



wwPDB EM Validation Summary Report ⓘ

Oct 2, 2023 – 08:15 pm BST

PDB ID : 8OXM
EMDB ID : EMD-17265
Title : ATM(Q2971A) activated by oxidative stress in complex with Mg AMP-PNP and p53 peptide
Authors : Howes, A.C.; Perisic, O.; Williams, R.L.
Deposited on : 2023-05-02
Resolution : 3.30 Å(reported)
Based on initial model : 7SIC

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.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

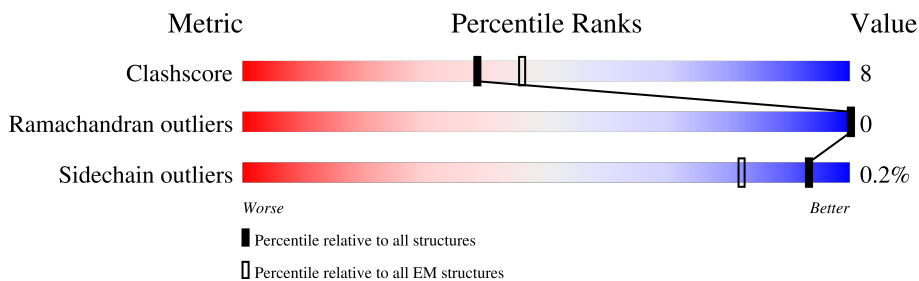
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	E	12	
1	F	12	
2	A	3184	
2	B	3184	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 44174 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	E	7	53	33	8	12	0	0
1	F	7	53	33	8	12	0	0

- Molecule 2 is a protein called Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	2748	22001	14066	3738	4046	151	0	0
2	B	2748	22001	14066	3738	4046	151	0	0

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP Q13315
A	-126	ASP	-	expression tag	UNP Q13315
A	-125	TYR	-	expression tag	UNP Q13315
A	-124	LYS	-	expression tag	UNP Q13315
A	-123	ASP	-	expression tag	UNP Q13315
A	-122	ASP	-	expression tag	UNP Q13315
A	-121	ASP	-	expression tag	UNP Q13315
A	-120	ASP	-	expression tag	UNP Q13315
A	-119	LYS	-	expression tag	UNP Q13315
A	-118	HIS	-	expression tag	UNP Q13315
A	-117	MET	-	expression tag	UNP Q13315
A	-116	GLY	-	expression tag	UNP Q13315
A	-115	VAL	-	expression tag	UNP Q13315
A	-114	GLN	-	expression tag	UNP Q13315
A	-113	VAL	-	expression tag	UNP Q13315
A	-112	GLU	-	expression tag	UNP Q13315
A	-111	THR	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-110	ILE	-	expression tag	UNP Q13315
A	-109	SER	-	expression tag	UNP Q13315
A	-108	PRO	-	expression tag	UNP Q13315
A	-107	GLY	-	expression tag	UNP Q13315
A	-106	ASP	-	expression tag	UNP Q13315
A	-105	GLY	-	expression tag	UNP Q13315
A	-104	ARG	-	expression tag	UNP Q13315
A	-103	THR	-	expression tag	UNP Q13315
A	-102	PHE	-	expression tag	UNP Q13315
A	-101	PRO	-	expression tag	UNP Q13315
A	-100	LYS	-	expression tag	UNP Q13315
A	-99	ARG	-	expression tag	UNP Q13315
A	-98	GLY	-	expression tag	UNP Q13315
A	-97	GLN	-	expression tag	UNP Q13315
A	-96	THR	-	expression tag	UNP Q13315
A	-95	CYS	-	expression tag	UNP Q13315
A	-94	VAL	-	expression tag	UNP Q13315
A	-93	VAL	-	expression tag	UNP Q13315
A	-92	HIS	-	expression tag	UNP Q13315
A	-91	TYR	-	expression tag	UNP Q13315
A	-90	THR	-	expression tag	UNP Q13315
A	-89	GLY	-	expression tag	UNP Q13315
A	-88	MET	-	expression tag	UNP Q13315
A	-87	LEU	-	expression tag	UNP Q13315
A	-86	GLU	-	expression tag	UNP Q13315
A	-85	ASP	-	expression tag	UNP Q13315
A	-84	GLY	-	expression tag	UNP Q13315
A	-83	LYS	-	expression tag	UNP Q13315
A	-82	LYS	-	expression tag	UNP Q13315
A	-81	PHE	-	expression tag	UNP Q13315
A	-80	ASP	-	expression tag	UNP Q13315
A	-79	SER	-	expression tag	UNP Q13315
A	-78	SER	-	expression tag	UNP Q13315
A	-77	ARG	-	expression tag	UNP Q13315
A	-76	ASP	-	expression tag	UNP Q13315
A	-75	ARG	-	expression tag	UNP Q13315
A	-74	ASN	-	expression tag	UNP Q13315
A	-73	LYS	-	expression tag	UNP Q13315
A	-72	PRO	-	expression tag	UNP Q13315
A	-71	PHE	-	expression tag	UNP Q13315
A	-70	LYS	-	expression tag	UNP Q13315
A	-69	PHE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-68	MET	-	expression tag	UNP Q13315
A	-67	LEU	-	expression tag	UNP Q13315
A	-66	GLY	-	expression tag	UNP Q13315
A	-65	LYS	-	expression tag	UNP Q13315
A	-64	GLN	-	expression tag	UNP Q13315
A	-63	GLU	-	expression tag	UNP Q13315
A	-62	VAL	-	expression tag	UNP Q13315
A	-61	ILE	-	expression tag	UNP Q13315
A	-60	ARG	-	expression tag	UNP Q13315
A	-59	GLY	-	expression tag	UNP Q13315
A	-58	TRP	-	expression tag	UNP Q13315
A	-57	GLU	-	expression tag	UNP Q13315
A	-56	GLU	-	expression tag	UNP Q13315
A	-55	GLY	-	expression tag	UNP Q13315
A	-54	VAL	-	expression tag	UNP Q13315
A	-53	ALA	-	expression tag	UNP Q13315
A	-52	GLN	-	expression tag	UNP Q13315
A	-51	MET	-	expression tag	UNP Q13315
A	-50	SER	-	expression tag	UNP Q13315
A	-49	VAL	-	expression tag	UNP Q13315
A	-48	GLY	-	expression tag	UNP Q13315
A	-47	GLN	-	expression tag	UNP Q13315
A	-46	ARG	-	expression tag	UNP Q13315
A	-45	ALA	-	expression tag	UNP Q13315
A	-44	LYS	-	expression tag	UNP Q13315
A	-43	LEU	-	expression tag	UNP Q13315
A	-42	THR	-	expression tag	UNP Q13315
A	-41	ILE	-	expression tag	UNP Q13315
A	-40	SER	-	expression tag	UNP Q13315
A	-39	PRO	-	expression tag	UNP Q13315
A	-38	ASP	-	expression tag	UNP Q13315
A	-37	TYR	-	expression tag	UNP Q13315
A	-36	ALA	-	expression tag	UNP Q13315
A	-35	TYR	-	expression tag	UNP Q13315
A	-34	GLY	-	expression tag	UNP Q13315
A	-33	ALA	-	expression tag	UNP Q13315
A	-32	THR	-	expression tag	UNP Q13315
A	-31	GLY	-	expression tag	UNP Q13315
A	-30	HIS	-	expression tag	UNP Q13315
A	-29	PRO	-	expression tag	UNP Q13315
A	-28	GLY	-	expression tag	UNP Q13315
A	-27	ILE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	ILE	-	expression tag	UNP Q13315
A	-25	PRO	-	expression tag	UNP Q13315
A	-24	PRO	-	expression tag	UNP Q13315
A	-23	HIS	-	expression tag	UNP Q13315
A	-22	ALA	-	expression tag	UNP Q13315
A	-21	THR	-	expression tag	UNP Q13315
A	-20	LEU	-	expression tag	UNP Q13315
A	-19	VAL	-	expression tag	UNP Q13315
A	-18	PHE	-	expression tag	UNP Q13315
A	-17	ASP	-	expression tag	UNP Q13315
A	-16	VAL	-	expression tag	UNP Q13315
A	-15	GLU	-	expression tag	UNP Q13315
A	-14	LEU	-	expression tag	UNP Q13315
A	-13	LEU	-	expression tag	UNP Q13315
A	-12	LYS	-	expression tag	UNP Q13315
A	-11	LEU	-	expression tag	UNP Q13315
A	-10	GLU	-	expression tag	UNP Q13315
A	-9	GLY	-	expression tag	UNP Q13315
A	-8	GLY	-	expression tag	UNP Q13315
A	-7	SER	-	expression tag	UNP Q13315
A	-6	ALA	-	expression tag	UNP Q13315
A	-5	GLY	-	expression tag	UNP Q13315
A	-4	SER	-	expression tag	UNP Q13315
A	-3	GLY	-	expression tag	UNP Q13315
A	-2	SER	-	expression tag	UNP Q13315
A	-1	ALA	-	expression tag	UNP Q13315
A	0	SER	-	expression tag	UNP Q13315
A	2971	ALA	GLN	engineered mutation	UNP Q13315
B	-127	MET	-	initiating methionine	UNP Q13315
B	-126	ASP	-	expression tag	UNP Q13315
B	-125	TYR	-	expression tag	UNP Q13315
B	-124	LYS	-	expression tag	UNP Q13315
B	-123	ASP	-	expression tag	UNP Q13315
B	-122	ASP	-	expression tag	UNP Q13315
B	-121	ASP	-	expression tag	UNP Q13315
B	-120	ASP	-	expression tag	UNP Q13315
B	-119	LYS	-	expression tag	UNP Q13315
B	-118	HIS	-	expression tag	UNP Q13315
B	-117	MET	-	expression tag	UNP Q13315
B	-116	GLY	-	expression tag	UNP Q13315
B	-115	VAL	-	expression tag	UNP Q13315
B	-114	GLN	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-113	VAL	-	expression tag	UNP Q13315
B	-112	GLU	-	expression tag	UNP Q13315
B	-111	THR	-	expression tag	UNP Q13315
B	-110	ILE	-	expression tag	UNP Q13315
B	-109	SER	-	expression tag	UNP Q13315
B	-108	PRO	-	expression tag	UNP Q13315
B	-107	GLY	-	expression tag	UNP Q13315
B	-106	ASP	-	expression tag	UNP Q13315
B	-105	GLY	-	expression tag	UNP Q13315
B	-104	ARG	-	expression tag	UNP Q13315
B	-103	THR	-	expression tag	UNP Q13315
B	-102	PHE	-	expression tag	UNP Q13315
B	-101	PRO	-	expression tag	UNP Q13315
B	-100	LYS	-	expression tag	UNP Q13315
B	-99	ARG	-	expression tag	UNP Q13315
B	-98	GLY	-	expression tag	UNP Q13315
B	-97	GLN	-	expression tag	UNP Q13315
B	-96	THR	-	expression tag	UNP Q13315
B	-95	CYS	-	expression tag	UNP Q13315
B	-94	VAL	-	expression tag	UNP Q13315
B	-93	VAL	-	expression tag	UNP Q13315
B	-92	HIS	-	expression tag	UNP Q13315
B	-91	TYR	-	expression tag	UNP Q13315
B	-90	THR	-	expression tag	UNP Q13315
B	-89	GLY	-	expression tag	UNP Q13315
B	-88	MET	-	expression tag	UNP Q13315
B	-87	LEU	-	expression tag	UNP Q13315
B	-86	GLU	-	expression tag	UNP Q13315
B	-85	ASP	-	expression tag	UNP Q13315
B	-84	GLY	-	expression tag	UNP Q13315
B	-83	LYS	-	expression tag	UNP Q13315
B	-82	LYS	-	expression tag	UNP Q13315
B	-81	PHE	-	expression tag	UNP Q13315
B	-80	ASP	-	expression tag	UNP Q13315
B	-79	SER	-	expression tag	UNP Q13315
B	-78	SER	-	expression tag	UNP Q13315
B	-77	ARG	-	expression tag	UNP Q13315
B	-76	ASP	-	expression tag	UNP Q13315
B	-75	ARG	-	expression tag	UNP Q13315
B	-74	ASN	-	expression tag	UNP Q13315
B	-73	LYS	-	expression tag	UNP Q13315
B	-72	PRO	-	expression tag	UNP Q13315

