



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 10:00 pm GMT

PDB ID : 7A98  
EMDB ID : EMD-11688  
Title : SARS-CoV-2 Spike Glycoprotein with 3 ACE2 Bound  
Authors : Benton, D.J.; Wrobel, A.G.; Rosenthal, P.B.; Gamblin, S.J.  
Deposited on : 2020-09-01  
Resolution : 5.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

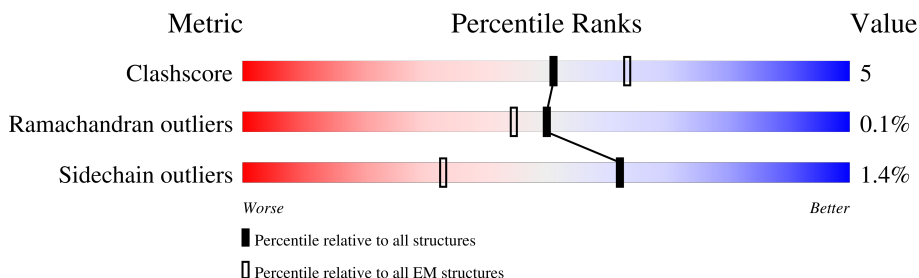
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1287	 71% 12% 17%
1	B	1287	 70% 12% 17%
1	C	1287	 71% 11% 17%
2	D	654	 78% 11% 10%
2	E	654	 78% 12% 10%
2	F	654	 78% 11% 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39435 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		
1	B	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		
1	C	1066	Total	C	N	O	S	0	0
			8344	5324	1394	1588	38		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP P0DTC2
A	-29	GLY	-	expression tag	UNP P0DTC2
A	-28	ILE	-	expression tag	UNP P0DTC2
A	-27	LEU	-	expression tag	UNP P0DTC2
A	-26	PRO	-	expression tag	UNP P0DTC2
A	-25	SER	-	expression tag	UNP P0DTC2
A	-24	PRO	-	expression tag	UNP P0DTC2
A	-23	GLY	-	expression tag	UNP P0DTC2
A	-22	MET	-	expression tag	UNP P0DTC2
A	-21	PRO	-	expression tag	UNP P0DTC2
A	-20	ALA	-	expression tag	UNP P0DTC2
A	-19	LEU	-	expression tag	UNP P0DTC2
A	-18	LEU	-	expression tag	UNP P0DTC2
A	-17	SER	-	expression tag	UNP P0DTC2
A	-16	LEU	-	expression tag	UNP P0DTC2
A	-15	VAL	-	expression tag	UNP P0DTC2
A	-14	SER	-	expression tag	UNP P0DTC2
A	-13	LEU	-	expression tag	UNP P0DTC2
A	-12	LEU	-	expression tag	UNP P0DTC2
A	-11	SER	-	expression tag	UNP P0DTC2
A	-10	VAL	-	expression tag	UNP P0DTC2
A	-9	LEU	-	expression tag	UNP P0DTC2
A	-8	LEU	-	expression tag	UNP P0DTC2
A	-7	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P0DTC2
A	-5	CYS	-	expression tag	UNP P0DTC2
A	-4	VAL	-	expression tag	UNP P0DTC2
A	-3	ALA	-	expression tag	UNP P0DTC2
A	-2	GLU	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	GLY	-	expression tag	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ASN	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	PHE	-	expression tag	UNP P0DTC2
A	1217	GLN	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
B	-30	MET	-	initiating methionine	UNP P0DTC2
B	-29	GLY	-	expression tag	UNP P0DTC2
B	-28	ILE	-	expression tag	UNP P0DTC2
B	-27	LEU	-	expression tag	UNP P0DTC2
B	-26	PRO	-	expression tag	UNP P0DTC2
B	-25	SER	-	expression tag	UNP P0DTC2
B	-24	PRO	-	expression tag	UNP P0DTC2
B	-23	GLY	-	expression tag	UNP P0DTC2
B	-22	MET	-	expression tag	UNP P0DTC2
B	-21	PRO	-	expression tag	UNP P0DTC2
B	-20	ALA	-	expression tag	UNP P0DTC2
B	-19	LEU	-	expression tag	UNP P0DTC2
B	-18	LEU	-	expression tag	UNP P0DTC2
B	-17	SER	-	expression tag	UNP P0DTC2
B	-16	LEU	-	expression tag	UNP P0DTC2
B	-15	VAL	-	expression tag	UNP P0DTC2
B	-14	SER	-	expression tag	UNP P0DTC2
B	-13	LEU	-	expression tag	UNP P0DTC2
B	-12	LEU	-	expression tag	UNP P0DTC2
B	-11	SER	-	expression tag	UNP P0DTC2
B	-10	VAL	-	expression tag	UNP P0DTC2
B	-9	LEU	-	expression tag	UNP P0DTC2
B	-8	LEU	-	expression tag	UNP P0DTC2
B	-7	MET	-	expression tag	UNP P0DTC2
B	-6	GLY	-	expression tag	UNP P0DTC2
B	-5	CYS	-	expression tag	UNP P0DTC2
B	-4	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ALA	-	expression tag	UNP P0DTC2
B	-2	GLU	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	GLY	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	ARG	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ASN	-	expression tag	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	PHE	-	expression tag	UNP P0DTC2
B	1217	GLN	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	ILE	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	ARG	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLN	-	expression tag	UNP P0DTC2
B	1234	ALA	-	expression tag	UNP P0DTC2
B	1235	TYR	-	expression tag	UNP P0DTC2
B	1236	VAL	-	expression tag	UNP P0DTC2
B	1237	ARG	-	expression tag	UNP P0DTC2
B	1238	LYS	-	expression tag	UNP P0DTC2
B	1239	ASP	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	TRP	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1245	LEU	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	THR	-	expression tag	UNP P0DTC2
B	1248	PHE	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
C	-30	MET	-	initiating methionine	UNP P0DTC2
C	-29	GLY	-	expression tag	UNP P0DTC2
C	-28	ILE	-	expression tag	UNP P0DTC2
C	-27	LEU	-	expression tag	UNP P0DTC2
C	-26	PRO	-	expression tag	UNP P0DTC2
C	-25	SER	-	expression tag	UNP P0DTC2
C	-24	PRO	-	expression tag	UNP P0DTC2
C	-23	GLY	-	expression tag	UNP P0DTC2
C	-22	MET	-	expression tag	UNP P0DTC2
C	-21	PRO	-	expression tag	UNP P0DTC2
C	-20	ALA	-	expression tag	UNP P0DTC2
C	-19	LEU	-	expression tag	UNP P0DTC2
C	-18	LEU	-	expression tag	UNP P0DTC2
C	-17	SER	-	expression tag	UNP P0DTC2
C	-16	LEU	-	expression tag	UNP P0DTC2
C	-15	VAL	-	expression tag	UNP P0DTC2
C	-14	SER	-	expression tag	UNP P0DTC2
C	-13	LEU	-	expression tag	UNP P0DTC2
C	-12	LEU	-	expression tag	UNP P0DTC2
C	-11	SER	-	expression tag	UNP P0DTC2
C	-10	VAL	-	expression tag	UNP P0DTC2
C	-9	LEU	-	expression tag	UNP P0DTC2
C	-8	LEU	-	expression tag	UNP P0DTC2
C	-7	MET	-	expression tag	UNP P0DTC2
C	-6	GLY	-	expression tag	UNP P0DTC2
C	-5	CYS	-	expression tag	UNP P0DTC2
C	-4	VAL	-	expression tag	UNP P0DTC2
C	-3	ALA	-	expression tag	UNP P0DTC2
C	-2	GLU	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	expression tag	UNP P0DTC2
C	1211	ARG	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ASN	-	expression tag	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	PHE	-	expression tag	UNP P0DTC2
C	1217	GLN	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLY	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	ILE	-	expression tag	UNP P0DTC2
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	ARG	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLN	-	expression tag	UNP P0DTC2
C	1234	ALA	-	expression tag	UNP P0DTC2
C	1235	TYR	-	expression tag	UNP P0DTC2
C	1236	VAL	-	expression tag	UNP P0DTC2
C	1237	ARG	-	expression tag	UNP P0DTC2
C	1238	LYS	-	expression tag	UNP P0DTC2
C	1239	ASP	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	TRP	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	LEU	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1248	PHE	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	588	Total	C	N	O	S	0	0
			4801	3076	794	902	29		
2	E	588	Total	C	N	O	S	0	0
			4801	3076	794	902	29		
2	F	588	Total	C	N	O	S	0	0
			4801	3076	794	902	29		

