



## Full wwPDB EM Validation Report ⓘ

Oct 2, 2023 – 08:11 pm BST

PDB ID : 8OXP  
EMDB ID : EMD-17267  
Title : ATM(Q2971A) in complex with Mg AMP-PNP  
Authors : Howes, A.C.; Perisic, O.; Williams, R.L.  
Deposited on : 2023-05-02  
Resolution : 2.60 Å(reported)  
Based on initial model : 7SIC

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

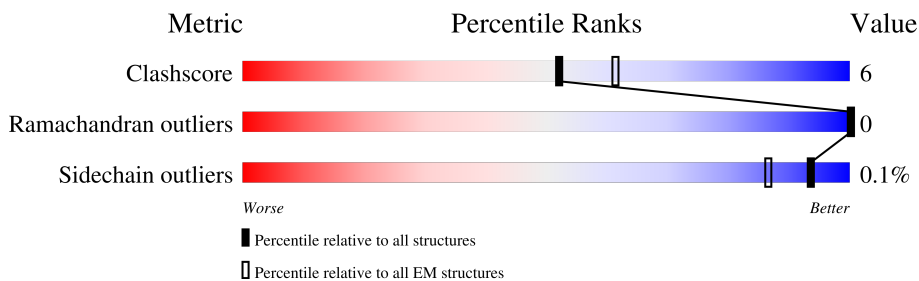
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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  $\geq 3$ , 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	3184	 17% 73% 14% 13%
1	B	3184	 17% 74% 13% 13%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 44460 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 Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2772	22197	14193	3772	4079	153	0	0
1	B	2772	22197	14193	3772	4079	153	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

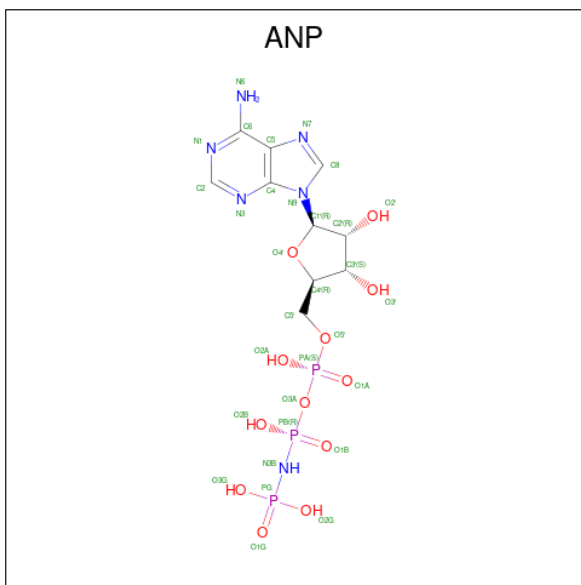
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	LEU	-	expression tag	UNP Q13315
B	-19	VAL	-	expression tag	UNP Q13315
B	-18	PHE	-	expression tag	UNP Q13315
B	-17	ASP	-	expression tag	UNP Q13315
B	-16	VAL	-	expression tag	UNP Q13315
B	-15	GLU	-	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 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

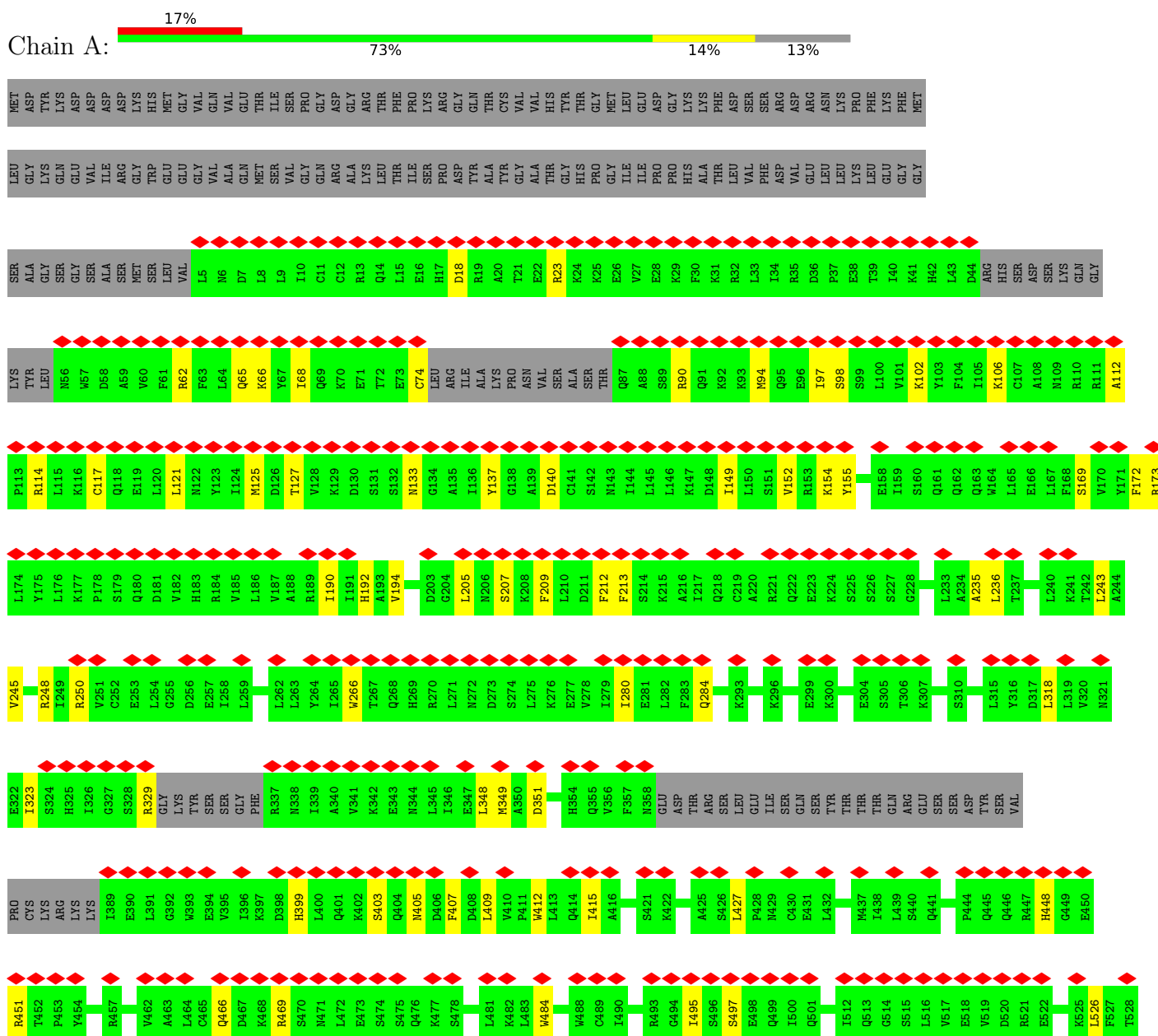
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

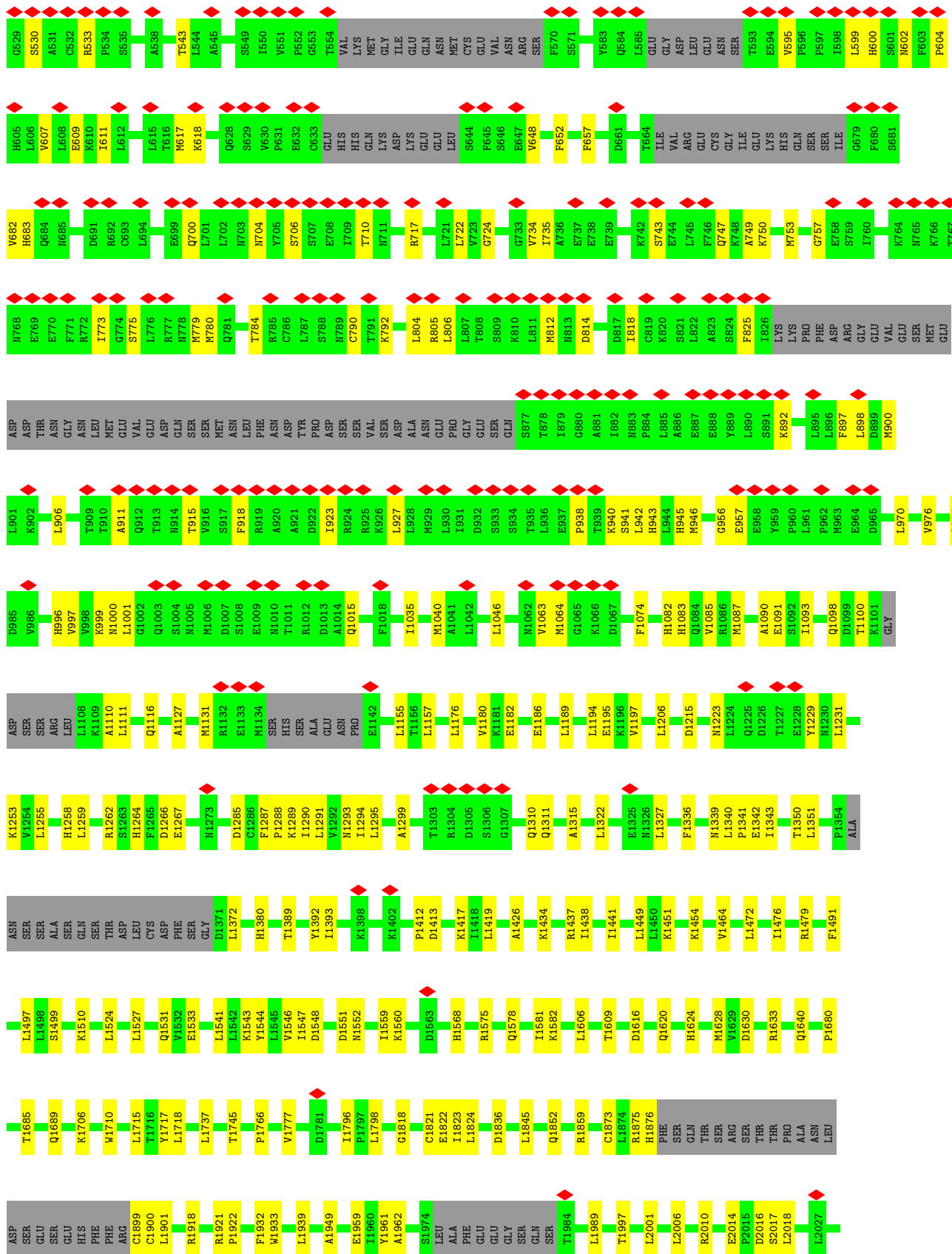
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	A	1	1	1	0
4	B	1	1	1	0

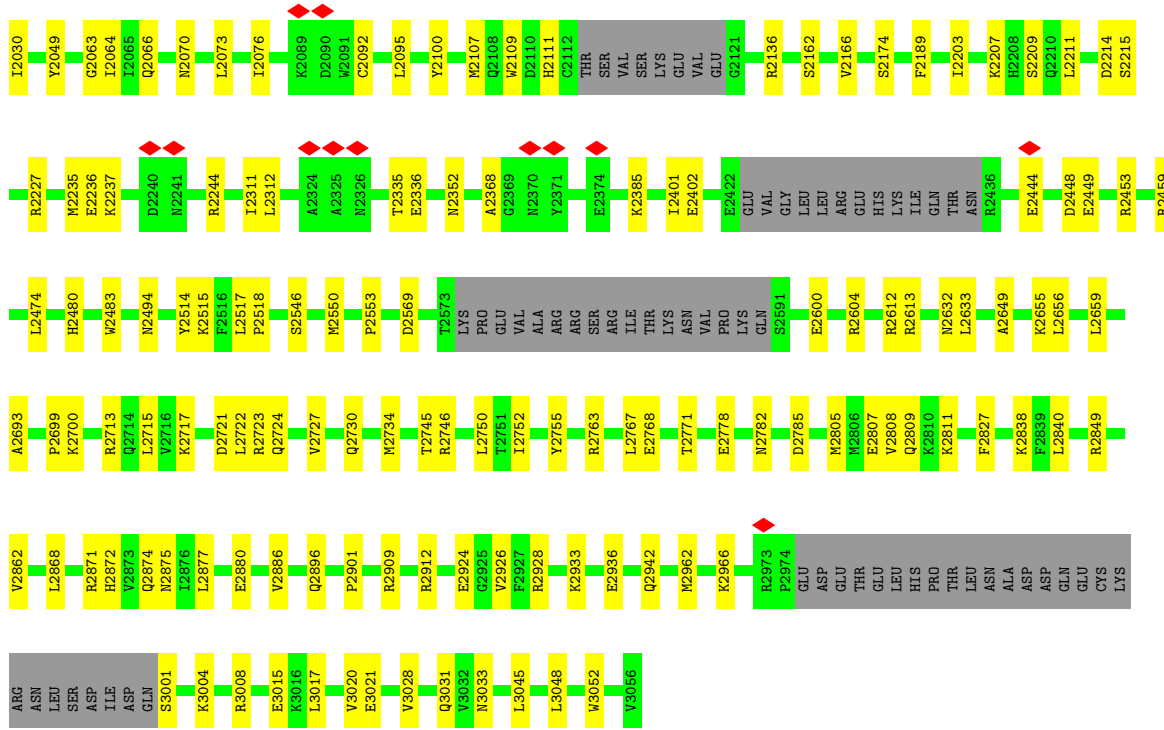
### 3 Residue-property plots

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

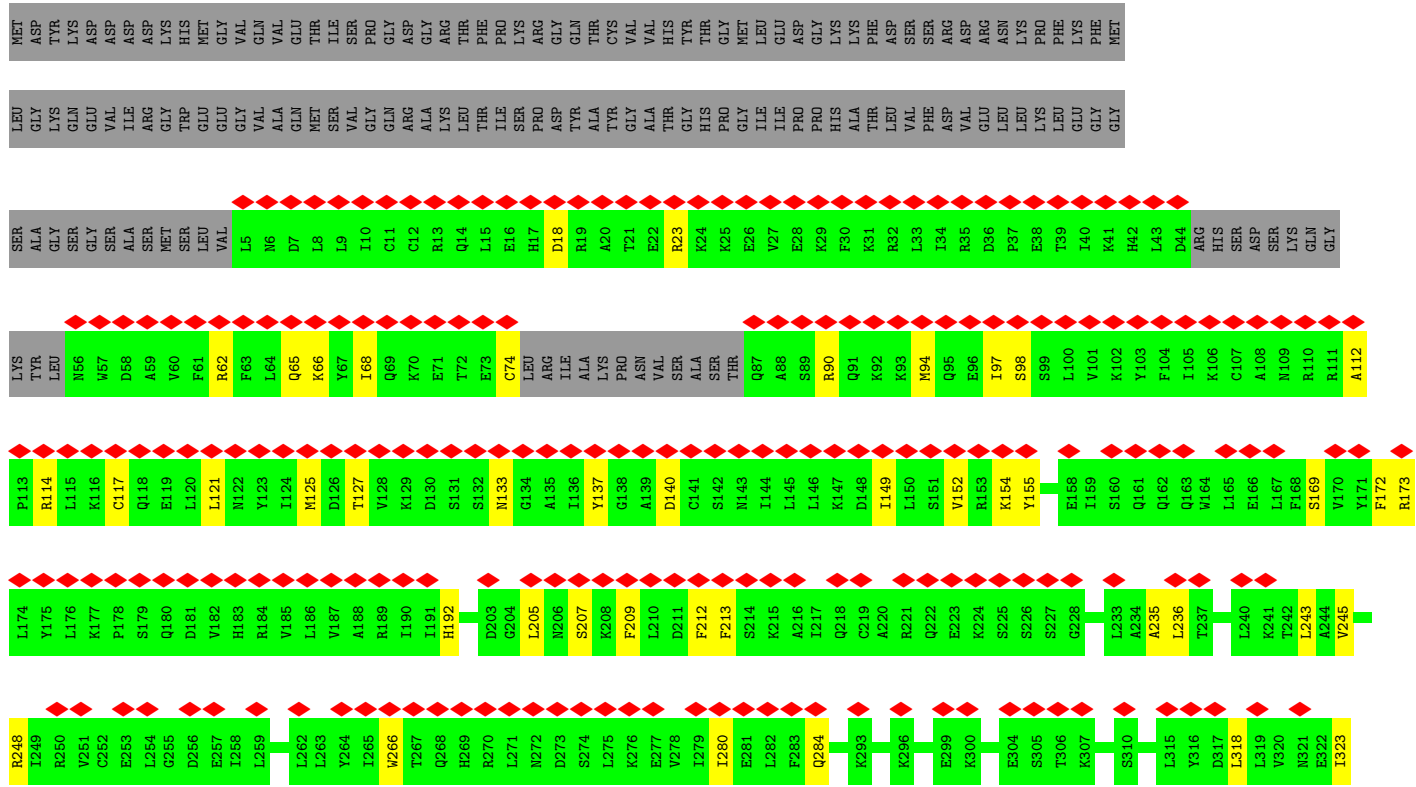
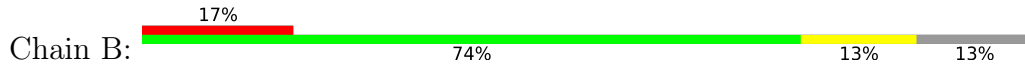
#### • Molecule 1: Serine-protein kinase ATM