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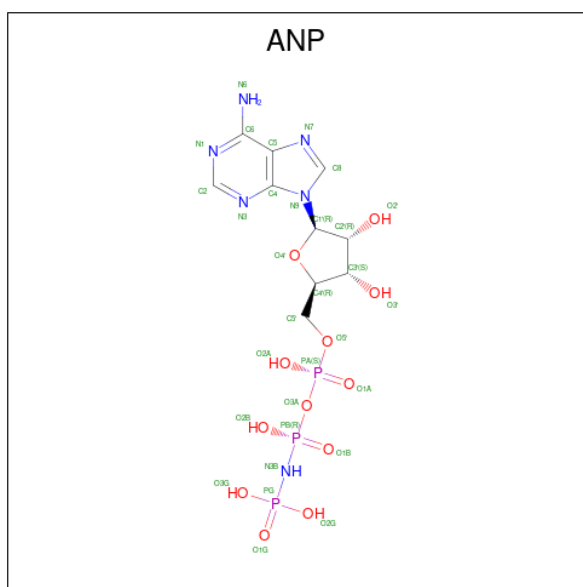
Chain	Residue	Modelled	Actual	Comment	Reference
B	-71	PHE	-	expression tag	UNP Q13315
B	-70	LYS	-	expression tag	UNP Q13315
B	-69	PHE	-	expression tag	UNP Q13315
B	-68	MET	-	expression tag	UNP Q13315
B	-67	LEU	-	expression tag	UNP Q13315
B	-66	GLY	-	expression tag	UNP Q13315
B	-65	LYS	-	expression tag	UNP Q13315
B	-64	GLN	-	expression tag	UNP Q13315
B	-63	GLU	-	expression tag	UNP Q13315
B	-62	VAL	-	expression tag	UNP Q13315
B	-61	ILE	-	expression tag	UNP Q13315
B	-60	ARG	-	expression tag	UNP Q13315
B	-59	GLY	-	expression tag	UNP Q13315
B	-58	TRP	-	expression tag	UNP Q13315
B	-57	GLU	-	expression tag	UNP Q13315
B	-56	GLU	-	expression tag	UNP Q13315
B	-55	GLY	-	expression tag	UNP Q13315
B	-54	VAL	-	expression tag	UNP Q13315
B	-53	ALA	-	expression tag	UNP Q13315
B	-52	GLN	-	expression tag	UNP Q13315
B	-51	MET	-	expression tag	UNP Q13315
B	-50	SER	-	expression tag	UNP Q13315
B	-49	VAL	-	expression tag	UNP Q13315
B	-48	GLY	-	expression tag	UNP Q13315
B	-47	GLN	-	expression tag	UNP Q13315
B	-46	ARG	-	expression tag	UNP Q13315
B	-45	ALA	-	expression tag	UNP Q13315
B	-44	LYS	-	expression tag	UNP Q13315
B	-43	LEU	-	expression tag	UNP Q13315
B	-42	THR	-	expression tag	UNP Q13315
B	-41	ILE	-	expression tag	UNP Q13315
B	-40	SER	-	expression tag	UNP Q13315
B	-39	PRO	-	expression tag	UNP Q13315
B	-38	ASP	-	expression tag	UNP Q13315
B	-37	TYR	-	expression tag	UNP Q13315
B	-36	ALA	-	expression tag	UNP Q13315
B	-35	TYR	-	expression tag	UNP Q13315
B	-34	GLY	-	expression tag	UNP Q13315
B	-33	ALA	-	expression tag	UNP Q13315
B	-32	THR	-	expression tag	UNP Q13315
B	-31	GLY	-	expression tag	UNP Q13315
B	-30	HIS	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	PRO	-	expression tag	UNP Q13315
B	-28	GLY	-	expression tag	UNP Q13315
B	-27	ILE	-	expression tag	UNP Q13315
B	-26	ILE	-	expression tag	UNP Q13315
B	-25	PRO	-	expression tag	UNP Q13315
B	-24	PRO	-	expression tag	UNP Q13315
B	-23	HIS	-	expression tag	UNP Q13315
B	-22	ALA	-	expression tag	UNP Q13315
B	-21	THR	-	expression tag	UNP Q13315
B	-20	LEU	-	expression tag	UNP Q13315
B	-19	VAL	-	expression tag	UNP Q13315
B	-18	PHE	-	expression tag	UNP Q13315
B	-17	ASP	-	expression tag	UNP Q13315
B	-16	VAL	-	expression tag	UNP Q13315
B	-15	GLU	-	expression tag	UNP Q13315
B	-14	LEU	-	expression tag	UNP Q13315
B	-13	LEU	-	expression tag	UNP Q13315
B	-12	LYS	-	expression tag	UNP Q13315
B	-11	LEU	-	expression tag	UNP Q13315
B	-10	GLU	-	expression tag	UNP Q13315
B	-9	GLY	-	expression tag	UNP Q13315
B	-8	GLY	-	expression tag	UNP Q13315
B	-7	SER	-	expression tag	UNP Q13315
B	-6	ALA	-	expression tag	UNP Q13315
B	-5	GLY	-	expression tag	UNP Q13315
B	-4	SER	-	expression tag	UNP Q13315
B	-3	GLY	-	expression tag	UNP Q13315
B	-2	SER	-	expression tag	UNP Q13315
B	-1	ALA	-	expression tag	UNP Q13315
B	0	SER	-	expression tag	UNP Q13315
B	2971	ALA	GLN	engineered mutation	UNP Q13315

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	31	10	6	12	3	0
3	B	1	31	10	6	12	3	0

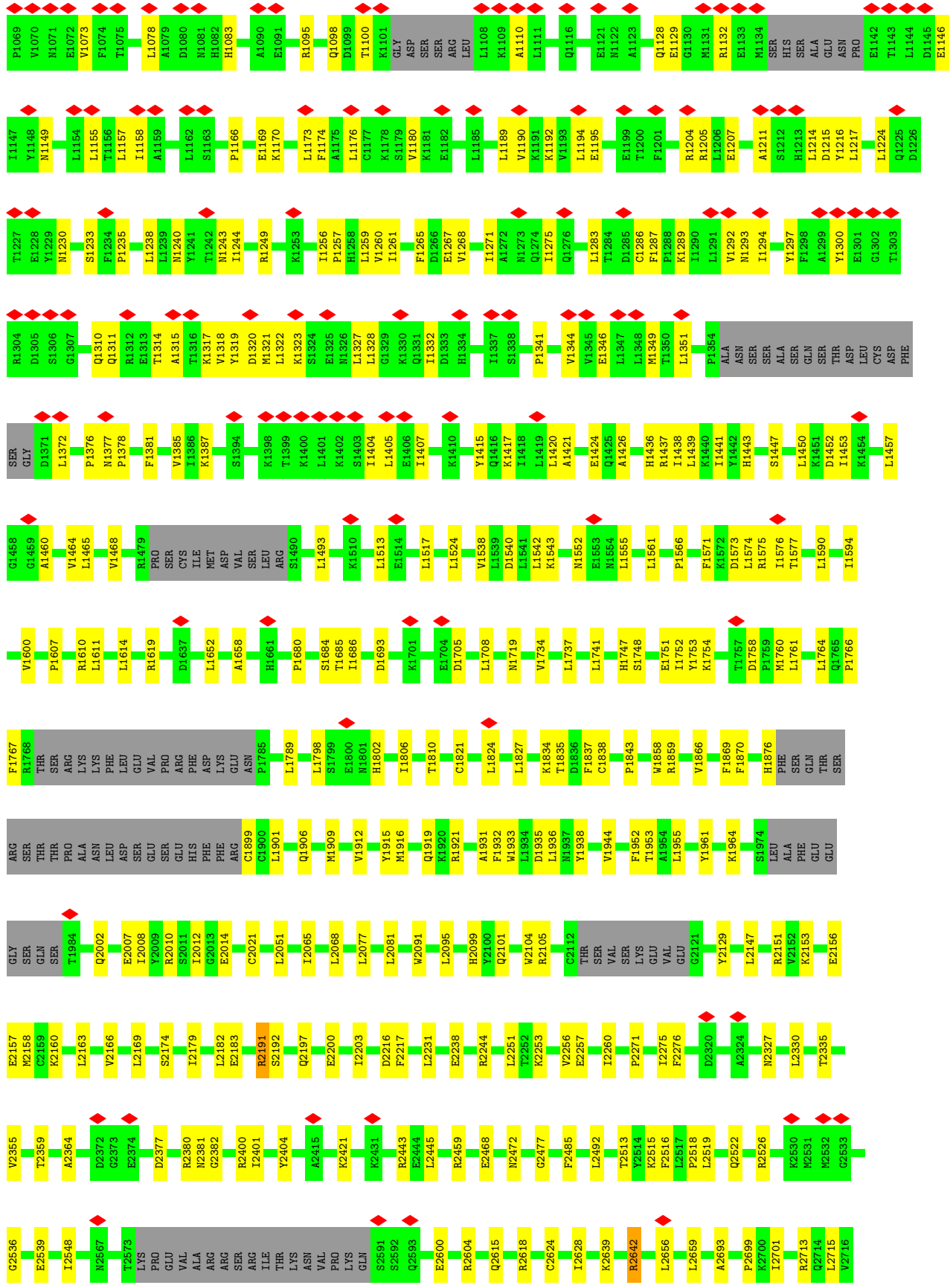
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	B	1	1	1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0
5	B	1	1	1	0