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	initiating methionine	UNP Q9BYF1
D	0	GLU	-	expression tag	UNP Q9BYF1
D	1	THR	-	expression tag	UNP Q9BYF1
D	2	ASP	-	expression tag	UNP Q9BYF1
D	3	THR	-	expression tag	UNP Q9BYF1
D	4	LEU	-	expression tag	UNP Q9BYF1
D	5	LEU	-	expression tag	UNP Q9BYF1
D	6	LEU	-	expression tag	UNP Q9BYF1
D	7	TRP	-	expression tag	UNP Q9BYF1
D	8	VAL	-	expression tag	UNP Q9BYF1
D	9	LEU	-	expression tag	UNP Q9BYF1
D	10	LEU	-	expression tag	UNP Q9BYF1
D	11	LEU	-	expression tag	UNP Q9BYF1
D	12	TRP	-	expression tag	UNP Q9BYF1
D	13	VAL	-	expression tag	UNP Q9BYF1
D	14	PRO	-	expression tag	UNP Q9BYF1
D	15	GLY	-	expression tag	UNP Q9BYF1
D	16	SER	-	expression tag	UNP Q9BYF1
D	17	THR	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	18	GLY	-	expression tag	UNP Q9BYF1
D	616	ASP	-	expression tag	UNP Q9BYF1
D	617	TYR	-	expression tag	UNP Q9BYF1
D	618	LYS	-	expression tag	UNP Q9BYF1
D	619	ASP	-	expression tag	UNP Q9BYF1
D	620	ASP	-	expression tag	UNP Q9BYF1
D	621	ASP	-	expression tag	UNP Q9BYF1
D	622	ASP	-	expression tag	UNP Q9BYF1
D	623	LYS	-	expression tag	UNP Q9BYF1
D	624	TRP	-	expression tag	UNP Q9BYF1
D	625	SER	-	expression tag	UNP Q9BYF1
D	626	HIS	-	expression tag	UNP Q9BYF1
D	627	PRO	-	expression tag	UNP Q9BYF1
D	628	GLN	-	expression tag	UNP Q9BYF1
D	629	PHE	-	expression tag	UNP Q9BYF1
D	630	GLU	-	expression tag	UNP Q9BYF1
D	631	LYS	-	expression tag	UNP Q9BYF1
D	632	GLY	-	expression tag	UNP Q9BYF1
D	633	GLY	-	expression tag	UNP Q9BYF1
D	634	GLY	-	expression tag	UNP Q9BYF1
D	635	SER	-	expression tag	UNP Q9BYF1
D	636	GLY	-	expression tag	UNP Q9BYF1
D	637	GLY	-	expression tag	UNP Q9BYF1
D	638	GLY	-	expression tag	UNP Q9BYF1
D	639	SER	-	expression tag	UNP Q9BYF1
D	640	GLY	-	expression tag	UNP Q9BYF1
D	641	GLY	-	expression tag	UNP Q9BYF1
D	642	SER	-	expression tag	UNP Q9BYF1
D	643	SER	-	expression tag	UNP Q9BYF1
D	644	ALA	-	expression tag	UNP Q9BYF1
D	645	TRP	-	expression tag	UNP Q9BYF1
D	646	SER	-	expression tag	UNP Q9BYF1
D	647	HIS	-	expression tag	UNP Q9BYF1
D	648	PRO	-	expression tag	UNP Q9BYF1
D	649	GLN	-	expression tag	UNP Q9BYF1
D	650	PHE	-	expression tag	UNP Q9BYF1
D	651	GLU	-	expression tag	UNP Q9BYF1
D	652	LYS	-	expression tag	UNP Q9BYF1
E	-1	MET	-	initiating methionine	UNP Q9BYF1
E	0	GLU	-	expression tag	UNP Q9BYF1
E	1	THR	-	expression tag	UNP Q9BYF1
E	2	ASP	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	3	THR	-	expression tag	UNP Q9BYF1
E	4	LEU	-	expression tag	UNP Q9BYF1
E	5	LEU	-	expression tag	UNP Q9BYF1
E	6	LEU	-	expression tag	UNP Q9BYF1
E	7	TRP	-	expression tag	UNP Q9BYF1
E	8	VAL	-	expression tag	UNP Q9BYF1
E	9	LEU	-	expression tag	UNP Q9BYF1
E	10	LEU	-	expression tag	UNP Q9BYF1
E	11	LEU	-	expression tag	UNP Q9BYF1
E	12	TRP	-	expression tag	UNP Q9BYF1
E	13	VAL	-	expression tag	UNP Q9BYF1
E	14	PRO	-	expression tag	UNP Q9BYF1
E	15	GLY	-	expression tag	UNP Q9BYF1
E	16	SER	-	expression tag	UNP Q9BYF1
E	17	THR	-	expression tag	UNP Q9BYF1
E	18	GLY	-	expression tag	UNP Q9BYF1
E	616	ASP	-	expression tag	UNP Q9BYF1
E	617	TYR	-	expression tag	UNP Q9BYF1
E	618	LYS	-	expression tag	UNP Q9BYF1
E	619	ASP	-	expression tag	UNP Q9BYF1
E	620	ASP	-	expression tag	UNP Q9BYF1
E	621	ASP	-	expression tag	UNP Q9BYF1
E	622	ASP	-	expression tag	UNP Q9BYF1
E	623	LYS	-	expression tag	UNP Q9BYF1
E	624	TRP	-	expression tag	UNP Q9BYF1
E	625	SER	-	expression tag	UNP Q9BYF1
E	626	HIS	-	expression tag	UNP Q9BYF1
E	627	PRO	-	expression tag	UNP Q9BYF1
E	628	GLN	-	expression tag	UNP Q9BYF1
E	629	PHE	-	expression tag	UNP Q9BYF1
E	630	GLU	-	expression tag	UNP Q9BYF1
E	631	LYS	-	expression tag	UNP Q9BYF1
E	632	GLY	-	expression tag	UNP Q9BYF1
E	633	GLY	-	expression tag	UNP Q9BYF1
E	634	GLY	-	expression tag	UNP Q9BYF1
E	635	SER	-	expression tag	UNP Q9BYF1
E	636	GLY	-	expression tag	UNP Q9BYF1
E	637	GLY	-	expression tag	UNP Q9BYF1
E	638	GLY	-	expression tag	UNP Q9BYF1
E	639	SER	-	expression tag	UNP Q9BYF1
E	640	GLY	-	expression tag	UNP Q9BYF1
E	641	GLY	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	642	SER	-	expression tag	UNP Q9BYF1
E	643	SER	-	expression tag	UNP Q9BYF1
E	644	ALA	-	expression tag	UNP Q9BYF1
E	645	TRP	-	expression tag	UNP Q9BYF1
E	646	SER	-	expression tag	UNP Q9BYF1
E	647	HIS	-	expression tag	UNP Q9BYF1
E	648	PRO	-	expression tag	UNP Q9BYF1
E	649	GLN	-	expression tag	UNP Q9BYF1
E	650	PHE	-	expression tag	UNP Q9BYF1
E	651	GLU	-	expression tag	UNP Q9BYF1
E	652	LYS	-	expression tag	UNP Q9BYF1
F	-1	MET	-	initiating methionine	UNP Q9BYF1
F	0	GLU	-	expression tag	UNP Q9BYF1
F	1	THR	-	expression tag	UNP Q9BYF1
F	2	ASP	-	expression tag	UNP Q9BYF1
F	3	THR	-	expression tag	UNP Q9BYF1
F	4	LEU	-	expression tag	UNP Q9BYF1
F	5	LEU	-	expression tag	UNP Q9BYF1
F	6	LEU	-	expression tag	UNP Q9BYF1
F	7	TRP	-	expression tag	UNP Q9BYF1
F	8	VAL	-	expression tag	UNP Q9BYF1
F	9	LEU	-	expression tag	UNP Q9BYF1
F	10	LEU	-	expression tag	UNP Q9BYF1
F	11	LEU	-	expression tag	UNP Q9BYF1
F	12	TRP	-	expression tag	UNP Q9BYF1
F	13	VAL	-	expression tag	UNP Q9BYF1
F	14	PRO	-	expression tag	UNP Q9BYF1
F	15	GLY	-	expression tag	UNP Q9BYF1
F	16	SER	-	expression tag	UNP Q9BYF1
F	17	THR	-	expression tag	UNP Q9BYF1
F	18	GLY	-	expression tag	UNP Q9BYF1
F	616	ASP	-	expression tag	UNP Q9BYF1
F	617	TYR	-	expression tag	UNP Q9BYF1
F	618	LYS	-	expression tag	UNP Q9BYF1
F	619	ASP	-	expression tag	UNP Q9BYF1
F	620	ASP	-	expression tag	UNP Q9BYF1
F	621	ASP	-	expression tag	UNP Q9BYF1
F	622	ASP	-	expression tag	UNP Q9BYF1
F	623	LYS	-	expression tag	UNP Q9BYF1
F	624	TRP	-	expression tag	UNP Q9BYF1
F	625	SER	-	expression tag	UNP Q9BYF1
F	626	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	627	PRO	-	expression tag	UNP Q9BYF1
F	628	GLN	-	expression tag	UNP Q9BYF1
F	629	PHE	-	expression tag	UNP Q9BYF1
F	630	GLU	-	expression tag	UNP Q9BYF1
F	631	LYS	-	expression tag	UNP Q9BYF1
F	632	GLY	-	expression tag	UNP Q9BYF1
F	633	GLY	-	expression tag	UNP Q9BYF1
F	634	GLY	-	expression tag	UNP Q9BYF1
F	635	SER	-	expression tag	UNP Q9BYF1
F	636	GLY	-	expression tag	UNP Q9BYF1
F	637	GLY	-	expression tag	UNP Q9BYF1
F	638	GLY	-	expression tag	UNP Q9BYF1
F	639	SER	-	expression tag	UNP Q9BYF1
F	640	GLY	-	expression tag	UNP Q9BYF1
F	641	GLY	-	expression tag	UNP Q9BYF1
F	642	SER	-	expression tag	UNP Q9BYF1
F	643	SER	-	expression tag	UNP Q9BYF1
F	644	ALA	-	expression tag	UNP Q9BYF1
F	645	TRP	-	expression tag	UNP Q9BYF1
F	646	SER	-	expression tag	UNP Q9BYF1
F	647	HIS	-	expression tag	UNP Q9BYF1
F	648	PRO	-	expression tag	UNP Q9BYF1
F	649	GLN	-	expression tag	UNP Q9BYF1
F	650	PHE	-	expression tag	UNP Q9BYF1
F	651	GLU	-	expression tag	UNP Q9BYF1
F	652	LYS	-	expression tag	UNP Q9BYF1