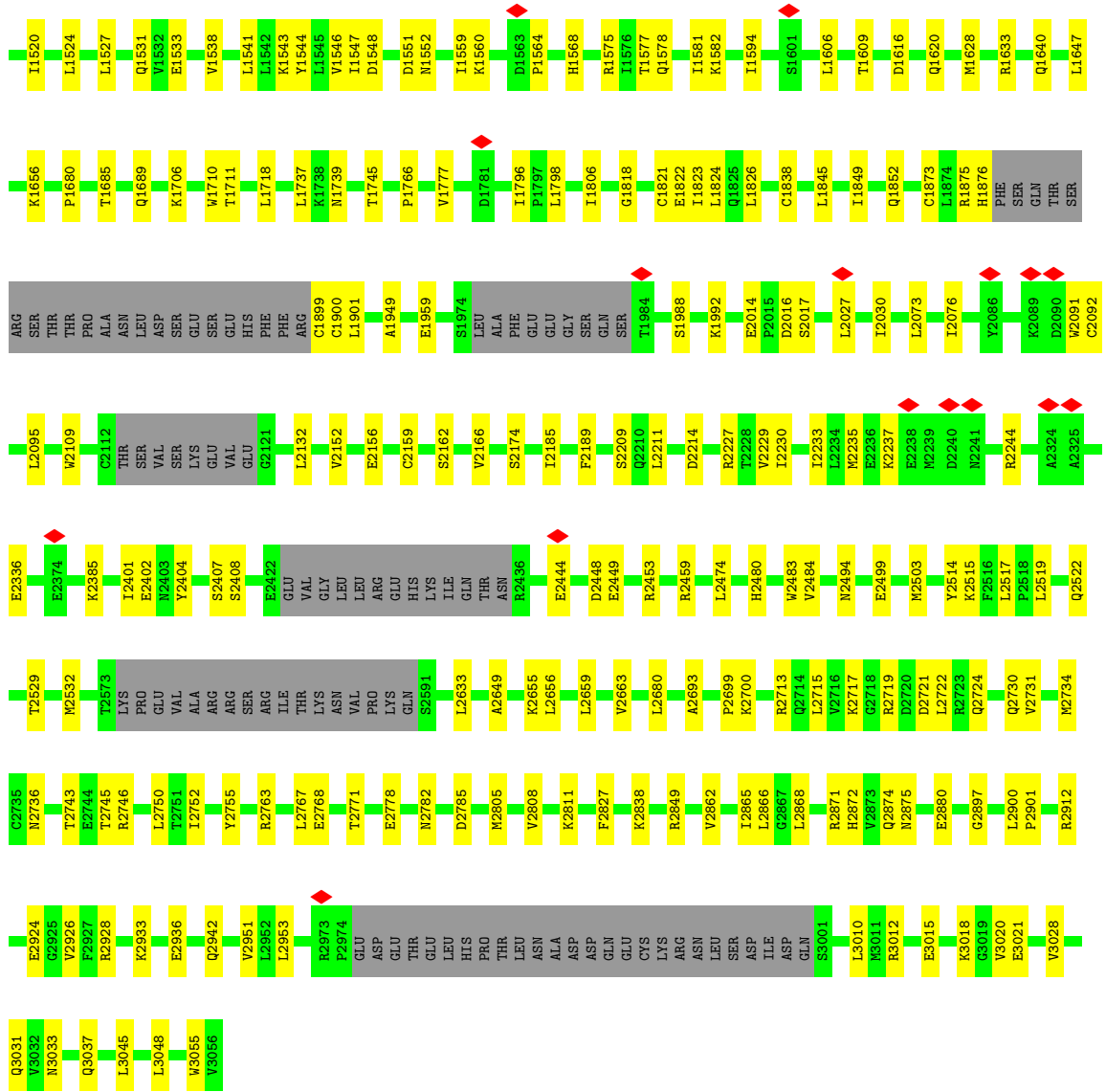




• Molecule 1: Serine-protein kinase ATM



S324	H325	I326	G327	S328	R329	GLY	LYS	TYR	SER	SER	GLY	PHE	R337	M338	I339	A340	V341	K342	E343	M344	L345	I346	E347	L348	M349	A350	D351	H354	Q355	V356	F357	N358	GLU	THR	ARG	SER	LEU	LEU	ILE	SER	GLN	SER	TYR	THR	THR	THR	THR	THR	GLN	ARG	GLU	SER	SER	ASP	TYR	VAL	PRO	CYS	
LYS	ARG	LYS	I389	E390	L391	G392	M393	E394	V395	I396	R469	K397	D398	H399	L400	Q401	K402	S403	Q404	M405	D406	F407	D408	L409	V410	P411	W412	I415	A416	S421	K422	A425	S426	L427	P428	M429	C430	E431	L432	M437	I438	L439	S440	Q441	P444	Q445	Q446	R447	H448	G449	E450	R451	T452	P453					
Y454	R457	V462	A463	L464	C465	Q466	D467	K468	R469	S470	M471	L472	E473	S474	Q475	Q476	K477	S478	L481	K482	L483	W484	W488	C489	I490	R493	G494	I495	S496	S497	E498	Q499	I500	Q501	I512	Q513	G514	S515	L516	E517	E518	V519	D520	Q446	R447	H448	G449	E450	R451	T452	G529	S530	A531						
C532	R533	P534	S535	A538	A545	S549	I550	V551	P552	G553	T554	VAL	LYS	MET	GLY	ILE	GLU	GLN	ASN	MET	CYS	GLU	VAL	ASN	ARG	SER	F570	S571	K578	Y583	Q584	L585	GLU	ASP	LEU	GLU	ASN	T593	E594	V595	P596	P597	I598	L599	H600	V519	D520	Q446	R447	H448	G449	E450	R451	T452	G529	S530	A531		
L608	E609	L612	L615	T616	M617	K618	A623	Q628	S629	V630	P631	E632	C633	GLU	HIS	GLU	GLN	LYS	ASP	LYS	GLU	GLU	LEU	S644	F645	S646	E647	V648	F652	F657	D661	T664	ILE	VAL	ARG	GLU	GLU	CYS	GLY	I676	G679	F680	N602	F603	P604	H605	L606	V607											
Q684	M685	R692	C693	L694	E699	Q700	L701	L702	M703	N704	V705	S706	S707	E708	I709	T710	M711	R717	L722	V723	G724	G733	V734	I735	A736	E737	E738	E739	K742	S743	E744	L745	E746	Q747	K748	A749	K750	E758	S759	I760	K764	N765	K766	T767	N768	E769	E770	F771	I773	G774									
S775	L776	R777	M778	M779	M780	Q781	T784	R785	C786	L787	S788	C790	T791	K792	L804	R805	L806	L807	S809	R810	L811	M812	N813	D814	D817	L818	C819	K820	S821	L822	A823	S824	F825	L826	LYS	LYS	PRO	PHE	ASP	ARG	GLY	VAL	VAL	GLU	SER	MET	GLU	ASP	THR	ASN	GLY	ASN	LEU						
MET	GLU	VAL	GLU	ASP	GLN	SER	MET	ASN	LEU	PHE	ASN	ASP	TYR	PRO	ASP	SER	VAL	SER	ALA	ALA	ASN	GLU	PRO	D808	S809	R810	L811	M812	N813	D814	D817	L818	C819	K820	S821	L822	A823	S824	F825	L826	LYS	LYS	PRO	PHE	ASP	ARG	GLY	VAL	VAL	GLU	SER	MET	GLU	ASP	THR	ASN	GLY	ASN	LEU
A911	Q912	T913	H914	T915	V916	S917	F918	R919	A920	A921	D922	I923	R924	R925	A926	L927	L928	M929	L930	I931	D932	S933	S934	T935	L936	E937	P938	T939	K940	S941	L942	H943	L944	H945	N946	G956	E957	E958	Y959	P960	L961	P962	H963	E964	D965	L970	H975	V976	Q984	D985	V986	H996	V997	V998					
K999	M1000	G1001	Q1003	S1004	N1005	M1006	D1007	S1008	E1009	N1010	T1011	R1012	D1013	A1014	Q1015	F1018	I1035	M1040	L1042	L1046	N1062	V1063	M1064	G1065	K1066	D1067	F1074	T1075	D1080	N1081	H1082	H1083	Q1084	V1085	R1086	I1089	Q1098	D1099	T1100	K1101	GLY	SER	SER	SER	ARG	LEU	L1108	K1109											
A1110	L1111	Q1116	K1126	R1132	E1133	M1134	SER	HIS	SER	ALA	SER	ALA	ASN	PRO	E1142	L1155	T1156	L1157	I1158	L1176	V1180	K1181	E1182	E1186	L1189	L1194	E1195	K1196	V1197	L1206	D1215	M1223	L1224	Q1225	D1226	T1227	E1228	Y1229	L1231	D1231	K1253	V1254	L1255	H1258	R1262														
D1266	E1267	H1273	D1285	C1286	F1287	P1288	P1289	I1290	L1291	V1292	M1293	I1294	L1295	A1299	T1303	R1304	D1305	S1306	G1307	Q1310	Q1311	A1315	L1322	E1325	M1326	L1327	F1336	M1339	L1340	P1341	E1342	I1343	L1351	P1354	ALA	ASN	SER	SER	ALA	SER	GLN	THR	THR	ASP	LEU	CYS													
ASP	PHE	SER	GLY	L1371	L1372	P1376	M1377	P1378	P1379	H1380	T1388	Y1392	I1393	K1398	K1402	P1412	D1413	S1414	K1417	L1418	L1419	K1435	L1438	L1441	L1444	F1445	V1446	L1449	L1457	V1464	L1472	I1473	I1476	R1479	F1491	L1497	L1498	S1499	K1510																				



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1207435	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	0.475	Depositor
Minimum map value	-0.192	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	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, ZN, ANP

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	0.23	0/22611	0.44	0/30548
1	B	0.23	0/22611	0.44	0/30548
All	All	0.23	0/45222	0.44	0/61096

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	A	22197	0	22381	261	0
1	B	22197	0	22381	252	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	44460	0	44788	508	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 6.

