wwPDB EM Validation Summary Report

Jan 16, 2025 – 03:16 am GMT

PDB ID	:	9F2A
EMDB ID	:	EMD-50143
Title	:	Pyrococcus abyssi PolD in complex with Rpa2 winged-helix domain class 2 (composite map)
Authors	:	Martinez-Carranza, M.; Sauguet, L.
Deposited on	:	2024-04-22
Resolution	:	2.91 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

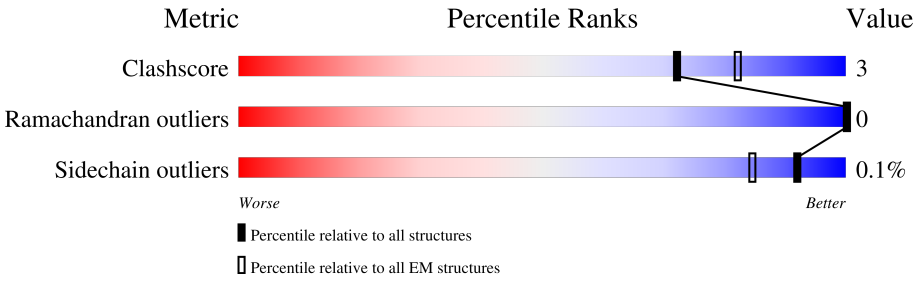
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	662	60% 8% 32%
2	B	1270	86% 7% 7%
3	C	132	36% 11% 52%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13557 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 polymerase II small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	447	3573	2322	588	656	7	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q9V2F3
A	-41	GLY	-	expression tag	UNP Q9V2F3
A	-40	LYS	-	expression tag	UNP Q9V2F3
A	-39	HIS	-	expression tag	UNP Q9V2F3
A	-38	HIS	-	expression tag	UNP Q9V2F3
A	-37	HIS	-	expression tag	UNP Q9V2F3
A	-36	HIS	-	expression tag	UNP Q9V2F3
A	-35	SER	-	expression tag	UNP Q9V2F3
A	-34	GLY	-	expression tag	UNP Q9V2F3
A	-33	HIS	-	expression tag	UNP Q9V2F3
A	-32	HIS	-	expression tag	UNP Q9V2F3
A	-31	HIS	-	expression tag	UNP Q9V2F3
A	-30	THR	-	expression tag	UNP Q9V2F3
A	-29	GLY	-	expression tag	UNP Q9V2F3
A	-28	HIS	-	expression tag	UNP Q9V2F3
A	-27	HIS	-	expression tag	UNP Q9V2F3
A	-26	HIS	-	expression tag	UNP Q9V2F3
A	-25	HIS	-	expression tag	UNP Q9V2F3
A	-24	SER	-	expression tag	UNP Q9V2F3
A	-23	GLY	-	expression tag	UNP Q9V2F3
A	-22	SER	-	expression tag	UNP Q9V2F3
A	-21	HIS	-	expression tag	UNP Q9V2F3
A	-20	HIS	-	expression tag	UNP Q9V2F3
A	-19	HIS	-	expression tag	UNP Q9V2F3
A	-18	THR	-	expression tag	UNP Q9V2F3
A	-17	SER	-	expression tag	UNP Q9V2F3
A	-16	SER	-	expression tag	UNP Q9V2F3
A	-15	SER	-	expression tag	UNP Q9V2F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP Q9V2F3
A	-13	SER	-	expression tag	UNP Q9V2F3
A	-12	THR	-	expression tag	UNP Q9V2F3
A	-11	GLY	-	expression tag	UNP Q9V2F3
A	-10	GLU	-	expression tag	UNP Q9V2F3
A	-9	ASN	-	expression tag	UNP Q9V2F3
A	-8	LEU	-	expression tag	UNP Q9V2F3
A	-7	TYR	-	expression tag	UNP Q9V2F3
A	-6	PHE	-	expression tag	UNP Q9V2F3
A	-5	GLN	-	expression tag	UNP Q9V2F3
A	-4	GLY	-	expression tag	UNP Q9V2F3
A	-3	THR	-	expression tag	UNP Q9V2F3
A	-2	GLY	-	expression tag	UNP Q9V2F3
A	-1	ASP	-	expression tag	UNP Q9V2F3
A	0	GLY	-	expression tag	UNP Q9V2F3
A	1	SER	-	expression tag	UNP Q9V2F3
A	451	ALA	HIS	engineered mutation	UNP Q9V2F3

- Molecule 2 is a protein called DNA polymerase II large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1182	Total	C	N	O	S	0	0
			9458	6052	1623	1741	42		

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	MET	ILE	conflict	UNP P81409
B	30	ALA	SER	conflict	UNP P81409
B	37	LEU	THR	conflict	UNP P81409
B	62	LYS	GLN	conflict	UNP P81409
B	68	VAL	LEU	conflict	UNP P81409
B	72	GLY	ASP	conflict	UNP P81409
B	76	ALA	VAL	conflict	UNP P81409
B	92	LEU	PHE	conflict	UNP P81409
B	95	ARG	LYS	conflict	UNP P81409
B	119	ILE	LEU	conflict	UNP P81409
B	124	ASN	ASP	conflict	UNP P81409
B	178	GLU	GLY	conflict	UNP P81409
B	196	THR	SER	conflict	UNP P81409
B	205	GLU	ASP	conflict	UNP P81409
B	234	PRO	GLU	conflict	UNP P81409