L233	A234	A235	L236	T237	I238	F239	L240	K241	T242	L243	A244	V245	N246	F247	R248	I249	R250	V251	C252	E253	L254	G255	D256	E257	I258	L259	P260	T261	L262	L263	Y264	L265	V266	T267	Q268	H269	R270	L271	N272	D273	S274	L275	K276	E277	V278	I279	I280	E281	L282	Q284	L285	Q286	I287	Y288	P292	K293				
K296	T297	Q298	E299	K300	F301	A302	Y303	E304	S305	T306	K307	W308	R309	S310	F311	L312	Y313	N314	L315	C252	Y316	D317	L318	L319	V320	N321	E322	I323	S324	H325	L326	G327	S328	R329	GLY	LYS	TTR	SER	SER	GLY	PHE	R337	N338	I339	S274	A340	V341	K342	E343	N344	L345	I346	E347	L348	N349	C353	H354	Q355	V356	F357
N358	GLU	L480	THR	ARG	SER	LEU	GLU	ILE	SER	GLN	TTR	THR	GLN	ARG	GLU	SER	SER	ASP	ASP	TTR	VAL	PRO	CYS	LYS	ARG	LYS	LYS	L389	E390	L391	G392	W393	E394	V395	I396	K397	D398	H399	L400	Q401	K402	S403	Q404	M405	D406	F407	D408	L409	V410	P411	W412	L413	Q414	A415	L416	A417	T417			
Q418	L419	I420	S421	K422	Y423	P424	L427	N428	M429	C430	E431	L432	S433	P434	L435	L436	M437	I438	L439	S440	Q441	L442	L443	P444	Q445	Q446	R447	H448	G449	E450	R451	T452	P453	Y454	Y455	L456	R457	C458	L459	T460	E461	A463	L464	C465	Q466	D467	K468	R469	S470	M471	L472	E473	S474	Q475	K477	S478				
D479	L480	L481	L482	W484	M485	K486	L487	W488	C489	I490	E491	F492	R493	S496	S497	E498	Q499	I500	Q501	N504	F505	G506	L507	L508	G509	A510	I511	I512	Q513	G514	S515	L516	V517	E518	V519	D520	R521	E522	K525	F527	T528	G529	S530	A531	C532	R533	P534	S535	A538	T543	L544	A545								
L546	T547	T548	S549	L550	V551	P552	M553	T554	VAL	LYS	MET	GLY	ILE	GLU	GLN	ASN	MET	CYS	GLU	HIS	VAL	GLN	LYS	ARG	SER	F570	S571	L572	K573	F582	Y583	Q584	L585	GLU	ASP	LEU	L653	G654	T655	L656	F657	D658	K659	M660	D661	F662	L663	T664	ILE	VAL	N602	F603	P604	H605	L606	V607	L608	E609	K610	V613
T616	M617	K618	K621	A622	A623	M624	N625	F626	S629	V630	P631	E632	GLU	HIS	HIS	GLN	LYS	ASP	LYS	GLU	LEU	S644	F645	S646	E647	V648	E649	L653	G654	T655	L656	F657	D658	K659	M660	D661	F662	L663	T664	ILE	VAL	ARG	GLU	CYS	GLY	ILE	GLU	LYS	HIS	SER	SER									
ILE	G679	F680	S681	V682	H683	Q684	N685	L686	R692	C693	L694	L695	G696	L697	S698	E699	Q700	M703	N704	Y705	S706	S707	E708	I709	T710	N711	S712	E713	T714	R717	C718	S719	R720	L721	L722	L726	M732	G733	V734	L735	A736	E737	E738	E739	L740	Y741	K742	S743	E744	L745	F746	K748								
Q754	C755	A756	G757	E758	S759	I760	T761	L762	F763	K764	N765	K766	M768	E769	E770	F771	R772	I773	G774	S775	L776	R777	M778	M779	K780	Q781	L782	C783	T784	R785	S788	M789	C790	T791	K792	K793	S794	F795	M796	K797	L798	F803	L804	L807	T808	S809	K810	L811	M812	D814	L815	A816	D817	L818						
C819	K820	S821	L822	A823	S824	F825	I826	LYS	LYS	PHE	ASP	ARG	GLY	VAL	GLU	SER	MET	GLU	ASP	THR	D899	M900	K902	F903	L904	C905	L906	C907	V908	T909	T910	A911	Q912	T913	N914	T915	V916	S917	F918	R919	A920	A921	D922	I923	R924	R925	K926	L927	L928	M929	L930	I931	D932	S933	T934	L936	E937	P938		
T939	K940	S941	L942	H943	L944	H945	H946	Y947	L948	M949	L950	L951	K952	E953	L954	P955	G956	E957	E958	Y959	P960	L961	P962	M963	E964	D965	V966	L967	E968	L969	L970	K971	L972	L973	S974	N975	V976	C977	Y980	R981	R982	D983	Y986	T990	L991	N992	H993	V994	L995	H996	K999	M1000	L1001	G1002	Q1003					
S1004	M1005	M1006	D1007	S1008	E1009	N1010	T1011	R1012	F1018	L1019	I1022	G1023	A1024	F1025	W1026	H1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	F1036	S1037	L1038	R1039	M1040	A1041	L1042	V1043	M1044	C1045	L1046	K1047	T1048	L1049	L1050	E1051	A1052	D1053	P1054	Y1055	S1056	K1057	W1058	A1059	I1060	L1061	M1062	V1063	M1064	G1065	K1066	D1067	F1068				



G494	I495	S496	S497	E498	Q499	I500	Q501	A502	E503	N504	F505	G506	L507	L508	G509	A510	I511	I512	Q513	G514	S515	L516	V517	E518	V519	D520	R521	E522	F523	W524	K525	L526	F527	T528	G529	S530	A531	C532	R533	F534	S535	C536	P537	A538	W539	C540	T543	L544	A545	L546	T547	I550	V551	P552	G553	T554	VAL																																																									
LYS	MET	GLY	ILE	GLU	GLN	ASP	ASN	GLU	ILE	GLY	GLU	VAL	ASN	ASN	ARG	SER	F570	F582	Y583	Q584	GLU	GLY	ASP	LEU	GLU	ASN	SER	T593	E594	V595	P596	I597	I598	L599	H600	S601	N602	F603	P604	H605	L606	V607	L608	E609	L612	L615	K618	N625	F626	F627	L695	G696	L697	S629	V630	P631	E632	C633																																																								
GLU	HIS	GLN	LYS	ASP	LYS	GLU	VAL	S644	F645	S646	E647	V648	E649	E650	Q654	T655	T656	F657	D658	K659	M660	D661	F662	L663	T664	I665	VAL	ARG	GLU	GLY	CYS	GLY	ILE	GLU	HIS	GLN	SER	SER	SER	I668	F679	F680	H683	Q684	N685	L686	R692	C693	L694	L695	G696	S698	L697	E699	Q700																																																											
L701	L702	N703	N704	Y705	S706	S707	E708	I709	T710	N711	S712	E713	T714	L715	V716	C718	S719	R720	L721	K659	M660	D661	F662	L663	T664	I665	VAL	ARG	GLU	GLY	CYS	GLY	ILE	GLU	HIS	GLN	SER	SER	SER	I668	F679	F680	H683	Q684	N685	L686	R692	C693	L694	L695	G696	S698	L697	E699	Q700																																																											
N769	E769	E770	F771	R772	I773	G774	S775	L776	R777	N778	M779	Q781	L782	R785	S788	N789	K792	K793	K797	I798	A799	S800	G801	F802	L804	R805	A736	L806	L807	T808	S809	K810	N813	D814	I815	A816	D817	I818	C819	K820	S821	L822	A823	S824	F825	I826	L826	L827	P828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	K892	Q893
GLU	VAL	GLU	SER	MET	GLU	ASP	THR	ASN	GLY	ASN	LEU	MET	GLU	GLU	GLU	ASP	GLN	SER	SER	MET	ASN	PHE	ASN	TYR	PRO	ASP	SER	SER	VAL	ASP	ALA	ASN	GLU	PRO	GLY	GLU	SER	SER	GLN	S877	T878	I879	G880	A881	I882	N883	P884	P885	A886	L887	E887	E888	Y889	S891	L890	S891	K892	Q893																																																								
D894	L895	L896	F897	L898	D899	H900	L901	K902	F903	L904	C905	V908	T909	T910	A911	Q912	T913	N914	T915	V916	S917	F918	R919	A920	A921	D922	I923	A924	R925	K926	L927	L928	N929	L930	I931	D932	S933	S934	T935	L936	E937	P938	T939	K940	S941	L942	H943	L944	Y947	L948	H949	L950	L951	K952	E953	L954	P955																																																									
G956	E957	E958	Y959	P960	L961	P962	M963	E964	D965	V966	L967	E968	L969	L970	K971	N975	V976	C977	Y980	R981	R982	D983	V986	C987	L991	V994	L995	H996	V997	V998	K999	M1000	L1001	G1002	Q1003	S1004	M1005	M1006	D1007	S1008	E1009	M1010	T1011	L1012	D1013	A1014	Q1015	F1018	L1019	G1023	W1026																																																															
H1027	L1028	T1029	K1030	E1031	R1032	K1033	Y1034	I1035	F1036	R1039	L1042	L1046	K1047	T1048	L1049	L1050	E1051	D1052	P1054	K1057	M1058	A1059	I1060	L1061	M1062	V1063	M1064	G1065	K1066	D1067	F1068	P1069	E1072	V1073	F1074	T1075	Q1076	F1077	L1078	A1079	D1080	M1081	H1082	L1083	H1084	V1085	A1090	E1091	M1094	R1095	L1096																																																															
F1097	Q1098	D1099	T1100	K1101	GLY	ASP	SER	ARG	LEU	L1108	K1109	A1110	L1111	Q1116	A1123	Y1124	L1125	K1126	A1127	Q1128	E1129	R1132	E1133	M1134	SER	HIS	ALA	GLU	ASN	PRO	E1142	T1143	L1144	D1145	E1146	M1149	V1153	L1154	L1155	L1156	I1158	A1159	V1160	V1161	P1166	E1169	K1170	Q1171	A1172	L1173																																																																
F1174	A1175	L1176	G1177	K1178	S1179	V1180	K1181	E1182	E1186	P1187	H1188	L1189	V1190	K1191	K1192	V1193	L1194	E1195	E1199	T1200	R1204	R1205	L1206	E1207	D1208	A1211	L1214	D1215	Y1216	L1217	V1218	L1219	F1220	W1221	L1222	M1223	L1224	Q1225	D1226	T1227	E1228	Y1229	M1230	L1231	S1232	S1233	F1234	I1237	L1238	L1239	M1240	Y1241	T1242																																																													
M1243	P1257	H1258	L1259	V1260	I1261	R1262	S1263	D1266	E1267	I1271	A1272	N1273	S1281	F1287	P1288	K1289	I1290	L1291	V1292	M1293	L1294	L1295	P1296	Y1300	E1301	G1302	T1303	R1304	L1305	S1306	G1307	Q1310	K1311	R1312	E1313	T1314	A1315	T1316	K1317	D1320	H1321	K1322	L1323	S1324	E1325	M1326	L1327	L1328	H1334	L1335																																																																
F1336	P1341	E1342	I1343	V1344	E1345	E1346	L1347	L1348	M1349	T1350	F1354	ALA	ASN	SER	SER	ALA	SER	GLN	SER	THR	ASP	LEU	CYS	ASP	PHE	SER	GLY	D1371	L1372	M1377	P1378	H1380	F1381	V1386	I1386	K1387	K1398	T1399	K1400	L1401	K1402	S1403	I1404	L1405	E1406	I1407	P1412	Q1416	L1419	L1420																																																																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30707	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 ($e^-/\text{\AA}^2$)	39.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.537	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	330.4, 330.4, 330.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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, ANP, 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	E	0.22	0/54	0.45	0/73
1	F	0.24	0/54	0.48	0/73
2	A	0.24	0/22409	0.45	0/30274
2	B	0.24	0/22409	0.45	0/30274
All	All	0.24	0/44926	0.45	0/60694

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	53	0	51	1	0
1	F	53	0	51	0	0
2	A	22001	0	22171	366	0
2	B	22001	0	22171	342	0
3	A	31	0	13	1	0
3	B	31	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
All	All	44174	0	44470	702	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 8.