All (508) 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:B:2514:TYR:HA	1:B:2517:LEU:HD23	1.65	0.78
1:A:2514:TYR:HA	1:A:2517:LEU:HD23	1.66	0.77
1:B:941:SER:O	1:B:945:HIS:ND1	2.22	0.71
1:B:940:LYS:HE2	1:B:942:LEU:HB3	1.73	0.71
1:A:1818:GLY:O	1:A:1852:GLN:NE2	2.24	0.70
1:B:1341:PRO:HG2	1:B:1417:LYS:HD2	1.73	0.70
1:B:1685:THR:HG23	1:B:2166:VAL:HG21	1.74	0.69
1:B:1739:ASN:HB3	1:B:1826:LEU:HD13	1.74	0.69
1:A:1685:THR:HG23	1:A:2166:VAL:HG21	1.75	0.68
1:A:940:LYS:HE2	1:A:942:LEU:HB3	1.75	0.68
1:B:3045:LEU:HA	1:B:3048:LEU:HD12	1.76	0.68
1:A:3045:LEU:HA	1:A:3048:LEU:HD12	1.76	0.68
1:A:1546:VAL:HG13	1:A:1559:ILE:HD11	1.75	0.68
1:B:2719:ARG:HA	1:B:2763:ARG:HE	1.58	0.67
1:A:2656:LEU:HD13	1:A:2659:LEU:HD11	1.76	0.67
1:B:1818:GLY:O	1:B:1852:GLN:NE2	2.25	0.67
1:A:349:MET:HG2	1:A:415:ILE:HG12	1.77	0.66
1:B:2649:ALA:O	1:B:2655:LYS:NZ	2.29	0.66
1:B:412:TRP:HA	1:B:415:ILE:HD12	1.78	0.66
1:B:2656:LEU:HD13	1:B:2659:LEU:HD11	1.76	0.66
1:A:412:TRP:HA	1:A:415:ILE:HD12	1.78	0.66
1:A:2136:ARG:NH1	1:A:2236:GLU:OE2	2.30	0.65
1:A:1294:ILE:HG23	1:A:1315:ALA:HB1	1.79	0.65
1:A:2649:ALA:O	1:A:2655:LYS:NZ	2.29	0.65
1:B:349:MET:HG2	1:B:415:ILE:HG12	1.77	0.65
1:A:2569:ASP:HB3	1:A:2763:ARG:HH21	1.62	0.65
1:B:2942:GLN:HE22	1:B:3018:LYS:HG3	1.62	0.64
1:B:2752:ILE:HD11	1:B:2862:VAL:HG21	1.80	0.64
1:A:2480:HIS:HB3	1:A:2483:TRP:HD1	1.63	0.64
1:B:1294:ILE:HG23	1:B:1315:ALA:HB1	1.79	0.64
1:A:722:LEU:HD22	1:A:749:ALA:HB2	1.79	0.64
1:A:1875:ARG:O	1:A:1876:HIS:ND1	2.31	0.64
1:B:722:LEU:HD22	1:B:749:ALA:HB2	1.79	0.64
1:A:280:ILE:HG23	1:A:348:LEU:HD22	1.81	0.63
1:B:2897:GLY:HA2	1:B:2900:LEU:HD23	1.79	0.63
1:B:897:PHE:HD1	1:B:900:MET:HE2	1.64	0.63
1:B:1546:VAL:HG13	1:B:1559:ILE:HD11	1.81	0.63
1:B:805:ARG:NH1	1:B:915:THR:O	2.32	0.62
1:B:2717:LYS:HD2	1:B:2722:LEU:HD21	1.79	0.62
1:B:1419:LEU:HD11	1:B:1464:VAL:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1875:ARG:O	1:B:1876:HIS:ND1	2.31	0.62
1:A:2752:ILE:HD11	1:A:2862:VAL:HG21	1.81	0.62
1:A:805:ARG:NH1	1:A:915:THR:O	2.32	0.62
1:A:2100:TYR:HE1	1:A:2111:HIS:HE1	1.48	0.62
1:B:169:SER:OG	1:B:173:ARG:NH1	2.33	0.62
1:B:329:ARG:NH2	1:B:407:PHE:O	2.33	0.62
1:A:169:SER:OG	1:A:173:ARG:NH1	2.33	0.61
1:B:2448:ASP:OD1	1:B:2449:GLU:N	2.33	0.61
1:A:1419:LEU:HD11	1:A:1464:VAL:HG23	1.81	0.61
1:B:280:ILE:HG23	1:B:348:LEU:HD22	1.81	0.61
1:B:1524:LEU:HD22	1:B:1538:VAL:HG23	1.81	0.61
1:A:2448:ASP:OD1	1:A:2449:GLU:N	2.33	0.61
1:A:1341:PRO:HG2	1:A:1417:LYS:HD2	1.82	0.61
1:A:329:ARG:NH2	1:A:407:PHE:O	2.33	0.61
1:B:1351:LEU:HB3	1:B:1441:ILE:HG22	1.83	0.61
1:B:1377:ASN:OD1	1:B:1379:PRO:HD2	2.01	0.60
1:B:1876:HIS:CE1	1:B:1900:CYS:H	2.20	0.60
1:B:825:PHE:O	1:B:940:LYS:NZ	2.34	0.60
1:B:1988:SER:OG	1:B:1992:LYS:NZ	2.34	0.60
1:B:248:ARG:HD2	1:B:652:PHE:CE1	2.37	0.59
1:B:2474:LEU:O	1:B:2515:LYS:NZ	2.35	0.59
1:A:248:ARG:HD2	1:A:652:PHE:CE1	2.37	0.59
1:A:2214:ASP:OD1	1:A:2746:ARG:NH1	2.36	0.59
1:B:617:MET:HA	1:B:682:VAL:HA	1.84	0.59
1:B:602:ASN:OD1	1:B:717:ARG:NH1	2.36	0.59
1:A:1876:HIS:CE1	1:A:1900:CYS:H	2.20	0.59
1:B:1412:PRO:HB2	1:B:1766:PRO:HA	1.85	0.58
1:A:2553:PRO:HG3	1:A:2613:ARG:NH1	2.18	0.58
1:B:205:LEU:HD12	1:B:209:PHE:HD2	1.68	0.58
1:B:1288:PRO:HA	1:B:1343:ILE:HG22	1.84	0.58
1:A:2474:LEU:O	1:A:2515:LYS:NZ	2.37	0.58
1:A:602:ASN:OD1	1:A:717:ARG:NH1	2.36	0.58
1:A:2896:GLN:HB3	1:A:2962:MET:HG2	1.84	0.58
1:B:1110:ALA:HB3	1:B:1372:LEU:HD21	1.86	0.58
1:B:1543:LYS:HG2	1:B:1547:ILE:HD12	1.85	0.58
1:B:1594:ILE:HG23	1:B:1647:LEU:HD12	1.84	0.58
1:A:205:LEU:HD12	1:A:209:PHE:HD2	1.68	0.57
1:A:1543:LYS:HG2	1:A:1547:ILE:HD12	1.86	0.57
1:B:938:PRO:HB3	1:B:976:VAL:HG22	1.86	0.57
1:B:2928:ARG:NH1	1:B:3033:ASN:OD1	2.37	0.57
1:A:1110:ALA:HB3	1:A:1372:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2871:ARG:NH2	1:B:2875:ASN:O	2.37	0.57
1:A:2612:ARG:NH1	1:A:2613:ARG:HH21	2.03	0.57
1:B:898:LEU:HD21	1:B:945:HIS:HB3	1.86	0.57
1:A:2632:ASN:OD1	1:A:2763:ARG:NH2	2.36	0.57
1:A:941:SER:O	1:A:945:HIS:ND1	2.38	0.57
1:A:2871:ARG:NH2	1:A:2875:ASN:O	2.38	0.56
1:A:825:PHE:O	1:A:940:LYS:NZ	2.38	0.56
1:A:956:GLY:O	1:A:1000:ASN:ND2	2.30	0.56
1:A:2066:GLN:NE2	1:A:2070:ASN:OD1	2.37	0.56
1:B:956:GLY:O	1:B:1000:ASN:ND2	2.30	0.56
1:B:1223:ASN:OD1	1:B:1262:ARG:NH2	2.38	0.56
1:B:1446:VAL:HG11	1:B:1497:LEU:HD21	1.86	0.56
1:B:1499:SER:HA	1:B:1541:LEU:HD13	1.86	0.56
1:A:1098:GLN:HG3	1:A:1100:THR:HG23	1.88	0.56
1:A:773:ILE:HG21	1:A:892:LYS:HB3	1.87	0.56
1:B:609:GLU:HG2	1:B:724:GLY:HA3	1.88	0.56
1:B:957:GLU:HB2	1:B:999:LYS:HD3	1.87	0.56
1:A:609:GLU:HG2	1:A:724:GLY:HA3	1.88	0.56
1:A:617:MET:HA	1:A:682:VAL:HA	1.89	0.55
1:A:2693:ALA:HB3	1:A:2699:PRO:HG2	1.88	0.55
1:B:2827:PHE:O	1:B:2912:ARG:NH1	2.34	0.55
1:A:1351:LEU:HB3	1:A:1441:ILE:HG22	1.89	0.55
1:B:747:GLN:HA	1:B:750:LYS:HZ3	1.71	0.55
1:B:1476:ILE:O	1:B:1479:ARG:NH1	2.38	0.55
1:A:2827:PHE:O	1:A:2912:ARG:NH1	2.34	0.55
1:A:2928:ARG:NH1	1:A:3033:ASN:OD1	2.37	0.55
1:B:1438:ILE:HA	1:B:1441:ILE:HG12	1.89	0.55
1:A:1223:ASN:OD1	1:A:1262:ARG:NH2	2.40	0.55
1:B:2092:CYS:SG	1:B:2095:LEU:HD23	2.46	0.55
1:A:599:LEU:O	1:A:717:ARG:NE	2.39	0.55
1:B:747:GLN:OE1	1:B:750:LYS:NZ	2.38	0.55
1:A:747:GLN:OE1	1:A:750:LYS:NZ	2.38	0.55
1:A:1544:TYR:HA	1:A:1548:ASP:HB2	1.89	0.55
1:A:1680:PRO:O	1:A:2215:SER:OG	2.24	0.55
1:B:1098:GLN:HG3	1:B:1100:THR:HG23	1.88	0.55
1:B:2480:HIS:HB3	1:B:2483:TRP:HD1	1.72	0.55
1:A:812:MET:SD	1:A:918:PHE:HB2	2.47	0.54
1:A:127:THR:O	1:A:133:ASN:ND2	2.40	0.54
1:A:938:PRO:HB3	1:A:976:VAL:HG22	1.88	0.54
1:B:127:THR:O	1:B:133:ASN:ND2	2.40	0.54
1:B:599:LEU:O	1:B:717:ARG:NE	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:VAL:HG12	1:B:735:ILE:HG13	1.88	0.54
1:B:812:MET:SD	1:B:918:PHE:HB2	2.47	0.54
1:B:2808:VAL:HG23	1:B:2811:LYS:HD2	1.90	0.54
1:A:2336:GLU:OE2	1:A:2385:LYS:NZ	2.39	0.54
1:B:1568:HIS:H	1:B:1575:ARG:NH2	2.06	0.54
1:B:2693:ALA:HB3	1:B:2699:PRO:HG2	1.89	0.54
1:A:2633:LEU:HB3	1:A:2700:LYS:HE2	1.89	0.54
1:A:1472:LEU:HD21	1:A:1497:LEU:HD23	1.89	0.54
1:A:747:GLN:HA	1:A:750:LYS:HZ2	1.73	0.54
1:B:2091:TRP:CZ2	1:B:2095:LEU:HB3	2.43	0.54
1:B:2336:GLU:OE2	1:B:2385:LYS:NZ	2.41	0.54
1:A:734:VAL:HG12	1:A:735:ILE:HG13	1.89	0.54
1:B:1253:LYS:HZ2	1:B:1285:ASP:HB3	1.72	0.53
1:B:1310:GLN:HE21	1:B:1311:GLN:NE2	2.06	0.53
1:A:1310:GLN:HE21	1:A:1311:GLN:NE2	2.06	0.53
1:B:1875:ARG:HD2	1:B:1899:CYS:HB2	1.91	0.53
1:A:957:GLU:HB2	1:A:999:LYS:HD3	1.91	0.53
1:A:1568:HIS:H	1:A:1575:ARG:NH2	2.07	0.53
1:A:1231:LEU:HD11	1:A:1255:LEU:HD22	1.91	0.53
1:A:1875:ARG:HD2	1:A:1899:CYS:HB2	1.91	0.53
1:A:2203:ILE:HG22	1:A:2207:LYS:HE2	1.90	0.53
1:B:1718:LEU:HB3	1:B:1737:LEU:HD21	1.90	0.53
1:A:1082:HIS:HB3	1:A:1085:VAL:HG23	1.91	0.53
1:A:1438:ILE:HA	1:A:1441:ILE:HG12	1.90	0.53
1:A:2073:LEU:HD22	1:A:2076:ILE:HD12	1.89	0.53
1:B:2014:GLU:OE1	1:B:2017:SER:N	2.39	0.53
1:A:2612:ARG:HH12	1:A:2613:ARG:HH21	1.56	0.53
1:A:2715:LEU:HD23	1:A:2767:LEU:HD11	1.91	0.53
1:A:2868:LEU:HG	1:A:2871:ARG:HD3	1.91	0.53
1:B:98:SER:OG	1:B:140:ASP:OD2	2.26	0.53
1:B:617:MET:SD	1:B:623:ALA:HB2	2.49	0.53
1:A:98:SER:OG	1:A:140:ASP:OD2	2.26	0.53
1:A:780:MET:HG2	1:A:900:MET:HA	1.91	0.53
1:A:1560:LYS:HG3	1:A:1582:LYS:HA	1.91	0.53
1:B:2745:THR:HG22	1:B:2750:LEU:HD12	1.91	0.53
1:B:466:GLN:OE1	1:B:484:TRP:NE1	2.38	0.52
1:B:2715:LEU:HD23	1:B:2767:LEU:HD11	1.90	0.52
1:A:530:SER:HA	1:A:533:ARG:HH22	1.74	0.52
1:B:1578:GLN:HA	1:B:1581:ILE:HG22	1.91	0.52
1:A:2235:MET:O	1:A:2244:ARG:NH2	2.42	0.52
1:B:2713:ARG:HD3	1:B:2771:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2073:LEU:HD22	1:B:2076:ILE:HD12	1.91	0.52
1:A:2713:ARG:HD3	1:A:2771:THR:HG22	1.91	0.52
1:B:2633:LEU:HB3	1:B:2700:LYS:HE2	1.91	0.52
1:A:1551:ASP:OD1	1:A:1551:ASP:N	2.42	0.52
1:B:2214:ASP:OD1	1:B:2746:ARG:NH1	2.42	0.52
1:A:2838:LYS:HE2	1:A:2880:GLU:HG2	1.92	0.52
1:A:1288:PRO:HA	1:A:1343:ILE:HG22	1.92	0.52
1:A:1340:LEU:HD23	1:A:1341:PRO:HD3	1.91	0.52
1:A:1253:LYS:HZ2	1:A:1285:ASP:HB3	1.73	0.51
1:B:1547:ILE:HG12	1:B:1577:THR:HG21	1.91	0.51
1:B:2484:VAL:HG13	1:B:2519:LEU:HD21	1.92	0.51
1:B:1291:LEU:HD12	1:B:1343:ILE:HG21	1.93	0.51
1:B:1544:TYR:HA	1:B:1548:ASP:HB2	1.92	0.51
1:A:245:VAL:HG12	1:A:1083:HIS:HB3	1.92	0.51
1:B:2402:GLU:OE2	1:B:2459:ARG:NE	2.34	0.51
1:B:2185:ILE:HG13	1:B:2230:ILE:HD12	1.92	0.51
1:B:1706:LYS:HE3	1:B:1710:TRP:HE1	1.75	0.51
1:B:1215:ASP:OD1	1:B:1258:HIS:NE2	2.32	0.51
1:B:2868:LEU:HG	1:B:2871:ARG:HD3	1.93	0.51
1:A:112:ALA:H	1:A:114:ARG:NH1	2.09	0.50
1:A:1087:MET:HA	1:A:1090:ALA:HB3	1.94	0.50
1:A:2401:ILE:HG21	1:A:2459:ARG:HB2	1.92	0.50
1:A:1628:MET:HE2	1:A:2211:LEU:HD13	1.94	0.50
1:B:112:ALA:H	1:B:114:ARG:NH1	2.09	0.50
1:A:2546:SER:O	1:A:2550:MET:HG2	2.12	0.50
1:B:780:MET:HG2	1:B:900:MET:HA	1.93	0.50
1:B:1551:ASP:OD1	1:B:1551:ASP:N	2.42	0.50
1:B:1082:HIS:HB3	1:B:1085:VAL:HG23	1.94	0.50
1:B:1063:VAL:HG13	1:B:1064:MET:SD	2.52	0.50
1:B:1231:LEU:HD11	1:B:1255:LEU:HD22	1.94	0.50
1:A:466:GLN:OE1	1:A:484:TRP:NE1	2.39	0.49
1:A:1182:GLU:OE2	1:A:1229:TYR:OH	2.30	0.49
1:B:1472:LEU:HD11	1:B:1497:LEU:HD22	1.94	0.49
1:B:530:SER:HA	1:B:533:ARG:HH22	1.77	0.49
1:B:2730:GLN:O	1:B:2734:MET:HG2	2.11	0.49
1:A:1426:ALA:HB2	1:A:1438:ILE:HG21	1.95	0.49
1:A:1195:GLU:HG2	1:A:1206:LEU:HD22	1.95	0.49
1:A:1859:ARG:NE	1:A:1933:TRP:O	2.42	0.49
1:A:1706:LYS:HE3	1:A:1710:TRP:HE1	1.76	0.49
1:A:1063:VAL:HG13	1:A:1064:MET:SD	2.52	0.49
1:B:1195:GLU:HG2	1:B:1206:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1351:LEU:HD12	1:B:1444:LEU:HD22	1.94	0.49
1:B:2152:VAL:O	1:B:2156:GLU:HG3	2.13	0.49
1:B:2719:ARG:HG3	1:B:2763:ARG:HH21	1.78	0.49
1:A:192:HIS:HA	1:A:235:ALA:HB2	1.95	0.49
1:A:1680:PRO:HG3	1:A:2174:SER:HB2	1.94	0.49
1:B:773:ILE:HG21	1:B:892:LYS:HB3	1.94	0.49
1:B:1182:GLU:OE2	1:B:1229:TYR:OH	2.30	0.49
1:A:18:ASP:O	1:A:23:ARG:NH1	2.46	0.49
1:A:2014:GLU:OE1	1:A:2017:SER:N	2.44	0.49
1:B:2401:ILE:HG21	1:B:2459:ARG:HB2	1.95	0.49
1:A:1322:LEU:HA	1:A:1327:LEU:HD12	1.95	0.49
1:A:2189:PHE:CE1	1:A:2237:LYS:HD3	2.48	0.49
1:B:942:LEU:HG	1:B:946:MET:HE1	1.94	0.49
1:B:1322:LEU:HA	1:B:1327:LEU:HD12	1.95	0.49
1:B:1339:ASN:HB2	1:B:1342:GLU:OE1	2.13	0.49
1:A:94:MET:CE	1:A:137:TYR:HB2	2.43	0.48
1:A:970:LEU:HD11	1:A:997:VAL:HG11	1.95	0.48
1:A:1412:PRO:HB2	1:A:1766:PRO:HA	1.95	0.48
1:B:1949:ALA:HB1	1:B:2162:SER:HB2	1.96	0.48
1:B:2189:PHE:CE1	1:B:2237:LYS:HD3	2.48	0.48
1:A:284:GLN:NE2	1:A:351:ASP:OD2	2.45	0.48
1:A:1959:GLU:OE2	1:A:2849:ARG:NH1	2.44	0.48
1:B:94:MET:CE	1:B:137:TYR:HB2	2.43	0.48
1:A:2942:GLN:HA	1:A:3017:LEU:HD13	1.96	0.48
1:B:18:ASP:O	1:B:23:ARG:NH1	2.46	0.48
1:B:970:LEU:HD11	1:B:997:VAL:HG11	1.96	0.48
1:B:2229:VAL:O	1:B:2233:ILE:HG12	2.12	0.48
1:A:1295:LEU:HD13	1:A:1393:ILE:HD11	1.95	0.48
1:A:2722:LEU:HD13	1:A:2767:LEU:HD23	1.95	0.48
1:B:2838:LYS:HE2	1:B:2880:GLU:HG2	1.94	0.48
1:B:192:HIS:HA	1:B:235:ALA:HB2	1.95	0.48
1:A:2924:GLU:OE2	1:A:2928:ARG:NH2	2.44	0.48
1:B:1824:LEU:HD13	1:B:1845:LEU:HD23	1.96	0.48
1:B:2924:GLU:OE2	1:B:2928:ARG:NH2	2.44	0.48
1:A:3015:GLU:HB2	1:A:3020:VAL:HB	1.95	0.48
1:B:1560:LYS:HG3	1:B:1582:LYS:HA	1.95	0.48
1:A:2402:GLU:OE2	1:A:2459:ARG:NE	2.39	0.48
1:A:2721:ASP:OD2	1:A:2724:GLN:NE2	2.43	0.48
1:B:1340:LEU:HD12	1:B:1343:ILE:HD11	1.94	0.48
1:A:1087:MET:O	1:A:1091:GLU:N	2.35	0.48
1:A:2444:GLU:OE1	1:B:2901:PRO:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1376:PRO:HG2	1:B:1380:HIS:CD2	2.49	0.48
1:B:1796:ILE:HG23	1:B:1798:LEU:HD23	1.96	0.47
1:B:2778:GLU:O	1:B:2782:ASN:HB2	2.14	0.47
1:A:706:SER:N	1:A:710:THR:OG1	2.47	0.47
1:B:1295:LEU:HD13	1:B:1393:ILE:HD11	1.95	0.47
1:B:1491:PHE:HZ	1:B:1527:LEU:HD22	1.79	0.47
1:A:2745:THR:HG22	1:A:2750:LEU:HD12	1.95	0.47