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Chain	Residue	Modelled	Actual	Comment	Reference
B	270	GLU	ASP	conflict	UNP P81409
B	287	PRO	GLU	conflict	UNP P81409
B	288	LYS	ILE	conflict	UNP P81409
B	291	GLY	SER	conflict	UNP P81409
B	292	LYS	GLU	conflict	UNP P81409
B	293	GLU	SER	conflict	UNP P81409
B	294	GLU	LYS	conflict	UNP P81409
B	295	SER	ALA	conflict	UNP P81409
B	296	LEU	GLU	conflict	UNP P81409
B	297	ALA	GLU	conflict	UNP P81409
B	298	GLU	SER	conflict	UNP P81409
B	299	SER	LYS	conflict	UNP P81409
B	300	THR	VAL	conflict	UNP P81409
B	301	LEU	-	insertion	UNP P81409
B	302	GLU	-	insertion	UNP P81409
B	305	LYS	ARG	conflict	UNP P81409
B	309	ASP	GLU	conflict	UNP P81409
B	310	MET	LYS	conflict	UNP P81409
B	315	SER	LYS	conflict	UNP P81409
B	318	GLN	GLU	conflict	UNP P81409
B	321	LYS	ARG	conflict	UNP P81409
B	322	GLU	ALA	conflict	UNP P81409
B	328	ASP	GLU	conflict	UNP P81409
B	334	VAL	ILE	conflict	UNP P81409
B	342	SER	ALA	conflict	UNP P81409
B	343	ASP	GLY	conflict	UNP P81409
B	346	LYS	GLU	conflict	UNP P81409
B	347	PRO	ASN	conflict	UNP P81409
B	359	ALA	VAL	conflict	UNP P81409
B	366	GLY	SER	conflict	UNP P81409
B	373	ILE	VAL	conflict	UNP P81409
B	385	LEU	MET	conflict	UNP P81409
B	399	VAL	ALA	conflict	UNP P81409
B	402	ILE	ALA	conflict	UNP P81409
B	415	LEU	VAL	conflict	UNP P81409
B	426	VAL	ILE	conflict	UNP P81409
B	428	GLU	ASP	conflict	UNP P81409
B	429	ASP	GLU	conflict	UNP P81409
B	440	VAL	ILE	conflict	UNP P81409
B	459	CYS	VAL	conflict	UNP P81409
B	465	LEU	GLN	conflict	UNP P81409
B	471	LEU	VAL	conflict	UNP P81409

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Chain	Residue	Modelled	Actual	Comment	Reference
B	472	LYS	ASN	conflict	UNP P81409
B	474	ILE	ALA	conflict	UNP P81409
B	478	HIS	GLU	conflict	UNP P81409
B	480	GLU	ARG	conflict	UNP P81409
B	483	THR	GLU	conflict	UNP P81409
B	486	GLU	PRO	conflict	UNP P81409
B	487	GLU	ARG	conflict	UNP P81409
B	490	ILE	VAL	conflict	UNP P81409
B	494	SER	ALA	conflict	UNP P81409
B	495	ASP	GLU	conflict	UNP P81409
B	499	ILE	VAL	conflict	UNP P81409
B	505	LYS	ALA	conflict	UNP P81409
B	506	GLU	LYS	conflict	UNP P81409
B	509	ARG	TYR	conflict	UNP P81409
B	527	VAL	ILE	conflict	UNP P81409
B	529	GLY	GLU	conflict	UNP P81409
B	542	SER	THR	conflict	UNP P81409
B	544	GLU	ASN	conflict	UNP P81409
B	550	LYS	ARG	conflict	UNP P81409
B	553	ARG	GLY	conflict	UNP P81409
B	554	LEU	VAL	conflict	UNP P81409
B	557	ASN	ASP	conflict	UNP P81409
B	558	TYR	LYS	conflict	UNP P81409
B	560	GLU	THR	conflict	UNP P81409
B	564	SER	GLY	conflict	UNP P81409
B	565	ASN	THR	conflict	UNP P81409
B	576	VAL	GLU	conflict	UNP P81409
B	579	GLN	LEU	conflict	UNP P81409
B	580	GLU	ASP	conflict	UNP P81409
B	581	LYS	ASP	conflict	UNP P81409
B	584	ASP	SER	conflict	UNP P81409
B	585	SER	LEU	conflict	UNP P81409
B	600	ASP	GLU	conflict	UNP P81409
B	602	ASN	ILE	conflict	UNP P81409
B	604	ILE	VAL	conflict	UNP P81409
B	610	ALA	SER	conflict	UNP P81409
B	621	ASN	GLU	conflict	UNP P81409
B	625	MET	LYS	conflict	UNP P81409
B	629	LEU	PHE	conflict	UNP P81409
B	631	ALA	THR	conflict	UNP P81409
B	632	THR	VAL	conflict	UNP P81409
B	641	GLU	GLN	conflict	UNP P81409

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Chain	Residue	Modelled	Actual	Comment	Reference
B	696	VAL	ILE	conflict	UNP P81409
B	716	HIS	THR	conflict	UNP P81409
B	720	ASN	GLU	conflict	UNP P81409
B	723	THR	ILE	conflict	UNP P81409
B	728	LEU	ILE	conflict	UNP P81409
B	730	VAL	THR	conflict	UNP P81409
B	733	ARG	LYS	conflict	UNP P81409
B	735	ASN	GLY	conflict	UNP P81409
B	739	PRO	THR	conflict	UNP P81409
B	740	GLU	ASN	conflict	UNP P81409
B	747	ASN	SER	conflict	UNP P81409
B	749	THR	SER	conflict	UNP P81409
B	758	ARG	LYS	conflict	UNP P81409
B	760	TYR	PHE	conflict	UNP P81409
B	761	ALA	THR	conflict	UNP P81409
B	766	ARG	LYS	conflict	UNP P81409
B	798	MET	ILE	conflict	UNP P81409
B	799	PRO	ALA	conflict	UNP P81409
B	812	ASP	GLU	conflict	UNP P81409
B	873	ILE	VAL	conflict	UNP P81409
B	881	ARG	LYS	conflict	UNP P81409
B	885	LYS	ARG	conflict	UNP P81409
B	888	LYS	ARG	conflict	UNP P81409
B	961	ALA	SER	conflict	UNP P81409
B	1009	ILE	VAL	conflict	UNP P81409
B	1050	LEU	ILE	conflict	UNP P81409
B	1079	ARG	LYS	conflict	UNP P81409
B	1083	GLU	THR	conflict	UNP P81409
B	1084	VAL	LEU	conflict	UNP P81409
B	1086	LYS	GLU	conflict	UNP P81409
B	1093	GLU	GLN	conflict	UNP P81409
B	1095	GLY	TYR	conflict	UNP P81409
B	1099	LYS	THR	conflict	UNP P81409
B	1130	PHE	TYR	conflict	UNP P81409
B	1136	ASN	ASP	conflict	UNP P81409
B	1167	THR	ALA	conflict	UNP P81409
B	1168	GLU	ASN	conflict	UNP P81409
B	1173	ASN	PRO	conflict	UNP P81409
B	1184	ARG	LYS	conflict	UNP P81409
B	1192	ASN	TYR	conflict	UNP P81409
B	1193	VAL	LEU	conflict	UNP P81409
B	1197	THR	ALA	conflict	UNP P81409