The worst 5 of 702 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)
2:B:1876:HIS:CE1	2:B:1899:CYS:SG	2.73	0.76
2:A:259:LEU:HD21	2:A:286:GLN:HE22	1.51	0.76
2:B:718:CYS:SG	2:B:748:LYS:NZ	2.59	0.76
2:A:954:LEU:HD23	2:A:969:LEU:HD22	1.69	0.75
2:A:1249:ARG:HE	2:A:1275:ILE:HG13	1.54	0.71

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	E	5/12 (42%)	5 (100%)	0	0	100	100
1	F	5/12 (42%)	5 (100%)	0	0	100	100
2	A	2708/3184 (85%)	2652 (98%)	56 (2%)	0	100	100
2	B	2708/3184 (85%)	2651 (98%)	57 (2%)	0	100	100
All	All	5426/6392 (85%)	5313 (98%)	113 (2%)	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	E	7/12 (58%)	7 (100%)	0	100	100
1	F	7/12 (58%)	7 (100%)	0	100	100
2	A	2444/2883 (85%)	2439 (100%)	5 (0%)	93	97
2	B	2444/2883 (85%)	2439 (100%)	5 (0%)	93	97
All	All	4902/5790 (85%)	4892 (100%)	10 (0%)	93	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1619	ARG
2	B	2191	ARG
2	B	2642	ARG
2	A	2191	ARG
2	A	2642	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1116	GLN
2	B	1310	GLN
2	B	1867	GLN
2	B	1416	GLN
2	A	2208	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	B	3101	4	29,33,33	1.09	4 (13%)	31,52,52	1.10	2 (6%)
3	ANP	A	3101	4	29,33,33	1.08	4 (13%)	31,52,52	1.08	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	B	3101	4	-	6/14/38/38	0/3/3/3
3	ANP	A	3101	4	-	6/14/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3101	ANP	PG-O1G	2.46	1.50	1.46
3	A	3101	ANP	PG-O1G	2.46	1.50	1.46
3	B	3101	ANP	PG-N3B	2.43	1.69	1.63
3	A	3101	ANP	PG-N3B	2.43	1.69	1.63
3	B	3101	ANP	PB-O1B	2.33	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3101	ANP	PB-O3A-PA	-3.75	119.42	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3101	ANP	PB-O3A-PA	-3.66	119.71	132.62
3	B	3101	ANP	C5-C6-N6	2.27	123.80	120.35
3	A	3101	ANP	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

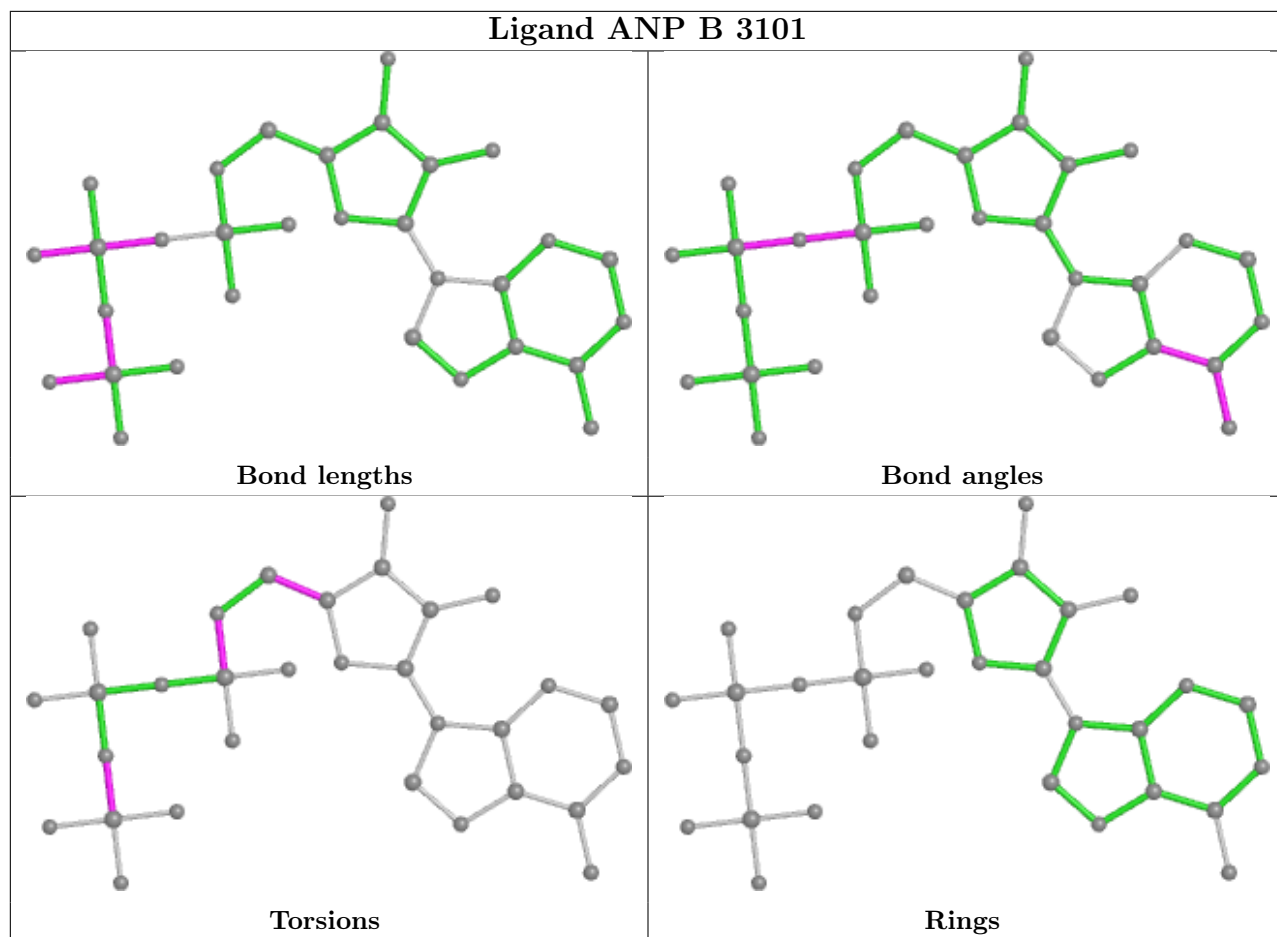
Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PB-N3B-PG-O1G
3	A	3101	ANP	C5'-O5'-PA-O1A
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	A	3101	ANP	C3'-C4'-C5'-O5'
3	B	3101	ANP	PB-N3B-PG-O1G

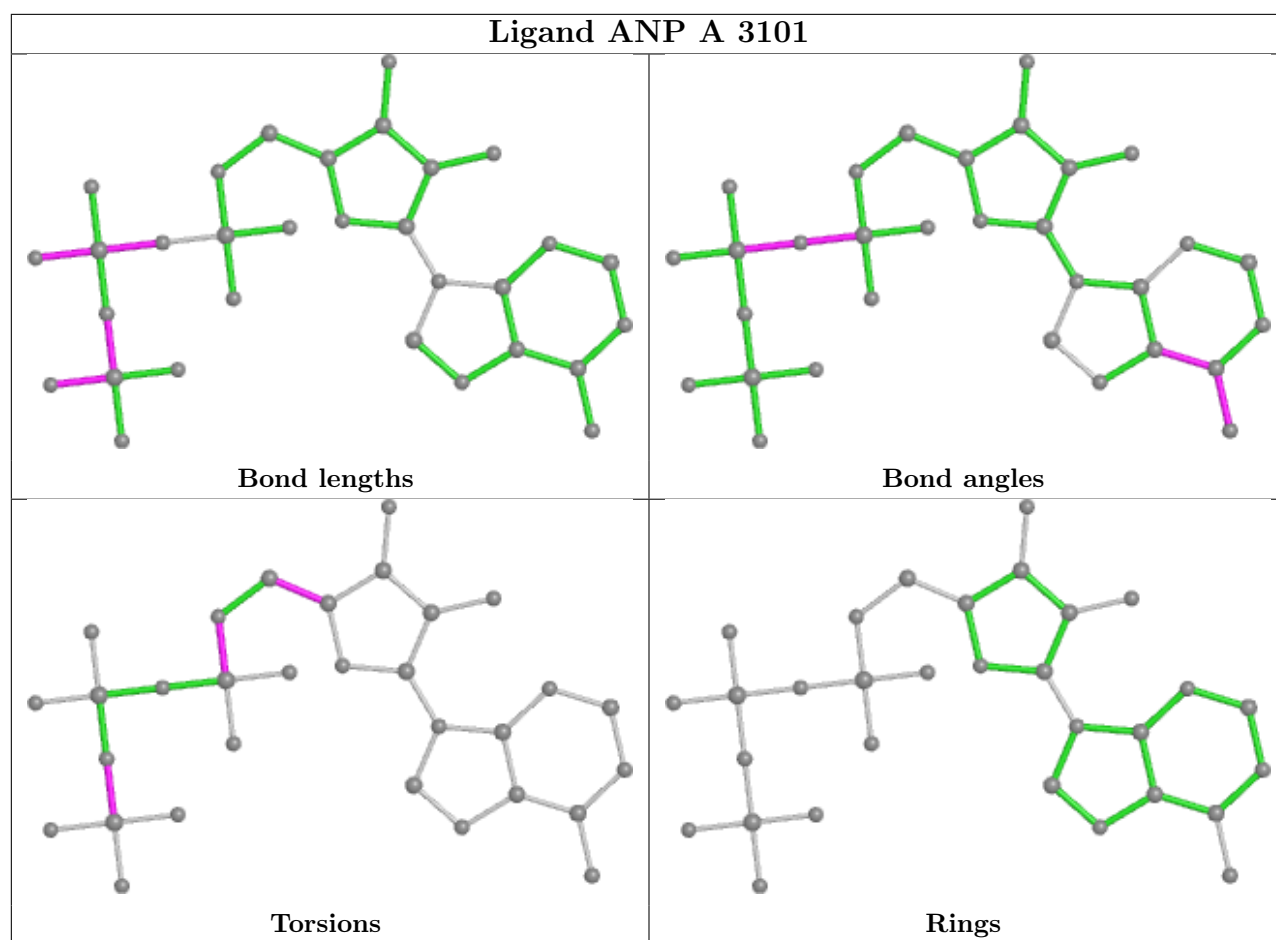
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3101	ANP	3	0
3	A	3101	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

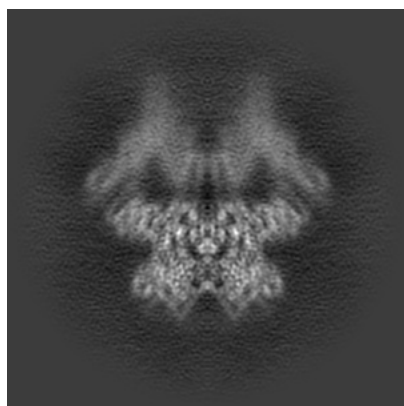
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17265. These allow visual inspection of the internal detail of the map and identification of artifacts.