1:B:1680:PRO:HG3	1:B:2174:SER:HB2	1.96	0.47
1:B:2404:TYR:O	1:B:2407:SER:OG	2.28	0.47
1:A:1215:ASP:OD1	1:A:1258:HIS:NE2	2.40	0.47
1:B:3012:ARG:NH1	1:B:3015:GLU:OE2	2.45	0.47
1:A:427:LEU:O	1:A:469:ARG:NH2	2.35	0.47
1:A:700:GLN:NE2	1:A:704:ASN:OD1	2.47	0.47
1:A:898:LEU:HD21	1:A:945:HIS:HB3	1.97	0.47
1:A:1413:ASP:OD1	1:A:1413:ASP:N	2.46	0.47
1:A:1796:ILE:HG23	1:A:1798:LEU:HD23	1.96	0.47
1:A:2352:ASN:HB3	1:B:3037:GLN:NE2	2.29	0.47
1:B:700:GLN:NE2	1:B:704:ASN:OD1	2.47	0.47
1:A:2449:GLU:OE1	1:A:2453:ARG:NH2	2.36	0.47
1:A:3021:GLU:OE2	1:A:3031:GLN:NE2	2.44	0.47
1:A:2962:MET:SD	1:A:2966:LYS:HD2	2.54	0.47
1:A:1259:LEU:HB3	1:A:1264:HIS:HB2	1.96	0.47
1:A:1640:GLN:O	1:A:1689:GLN:NE2	2.48	0.47
1:B:284:GLN:NE2	1:B:351:ASP:OD2	2.46	0.47
1:B:1473:ILE:HD11	1:B:1520:ILE:HG22	1.96	0.47
1:A:2311:ILE:HD11	1:B:2027:LEU:HD11	1.97	0.46
1:B:1821:CYS:SG	1:B:1823:ILE:HG12	2.54	0.46
1:A:1491:PHE:HZ	1:A:1527:LEU:HD22	1.80	0.46
1:A:1339:ASN:HB2	1:A:1342:GLU:OE1	2.14	0.46
1:A:2335:THR:HG21	1:A:2368:ALA:HB2	1.97	0.46
1:A:2778:GLU:O	1:A:2782:ASN:HB2	2.15	0.46
1:B:706:SER:N	1:B:710:THR:OG1	2.47	0.46
1:A:207:SER:HB2	1:A:243:LEU:HD21	1.97	0.46
1:B:1711:THR:HG22	1:B:1823:ILE:HG21	1.97	0.46
1:B:448:HIS:CE1	1:B:497:SER:HG	2.28	0.46
1:B:1413:ASP:N	1:B:1413:ASP:OD1	2.47	0.46
1:B:1640:GLN:O	1:B:1689:GLN:NE2	2.48	0.46
1:B:2936:GLU:HG3	1:B:3028:VAL:HG11	1.97	0.46
1:A:448:HIS:CE1	1:A:497:SER:HG	2.30	0.46
1:A:1499:SER:HA	1:A:1541:LEU:HD13	1.96	0.46
1:B:1457:LEU:HD22	1:B:1464:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1606:LEU:HD23	1:B:1609:THR:HG23	1.98	0.46
1:A:1451:LYS:O	1:A:1454:LYS:NZ	2.42	0.46
1:A:399:HIS:O	1:A:403:SER:OG	2.22	0.46
1:A:2209:SER:HG	1:A:2227:ARG:HH12	1.63	0.46
1:A:943:HIS:HA	1:A:946:MET:HE1	1.99	0.45
1:A:1578:GLN:HA	1:A:1581:ILE:HG22	1.97	0.45
1:A:2936:GLU:HG3	1:A:3028:VAL:HG11	1.98	0.45
1:B:1336:PHE:HZ	1:B:1393:ILE:HG23	1.80	0.45
1:B:1568:HIS:H	1:B:1575:ARG:HH22	1.64	0.45
1:B:2522:GLN:HG2	1:B:2951:VAL:HG12	1.98	0.45
1:A:2808:VAL:HG23	1:A:2811:LYS:HD2	1.98	0.45
1:A:604:PRO:HB2	1:A:607:VAL:HG21	1.97	0.45
1:B:1628:MET:HE2	1:B:2211:LEU:HD13	1.99	0.45
1:B:1656:LYS:NZ	1:B:2159:CYS:O	2.34	0.45
1:A:1949:ALA:HB1	1:A:2162:SER:HB2	1.98	0.45
1:B:172:PHE:CE2	1:B:212:PHE:HB3	2.52	0.45
1:B:1040:MET:SD	1:B:1085:VAL:HG22	2.57	0.45
1:B:1435:LYS:HA	1:B:1438:ILE:HG12	1.98	0.45
1:B:773:ILE:HG12	1:B:896:LEU:HD22	1.99	0.45
1:B:1389:THR:O	1:B:1393:ILE:HG12	2.16	0.45
1:A:1921:ARG:HA	1:A:1933:TRP:CZ2	2.51	0.45
1:B:3021:GLU:OE2	1:B:3031:GLN:NE2	2.46	0.45
1:A:172:PHE:CE2	1:A:212:PHE:HB3	2.52	0.45
1:A:1821:CYS:SG	1:A:1823:ILE:HG12	2.57	0.45
1:B:323:ILE:O	1:B:329:ARG:NH1	2.50	0.45
1:B:604:PRO:HB2	1:B:607:VAL:HG21	1.97	0.45
1:B:2755:TYR:HB2	1:B:2768:GLU:HB3	1.98	0.45
1:A:543:THR:HB	1:A:611:ILE:HD11	1.99	0.45
1:A:648:VAL:HG12	1:A:652:PHE:CE2	2.52	0.45
1:A:1568:HIS:H	1:A:1575:ARG:HH22	1.64	0.45
1:A:2459:ARG:NH2	1:A:2494:ASN:OD1	2.50	0.45
1:B:2721:ASP:OD2	1:B:2724:GLN:NE2	2.47	0.45
1:A:1291:LEU:HD12	1:A:1343:ILE:HG21	1.99	0.44
1:A:1434:LYS:O	1:A:1437:ARG:HG2	2.16	0.44
1:B:1633:ARG:HG2	1:B:1633:ARG:HH11	1.82	0.44
1:B:1745:THR:OG1	1:B:1822:GLU:OE2	2.28	0.44
1:A:1718:LEU:HB3	1:A:1737:LEU:HD21	1.99	0.44
1:A:2755:TYR:HB2	1:A:2768:GLU:HB3	1.98	0.44
1:B:207:SER:HB2	1:B:243:LEU:HD21	1.98	0.44
1:A:1336:PHE:HZ	1:A:1393:ILE:HG23	1.82	0.44
1:A:2901:PRO:HB3	1:B:2444:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:VAL:HG12	1:B:652:PHE:CE2	2.52	0.44
1:B:1564:PRO:HA	1:B:1578:GLN:OE1	2.17	0.44
1:B:2736:ASN:OD1	1:B:2752:ILE:N	2.45	0.44
1:A:266:TRP:CG	1:A:318:LEU:HD21	2.52	0.44
1:A:323:ILE:O	1:A:329:ARG:NH1	2.50	0.44
1:A:530:SER:O	1:A:530:SER:OG	2.33	0.44
1:B:2953:LEU:HD12	1:B:3010:LEU:HG	1.99	0.44
1:A:117:CYS:HB2	1:A:155:TYR:CD1	2.53	0.44
1:A:749:ALA:HB1	1:A:806:LEU:HD11	2.00	0.44
1:A:1745:THR:OG1	1:A:1822:GLU:OE2	2.28	0.44
1:B:266:TRP:CG	1:B:318:LEU:HD21	2.52	0.44
1:A:1476:ILE:O	1:A:1479:ARG:NH1	2.44	0.44
1:A:1717:TYR:OH	1:A:1836:ASP:OD2	2.27	0.44
1:B:495:ILE:HG21	1:B:526:LEU:HD21	1.99	0.44
1:A:1389:THR:O	1:A:1393:ILE:HG12	2.17	0.44
1:A:1176:LEU:O	1:A:1180:VAL:HG23	2.19	0.43
1:B:117:CYS:HB2	1:B:155:TYR:CD1	2.53	0.43
1:B:149:ILE:HA	1:B:155:TYR:HD2	1.83	0.43
1:B:996:HIS:O	1:B:999:LYS:HG2	2.18	0.43
1:B:1194:LEU:HA	1:B:1197:VAL:HG12	2.00	0.43
1:A:403:SER:HB2	1:A:409:LEU:HD13	2.01	0.43
1:A:775:SER:O	1:A:779:MET:HG2	2.18	0.43
1:A:1510:LYS:HG2	1:A:1552:ASN:HD21	1.81	0.43
1:B:595:VAL:HG13	1:B:600:HIS:HB2	2.00	0.43
1:B:749:ALA:HB1	1:B:806:LEU:HD11	2.00	0.43
1:B:1080:ASP:O	1:B:1086:ARG:NE	2.52	0.43
1:B:1176:LEU:O	1:B:1180:VAL:HG23	2.18	0.43
1:A:2600:GLU:OE2	1:A:2604:ARG:NH2	2.51	0.43
1:B:527:PHE:HE1	1:B:538:ALA:HB1	1.82	0.43
1:A:213:PHE:CG	1:A:236:LEU:HD13	2.53	0.43
1:A:1961:TYR:CE2	1:A:2001:LEU:HD12	2.54	0.43
1:A:1873:CYS:HA	1:A:1901:LEU:HD13	2.01	0.43
1:A:1918:ARG:HG2	1:A:2840:LEU:HD13	2.01	0.43
1:A:2092:CYS:SG	1:A:2095:LEU:HD23	2.58	0.43
1:A:3004:LYS:HD2	1:A:3008:ARG:HH21	1.83	0.43
1:A:2730:GLN:O	1:A:2734:MET:HG2	2.19	0.43
1:B:2722:LEU:HD13	1:B:2767:LEU:HD23	2.00	0.43
1:A:2872:HIS:CE1	1:A:2874:GLN:HB2	2.54	0.43
1:B:74:CYS:O	1:B:90:ARG:NH1	2.45	0.43
1:B:213:PHE:CG	1:B:236:LEU:HD13	2.53	0.43
1:B:403:SER:HB2	1:B:409:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:SER:O	1:B:779:MET:HG2	2.19	0.43
1:B:1873:CYS:HA	1:B:1901:LEU:HD13	2.01	0.43
1:A:996:HIS:O	1:A:999:LYS:HG2	2.18	0.43
1:B:248:ARG:HD2	1:B:652:PHE:CD1	2.54	0.43
1:B:1287:PHE:HD1	1:B:1290:ILE:HD11	1.84	0.43
1:B:2459:ARG:NH2	1:B:2494:ASN:OD1	2.51	0.43
1:B:3015:GLU:HB2	1:B:3020:VAL:HB	1.99	0.43
1:A:405:ASN:OD1	1:A:405:ASN:N	2.52	0.43
1:A:2312:LEU:HD12	1:A:2312:LEU:HA	1.88	0.43
1:B:1093:ILE:HG21	1:B:1157:LEU:HD12	2.01	0.43
1:B:2109:TRP:HH2	1:B:2132:LEU:HD13	1.84	0.43
1:B:405:ASN:OD1	1:B:405:ASN:N	2.52	0.42
1:B:1510:LYS:HG2	1:B:1552:ASN:HD21	1.83	0.42
1:B:2731:VAL:HG11	1:B:2866:LEU:HD11	2.01	0.42
1:A:1194:LEU:HA	1:A:1197:VAL:HG12	2.00	0.42
1:A:1266:ASP:OD1	1:A:1267:GLU:N	2.52	0.42
1:A:1630:ASP:OD1	1:A:1633:ARG:NH2	2.46	0.42
1:B:2942:GLN:NE2	1:B:3018:LYS:HG3	2.30	0.42
1:A:68:ILE:HD12	1:A:97:ILE:HD12	2.01	0.42
1:A:1299:ALA:HB2	1:A:1392:TYR:HB2	2.02	0.42
1:A:2107:MET:HG2	1:A:2109:TRP:CZ2	2.54	0.42
1:B:814:ASP:O	1:B:818:ILE:HG13	2.20	0.42
1:B:1531:GLN:OE1	1:B:1533:GLU:HB3	2.18	0.42
1:A:248:ARG:HD2	1:A:652:PHE:CD1	2.55	0.42
1:A:657:PHE:CZ	1:A:1155:LEU:HB3	2.54	0.42
1:A:1111:LEU:H	1:A:1116:GLN:HE21	1.67	0.42
1:A:1859:ARG:NH2	1:A:1932:PHE:O	2.45	0.42
1:A:1922:PRO:HD3	1:A:1933:TRP:CH2	2.55	0.42
1:A:2717:LYS:HD3	1:A:2722:LEU:HD21	2.01	0.42
1:B:748:LYS:HA	1:B:748:LYS:HD3	1.88	0.42
1:B:1398:LYS:H	1:B:1398:LYS:HG2	1.69	0.42
1:B:2872:HIS:CE1	1:B:2874:GLN:HB2	2.54	0.42
1:B:2529:THR:O	1:B:2532:MET:HG2	2.20	0.42
1:A:804:LEU:HD13	1:A:911:ALA:HA	2.01	0.42
1:A:1350:THR:HB	1:A:1380:HIS:HA	2.00	0.42
1:A:2006:LEU:O	1:A:2010:ARG:HG3	2.19	0.42
1:A:2933:LYS:HA	1:A:2933:LYS:HD3	1.85	0.42
1:B:62:ARG:HA	1:B:65:GLN:HB2	2.01	0.42
1:B:68:ILE:HD12	1:B:97:ILE:HD12	2.01	0.42
1:A:595:VAL:HG13	1:A:600:HIS:HB2	2.01	0.42
1:A:814:ASP:O	1:A:818:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ALA:O	1:A:1131:MET:HG2	2.20	0.42
1:A:2010:ARG:HG2	1:A:2018:LEU:HD11	2.02	0.42
1:B:657:PHE:CZ	1:B:1155:LEU:HB3	2.54	0.42
1:B:1777:VAL:HG21	1:B:1822:GLU:HB2	2.02	0.42
1:A:618:LYS:HG2	1:A:683:HIS:CD2	2.55	0.42
1:A:1989:LEU:HD22	1:A:2001:LEU:HD13	2.02	0.42
1:A:2723:ARG:O	1:A:2727:VAL:HG23	2.19	0.42
1:B:1449:LEU:HD22	1:B:1457:LEU:HD21	2.01	0.42
1:B:2209:SER:HG	1:B:2227:ARG:HH12	1.64	0.42
1:B:2235:MET:O	1:B:2244:ARG:NH2	2.53	0.42
1:A:149:ILE:HA	1:A:155:TYR:HD2	1.83	0.42
1:A:495:ILE:HG21	1:A:526:LEU:HD21	2.00	0.42
1:A:1093:ILE:HG21	1:A:1157:LEU:HD12	2.01	0.42
1:A:2517:LEU:N	1:A:2518:PRO:HD2	2.35	0.42
1:A:2909:ARG:HG3	1:A:3052:TRP:CZ2	2.55	0.42
1:B:1959:GLU:OE2	1:B:2849:ARG:NH1	2.44	0.42
1:A:1531:GLN:OE1	1:A:1533:GLU:HB3	2.20	0.41
1:A:1606:LEU:HD23	1:A:1609:THR:HG23	2.02	0.41
1:A:1777:VAL:HG21	1:A:1822:GLU:HB2	2.02	0.41
1:A:2016:ASP:HB3	1:A:2926:VAL:HA	2.02	0.41
1:B:2663:VAL:HG21	1:B:2680:LEU:HD13	2.02	0.41
1:B:2865:ILE:HD13	1:B:2865:ILE:HA	1.92	0.41
1:B:2933:LYS:HA	1:B:2933:LYS:HD3	1.85	0.41
1:A:984:GLN:HB3	1:A:1035:ILE:HG12	2.02	0.41
1:A:1046:LEU:HD22	1:A:1074:PHE:HD1	1.84	0.41
1:A:1289:LYS:O	1:A:1293:ASN:ND2	2.52	0.41
1:A:1524:LEU:HD23	1:A:1527:LEU:HD12	2.02	0.41
1:A:3001:SER:HB3	1:A:3004:LYS:HG2	2.01	0.41
1:B:245:VAL:HG12	1:B:1083:HIS:HB3	2.02	0.41
1:B:1299:ALA:HB2	1:B:1392:TYR:HB2	2.01	0.41
1:B:1449:LEU:HD23	1:B:1449:LEU:HA	1.91	0.41
1:A:250:ARG:HA	1:A:250:ARG:HD2	1.84	0.41
1:A:2807:GLU:O	1:A:2811:LYS:NZ	2.53	0.41
1:A:3008:ARG:HH12	1:B:2408:SER:CB	2.33	0.41
1:B:940:LYS:HD3	1:B:943:HIS:CD2	2.55	0.41
1:B:2743:THR:HG22	1:B:2746:ARG:HH12	1.85	0.41
1:A:62:ARG:HA	1:A:65:GLN:HB2	2.02	0.41
1:A:1001:LEU:HD21	1:A:1015:GLN:HA	2.01	0.41
1:A:1287:PHE:HD1	1:A:1290:ILE:HD11	1.85	0.41
1:A:1962:ALA:HB2	1:A:2001:LEU:HD11	2.01	0.41
1:B:790:CYS:SG	1:B:792:LYS:HG2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1046:LEU:HD22	1:B:1074:PHE:HD1	1.85	0.41
1:B:2449:GLU:OE1	1:B:2453:ARG:NH2	2.38	0.41
1:B:2499:GLU:O	1:B:2503:MET:HG3	2.21	0.41
1:A:790:CYS:SG	1:A:792:LYS:HG2	2.60	0.41
1:A:2877:LEU:HB2	1:A:2886:VAL:HB	2.03	0.41
1:A:74:CYS:O	1:A:90:ARG:NH1	2.45	0.41
1:A:121:LEU:O	1:A:125:MET:HG2	2.20	0.41
1:A:784:THR:HG23	1:A:906:LEU:HD12	2.03	0.41
1:A:1040:MET:SD	1:A:1085:VAL:HG22	2.60	0.41
1:A:1715:LEU:HD22	1:A:1737:LEU:HD13	2.02	0.41
1:A:1961:TYR:CD2	1:A:2001:LEU:HD12	2.55	0.41
1:A:2782:ASN:ND2	1:A:2785:ASP:OD1	2.54	0.41
1:B:427:LEU:O	1:B:469:ARG:NH2	2.34	0.41
1:B:804:LEU:HD13	1:B:911:ALA:HA	2.02	0.41
1:B:1289:LYS:O	1:B:1293:ASN:ND2	2.52	0.41
1:A:409:LEU:HD23	1:A:451:ARG:HD3	2.03	0.41
1:A:1449:LEU:HD23	1:A:1449:LEU:HA	1.90	0.41
1:B:784:THR:HG23	1:B:906:LEU:HD12	2.03	0.41
1:B:984:GLN:HB3	1:B:1035:ILE:HG12	2.02	0.41
1:A:1620:GLN:O	1:A:1624:HIS:HB2	2.21	0.41
1:B:1075:THR:O	1:B:1126:LYS:HG2	2.20	0.41
1:B:1158:ILE:HG21	1:B:1176:LEU:HB2	2.03	0.41
1:B:1186:GLU:HB2	1:B:1189:LEU:HB2	2.02	0.41
1:B:2805:MET:HG3	1:B:3055:TRP:CZ3	2.56	0.41
1:B:812:MET:HB2	1:B:923:ILE:HD11	2.03	0.41
1:B:1111:LEU:H	1:B:1116:GLN:HE21	1.67	0.41
1:B:2016:ASP:HB3	1:B:2926:VAL:HA	2.02	0.41
1:B:2030:ILE:HD12	1:B:2030:ILE:H	1.86	0.41
1:A:102:LYS:HZ1	1:A:106:LYS:HD3	1.85	0.41
1:A:1824:LEU:HD13	1:A:1845:LEU:HD23	2.02	0.41
1:A:2805:MET:O	1:A:2809:GLN:HG2	2.21	0.41
1:B:1001:LEU:HD21	1:B:1015:GLN:HA	2.01	0.41
1:A:152:VAL:HG12	1:A:154:LYS:H	1.86	0.40
1:A:897:PHE:HA	1:A:900:MET:SD	2.61	0.40
1:A:923:ILE:O	1:A:927:LEU:HG	2.20	0.40
1:A:1186:GLU:HB2	1:A:1189:LEU:HB2	2.03	0.40
1:B:152:VAL:HG12	1:B:154:LYS:H	1.86	0.40
1:B:1706:LYS:HE3	1:B:1710:TRP:NE1	2.36	0.40
1:A:743:SER:O	1:A:747:GLN:HG2	2.22	0.40
1:A:812:MET:HB2	1:A:923:ILE:HD11	2.04	0.40
1:A:1939:LEU:HD23	1:A:1997:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:LEU:HG	1:B:946:MET:CE	2.51	0.40
1:B:1266:ASP:OD1	1:B:1267:GLU:N	2.54	0.40
1:B:1845:LEU:O	1:B:1849:ILE:HG12	2.21	0.40
1:A:190:ILE:O	1:A:194:VAL:HG23	2.22	0.40
1:A:753:MET:O	1:A:757:GLY:N	2.55	0.40
1:A:1291:LEU:O	1:A:1295:LEU:HB2	2.22	0.40
1:B:2782:ASN:ND2	1:B:2785:ASP:OD1	2.54	0.40
1:A:1616:ASP:O	1:A:1620:GLN:HG2	2.21	0.40
1:A:2030:ILE:H	1:A:2030:ILE:HD12	1.87	0.40
1:A:2049:TYR:CZ	1:A:2063:GLY:HA3	2.56	0.40
1:A:2049:TYR:HB3	1:A:2064:ILE:HG13	2.04	0.40
1:B:121:LEU:O	1:B:125:MET:HG2	2.21	0.40
1:B:1082:HIS:HD2	1:B:1084:GLN:HB3	1.86	0.40
1:B:1341:PRO:HG3	1:B:1414:SER:HB2	2.03	0.40
1:B:1472:LEU:HD11	1:B:1497:LEU:CD2	2.51	0.40
1:B:1616:ASP:O	1:B:1620:GLN:HG2	2.21	0.40
1:B:1806:ILE:HG13	1:B:1838:CYS:HB3	2.04	0.40