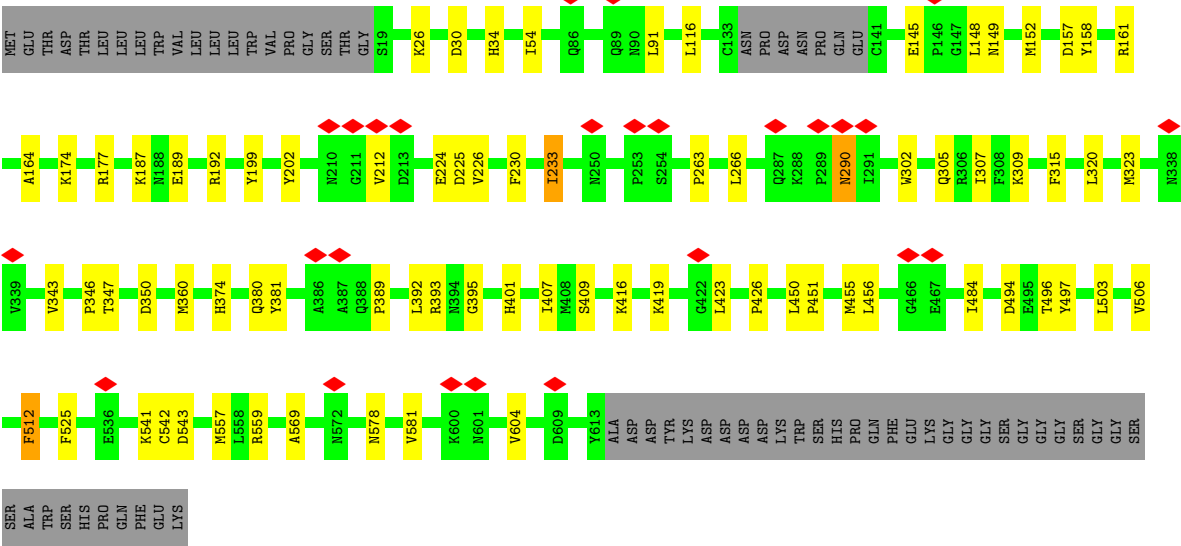
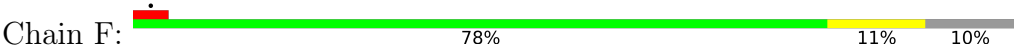






SER  
SER  
SER  
ALA  
TRP  
TRP  
SER  
HIS  
HIS  
PRO  
PRO  
GLN  
PHE  
GLU  
GLU  
LYS

● Molecule 2: Angiotensin-converting enzyme 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	8000	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 ( $e^-/\text{\AA}^2$ )	54.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.559	Depositor
Minimum map value	-0.727	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	551.936, 551.936, 551.936	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.078, 1.078, 1.078	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/8538	0.42	0/11618
1	B	0.28	0/8538	0.42	0/11618
1	C	0.28	0/8538	0.42	0/11618
2	D	0.27	0/4935	0.39	0/6701
2	E	0.27	0/4935	0.39	0/6701
2	F	0.27	0/4935	0.39	0/6701
All	All	0.27	0/40419	0.41	0/54957

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	8344	0	8136	115	0
1	B	8344	0	8136	134	0
1	C	8344	0	8136	114	0
2	D	4801	0	4589	40	0
2	E	4801	0	4589	48	0
2	F	4801	0	4589	40	0
All	All	39435	0	38175	409	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 5.