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1204	ASN	ASP	conflict	UNP P81409
B	1210	GLN	MET	conflict	UNP P81409
B	1211	ARG	LYS	conflict	UNP P81409
B	1212	LEU	MET	conflict	UNP P81409
B	1213	VAL	ILE	conflict	UNP P81409
B	1214	MET	LYS	conflict	UNP P81409
B	1215	ALA	GLU	conflict	UNP P81409
B	1220	VAL	THR	conflict	UNP P81409
B	1221	ASN	VAL	conflict	UNP P81409
B	1222	LYS	GLN	conflict	UNP P81409
B	1223	SER	GLY	conflict	UNP P81409
B	1229	LEU	PHE	conflict	UNP P81409
B	1230	SER	ASN	conflict	UNP P81409
B	1231	ASN	SER	conflict	UNP P81409
B	1232	GLY	SER	conflict	UNP P81409
B	1233	SER	GLY	conflict	UNP P81409
B	1234	LYS	ASN	conflict	UNP P81409
B	1235	LYS	-	insertion	UNP P81409
B	1236	THR	-	insertion	UNP P81409
B	1237	GLU	-	insertion	UNP P81409
B	1238	LYS	ASN	conflict	UNP P81409
B	1239	ALA	GLY	conflict	UNP P81409
B	1240	GLU	LYS	conflict	UNP P81409
B	1242	ALA	ILE	conflict	UNP P81409
B	1245	PRO	LYS	conflict	UNP P81409
B	1246	ARG	GLU	conflict	UNP P81409
B	1249	SER	ALA	conflict	UNP P81409
B	1250	ASP	LYS	conflict	UNP P81409
B	1257	ARG	LYS	conflict	UNP P81409
B	1262	GLU	ASP	conflict	UNP P81409
B	1263	GLU	ASP	conflict	UNP P81409
B	1267	ARG	LYS	conflict	UNP P81409
B	1268	LYS	ARG	conflict	UNP P81409
B	1269	SER	-	expression tag	UNP P81409
B	1270	LYS	-	expression tag	UNP P81409

- Molecule 3 is a protein called RPA32 subunit of the hetero-oligomeric complex involved in homologous recombination.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	63	Total	C	N	O	0	0
			522	334	83	105		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	MET	-	initiating methionine	UNP Q9V1Z1
C	138	GLY	-	expression tag	UNP Q9V1Z1
C	139	LYS	-	expression tag	UNP Q9V1Z1
C	140	HIS	-	expression tag	UNP Q9V1Z1
C	141	HIS	-	expression tag	UNP Q9V1Z1
C	142	HIS	-	expression tag	UNP Q9V1Z1
C	143	HIS	-	expression tag	UNP Q9V1Z1
C	144	SER	-	expression tag	UNP Q9V1Z1
C	145	GLY	-	expression tag	UNP Q9V1Z1
C	146	HIS	-	expression tag	UNP Q9V1Z1
C	147	HIS	-	expression tag	UNP Q9V1Z1
C	148	HIS	-	expression tag	UNP Q9V1Z1
C	149	THR	-	expression tag	UNP Q9V1Z1
C	150	GLY	-	expression tag	UNP Q9V1Z1
C	151	HIS	-	expression tag	UNP Q9V1Z1
C	152	HIS	-	expression tag	UNP Q9V1Z1
C	153	HIS	-	expression tag	UNP Q9V1Z1
C	154	HIS	-	expression tag	UNP Q9V1Z1
C	155	SER	-	expression tag	UNP Q9V1Z1
C	156	GLY	-	expression tag	UNP Q9V1Z1
C	157	SER	-	expression tag	UNP Q9V1Z1
C	158	HIS	-	expression tag	UNP Q9V1Z1
C	159	HIS	-	expression tag	UNP Q9V1Z1
C	160	HIS	-	expression tag	UNP Q9V1Z1
C	161	THR	-	expression tag	UNP Q9V1Z1
C	162	SER	-	expression tag	UNP Q9V1Z1
C	163	SER	-	expression tag	UNP Q9V1Z1
C	164	SER	-	expression tag	UNP Q9V1Z1
C	165	ALA	-	expression tag	UNP Q9V1Z1
C	166	SER	-	expression tag	UNP Q9V1Z1
C	167	THR	-	expression tag	UNP Q9V1Z1
C	168	GLY	-	expression tag	UNP Q9V1Z1
C	169	GLU	-	expression tag	UNP Q9V1Z1
C	170	ASN	-	expression tag	UNP Q9V1Z1
C	171	LEU	-	expression tag	UNP Q9V1Z1
C	172	TYR	-	expression tag	UNP Q9V1Z1
C	173	PHE	-	expression tag	UNP Q9V1Z1
C	174	GLN	-	expression tag	UNP Q9V1Z1
C	175	GLY	-	expression tag	UNP Q9V1Z1
C	176	THR	-	expression tag	UNP Q9V1Z1
C	177	GLY	-	expression tag	UNP Q9V1Z1

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
4	A	1	1	1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

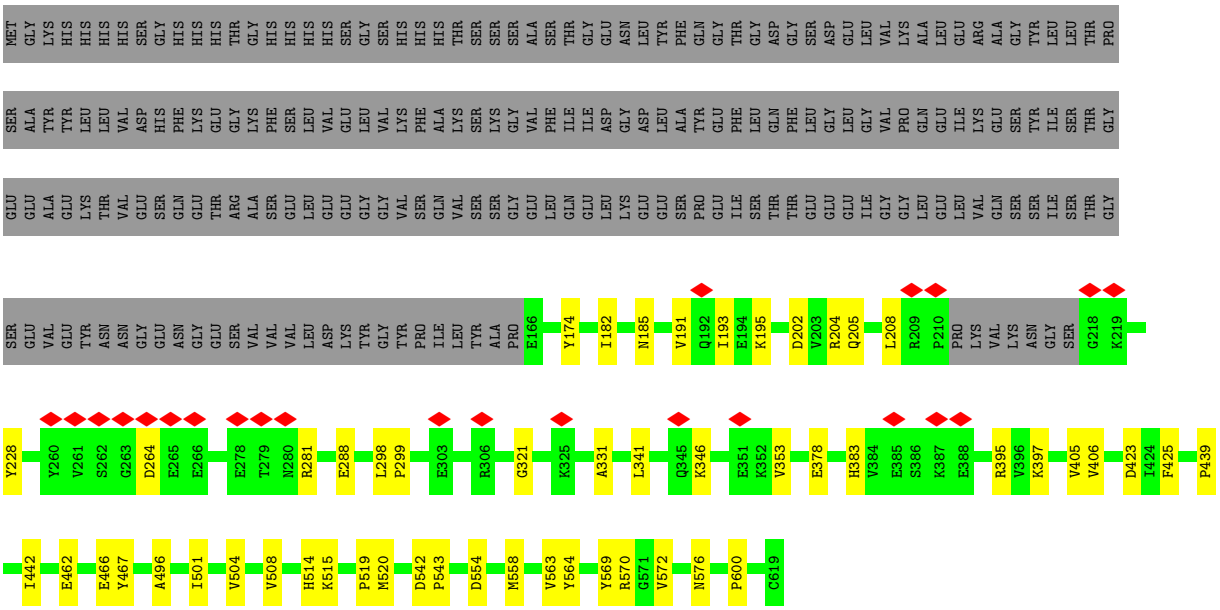
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	B	3	3	3	0