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	2734/3184 (86%)	2684 (98%)	50 (2%)	0	100	100
1	B	2734/3184 (86%)	2687 (98%)	47 (2%)	0	100	100
All	All	5468/6368 (86%)	5371 (98%)	97 (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	A	2467/2883 (86%)	2466 (100%)	1 (0%)	100	100
1	B	2467/2883 (86%)	2465 (100%)	2 (0%)	93	98
All	All	4934/5766 (86%)	4931 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	B	66	LYS
1	B	578	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1310	GLN
1	A	1578	GLN
1	A	2066	GLN
1	A	2111	HIS
1	A	2714	GLN
1	A	3014	GLN
1	B	1310	GLN
1	B	2942	GLN
1	B	3014	GLN

### 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
2	ANP	B	3101	-	29,33,33	1.09	4 (13%)	31,52,52	1.10	2 (6%)
2	ANP	A	3101	-	29,33,33	1.09	4 (13%)	31,52,52	1.12	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
2	ANP	B	3101	-	-	1/14/38/38	0/3/3/3
2	ANP	A	3101	-	-	1/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3101	ANP	PG-O1G	2.46	1.50	1.46
2	B	3101	ANP	PG-O1G	2.45	1.50	1.46
2	A	3101	ANP	PG-N3B	2.43	1.69	1.63
2	B	3101	ANP	PG-N3B	2.43	1.69	1.63
2	B	3101	ANP	PB-O1B	2.33	1.49	1.46
2	A	3101	ANP	PB-O1B	2.33	1.49	1.46
2	B	3101	ANP	PB-O3A	-2.27	1.56	1.59
2	A	3101	ANP	PB-O3A	-2.27	1.56	1.59

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3101	ANP	PB-O3A-PA	-3.76	119.37	132.62
2	A	3101	ANP	PB-O3A-PA	-3.73	119.48	132.62
2	A	3101	ANP	C5-C6-N6	2.41	124.01	120.35
2	B	3101	ANP	C5-C6-N6	2.28	123.82	120.35

There are no chirality outliers.

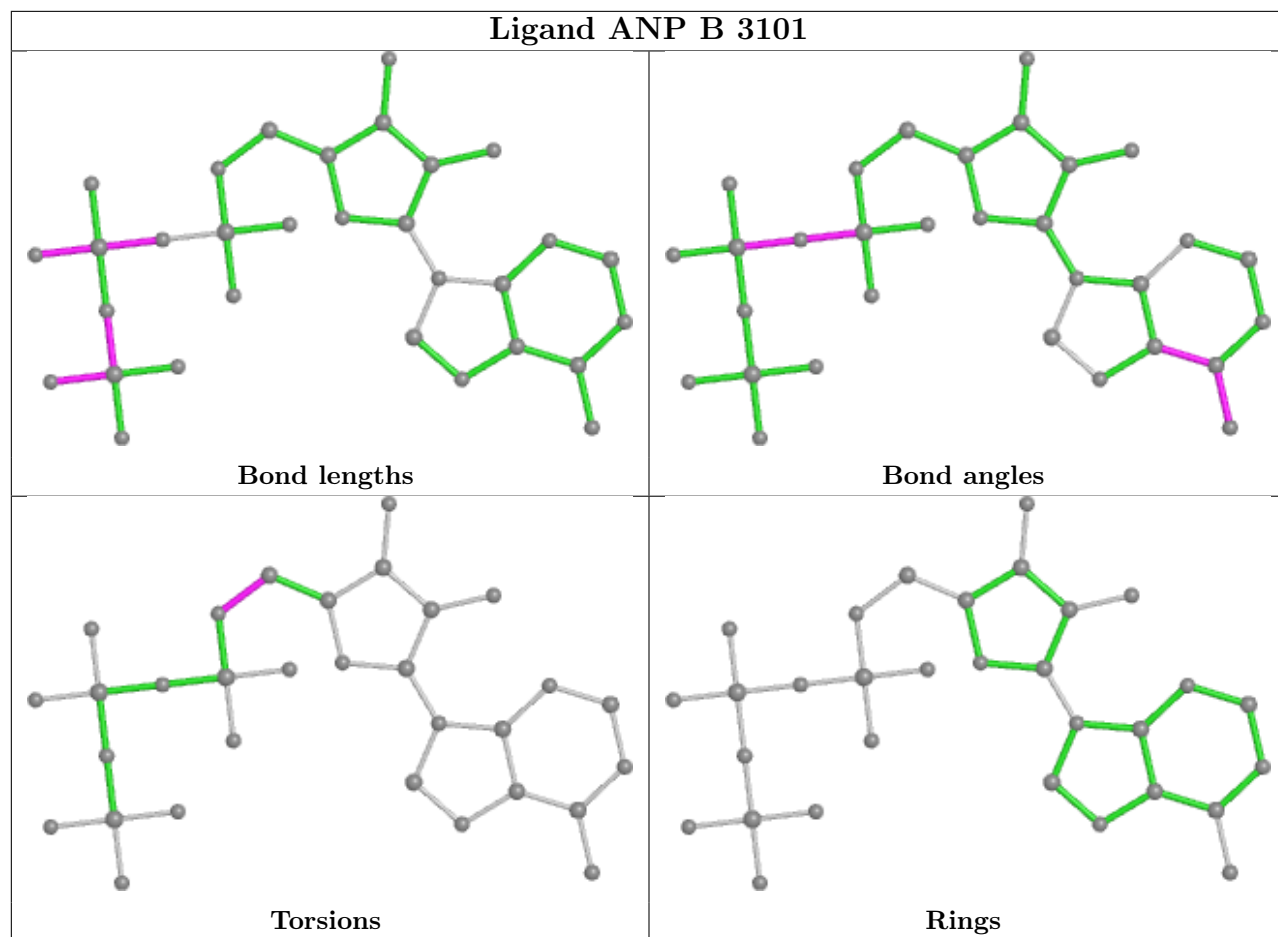
All (2) torsion outliers are listed below:

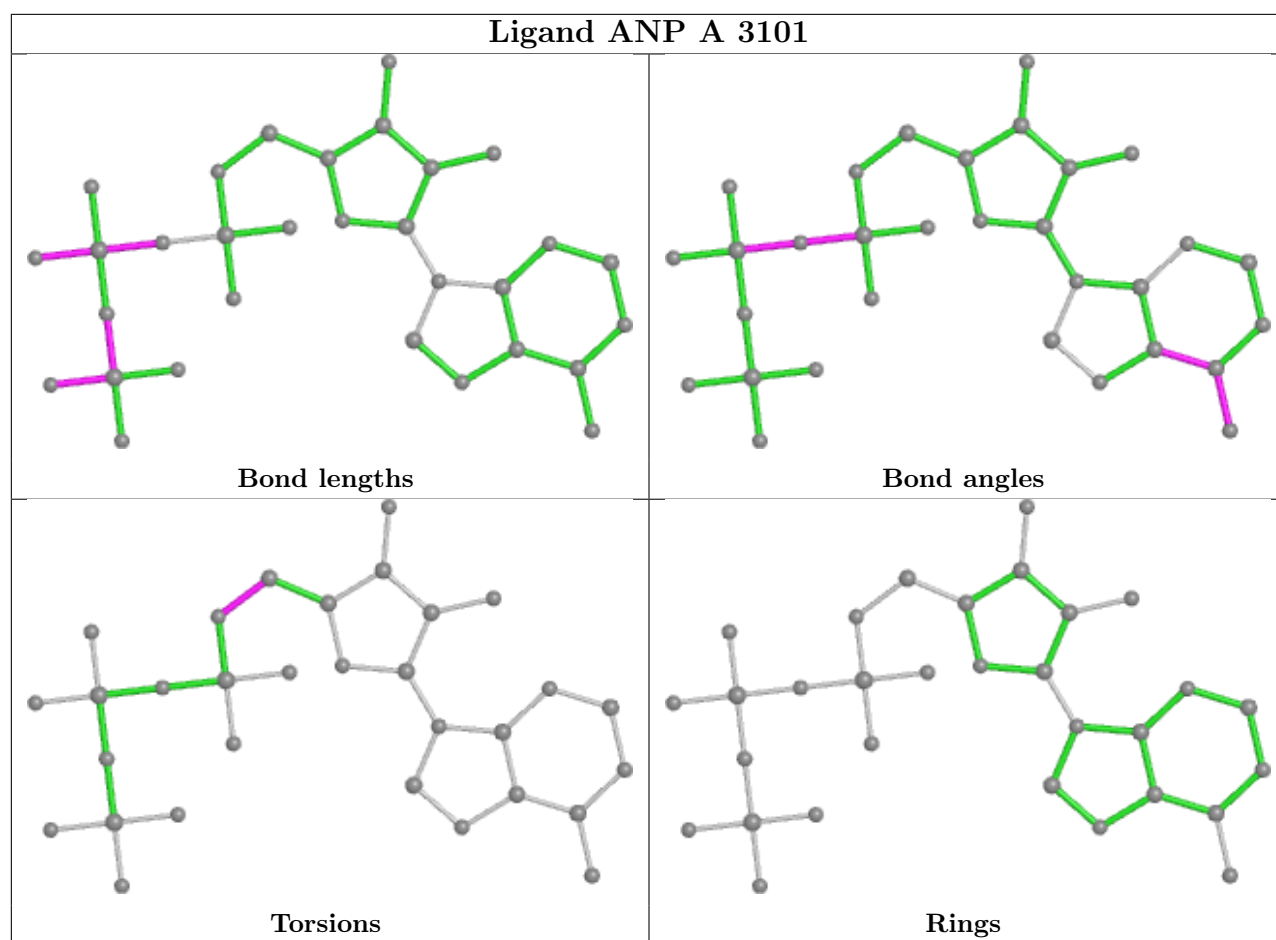
Mol	Chain	Res	Type	Atoms
2	A	3101	ANP	C4'-C5'-O5'-PA
2	B	3101	ANP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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.

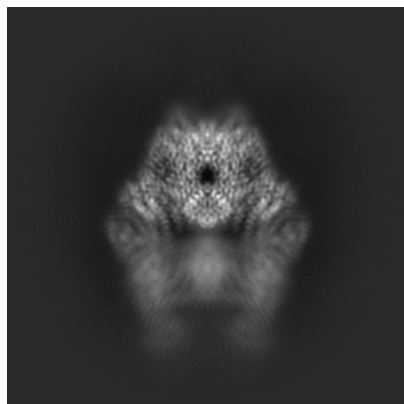
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17267. These allow visual inspection of the internal detail of the map and identification of artifacts.

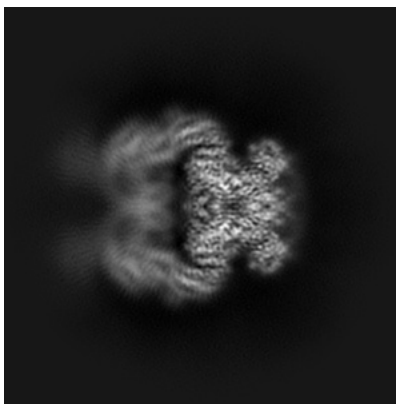
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

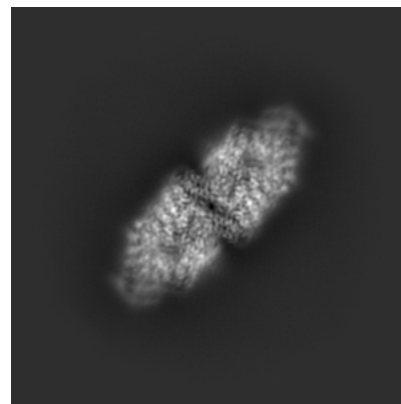
#### 6.1.1 Primary map



X

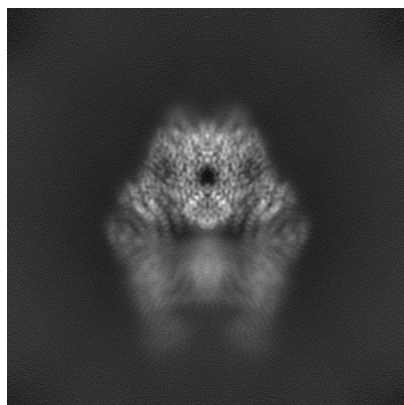


Y

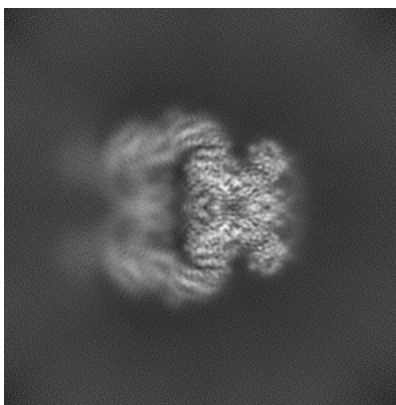


Z

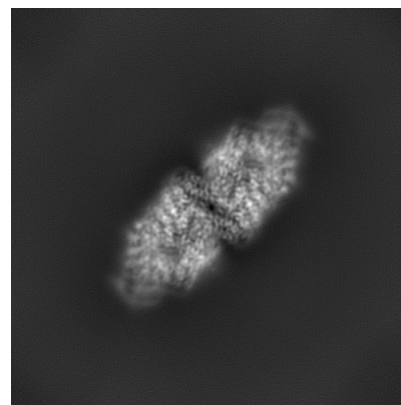
#### 6.1.2 Raw map



X



Y

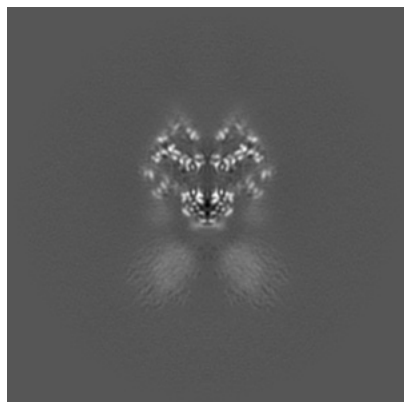


Z

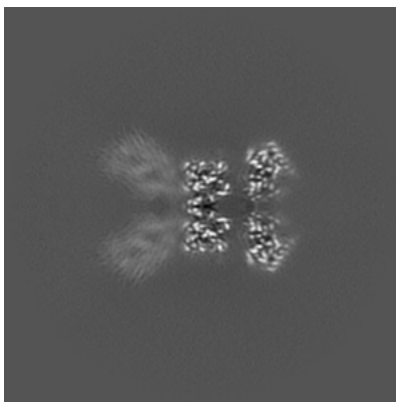
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

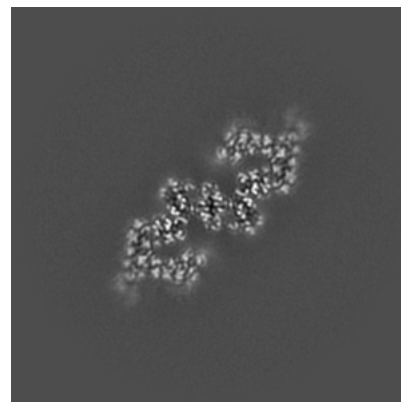
### 6.2.1 Primary map



X Index: 200

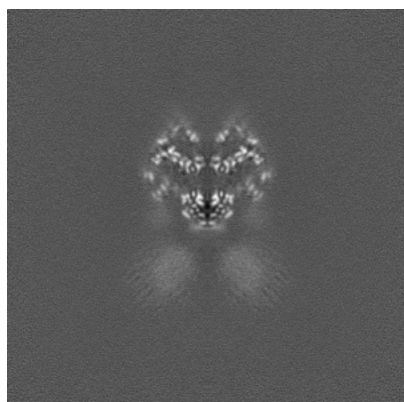


Y Index: 200

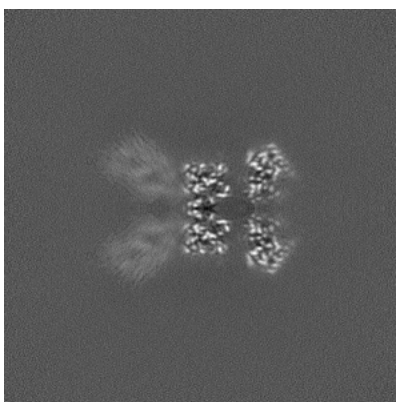


Z Index: 200

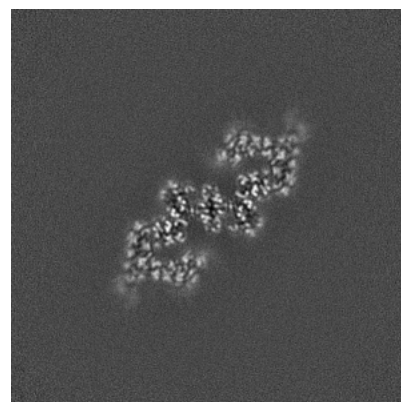
### 6.2.2 Raw map



X Index: 200



Y Index: 200

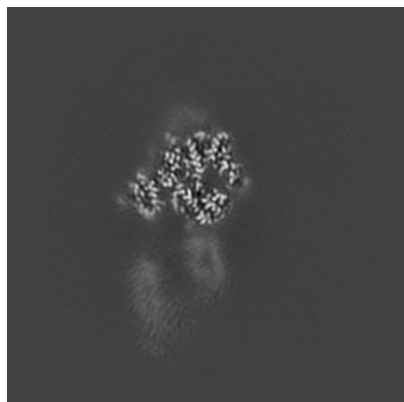


Z Index: 200

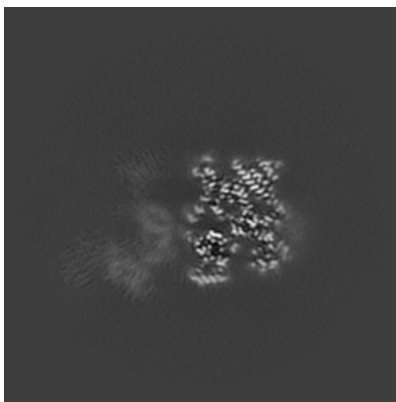
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

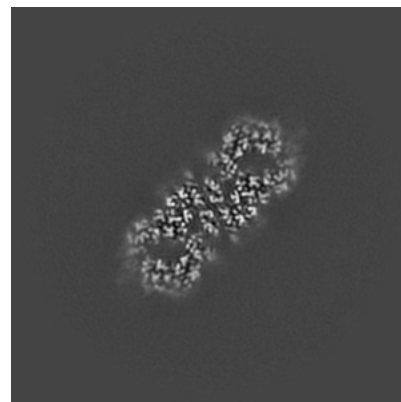
### 6.3.1 Primary map



X Index: 171

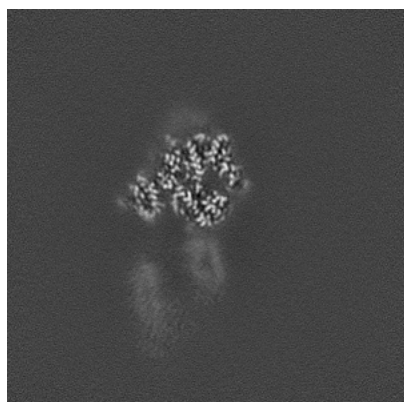


Y Index: 182

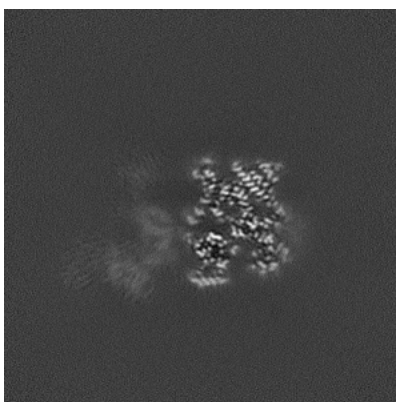


Z Index: 211

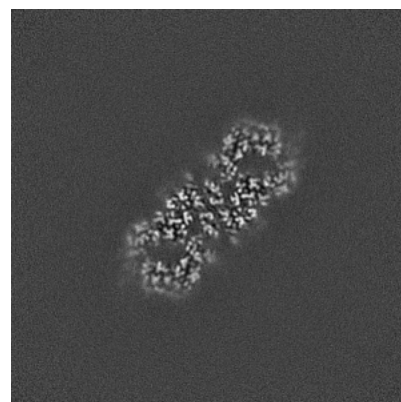
### 6.3.2 Raw map



X Index: 171



Y Index: 182

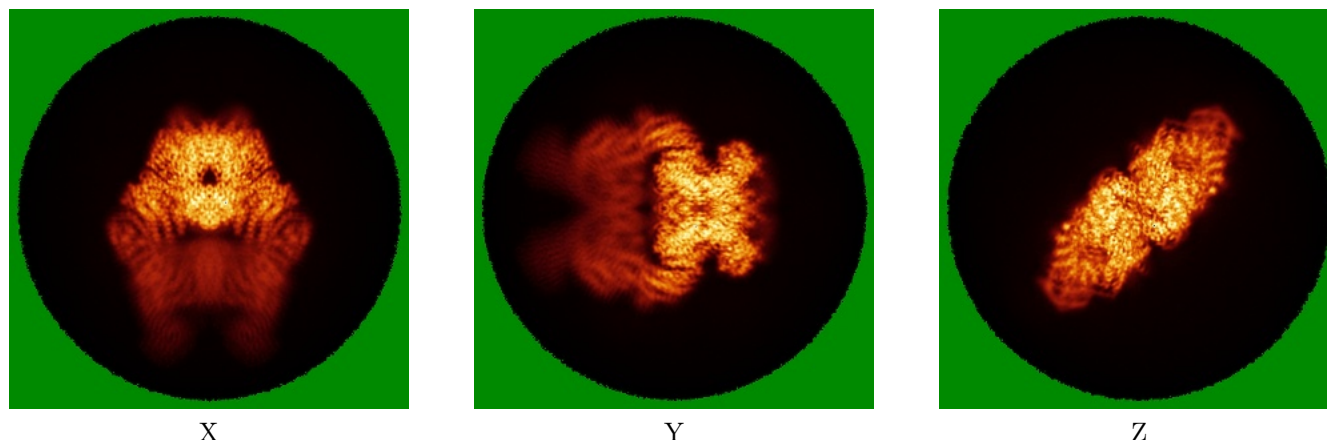


Z Index: 211

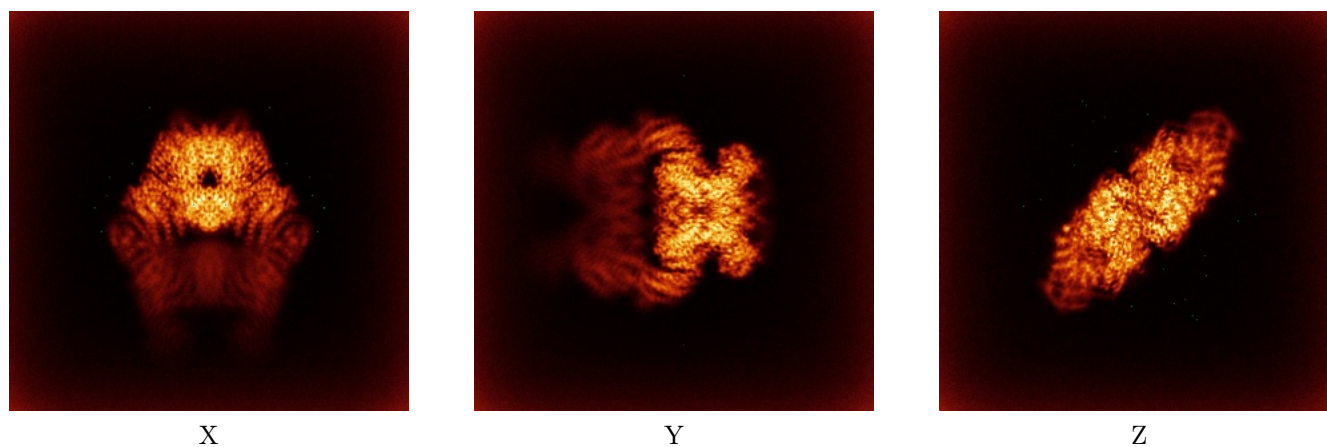
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