All (409) 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:E:19:SER:OG	1:B:476:GLY:HA2	1.60	1.01
2:E:27:THR:HG22	1:B:489:TYR:CD1	2.14	0.83
1:A:895:GLN:HB3	1:C:705:VAL:HG11	1.58	0.82
1:A:705:VAL:HG11	1:B:895:GLN:HB3	1.61	0.82
1:B:705:VAL:HG11	1:C:895:GLN:HB3	1.65	0.79
1:B:969:ASN:HB2	1:C:755:GLN:NE2	1.99	0.78
2:E:83:TYR:CE2	1:B:486:PHE:CZ	2.74	0.75
1:A:953:ASN:O	1:A:957:GLN:HG2	1.92	0.70
1:B:953:ASN:O	1:B:957:GLN:HG2	1.92	0.69
1:A:969:ASN:HB2	1:B:755:GLN:NE2	2.07	0.69
1:C:953:ASN:O	1:C:957:GLN:HG2	1.92	0.69
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.75	0.69
1:B:1002:GLN:HE21	1:C:1005:GLN:HG3	1.58	0.68
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.75	0.68
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.75	0.68
1:A:592:PHE:HZ	1:B:855:PHE:HE1	1.42	0.67
2:E:27:THR:CG2	1:B:489:TYR:CD1	2.77	0.67
1:B:1002:GLN:NE2	1:C:1005:GLN:HG3	2.10	0.67
1:A:329:PHE:HB3	1:A:528:LYS:HE3	1.79	0.65
1:A:895:GLN:HB3	1:C:705:VAL:CG1	2.26	0.65
1:C:329:PHE:HB3	1:C:528:LYS:HE3	1.78	0.65
1:B:329:PHE:HB3	1:B:528:LYS:HE3	1.79	0.65
1:A:1006:THR:HG21	1:B:762:GLN:NE2	2.12	0.64
1:A:1002:GLN:HG3	1:B:759:PHE:HE1	1.62	0.64
1:A:855:PHE:HE1	1:C:592:PHE:HZ	1.43	0.64
1:B:329:PHE:HE2	1:B:527:PRO:HG2	1.64	0.63
1:C:329:PHE:HE2	1:C:527:PRO:HG2	1.64	0.63
1:B:592:PHE:HZ	1:C:855:PHE:HE1	1.46	0.63
1:A:329:PHE:HE2	1:A:527:PRO:HG2	1.64	0.63
1:B:697:MET:HG3	1:C:869:MET:HE2	1.79	0.63
1:A:168:PHE:HE1	1:C:360:ASN:HD21	1.44	0.63
2:E:83:TYR:CE2	1:B:486:PHE:HZ	2.17	0.62
1:A:232:GLY:HA3	1:C:521:PRO:HD2	1.82	0.62
1:C:822:LEU:HD21	1:C:938:LEU:HD13	1.83	0.61
2:D:177:ARG:NH1	2:D:497:TYR:O	2.34	0.60
2:F:177:ARG:NH1	2:F:497:TYR:O	2.34	0.60
1:A:705:VAL:CG1	1:B:895:GLN:HB3	2.31	0.60
2:E:177:ARG:NH1	2:E:497:TYR:O	2.34	0.60
2:E:30:ASP:O	2:E:34:HIS:ND1	2.35	0.60
2:E:19:SER:OG	1:B:476:GLY:CA	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:ASP:O	2:D:34:HIS:ND1	2.35	0.59
2:F:30:ASP:O	2:F:34:HIS:ND1	2.35	0.59
1:C:129:LYS:HG2	1:C:169:GLU:HG3	1.84	0.59
1:B:822:LEU:HD21	1:B:938:LEU:HD13	1.83	0.59
1:A:822:LEU:HD21	1:A:938:LEU:HD13	1.83	0.59
2:D:323:MET:SD	2:D:380:GLN:NE2	2.76	0.59
2:D:423:LEU:HD23	2:D:423:LEU:H	1.67	0.59
2:E:323:MET:SD	2:E:380:GLN:NE2	2.76	0.59
2:E:423:LEU:H	2:E:423:LEU:HD23	1.67	0.59
1:A:869:MET:HE2	1:C:697:MET:HG3	1.84	0.59
2:F:423:LEU:HD23	2:F:423:LEU:H	1.67	0.58
1:B:129:LYS:HG2	1:B:169:GLU:HG3	1.84	0.58
2:F:323:MET:SD	2:F:380:GLN:NE2	2.76	0.58
2:E:83:TYR:HE2	1:B:486:PHE:CZ	2.22	0.58
1:A:129:LYS:HG2	1:A:169:GLU:HG3	1.84	0.58
1:A:697:MET:HG3	1:B:869:MET:HE2	1.86	0.58
2:F:389:PRO:HD2	2:F:392:LEU:HD12	1.85	0.57
2:E:389:PRO:HD2	2:E:392:LEU:HD12	1.85	0.57
1:A:855:PHE:CE1	1:C:592:PHE:HZ	2.21	0.57
2:D:389:PRO:HD2	2:D:392:LEU:HD12	1.85	0.57
1:A:379:CYS:HA	1:A:432:CYS:HA	1.87	0.57
1:C:731:MET:HB2	1:C:955:ASN:HD21	1.69	0.57
1:B:705:VAL:CG1	1:C:895:GLN:HB3	2.35	0.57
1:B:731:MET:HB2	1:B:955:ASN:HD21	1.69	0.57
2:E:189:GLU:OE1	2:E:192:ARG:NH1	2.38	0.56
1:A:855:PHE:HE1	1:C:592:PHE:CZ	2.22	0.56
1:A:731:MET:HB2	1:A:955:ASN:HD21	1.69	0.56
2:D:224:GLU:O	2:D:226:VAL:N	2.36	0.56
1:B:379:CYS:HA	1:B:432:CYS:HA	1.87	0.56
1:A:592:PHE:CZ	1:B:855:PHE:HE1	2.23	0.56
1:C:379:CYS:HA	1:C:432:CYS:HA	1.87	0.56
1:C:391:CYS:HA	1:C:525:CYS:HA	1.87	0.56
1:C:725:GLU:HB3	1:C:1062:PHE:HB2	1.88	0.56
2:D:189:GLU:OE1	2:D:192:ARG:NH1	2.38	0.56
2:F:189:GLU:OE1	2:F:192:ARG:NH1	2.38	0.56
1:B:391:CYS:HA	1:B:525:CYS:HA	1.87	0.56
1:B:697:MET:SD	1:C:869:MET:HE1	2.46	0.56
1:A:360:ASN:HD21	1:B:168:PHE:HE1	1.53	0.56
1:A:391:CYS:HA	1:A:525:CYS:HA	1.87	0.56
2:E:224:GLU:O	2:E:226:VAL:N	2.36	0.56
2:F:224:GLU:O	2:F:226:VAL:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:PHE:HB3	1:A:911:VAL:HB	1.88	0.56
1:A:981:LEU:HD21	1:A:993:ILE:HD11	1.88	0.56
2:E:290:ASN:HD22	2:E:290:ASN:H	1.53	0.56
1:C:131:CYS:HA	1:C:166:CYS:HA	1.88	0.56
1:A:42:VAL:HG13	1:C:565:PHE:HB2	1.86	0.55
1:B:906:PHE:HB3	1:B:911:VAL:HB	1.88	0.55
1:A:592:PHE:HZ	1:B:855:PHE:CE1	2.22	0.55
1:A:725:GLU:HB3	1:A:1062:PHE:HB2	1.88	0.55
1:B:68:ILE:HA	1:B:262:ALA:HA	1.88	0.55
1:C:906:PHE:HB3	1:C:911:VAL:HB	1.88	0.55
2:F:290:ASN:H	2:F:290:ASN:HD22	1.53	0.55
1:B:725:GLU:HB3	1:B:1062:PHE:HB2	1.88	0.55
1:C:68:ILE:HA	1:C:262:ALA:HA	1.88	0.55
1:B:131:CYS:HA	1:B:166:CYS:HA	1.88	0.55
2:D:290:ASN:H	2:D:290:ASN:HD22	1.53	0.55
1:B:592:PHE:CZ	1:C:855:PHE:HE1	2.23	0.55
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.89	0.54
1:A:131:CYS:HA	1:A:166:CYS:HA	1.88	0.54
1:A:780:GLU:O	1:A:784:GLN:NE2	2.41	0.54
1:B:981:LEU:HD21	1:B:993:ILE:HD11	1.88	0.54
1:C:981:LEU:HD21	1:C:993:ILE:HD11	1.88	0.54
2:E:28:PHE:HB2	1:B:489:TYR:OH	2.08	0.54
1:A:68:ILE:HA	1:A:262:ALA:HA	1.88	0.54
1:B:697:MET:SD	1:C:869:MET:CE	2.96	0.54
1:B:360:ASN:HD21	1:C:168:PHE:HE1	1.56	0.54
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.90	0.54
1:B:103:GLY:HA3	1:B:120:VAL:HA	1.90	0.54
1:A:1002:GLN:CG	1:B:759:PHE:HE1	2.21	0.53
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.89	0.53
1:C:56:LEU:HD12	1:C:57:PRO:HD2	1.89	0.53
1:B:780:GLU:O	1:B:784:GLN:NE2	2.41	0.53
2:D:116:LEU:HD11	2:D:187:LYS:HE2	1.91	0.53
2:E:174:LYS:HE3	2:E:496:THR:HB	1.90	0.53
2:E:263:PRO:HD2	2:E:266:LEU:HD12	1.91	0.53
2:F:148:LEU:HD11	2:F:164:ALA:HB1	1.91	0.53
1:C:780:GLU:O	1:C:784:GLN:NE2	2.41	0.53
1:A:457:ARG:NH2	1:A:460:ASN:O	2.42	0.53
2:D:148:LEU:HD11	2:D:164:ALA:HB1	1.91	0.53
1:B:598:ILE:HD11	1:B:611:LEU:HD22	1.90	0.53
1:A:598:ILE:HD11	1:A:611:LEU:HD22	1.90	0.53
1:C:457:ARG:NH2	1:C:460:ASN:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:ILE:HD11	1:C:611:LEU:HD22	1.90	0.53
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.91	0.53
1:B:713:ALA:HB2	1:C:895:GLN:NE2	2.24	0.53
2:F:145:GLU:HG2	2:F:149:ASN:HB2	1.92	0.52
1:B:457:ARG:NH2	1:B:460:ASN:O	2.42	0.52
2:E:148:LEU:HD11	2:E:164:ALA:HB1	1.91	0.52
1:A:755:GLN:NE2	1:C:969:ASN:HB2	2.25	0.52
2:E:116:LEU:HD11	2:E:187:LYS:HE2	1.91	0.52
1:B:1002:GLN:HG3	1:C:759:PHE:HE1	1.72	0.52
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.90	0.52
2:E:145:GLU:HG2	2:E:149:ASN:HB2	1.92	0.52
2:E:559:ARG:HB3	2:E:559:ARG:CZ	2.39	0.52
2:F:174:LYS:HE3	2:F:496:THR:HB	1.90	0.52
1:B:328:ARG:HB2	1:B:328:ARG:CZ	2.40	0.52
2:F:116:LEU:HD11	2:F:187:LYS:HE2	1.91	0.52
2:D:559:ARG:HB3	2:D:559:ARG:CZ	2.39	0.52
2:F:559:ARG:HB3	2:F:559:ARG:CZ	2.39	0.52