3 Residue-property plots (i)

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

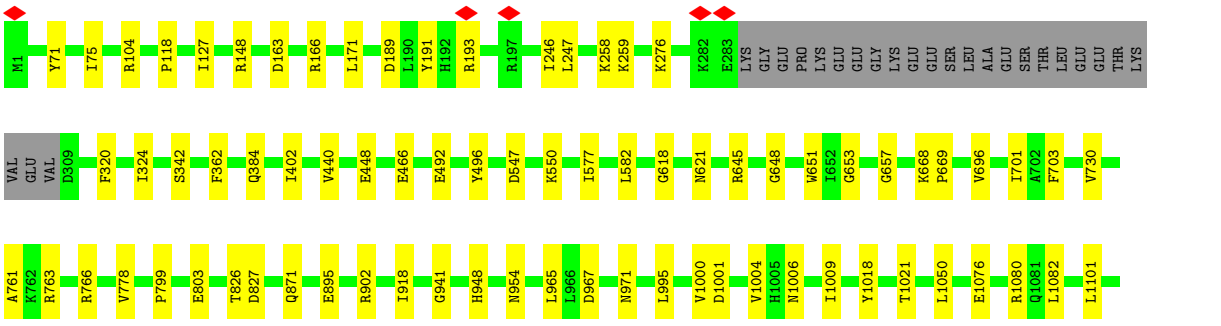
• Molecule 1: DNA polymerase II small subunit

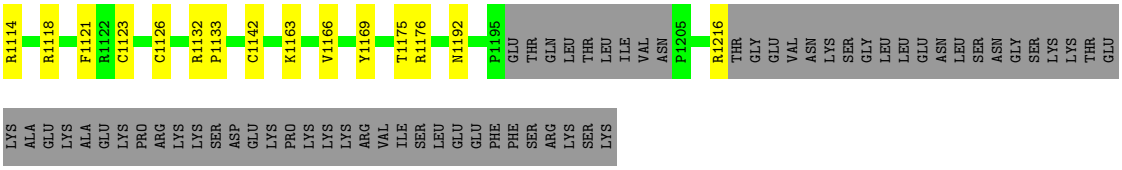
Chain A:



• Molecule 2: DNA polymerase II large subunit

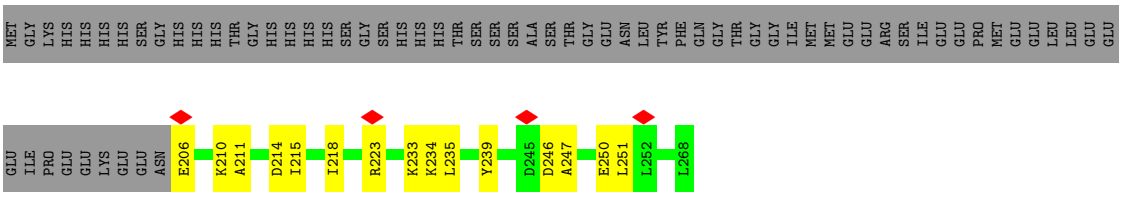
Chain B:





• Molecule 3: RPA32 subunit of the hetero-oligomeric complex involved in homologous recombination

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174709	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.833	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.28	0/3659	0.47	0/4964
2	B	0.27	0/9660	0.48	0/13048
3	C	0.25	0/527	0.46	0/705
All	All	0.27	0/13846	0.48	0/18717

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	3573	0	3614	32	0
2	B	9458	0	9566	51	0
3	C	522	0	539	9	0
4	A	1	0	0	0	0
5	B	3	0	0	0	0
All	All	13557	0	13719	87	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 3.

The worst 5 of 87 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)
1:A:204:ARG:HH21	1:A:462:GLU:HB3	1.53	0.72
1:A:514:HIS:HA	1:A:563:VAL:HG11	1.75	0.69
2:B:1166:VAL:HG13	2:B:1176:ARG:HG2	1.76	0.66
1:A:185:ASN:OD1	1:A:383:HIS:ND1	2.29	0.65
2:B:1114:ARG:HG2	2:B:1118:ARG:HH21	1.60	0.64

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/662 (67%)	429 (97%)	14 (3%)	0	100	100
2	B	1176/1270 (93%)	1145 (97%)	31 (3%)	0	100	100
3	C	61/132 (46%)	60 (98%)	1 (2%)	0	100	100
All	All	1680/2064 (81%)	1634 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/573 (68%)	391 (100%)	1 (0%)	91	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	1014/1094 (93%)	1014 (100%)	0	100 100
3	C	56/116 (48%)	56 (100%)	0	100 100
All	All	1462/1783 (82%)	1461 (100%)	1 (0%)	92 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1104	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 (i)

Of 4 ligands modelled in this entry, 4 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.

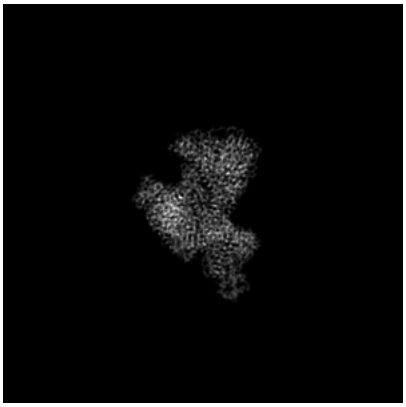
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50143. These allow visual inspection of the internal detail of the map and identification of artifacts.