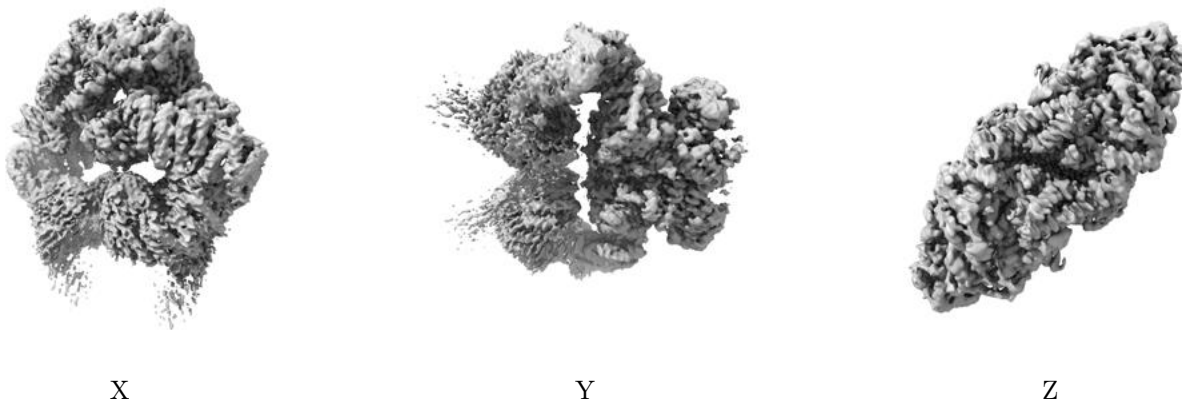
### 6.4.2 Raw map



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.

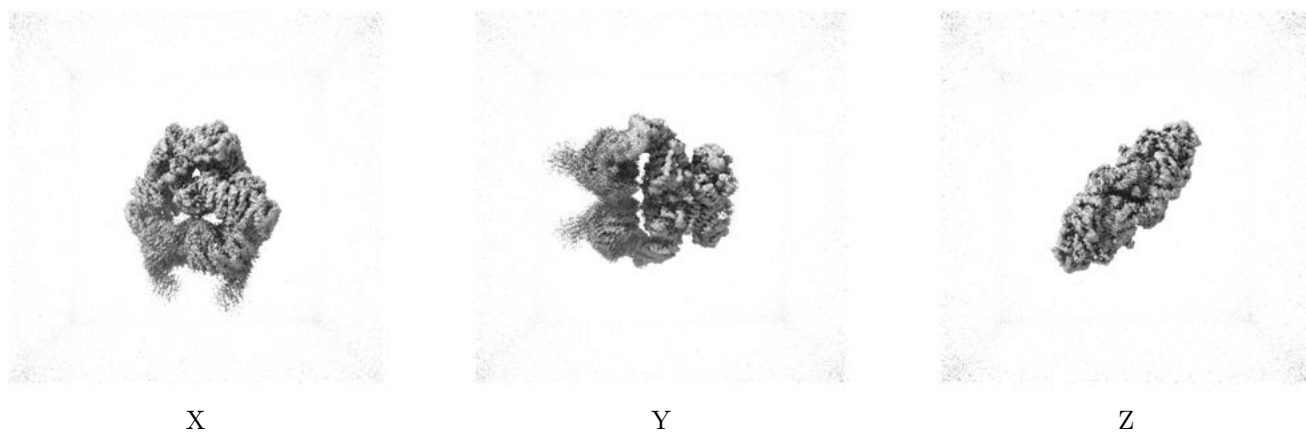
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.



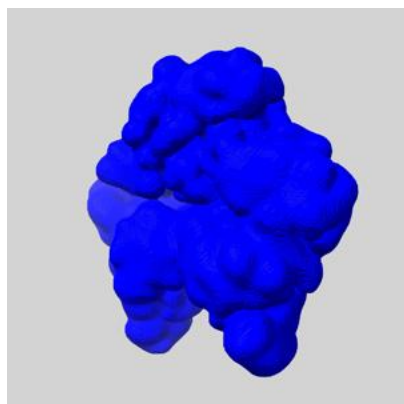
## 6.6 Mask visualisation [i](#)

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

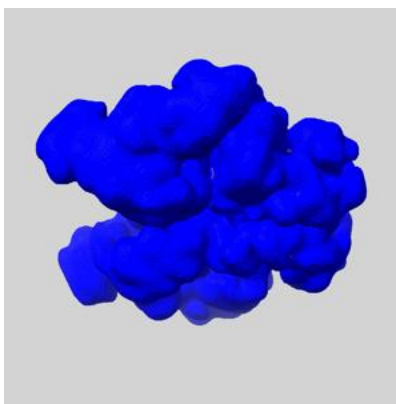
A mask typically either:

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

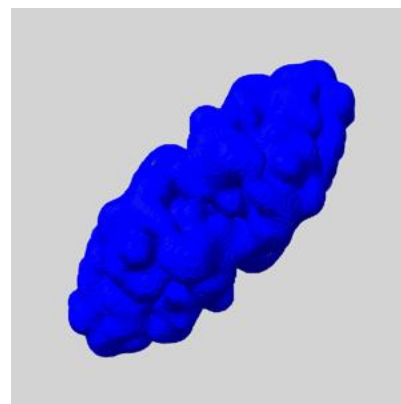
### 6.6.1 emd\_17267\_msk\_1.map [i](#)



X



Y

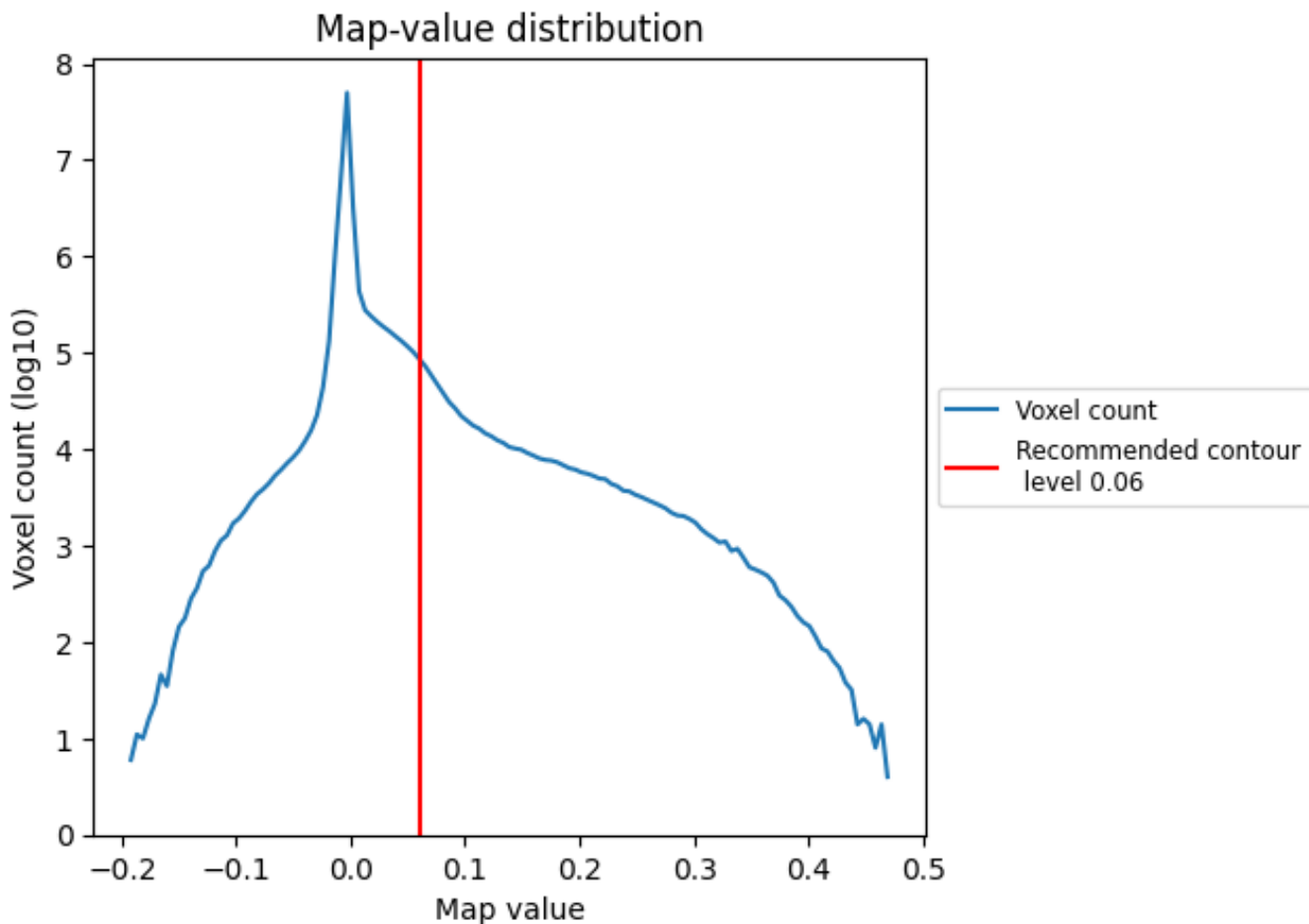


Z

## 7 Map analysis [i](#)

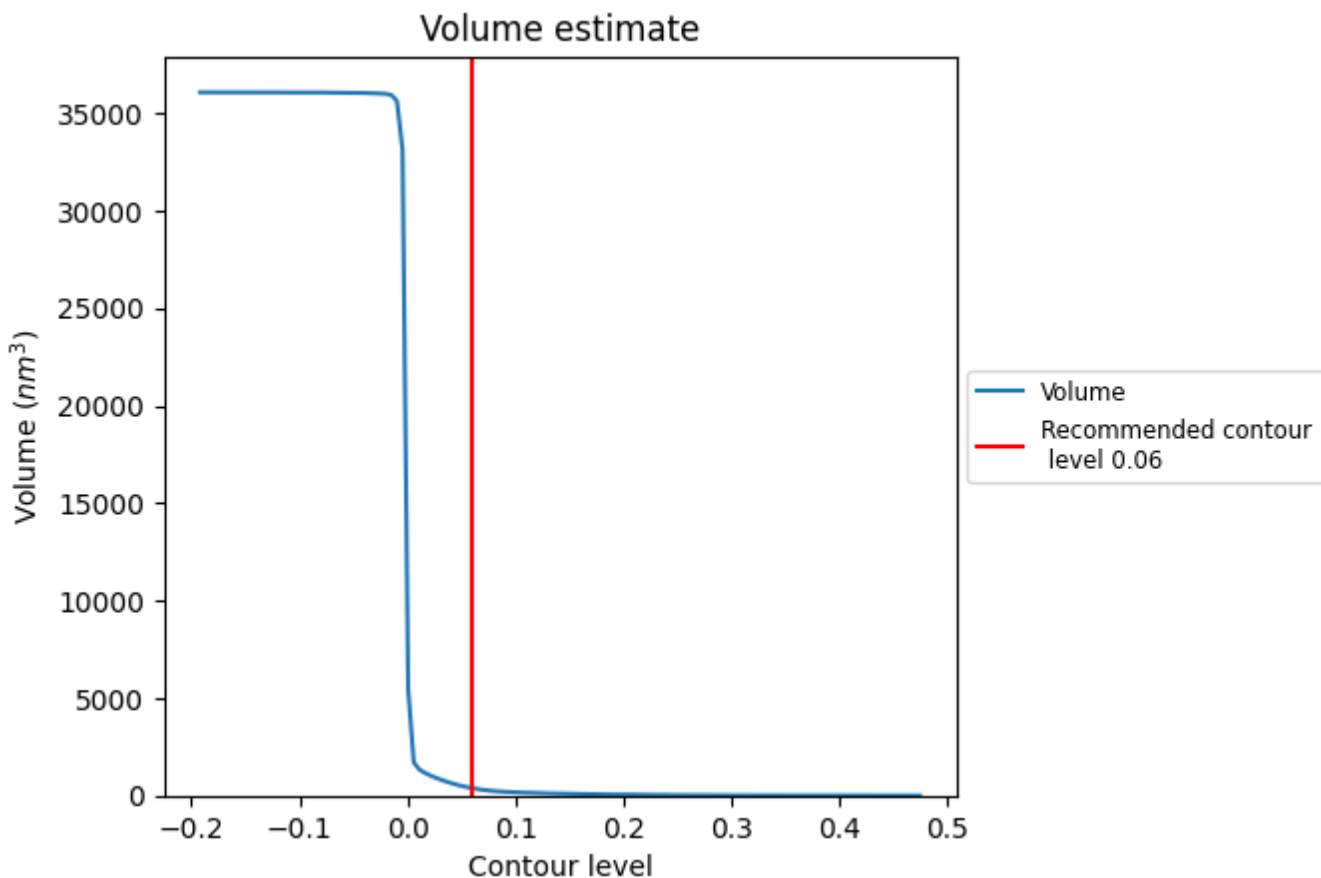
This section contains the results of statistical analysis of the map.