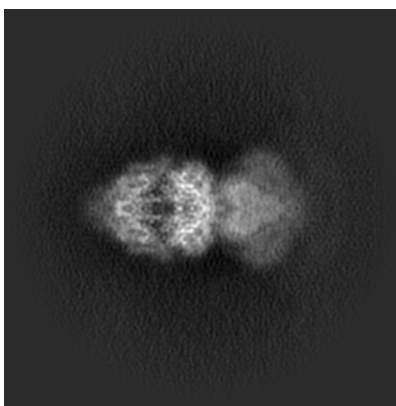
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

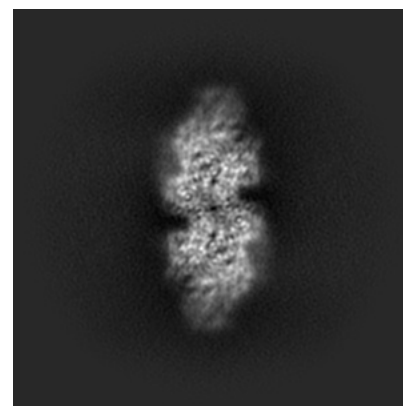
6.1.1 Primary map



X

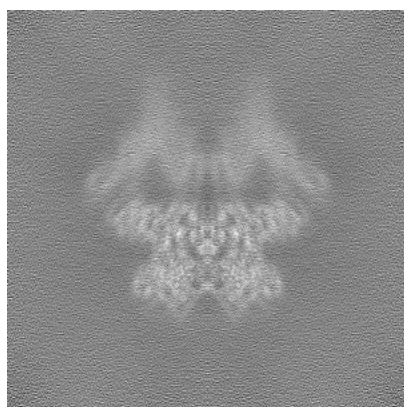


Y

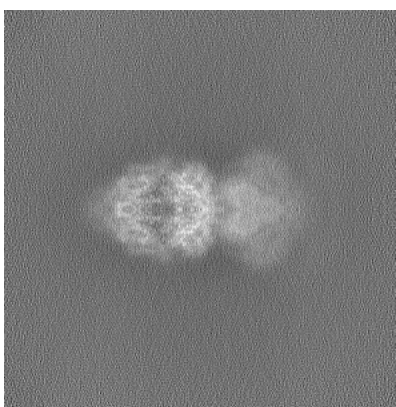


Z

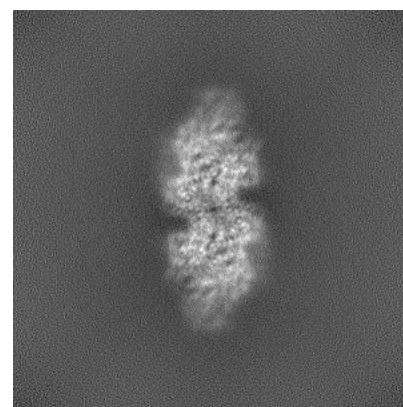
6.1.2 Raw map



X



Y

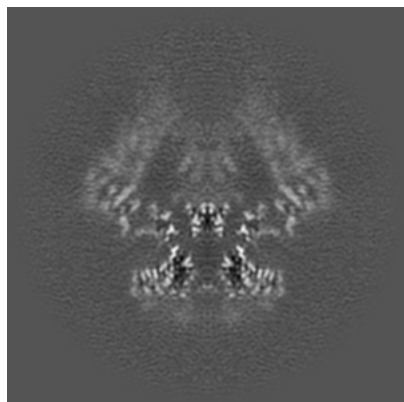


Z

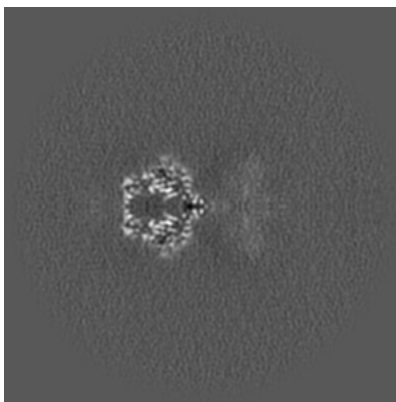
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

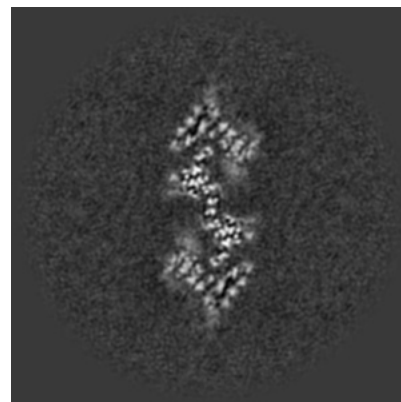
6.2.1 Primary map



X Index: 200

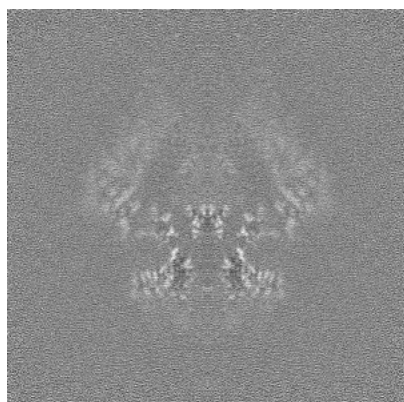


Y Index: 200

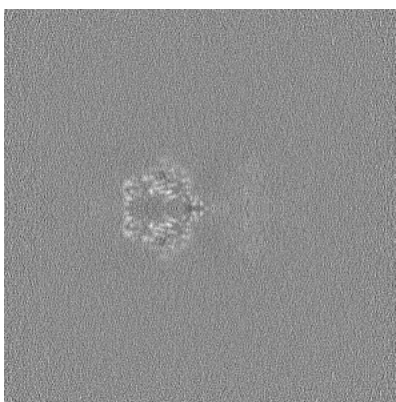


Z Index: 200

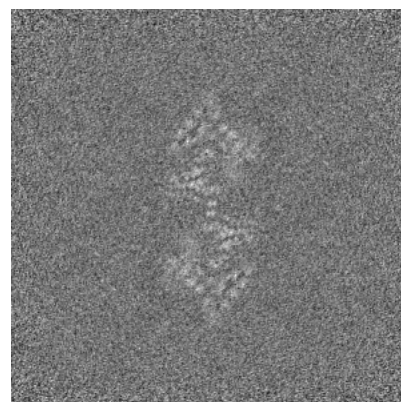
6.2.2 Raw map



X Index: 200



Y Index: 200

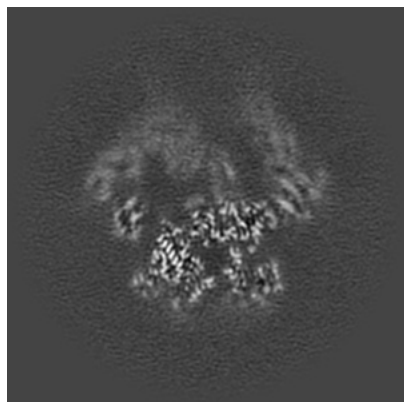


Z Index: 200

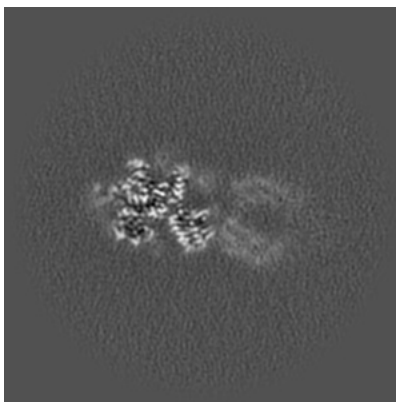
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

