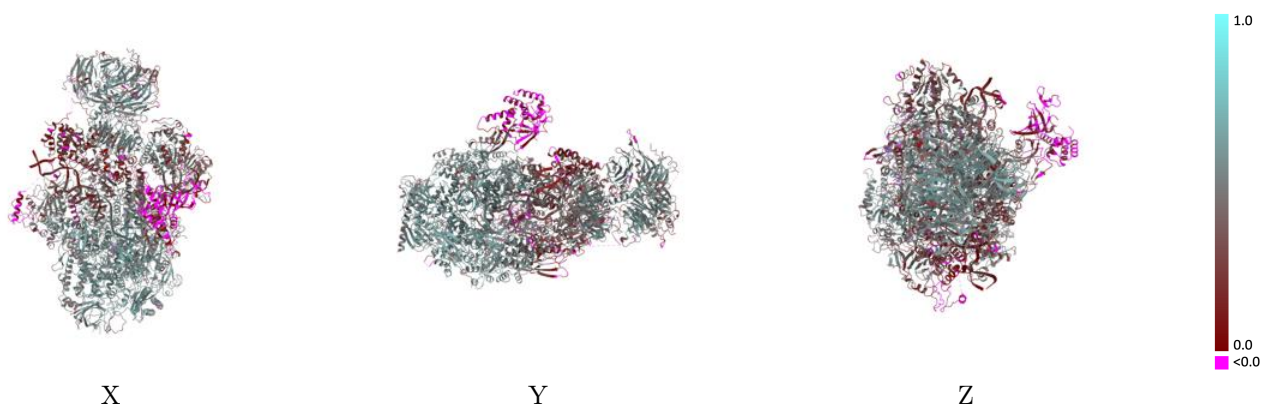
Y



Z

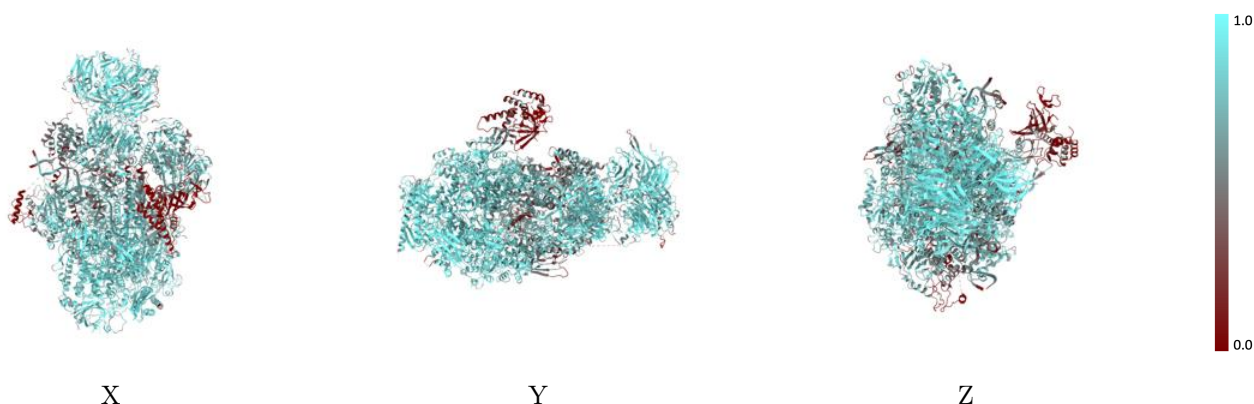
The images above show the 3D surface view of the map at the recommended contour level 4.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