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.92	0.52
1:A:327:VAL:HB	1:A:528:LYS:HE2	1.93	0.51
2:D:174:LYS:HE3	2:D:496:THR:HB	1.90	0.51
1:B:1006:THR:HG21	1:C:762:GLN:NE2	2.25	0.51
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.91	0.51
1:C:89:GLY:HA2	1:C:195:LYS:HG2	1.93	0.51
2:D:145:GLU:HG2	2:D:149:ASN:HB2	1.92	0.51
2:D:263:PRO:HD2	2:D:266:LEU:HD12	1.91	0.51
2:D:290:ASN:HD22	2:D:290:ASN:N	2.08	0.51
2:F:263:PRO:HD2	2:F:266:LEU:HD12	1.91	0.51
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.91	0.51
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.92	0.51
1:C:327:VAL:HB	1:C:528:LYS:HE2	1.92	0.51
2:E:290:ASN:HD22	2:E:290:ASN:N	2.08	0.51
1:C:328:ARG:CZ	1:C:328:ARG:HB2	2.40	0.51
2:D:559:ARG:HB3	2:D:559:ARG:NH1	2.25	0.51
2:E:559:ARG:HB3	2:E:559:ARG:NH1	2.25	0.51
2:F:290:ASN:HD22	2:F:290:ASN:N	2.08	0.51
2:F:559:ARG:HB3	2:F:559:ARG:NH1	2.25	0.51
1:A:1002:GLN:NE2	1:B:1005:GLN:HG3	2.27	0.51
2:E:19:SER:CB	1:B:476:GLY:HA2	2.40	0.50
1:B:251:PRO:HD2	1:B:257:GLY:HA3	1.94	0.50
1:A:697:MET:SD	1:B:869:MET:HE1	2.52	0.50
1:C:251:PRO:HD2	1:C:257:GLY:HA3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PRO:HD2	1:A:257:GLY:HA3	1.94	0.50
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.92	0.50
1:B:89:GLY:HA2	1:B:195:LYS:HG2	1.93	0.50
1:C:276:LEU:HD22	1:C:301:CYS:HA	1.94	0.50
1:A:89:GLY:HA2	1:A:195:LYS:HG2	1.93	0.49
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.93	0.49
1:B:327:VAL:HB	1:B:528:LYS:HE2	1.92	0.49
1:B:329:PHE:CE2	1:B:527:PRO:HG2	2.47	0.49
1:A:328:ARG:HB2	1:A:328:ARG:CZ	2.40	0.49
1:A:1002:GLN:CG	1:B:759:PHE:CE1	2.95	0.49
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.93	0.49
2:D:350:ASP:OD2	2:D:393:ARG:NH2	2.46	0.49
1:B:276:LEU:HD22	1:B:301:CYS:HA	1.94	0.49
1:B:697:MET:CG	1:C:869:MET:HE2	2.42	0.49
2:E:416:LYS:O	2:E:419:LYS:NZ	2.41	0.49
1:B:521:PRO:HD2	1:C:232:GLY:HA3	1.94	0.49
1:A:565:PHE:HB2	1:B:42:VAL:HG13	1.94	0.49
2:F:91:LEU:HD13	2:F:212:VAL:HA	1.95	0.49
2:F:350:ASP:OD2	2:F:393:ARG:NH2	2.46	0.49
1:A:276:LEU:HD22	1:A:301:CYS:HA	1.94	0.49
2:D:416:LYS:O	2:D:419:LYS:NZ	2.41	0.49
2:D:91:LEU:HD13	2:D:212:VAL:HA	1.95	0.49
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.93	0.48
1:A:1005:GLN:HG3	1:C:1002:GLN:HE21	1.77	0.48
2:E:395:GLY:H	2:E:401:HIS:CE1	2.31	0.48
1:A:521:PRO:HD2	1:B:232:GLY:HA3	1.96	0.48
2:D:395:GLY:H	2:D:401:HIS:CE1	2.31	0.48
1:A:855:PHE:CE1	1:C:592:PHE:CZ	3.01	0.48
2:E:419:LYS:HB2	2:E:426:PRO:HA	1.96	0.48
1:A:329:PHE:CE2	1:A:527:PRO:HG2	2.47	0.48
2:E:350:ASP:OD2	2:E:393:ARG:NH2	2.46	0.48
2:E:91:LEU:HD13	2:E:212:VAL:HA	1.95	0.48
1:A:454:ARG:HH21	1:A:457:ARG:HG3	1.79	0.48
2:F:395:GLY:H	2:F:401:HIS:CE1	2.31	0.48
1:B:805:ILE:HB	1:B:878:LEU:HD13	1.95	0.48
1:A:822:LEU:HD13	1:A:1061:VAL:HG21	1.96	0.47
1:C:329:PHE:CE2	1:C:527:PRO:HG2	2.47	0.47
2:E:302:TRP:CE3	2:E:307:ILE:HG12	2.49	0.47
2:F:302:TRP:CE3	2:F:307:ILE:HG12	2.49	0.47
2:F:416:LYS:O	2:F:419:LYS:NZ	2.41	0.47
2:D:157:ASP:OD1	2:D:158:TYR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:157:ASP:OD1	2:E:158:TYR:N	2.48	0.47
1:A:805:ILE:HB	1:A:878:LEU:HD13	1.95	0.47
2:D:419:LYS:HB2	2:D:426:PRO:HA	1.96	0.47
2:D:557:MET:HB2	2:D:569:ALA:HB1	1.96	0.47
2:E:542:CYS:SG	2:E:543:ASP:N	2.88	0.47
1:C:822:LEU:HD13	1:C:1061:VAL:HG21	1.96	0.47
2:E:557:MET:HB2	2:E:569:ALA:HB1	1.96	0.47
1:B:452:LEU:HD23	1:B:492:LEU:HB3	1.97	0.47
1:B:985:ASP:HB2	1:B:987:PRO:HD2	1.97	0.47
1:B:1090:PRO:O	1:C:913:GLN:OE1	2.33	0.47
1:B:454:ARG:HH21	1:B:457:ARG:HG3	1.79	0.47
1:A:976:VAL:HG12	1:A:978:ASN:H	1.80	0.47
1:B:334:ASN:H	1:B:362:VAL:HG21	1.80	0.47
1:B:976:VAL:HG12	1:B:978:ASN:H	1.80	0.47
1:C:454:ARG:HH21	1:C:457:ARG:HG3	1.79	0.47
1:C:805:ILE:HB	1:C:878:LEU:HD13	1.95	0.47
2:D:302:TRP:CE3	2:D:307:ILE:HG12	2.49	0.46
2:D:542:CYS:SG	2:D:543:ASP:N	2.88	0.46
2:F:542:CYS:SG	2:F:543:ASP:N	2.88	0.46
1:A:452:LEU:HD23	1:A:492:LEU:HB3	1.97	0.46
2:F:157:ASP:OD1	2:F:158:TYR:N	2.48	0.46
2:F:557:MET:HB2	2:F:569:ALA:HB1	1.96	0.46
2:E:27:THR:HG22	1:B:489:TYR:CE1	2.49	0.46
1:C:976:VAL:HG12	1:C:978:ASN:H	1.80	0.46
1:A:1002:GLN:HE21	1:B:1005:GLN:HG3	1.79	0.46
2:F:419:LYS:HB2	2:F:426:PRO:HA	1.96	0.46
1:B:592:PHE:HZ	1:C:855:PHE:CE1	2.28	0.46
1:A:713:ALA:HB2	1:B:895:GLN:NE2	2.31	0.46
1:B:357:ARG:NH1	1:C:167:THR:O	2.49	0.46
1:C:985:ASP:HB2	1:C:987:PRO:HD2	1.97	0.46
1:C:452:LEU:HD23	1:C:492:LEU:HB3	1.97	0.46
1:A:985:ASP:HB2	1:A:987:PRO:HD2	1.97	0.46
1:B:697:MET:CG	1:C:869:MET:CE	2.94	0.46
1:C:334:ASN:H	1:C:362:VAL:HG21	1.80	0.46
2:F:455:MET:HG2	2:F:484:ILE:HD12	1.98	0.46
1:B:565:PHE:HB2	1:C:42:VAL:HG13	1.97	0.46
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.49	0.46
1:B:336:CYS:O	1:B:338:PHE:N	2.49	0.46
1:A:334:ASN:H	1:A:362:VAL:HG21	1.80	0.45
1:B:822:LEU:HD13	1:B:1061:VAL:HG21	1.96	0.45
2:D:225:ASP:OD2	2:D:578:ASN:ND2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.49	0.45
1:A:721:SER:OG	1:A:1066:THR:OG1	2.34	0.45
1:A:790:LYS:HG2	1:A:791:THR:N	2.32	0.45
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.49	0.45
2:E:225:ASP:OD2	2:E:578:ASN:ND2	2.46	0.45
2:E:455:MET:HG2	2:E:484:ILE:HD12	1.98	0.45
1:C:721:SER:OG	1:C:1066:THR:OG1	2.34	0.45
2:F:305:GLN:HE22	2:F:309:LYS:HG2	1.82	0.45
1:B:790:LYS:HG2	1:B:791:THR:N	2.32	0.45
1:C:790:LYS:HG2	1:C:791:THR:N	2.31	0.45
1:A:563:GLN:OE1	1:B:43:PHE:CA	2.65	0.45
1:B:563:GLN:OE1	1:C:43:PHE:HB2	2.16	0.45
1:A:1005:GLN:HG3	1:C:1002:GLN:NE2	2.31	0.45
2:E:305:GLN:HE22	2:E:309:LYS:HG2	1.82	0.45
2:E:346:PRO:HA	2:E:360:MET:HG2	1.99	0.45
1:A:855:PHE:CZ	1:C:588:THR:HG23	2.53	0.44
2:D:455:MET:HG2	2:D:484:ILE:HD12	1.98	0.44
1:B:126:VAL:HB	1:B:172:SER:HB3	1.99	0.44
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.99	0.44
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.99	0.44
1:A:1090:PRO:O	1:B:913:GLN:OE1	2.36	0.44
2:E:233:ILE:HB	2:E:581:VAL:HG21	1.99	0.44
1:A:1078:ALA:HB3	1:A:1095:PHE:HB2	2.00	0.44
1:B:721:SER:OG	1:B:1066:THR:OG1	2.34	0.44
1:B:743:CYS:HA	1:B:977:LEU:HD21	1.99	0.44
1:B:1142:GLN:O	1:B:1142:GLN:NE2	2.51	0.44
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.99	0.44
1:A:375:SER:H	1:A:436:TRP:HA	1.83	0.44
1:A:592:PHE:CZ	1:B:855:PHE:CE1	3.03	0.44
1:A:1142:GLN:O	1:A:1142:GLN:NE2	2.51	0.44
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.99	0.44
1:C:1078:ALA:HB3	1:C:1095:PHE:HB2	2.00	0.44
1:A:336:CYS:O	1:A:338:PHE:N	2.49	0.44