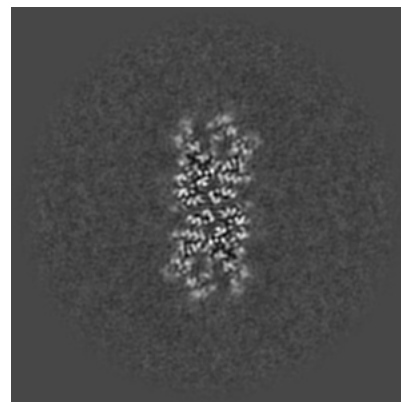
6.3.1 Primary map



X Index: 191

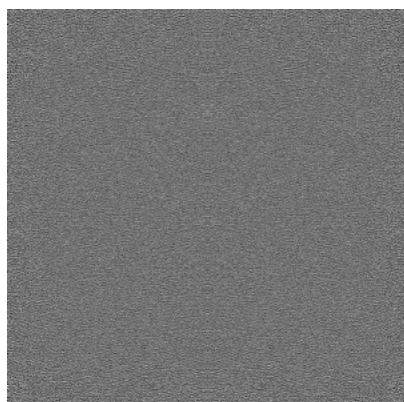


Y Index: 229

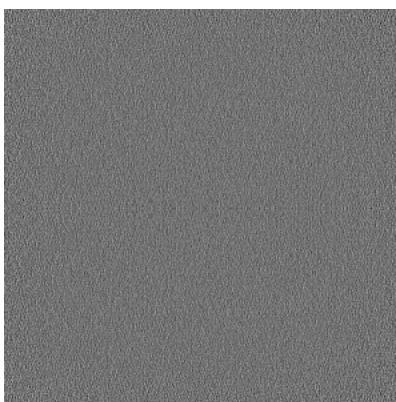


Z Index: 177

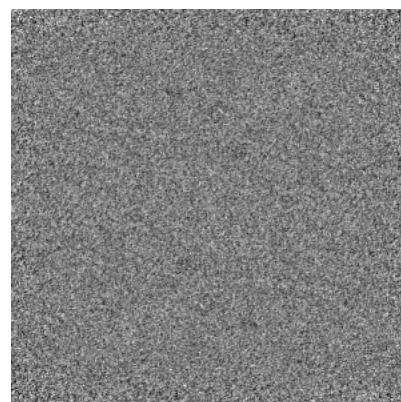
6.3.2 Raw map



X Index: 0



Y Index: 0

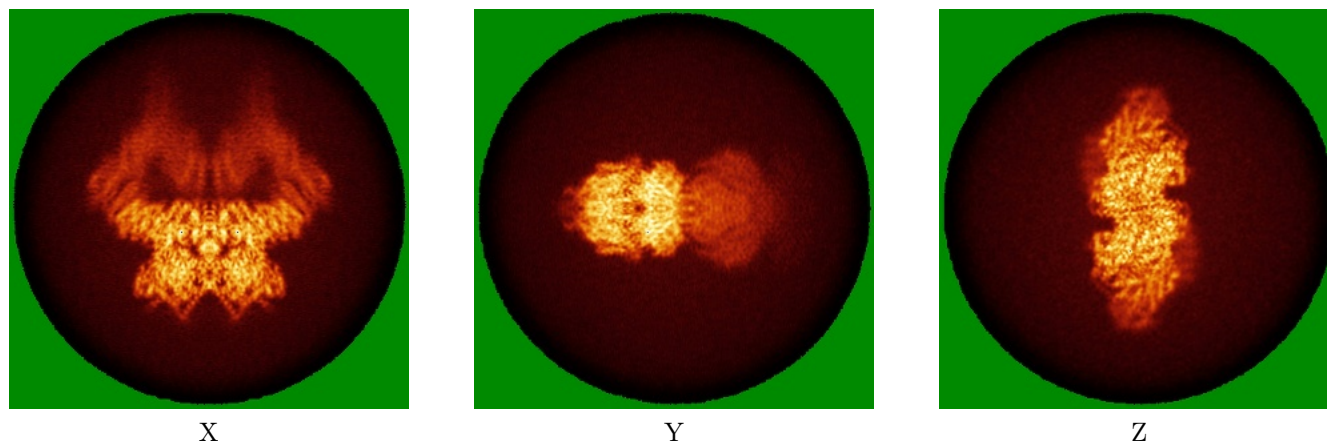


Z Index: 0

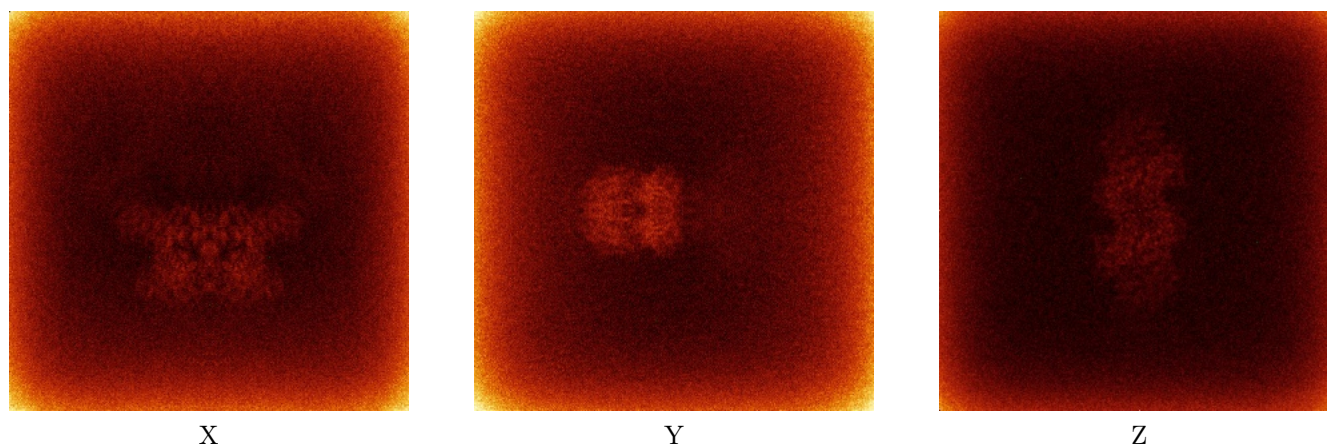
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



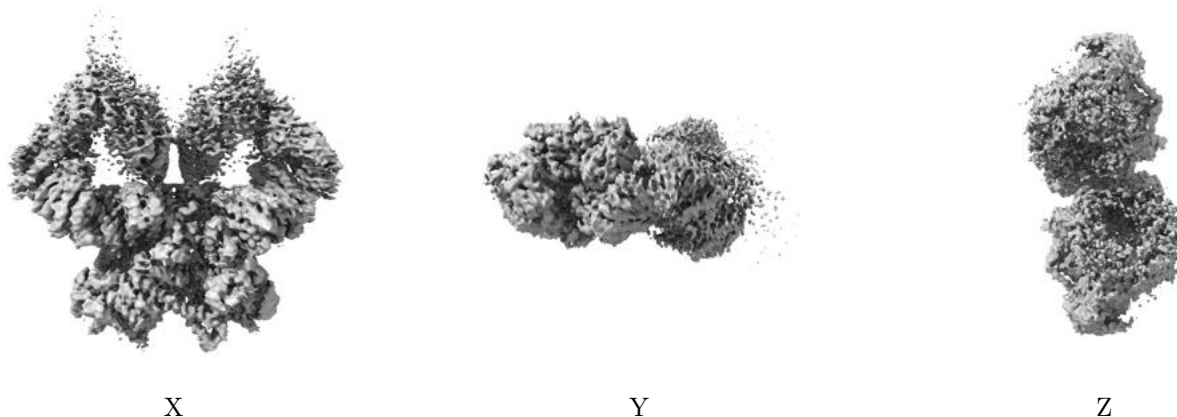
6.4.2 Raw map



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.

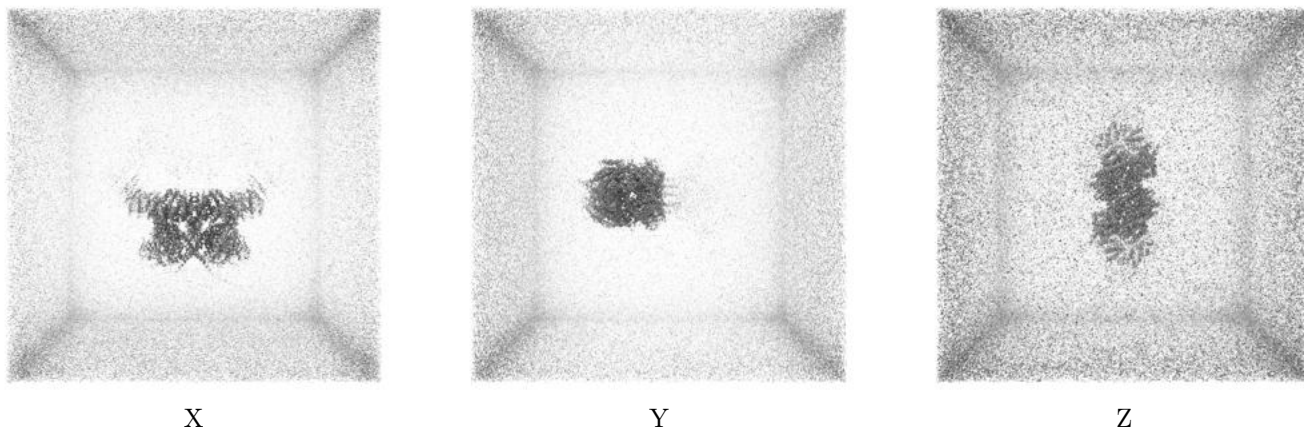
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

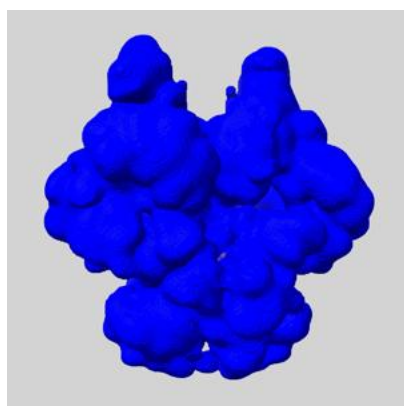
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

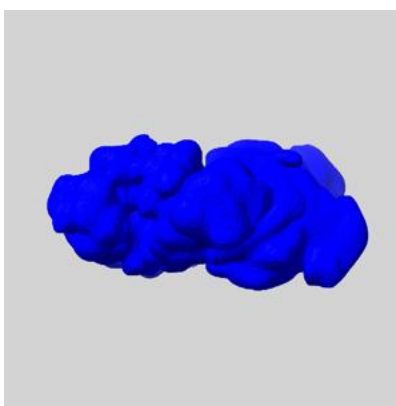
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

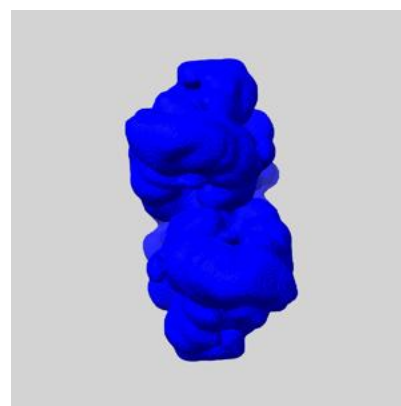
6.6.1 emd_17265_msk_1.map [i](#)