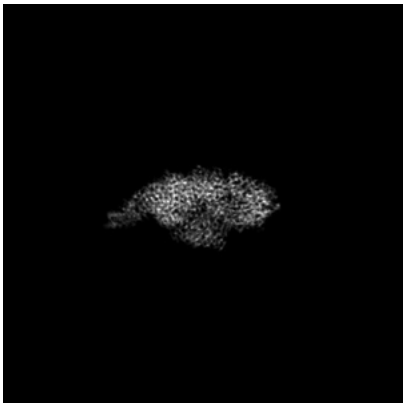
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

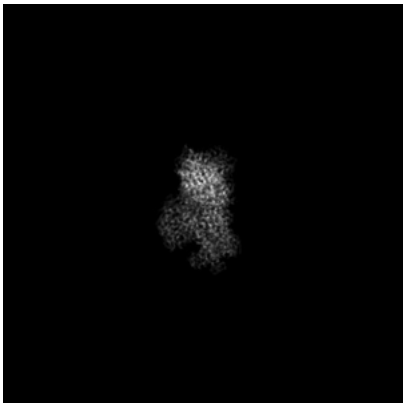
6.1.1 Primary map



X



Y



Z

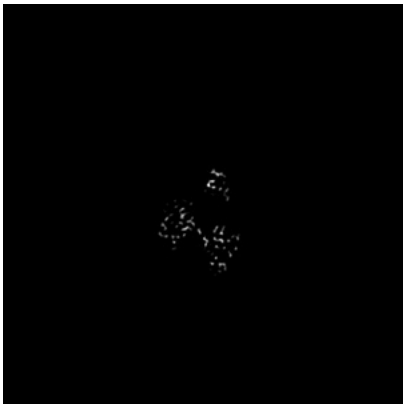
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 175

Y Index: 175

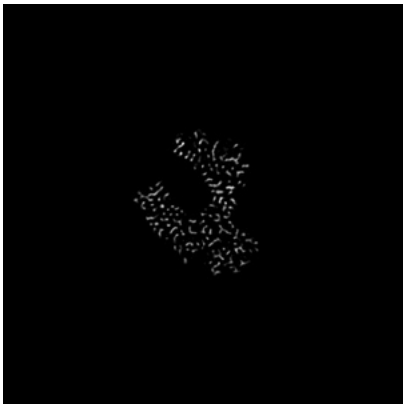


Z Index: 175

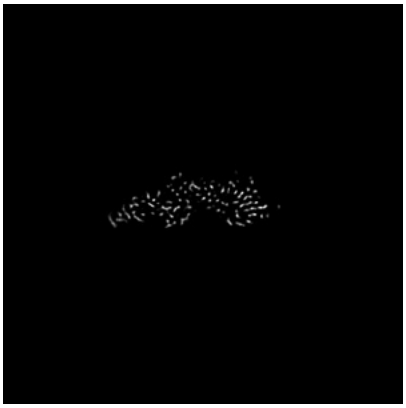
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

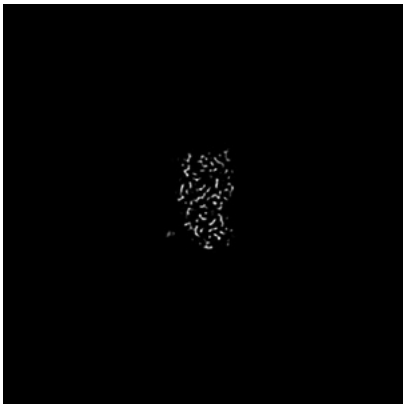
6.3.1 Primary map



X Index: 182



Y Index: 192

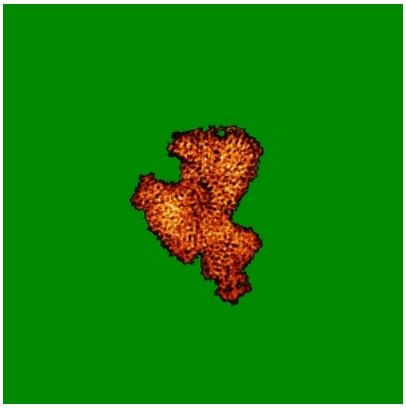


Z Index: 148

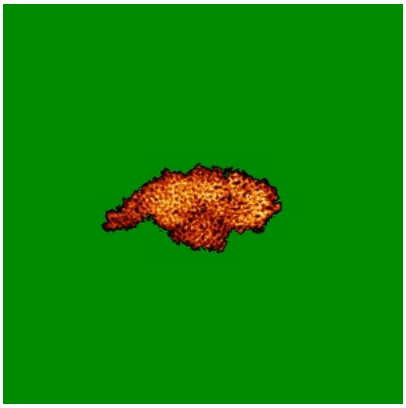
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

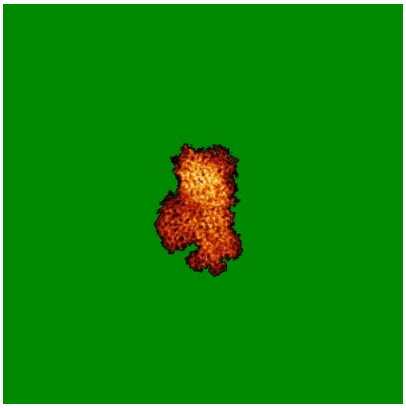
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