### 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.

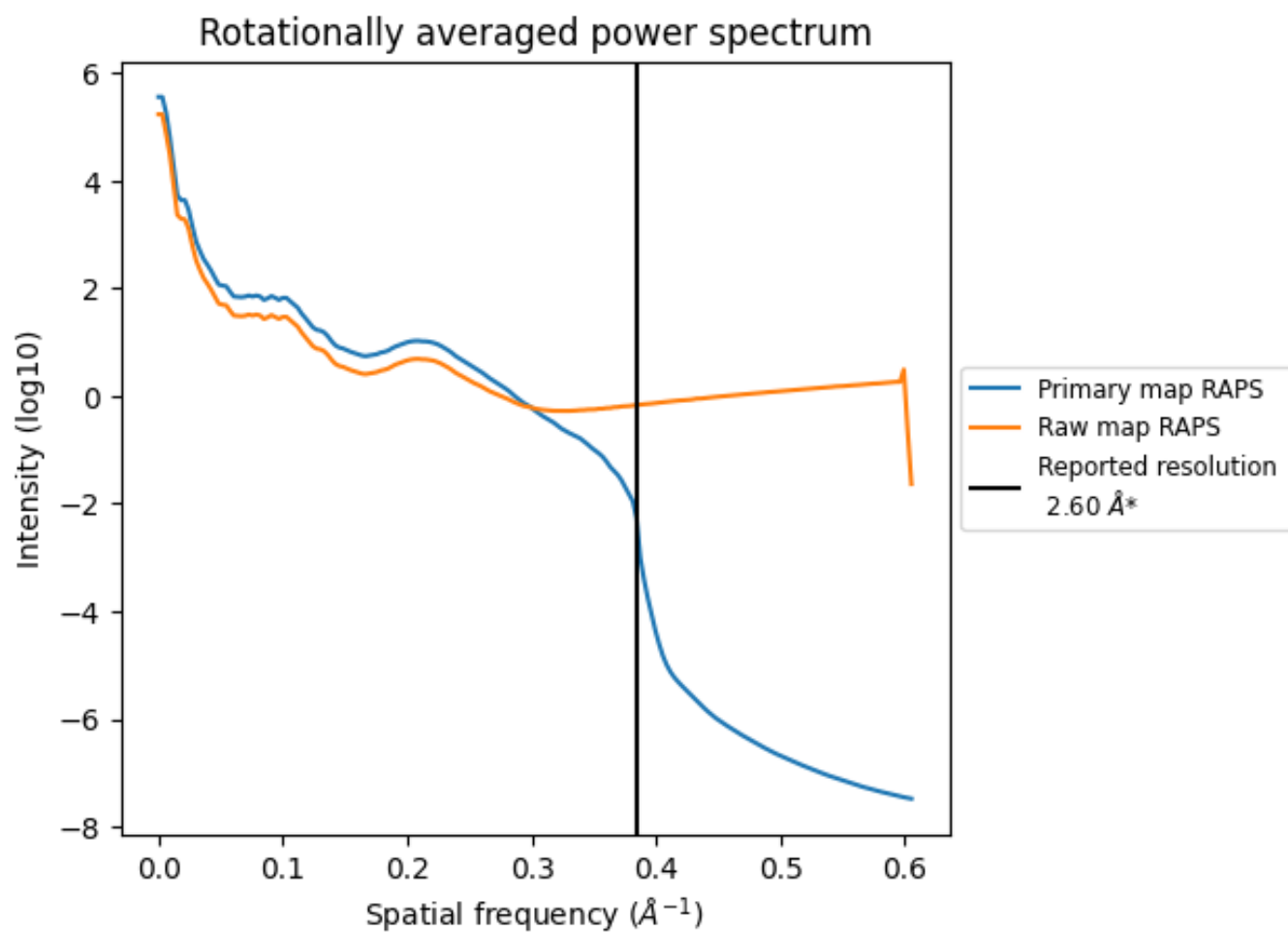
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm<sup>3</sup>; this corresponds to an approximate mass of 342 kDa.

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

### 7.3 Rotationally averaged power spectrum i

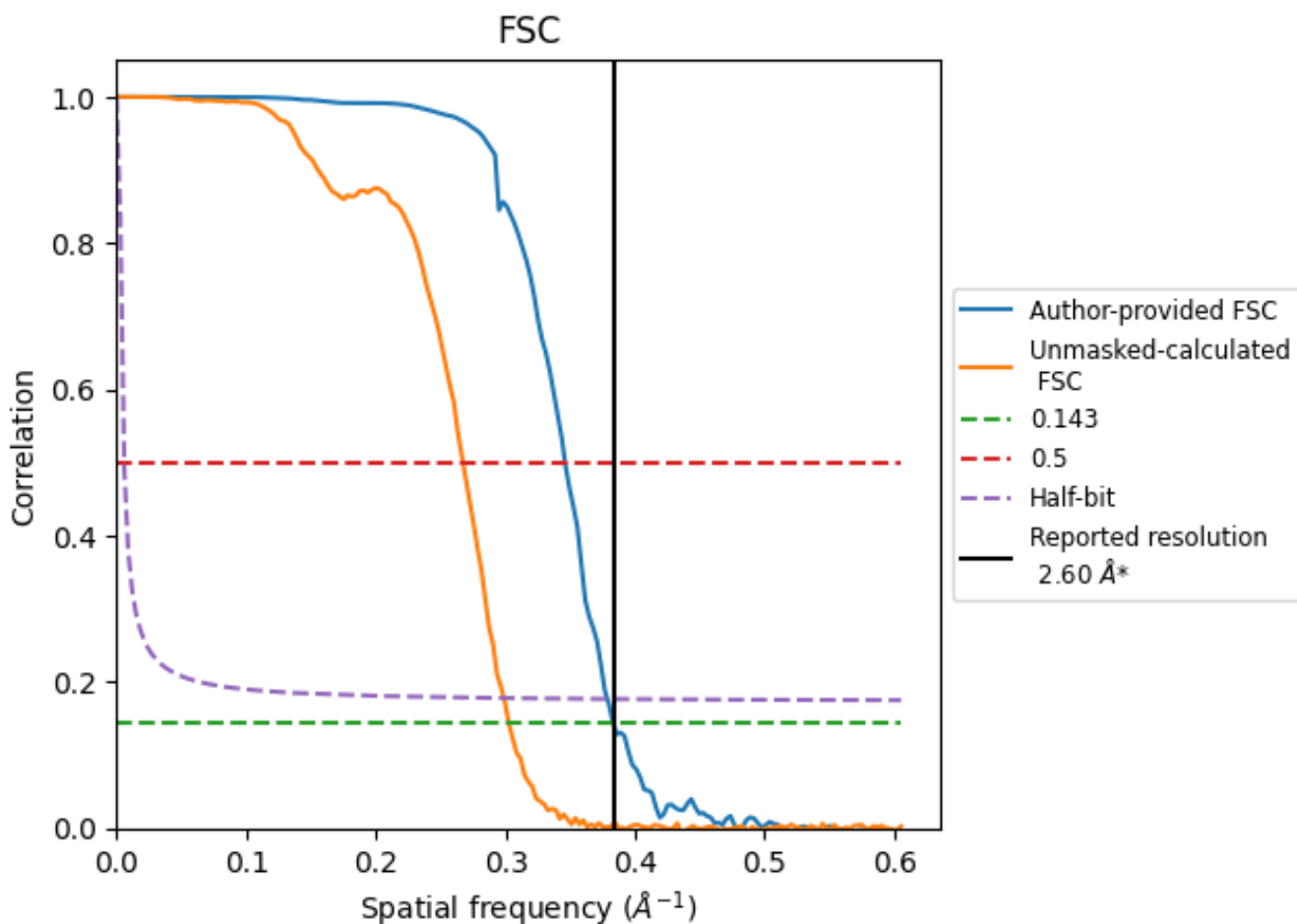


\*Reported resolution corresponds to spatial frequency of  $0.385 \text{ \AA}^{-1}$

## 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 0.385 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

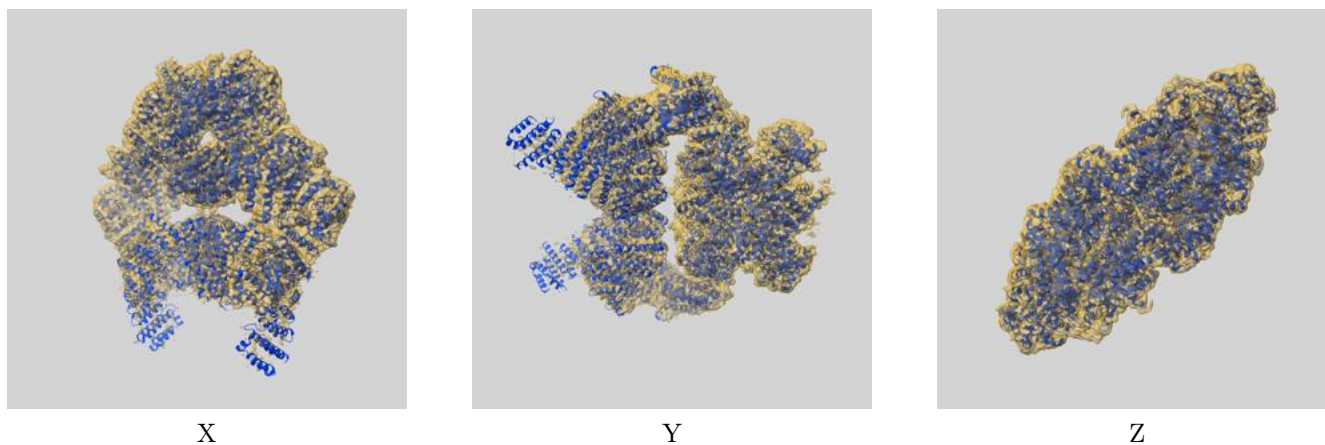
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.89	2.64
Unmasked-calculated*	3.30	3.74	3.35

\*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 3.30 differs from the reported value 2.6 by more than 10 %

## 9 Map-model fit [i](#)

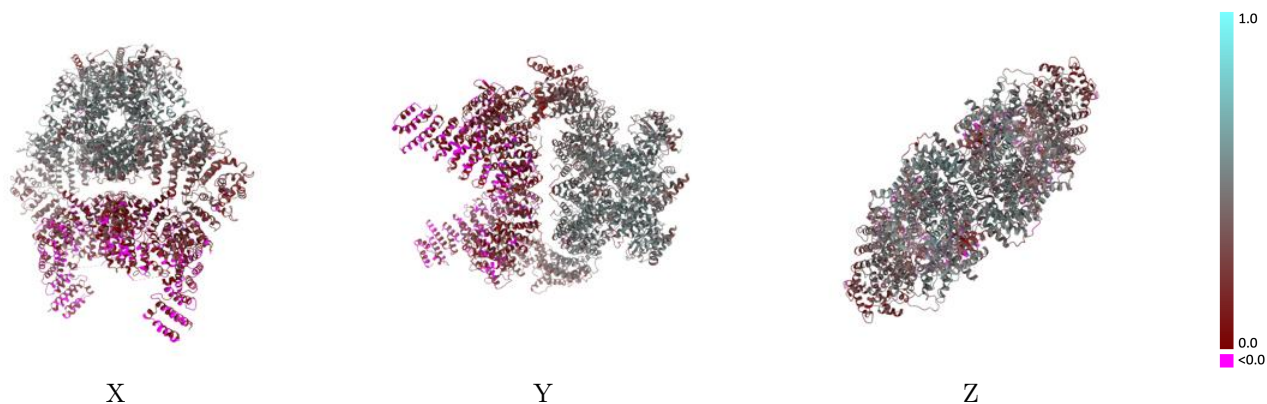
This section contains information regarding the fit between EMDB map EMD-17267 and PDB model 8OXP. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



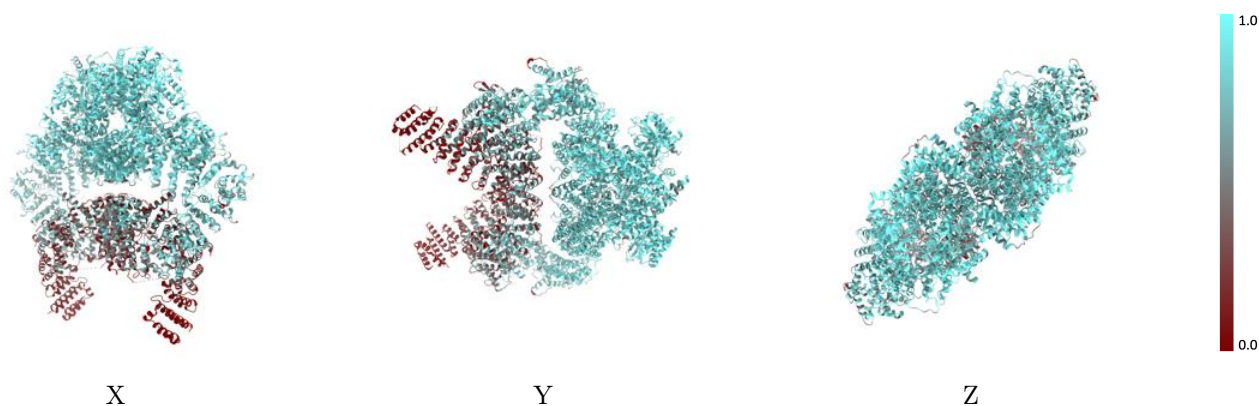
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

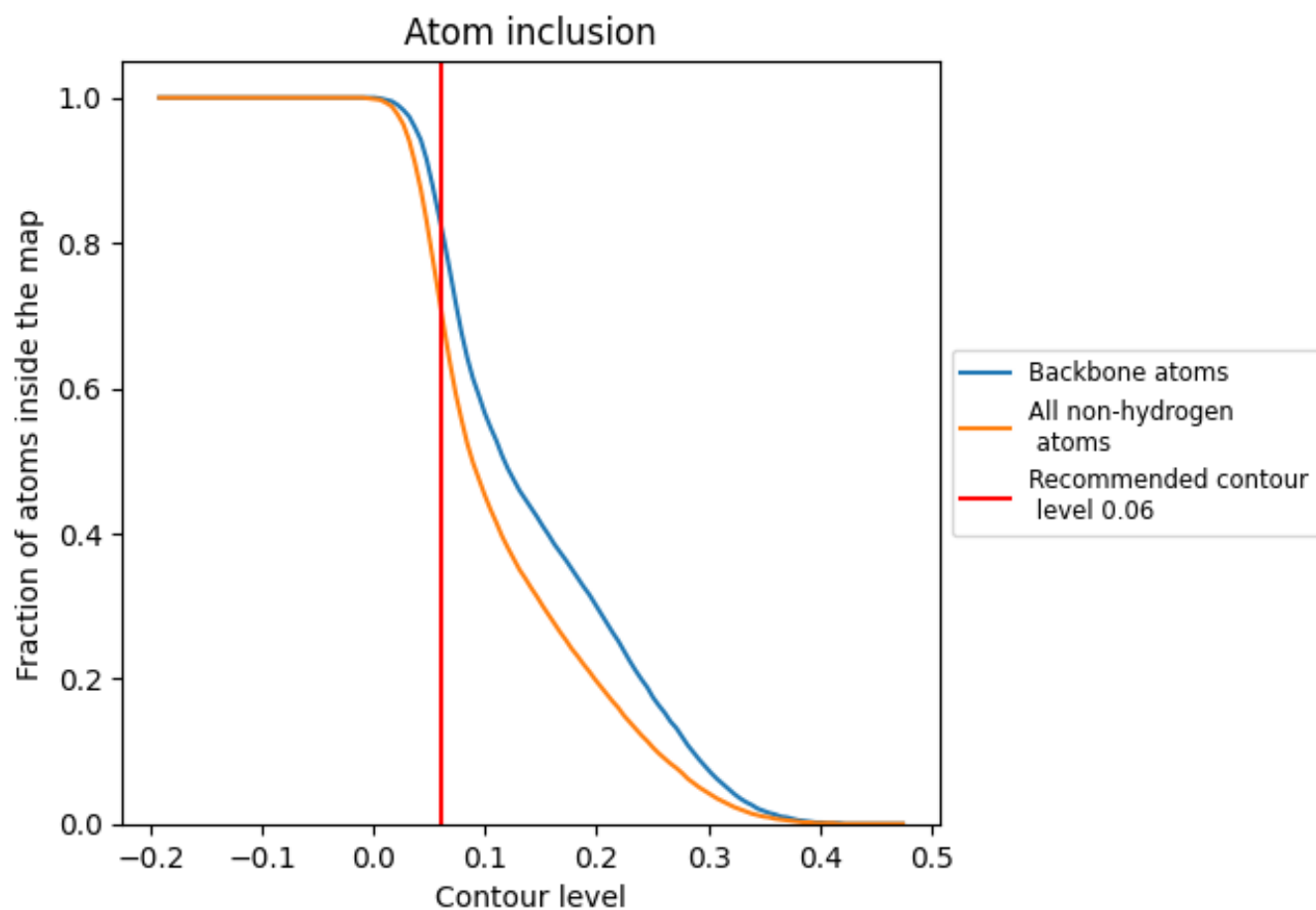
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.06).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 71% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.3200
A	 0.7140	 0.3250
B	 0.7090	 0.3140