X



Y

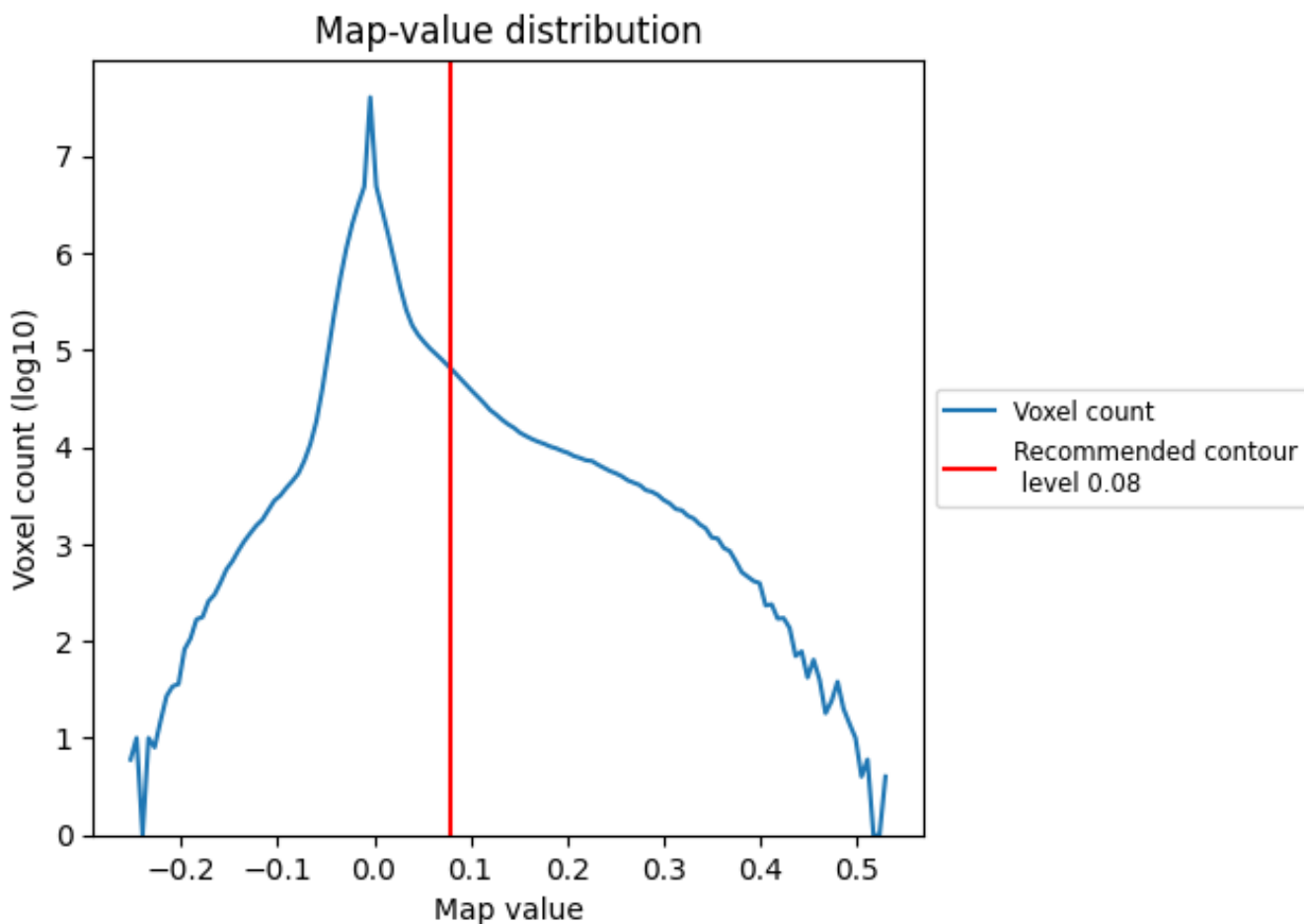


Z

7 Map analysis [i](#)

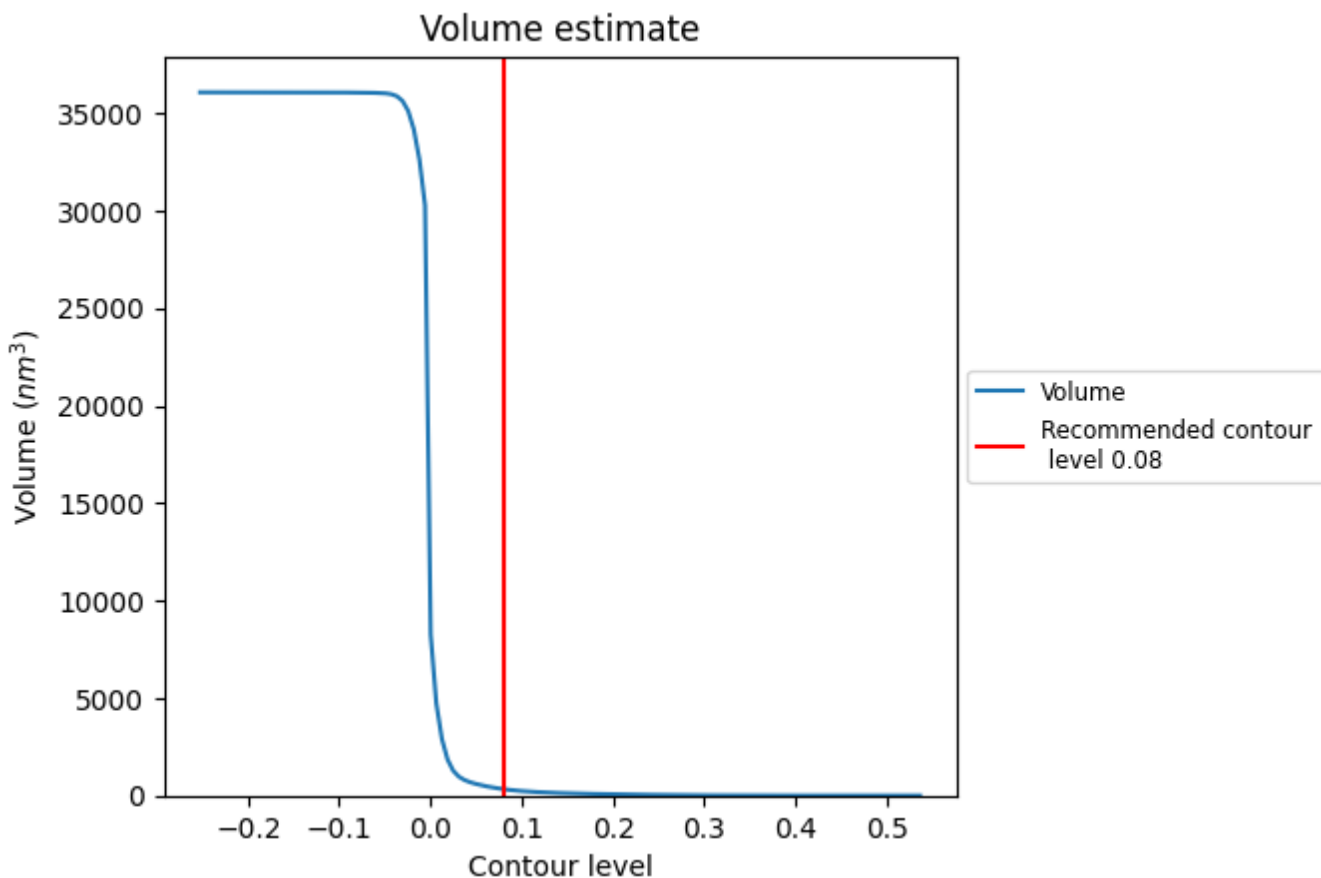
This section contains the results of statistical analysis of the map.

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.

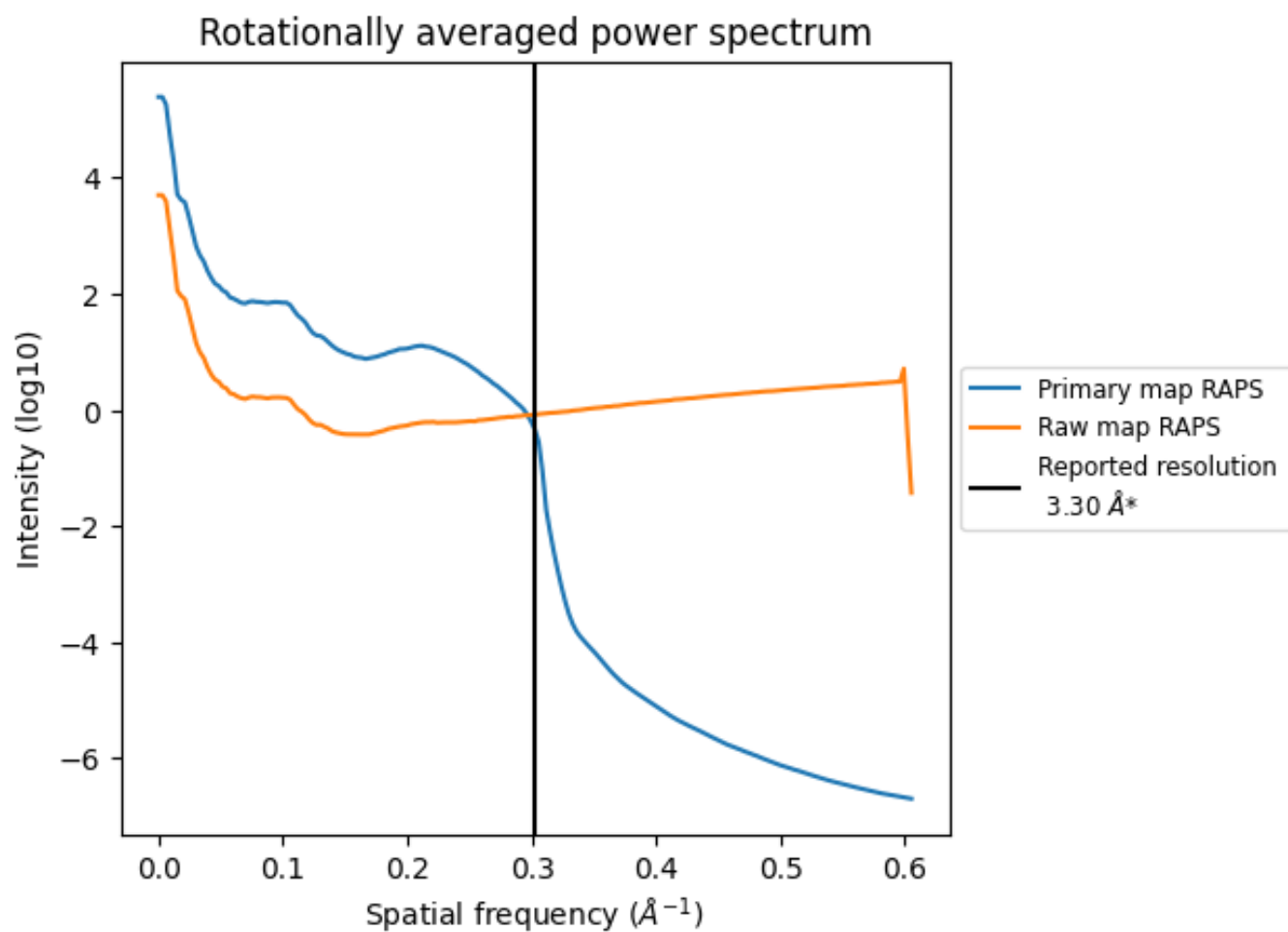
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 331 nm^3 ; this corresponds to an approximate mass of 299 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](#)