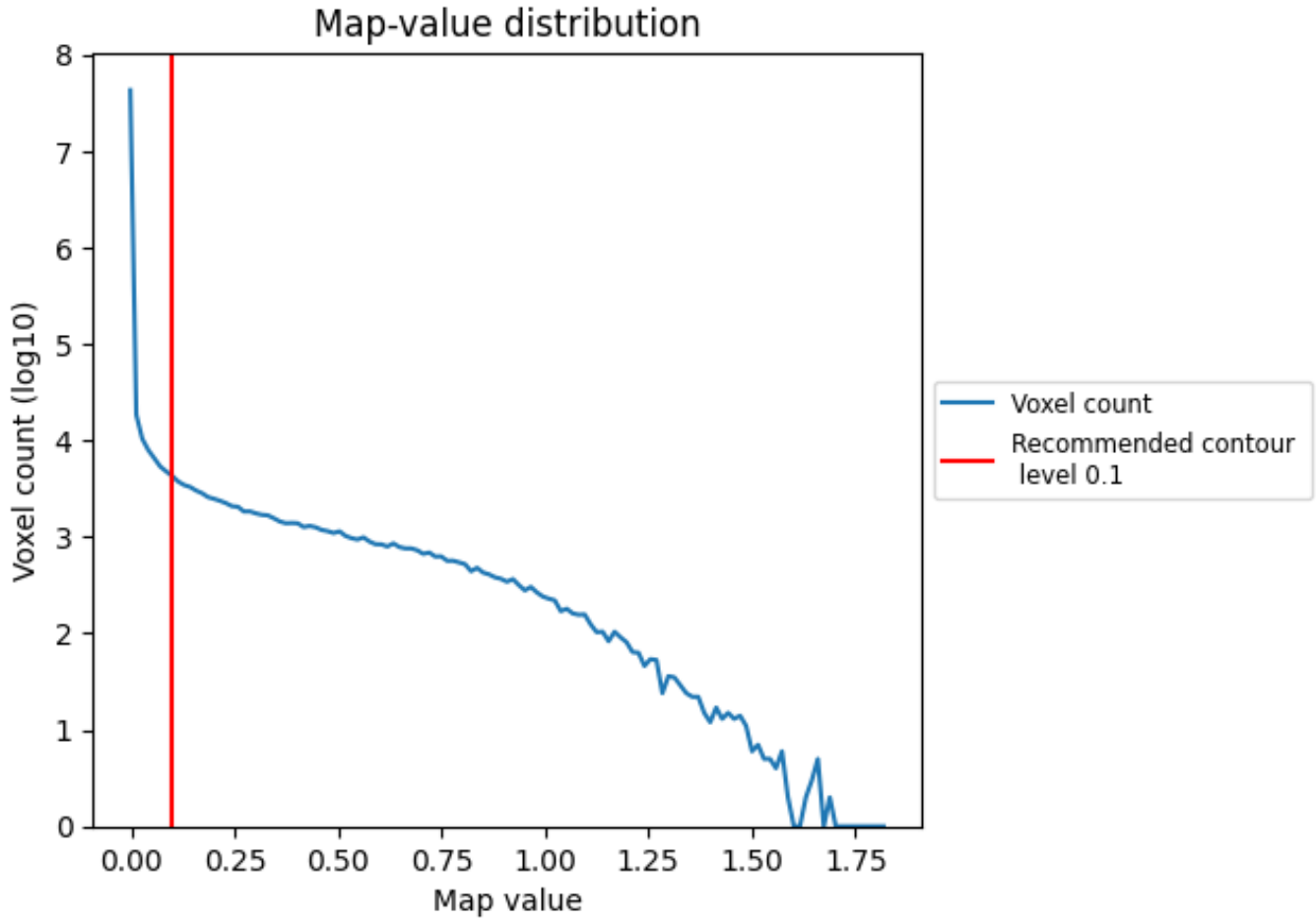
6.6 Mask visualisation (i)

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

7 Map analysis

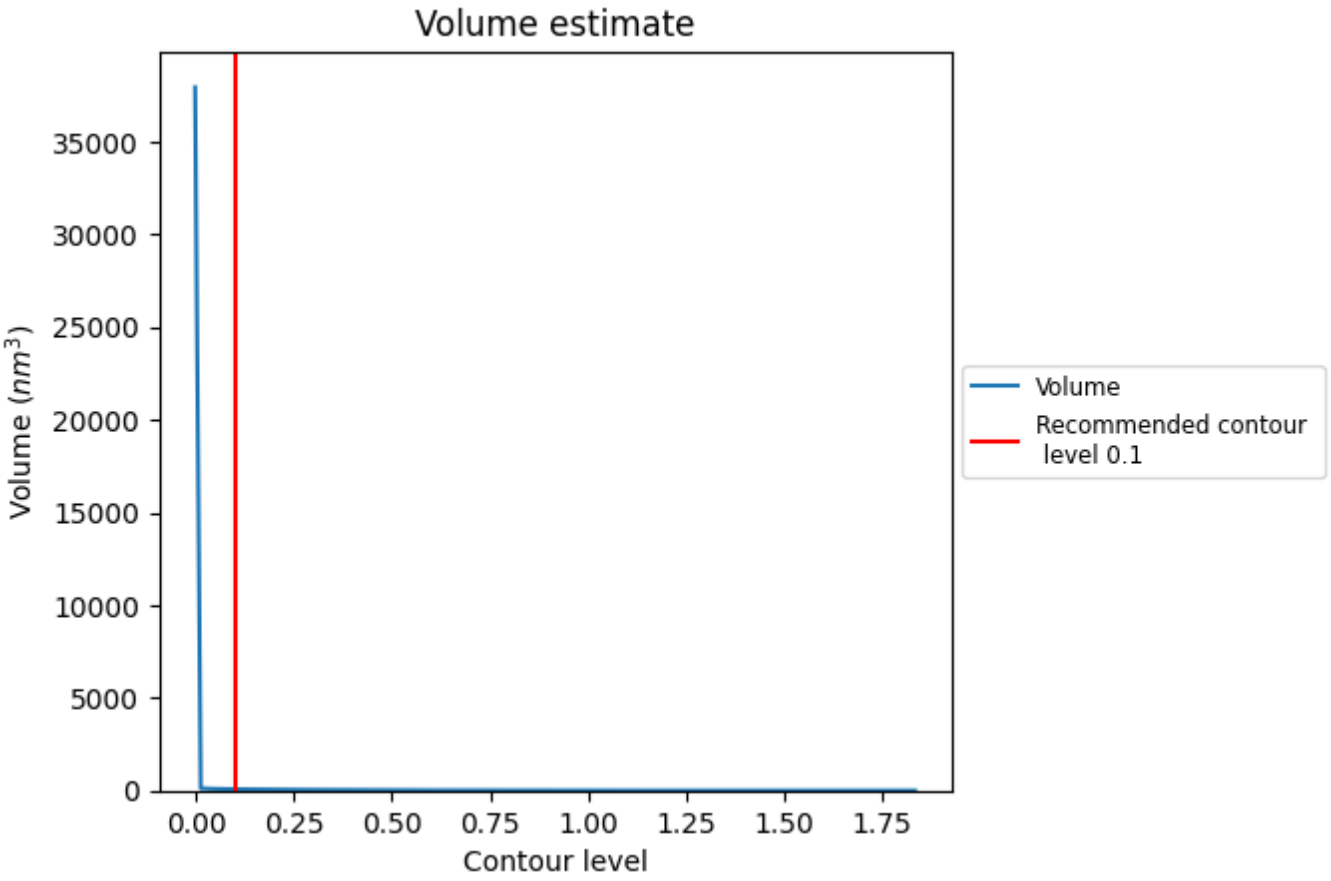
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