1:A:983:ARG:HG3	1:A:984:LEU:HG	1.99	0.44
1:B:328:ARG:HB3	1:B:543:PHE:HD1	1.82	0.44
1:A:328:ARG:HB3	1:A:543:PHE:HD1	1.82	0.44
2:F:233:ILE:HB	2:F:581:VAL:HG21	1.99	0.44
1:B:983:ARG:HG3	1:B:984:LEU:HG	1.99	0.44
1:A:43:PHE:CA	1:C:563:GLN:OE1	2.66	0.44
1:A:126:VAL:HB	1:A:172:SER:HB3	1.99	0.44
2:F:346:PRO:HA	2:F:360:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:SER:H	1:B:436:TRP:HA	1.83	0.44
1:B:1002:GLN:CG	1:C:759:PHE:HE1	2.31	0.44
1:C:743:CYS:HA	1:C:977:LEU:HD21	1.99	0.44
1:C:1142:GLN:NE2	1:C:1142:GLN:O	2.51	0.44
1:A:697:MET:SD	1:B:869:MET:CE	3.06	0.44
1:B:1078:ALA:HB3	1:B:1095:PHE:HB2	2.00	0.44
1:C:328:ARG:HB3	1:C:543:PHE:HD1	1.82	0.44
1:C:478:THR:HB	1:C:487:ASN:HB2	2.00	0.44
1:C:336:CYS:O	1:C:338:PHE:N	2.49	0.43
1:A:743:CYS:HA	1:A:977:LEU:HD21	1.99	0.43
1:A:869:MET:CE	1:C:697:MET:CG	2.97	0.43
1:C:375:SER:H	1:C:436:TRP:HA	1.83	0.43
1:A:418:ILE:HG23	1:A:422:ASN:HD22	1.84	0.43
1:A:869:MET:HE1	1:C:697:MET:SD	2.58	0.43
2:D:233:ILE:HB	2:D:581:VAL:HG21	1.99	0.43
2:D:305:GLN:HE22	2:D:309:LYS:HG2	1.82	0.43
2:D:503:LEU:HD23	2:D:506:VAL:HG23	2.00	0.43
1:A:328:ARG:NH2	1:A:532:ASN:O	2.52	0.43
1:A:410:ILE:HG23	1:A:425:LEU:HD11	2.01	0.43
2:E:374:HIS:HB2	2:E:409:SER:HB2	2.00	0.43
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.99	0.43
1:C:328:ARG:NH2	1:C:532:ASN:O	2.52	0.43
1:C:418:ILE:HG23	1:C:422:ASN:HD22	1.84	0.43
2:D:346:PRO:HA	2:D:360:MET:HG2	1.99	0.43
1:A:1143:PRO:C	1:A:1145:LEU:H	2.22	0.43
2:D:407:ILE:HG21	2:D:525:PHE:HB2	2.00	0.43
1:B:328:ARG:NH2	1:B:532:ASN:O	2.52	0.43
1:B:410:ILE:HG23	1:B:425:LEU:HD11	2.01	0.43
1:C:85:PRO:HA	1:C:237:ARG:HG2	2.01	0.43
1:C:126:VAL:HB	1:C:172:SER:HB3	1.99	0.43
1:C:983:ARG:HG3	1:C:984:LEU:HG	1.99	0.43
1:B:1143:PRO:C	1:B:1145:LEU:H	2.22	0.43
1:A:478:THR:HB	1:A:487:ASN:HB2	2.00	0.43
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.99	0.43
2:E:407:ILE:HG21	2:E:525:PHE:HB2	2.00	0.43
2:E:450:LEU:HB3	2:E:451:PRO:HD3	2.01	0.43
1:B:119:ILE:HG12	1:B:128:ILE:HG23	2.01	0.43
1:B:478:THR:HB	1:B:487:ASN:HB2	2.00	0.43
1:C:647:ALA:HB2	1:C:668:ALA:HB3	2.01	0.43
1:C:1143:PRO:C	1:C:1145:LEU:H	2.22	0.43
2:F:503:LEU:HD23	2:F:506:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PRO:HA	1:B:237:ARG:HG2	2.01	0.42
1:A:125:ASN:HA	1:A:174:PRO:HA	2.00	0.42
1:A:707:TYR:CE2	1:B:796:ASP:O	2.73	0.42
1:A:1056:ALA:HB2	1:A:1061:VAL:HG23	2.00	0.42
2:D:152:MET:O	2:D:161:ARG:NH2	2.52	0.42
2:E:503:LEU:HD23	2:E:506:VAL:HG23	2.00	0.42
1:B:647:ALA:HB2	1:B:668:ALA:HB3	2.01	0.42
1:B:920:GLN:HE21	1:B:920:GLN:HB3	1.67	0.42
1:C:410:ILE:HG23	1:C:425:LEU:HD11	2.01	0.42
1:A:647:ALA:HB2	1:A:668:ALA:HB3	2.01	0.42
2:D:374:HIS:HB2	2:D:409:SER:HB2	2.00	0.42
2:D:450:LEU:HB3	2:D:451:PRO:HD3	2.01	0.42
2:F:407:ILE:HG21	2:F:525:PHE:HB2	2.00	0.42
1:A:490:PHE:CE1	1:A:492:LEU:HB2	2.55	0.42
2:F:152:MET:O	2:F:161:ARG:NH2	2.52	0.42
1:C:920:GLN:HE21	1:C:920:GLN:HB3	1.67	0.42
1:C:1107:ARG:H	1:C:1107:ARG:HD3	1.85	0.42
1:A:85:PRO:HA	1:A:237:ARG:HG2	2.01	0.42
2:F:374:HIS:HB2	2:F:409:SER:HB2	2.00	0.42
1:B:125:ASN:HA	1:B:174:PRO:HA	2.00	0.42
1:B:717:ASN:HB3	1:B:1071:GLN:H	1.85	0.42
1:B:1002:GLN:CG	1:C:759:PHE:CE1	3.02	0.42
1:C:125:ASN:HA	1:C:174:PRO:HA	2.00	0.42
1:C:490:PHE:CE1	1:C:492:LEU:HB2	2.55	0.42
1:A:259:THR:HG22	1:A:261:GLY:H	1.84	0.42
1:A:330:PRO:HG3	1:A:528:LYS:O	2.20	0.42
1:A:717:ASN:HB3	1:A:1071:GLN:H	1.85	0.42
2:F:450:LEU:HB3	2:F:451:PRO:HD3	2.01	0.42
1:B:490:PHE:CE1	1:B:492:LEU:HB2	2.55	0.42
1:B:1056:ALA:HB2	1:B:1061:VAL:HG23	2.00	0.42
1:C:717:ASN:HB3	1:C:1071:GLN:H	1.85	0.42
2:D:423:LEU:HD23	2:D:423:LEU:N	2.34	0.42
1:B:330:PRO:HG3	1:B:528:LYS:O	2.20	0.42
1:B:592:PHE:CZ	1:C:855:PHE:CE1	3.06	0.42
1:B:718:PHE:HA	1:B:1069:PRO:HA	2.02	0.42
1:B:1107:ARG:H	1:B:1107:ARG:HD3	1.85	0.42
1:C:718:PHE:HA	1:C:1069:PRO:HA	2.02	0.42
1:C:1056:ALA:HB2	1:C:1061:VAL:HG23	2.00	0.42
1:A:43:PHE:HB2	1:C:563:GLN:OE1	2.19	0.42
1:A:697:MET:CG	1:B:869:MET:CE	2.98	0.42
2:E:152:MET:O	2:E:161:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:423:LEU:HD23	2:F:423:LEU:N	2.34	0.42
1:A:561:PRO:HA	1:A:577:ARG:HH12	1.85	0.41
1:B:329:PHE:HE2	1:B:527:PRO:CG	2.32	0.41
2:E:54:ILE:HD11	2:E:343:VAL:HG13	2.02	0.41
2:F:54:ILE:HD11	2:F:343:VAL:HG13	2.02	0.41
1:B:259:THR:HG22	1:B:261:GLY:H	1.84	0.41
1:B:418:ILE:HG23	1:B:422:ASN:HD22	1.84	0.41
1:C:119:ILE:HG12	1:C:128:ILE:HG23	2.01	0.41
1:C:259:THR:HG22	1:C:261:GLY:H	1.84	0.41
1:C:561:PRO:HA	1:C:577:ARG:HH12	1.85	0.41
1:A:718:PHE:HA	1:A:1069:PRO:HA	2.02	0.41
2:F:225:ASP:OD2	2:F:578:ASN:ND2	2.46	0.41
1:B:561:PRO:HA	1:B:577:ARG:HH12	1.85	0.41
1:C:330:PRO:HG3	1:C:528:LYS:O	2.20	0.41
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.52	0.41
1:A:1107:ARG:HD3	1:A:1107:ARG:H	1.85	0.41
2:F:315:PHE:HD2	2:F:320:LEU:HD12	1.85	0.41
1:A:345:THR:HA	1:A:509:ARG:HH12	1.86	0.41
1:A:119:ILE:HG12	1:A:128:ILE:HG23	2.01	0.41
1:A:563:GLN:OE1	1:B:43:PHE:HB2	2.20	0.41
2:E:27:THR:CG2	1:B:489:TYR:CE1	3.03	0.41
2:E:315:PHE:HD2	2:E:320:LEU:HD12	1.85	0.41
1:A:689:SER:OG	1:A:690:GLN:N	2.52	0.41
1:B:1033:VAL:HA	1:B:1051:SER:HB2	2.03	0.41
1:A:913:GLN:OE1	1:C:1090:PRO:O	2.38	0.41
2:D:54:ILE:HD11	2:D:343:VAL:HG13	2.02	0.41
2:D:315:PHE:HD2	2:D:320:LEU:HD12	1.85	0.41
2:F:230:PHE:HA	2:F:233:ILE:HG22	2.03	0.41
1:B:689:SER:OG	1:B:690:GLN:N	2.52	0.41
1:B:707:TYR:CE2	1:C:796:ASP:O	2.74	0.41
1:C:344:ALA:O	1:C:509:ARG:NH1	2.52	0.41
2:F:456:LEU:HD23	2:F:512:PHE:HD1	1.86	0.40
1:A:1033:VAL:HA	1:A:1051:SER:HB2	2.03	0.40
1:B:344:ALA:O	1:B:509:ARG:NH1	2.52	0.40
1:A:869:MET:CE	1:C:697:MET:SD	3.09	0.40
2:D:456:LEU:HD23	2:D:512:PHE:HD1	1.86	0.40
1:B:345:THR:HA	1:B:509:ARG:HH12	1.86	0.40
1:A:152:TRP:CD1	1:A:180:GLU:HG2	2.56	0.40
1:C:188:ASN:HA	1:C:209:PRO:HA	2.04	0.40
2:D:239:HIS:O	2:D:599:ASN:ND2	2.55	0.40
1:B:792:PRO:HA	1:B:793:PRO:HD3	1.99	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	1054/1287 (82%)	942 (89%)	110 (10%)	2 (0%)	44	78
1	B	1054/1287 (82%)	942 (89%)	110 (10%)	2 (0%)	44	78
1	C	1054/1287 (82%)	942 (89%)	110 (10%)	2 (0%)	44	78
2	D	584/654 (89%)	536 (92%)	48 (8%)	0	100	100
2	E	584/654 (89%)	536 (92%)	48 (8%)	0	100	100
2	F	584/654 (89%)	536 (92%)	48 (8%)	0	100	100
All	All	4914/5823 (84%)	4434 (90%)	474 (10%)	6 (0%)	50	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	PRO
1	B	527	PRO
1	C	527	PRO
1	A	330	PRO
1	B	330	PRO
1	C	330	PRO