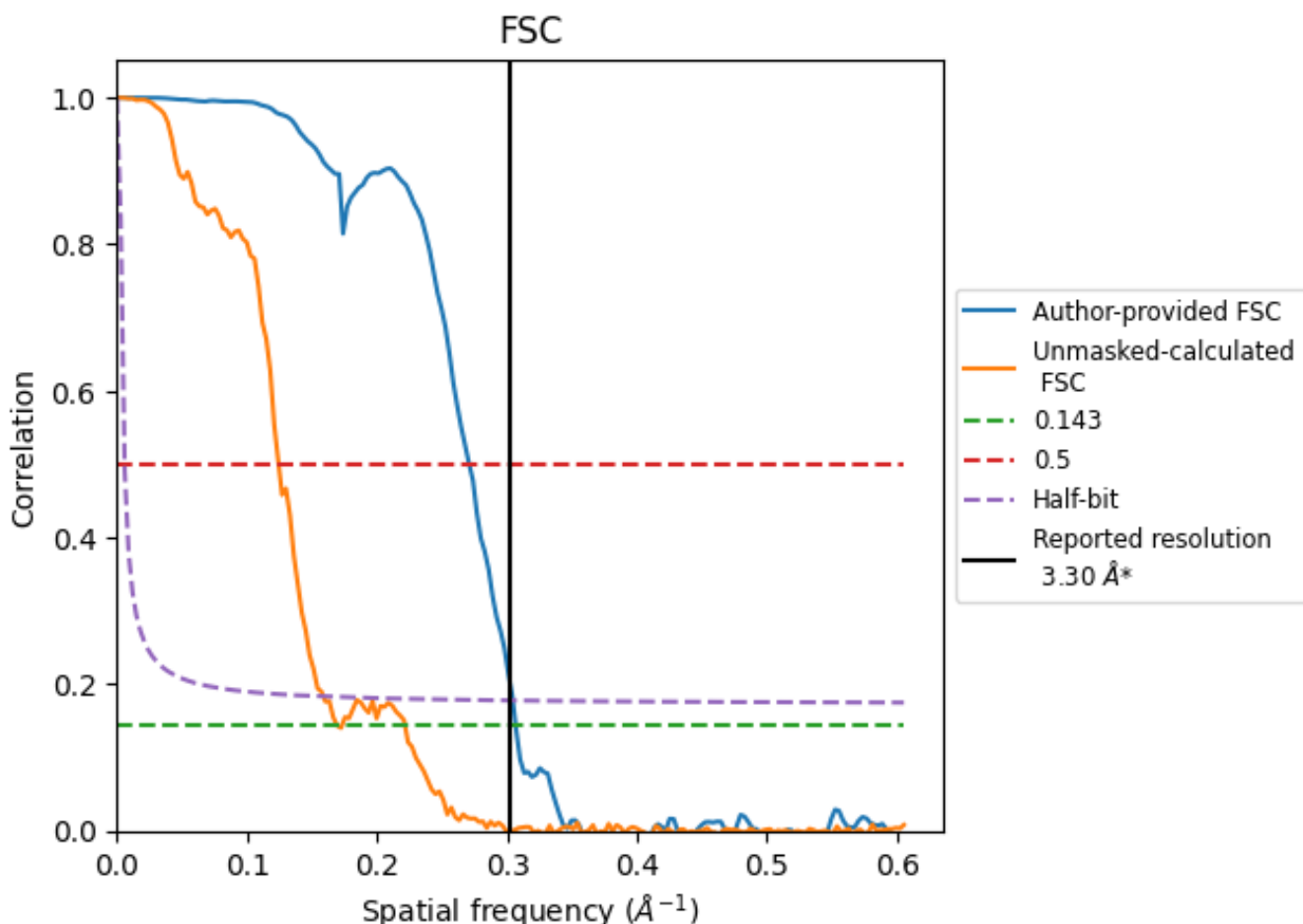


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

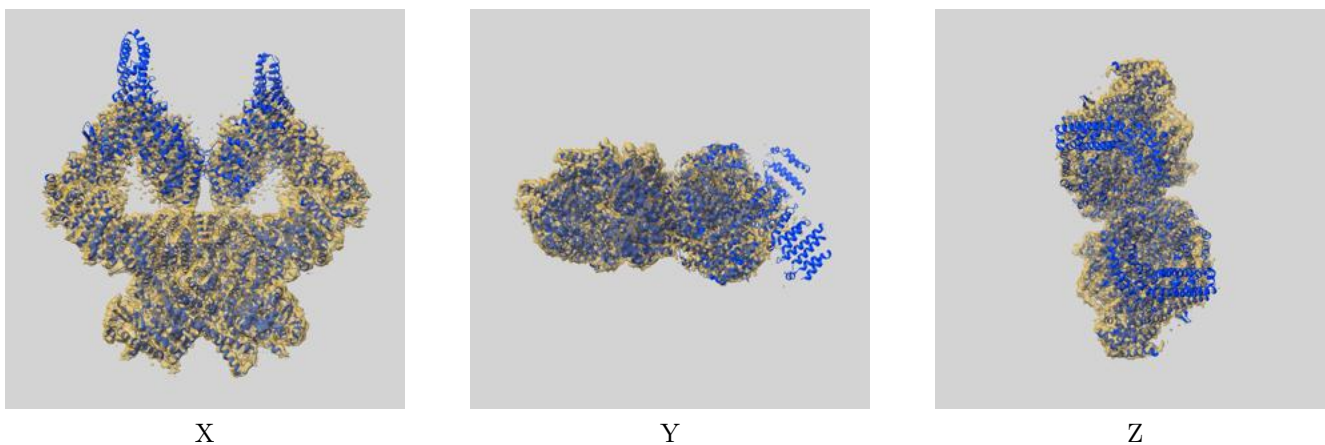
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.69	3.28
Unmasked-calculated*	5.90	8.04	6.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.90 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

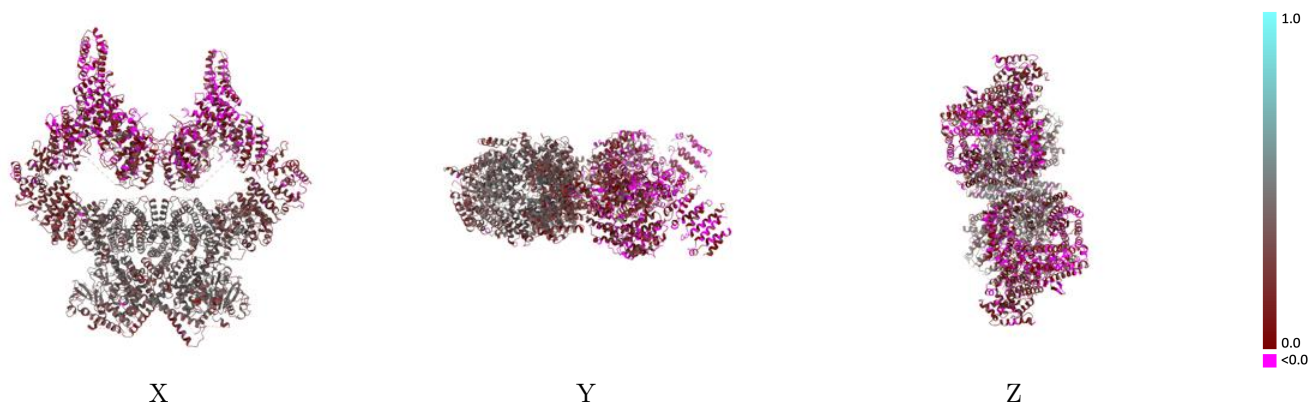
This section contains information regarding the fit between EMDB map EMD-17265 and PDB model 8OXM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



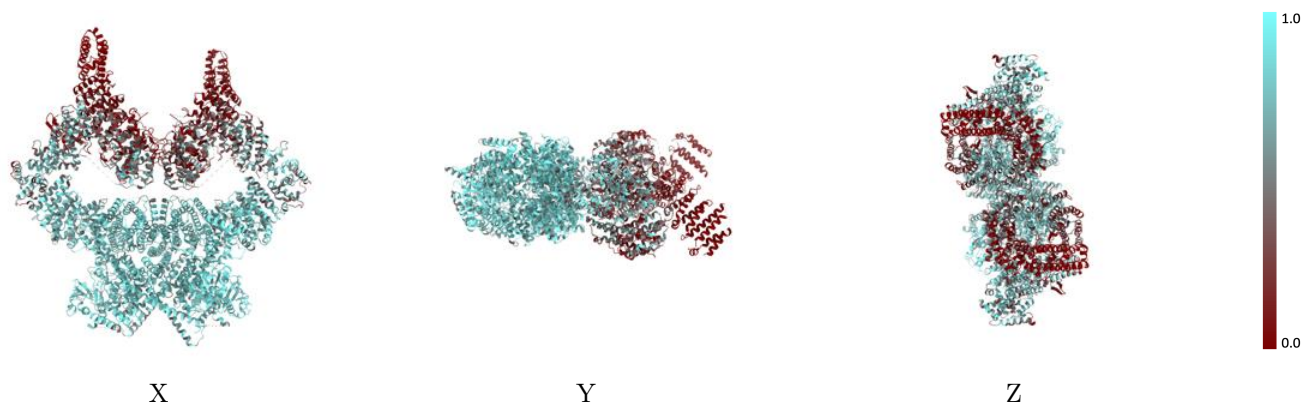
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



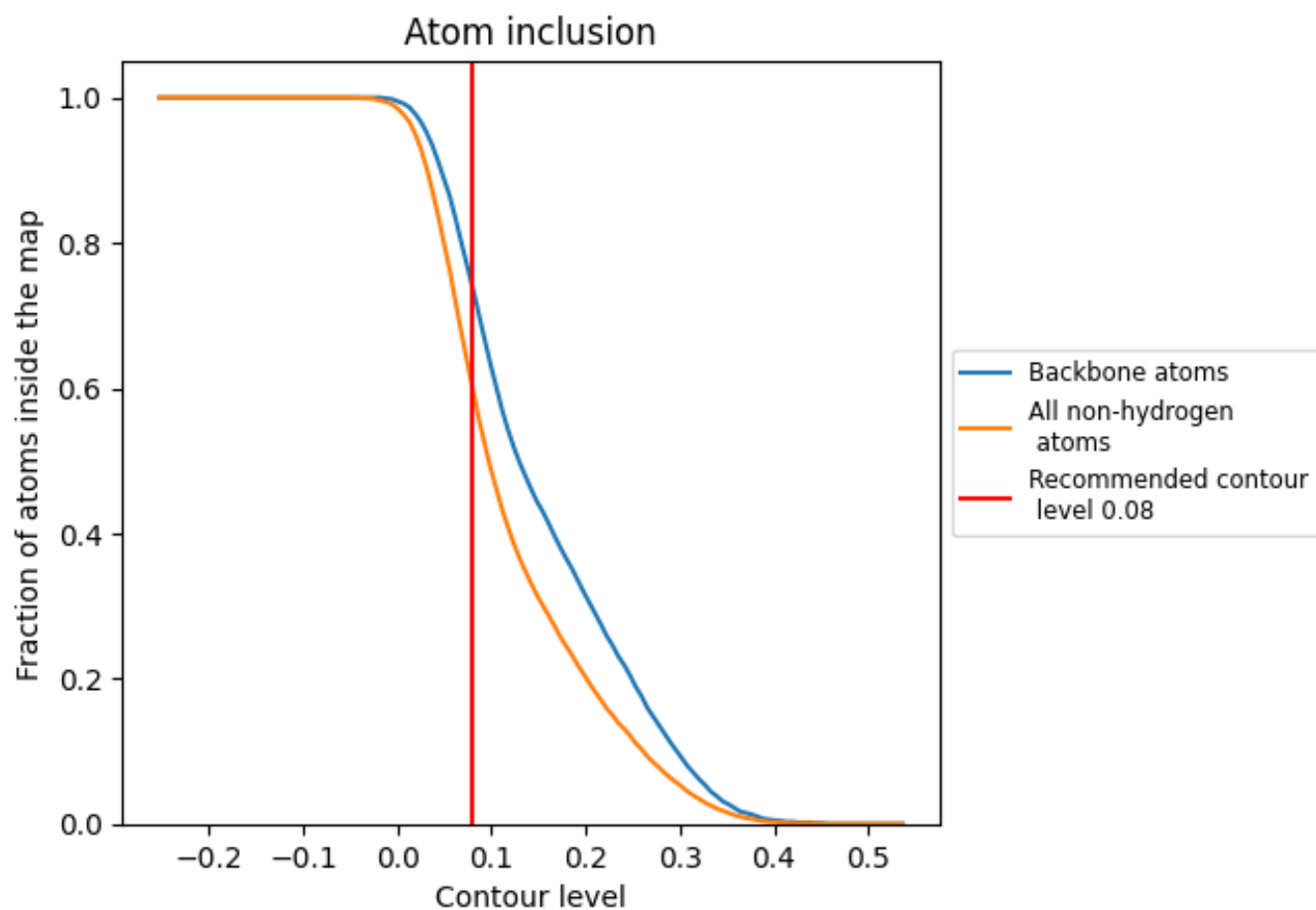
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).











9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5980	 0.2450
A	 0.5960	 0.2410
B	 0.6020	 0.2480
E	 0.2830	 0.2750
F	 0.2830	 0.2820