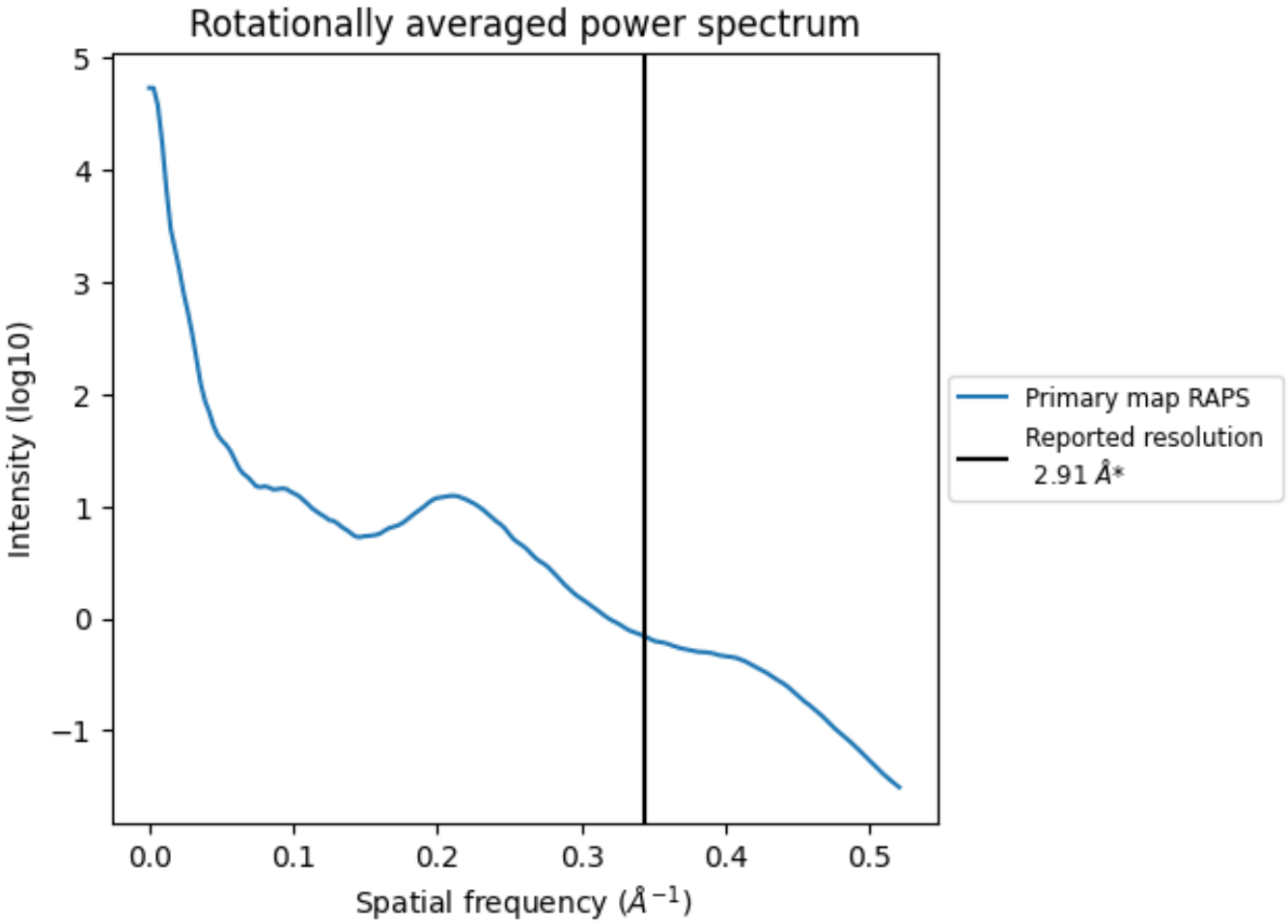
7.2 Volume estimate (i)



The volume at the recommended contour level is 72 nm^3; this corresponds to an approximate mass of 65 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.344 Å^{-1}

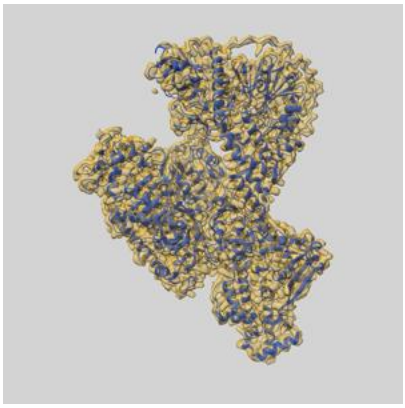
8 Fourier-Shell correlation

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

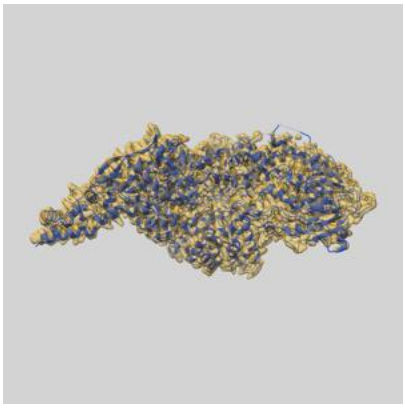
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50143 and PDB model 9F2A. Per-residue inclusion information can be found in section 3 on page 11.

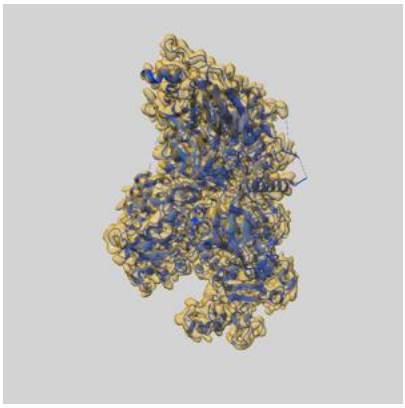
9.1 Map-model overlay



X



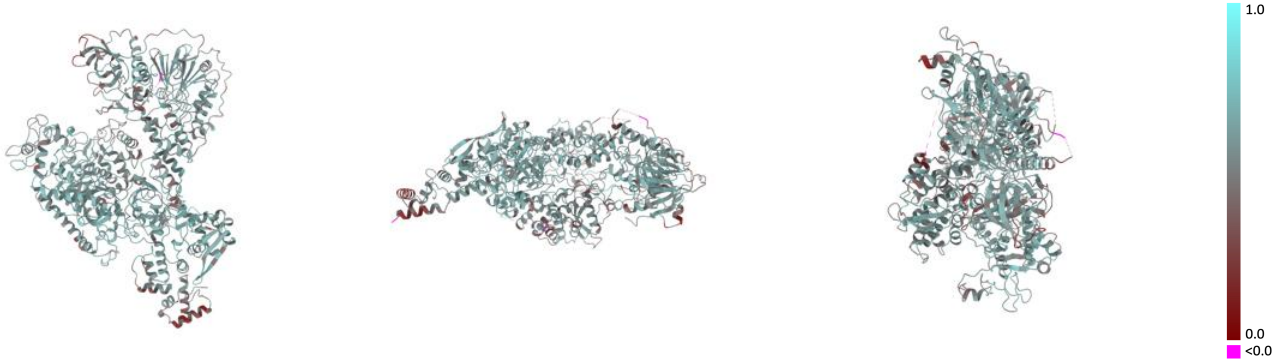
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