### 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	932/1116 (84%)	923 (99%)	9 (1%)	73	81
1	B	932/1116 (84%)	923 (99%)	9 (1%)	73	81
1	C	932/1116 (84%)	923 (99%)	9 (1%)	73	81
2	D	519/573 (91%)	508 (98%)	11 (2%)	48	66
2	E	519/573 (91%)	508 (98%)	11 (2%)	48	66
2	F	519/573 (91%)	508 (98%)	11 (2%)	48	66
All	All	4353/5067 (86%)	4293 (99%)	60 (1%)	62	76

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	97	LYS
1	A	145	TYR
1	A	387	LEU
1	A	787	GLN
1	A	920	GLN
1	A	977	LEU
1	A	1107	ARG
1	A	1110	TYR
2	D	26	LYS
2	D	199	TYR
2	D	202	TYR
2	D	233	ILE
2	D	290	ASN
2	D	347	THR
2	D	381	TYR
2	D	494	ASP
2	D	512	PHE
2	D	541	LYS
2	D	604	VAL
2	E	26	LYS
2	E	199	TYR
2	E	202	TYR
2	E	233	ILE
2	E	290	ASN
2	E	347	THR
2	E	381	TYR
2	E	494	ASP
2	E	512	PHE
2	E	541	LYS

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Mol	Chain	Res	Type
2	E	604	VAL
2	F	26	LYS
2	F	199	TYR
2	F	202	TYR
2	F	233	ILE
2	F	290	ASN
2	F	347	THR
2	F	381	TYR
2	F	494	ASP
2	F	512	PHE
2	F	541	LYS
2	F	604	VAL
1	B	21	ARG
1	B	97	LYS
1	B	145	TYR
1	B	387	LEU
1	B	787	GLN
1	B	920	GLN
1	B	977	LEU
1	B	1107	ARG
1	B	1110	TYR
1	C	21	ARG
1	C	97	LYS
1	C	145	TYR
1	C	387	LEU
1	C	787	GLN
1	C	920	GLN
1	C	977	LEU
1	C	1107	ARG
1	C	1110	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	52	GLN
1	A	69	HIS
1	A	271	GLN
1	A	321	GLN
1	A	409	GLN
1	A	448	ASN
1	A	450	ASN