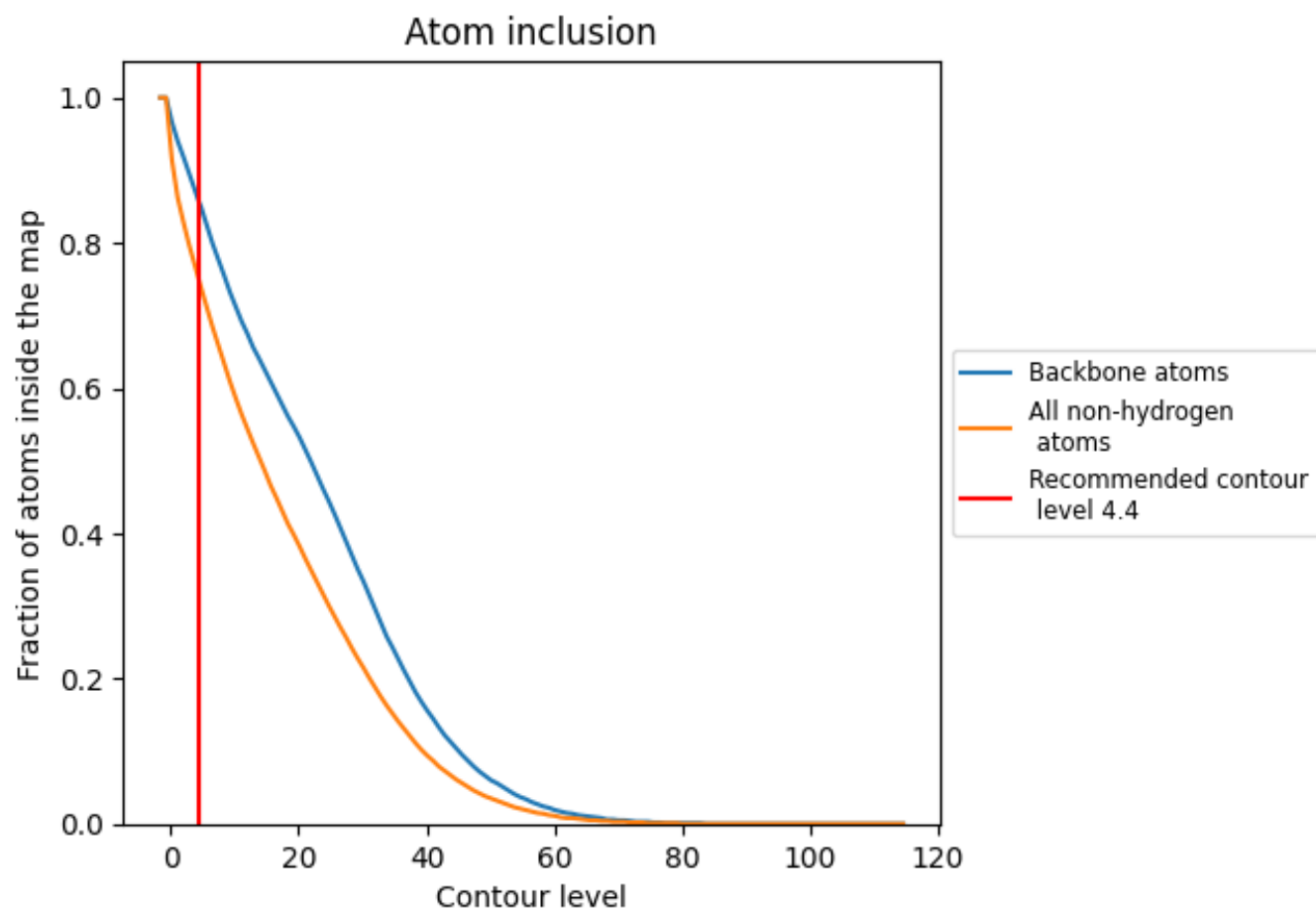
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.4).















































9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 75% 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 (4.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.4360
A	 0.7920	 0.4980
B	 0.8130	 0.5090
C	 0.8510	 0.5400
D	 0.1360	 -0.0040
E	 0.7950	 0.4840
F	 0.8290	 0.5120
G	 0.3060	 0.1540
H	 0.8190	 0.5180
I	 0.6570	 0.3880
J	 0.8870	 0.5680
K	 0.8580	 0.5480
L	 0.7290	 0.4390
M	 0.8910	 0.4930
N	 0.6400	 0.2460
T	 0.7120	 0.3270
a	 0.8710	 0.5110
b	 0.8450	 0.4820
c	 0.5360	 0.3050
d	 0.3510	 0.1260
e	 0.7330	 0.3740
f	 0.6370	 0.3180
g	 0.6310	 0.2400