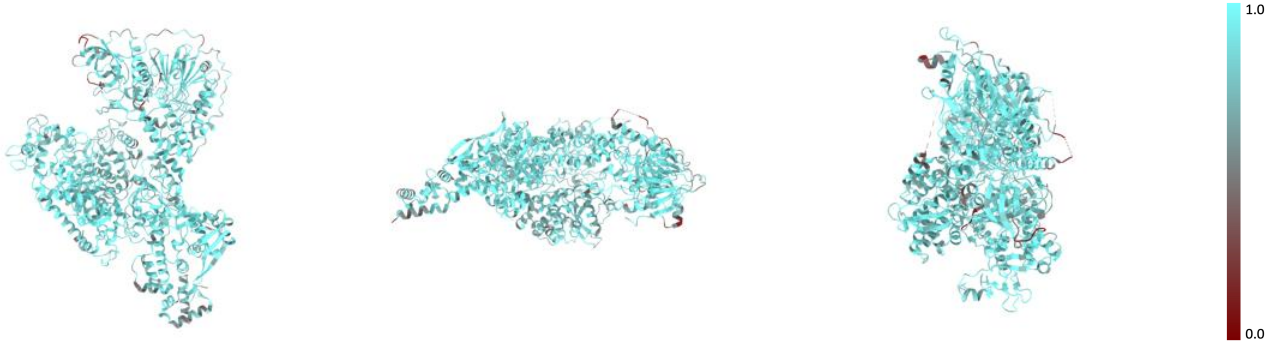
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

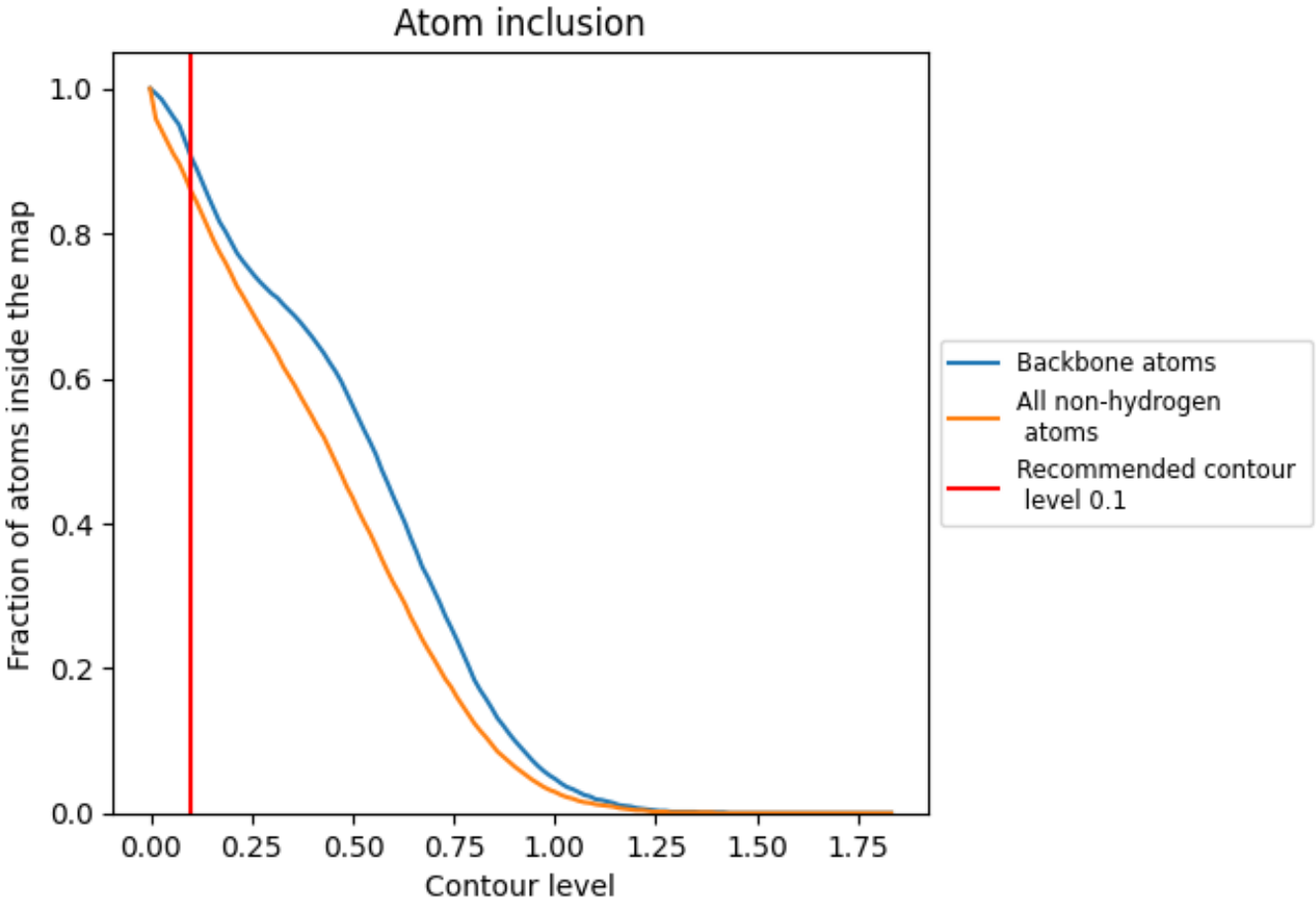
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8580	0.5580
A	0.8210	0.5290
B	0.8810	0.5780
C	0.7120	0.3870