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Mol	Chain	Res	Type
1	A	544	ASN
1	A	675	GLN
1	A	690	GLN
1	A	755	GLN
1	A	787	GLN
1	A	804	GLN
1	A	920	GLN
1	A	926	GLN
1	A	935	GLN
1	A	992	GLN
1	A	1002	GLN
1	A	1064	HIS
1	A	1134	ASN
1	A	1142	GLN
2	D	58	ASN
2	D	60	GLN
2	D	86	GLN
2	D	96	GLN
2	D	98	GLN
2	D	101	GLN
2	D	102	GLN
2	D	175	GLN
2	D	194	ASN
2	D	221	GLN
2	D	290	ASN
2	D	305	GLN
2	D	325	GLN
2	D	378	HIS
2	D	388	GLN
2	D	437	ASN
2	D	598	GLN
2	E	58	ASN
2	E	60	GLN
2	E	86	GLN
2	E	96	GLN
2	E	98	GLN
2	E	101	GLN
2	E	102	GLN
2	E	175	GLN
2	E	194	ASN
2	E	221	GLN
2	E	290	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
2	E	305	GLN
2	E	325	GLN
2	E	378	HIS
2	E	388	GLN
2	E	437	ASN
2	E	598	GLN
2	F	58	ASN
2	F	60	GLN
2	F	86	GLN
2	F	96	GLN
2	F	98	GLN
2	F	101	GLN
2	F	102	GLN
2	F	175	GLN
2	F	194	ASN
2	F	221	GLN
2	F	290	ASN
2	F	305	GLN
2	F	325	GLN
2	F	378	HIS
2	F	388	GLN
2	F	437	ASN
2	F	598	GLN
1	B	14	GLN
1	B	52	GLN
1	B	69	HIS
1	B	271	GLN
1	B	321	GLN
1	B	409	GLN
1	B	448	ASN
1	B	450	ASN
1	B	493	GLN
1	B	544	ASN
1	B	675	GLN
1	B	690	GLN
1	B	755	GLN
1	B	762	GLN
1	B	787	GLN
1	B	804	GLN
1	B	920	GLN
1	B	926	GLN
1	B	935	GLN

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Mol	Chain	Res	Type
1	B	992	GLN
1	B	1002	GLN
1	B	1064	HIS
1	B	1134	ASN
1	B	1142	GLN
1	C	14	GLN
1	C	52	GLN
1	C	69	HIS
1	C	271	GLN
1	C	321	GLN
1	C	409	GLN
1	C	448	ASN
1	C	450	ASN
1	C	544	ASN
1	C	675	GLN
1	C	690	GLN
1	C	755	GLN
1	C	787	GLN
1	C	804	GLN
1	C	920	GLN
1	C	926	GLN
1	C	935	GLN
1	C	992	GLN
1	C	1002	GLN
1	C	1064	HIS
1	C	1134	ASN
1	C	1142	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



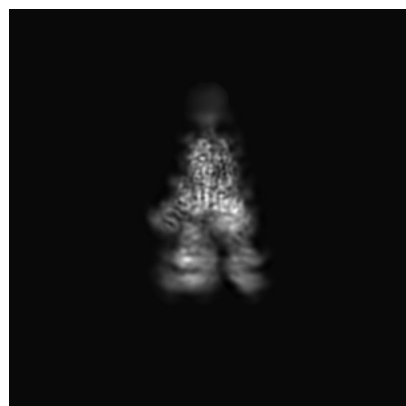
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11688. These allow visual inspection of the internal detail of the map and identification of artifacts.

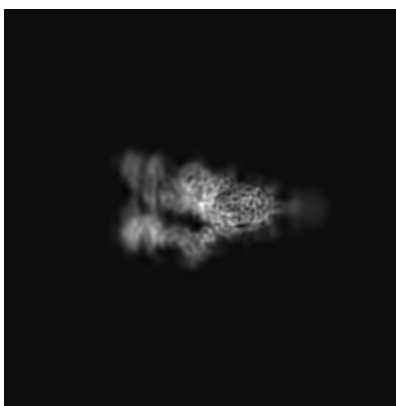
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

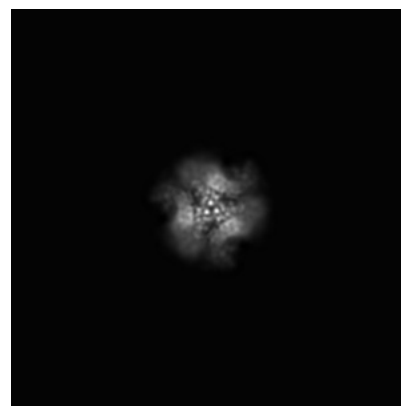
#### 6.1.1 Primary map



X

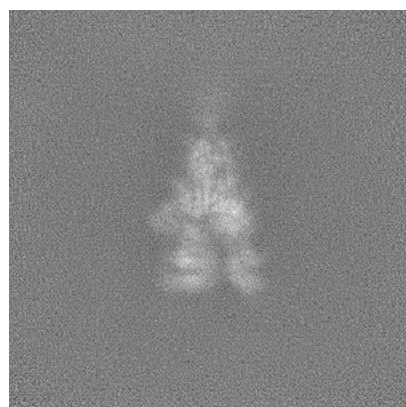


Y

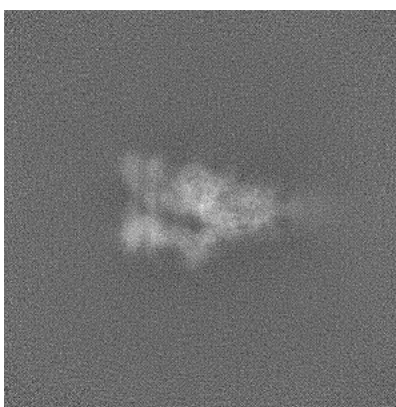


Z

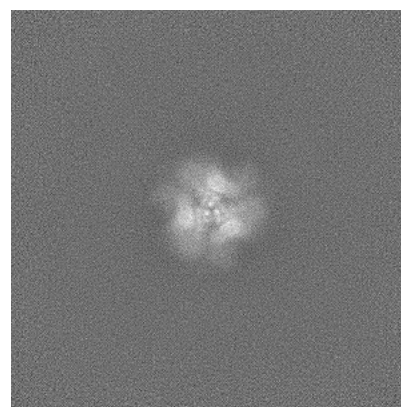
#### 6.1.2 Raw map



X



Y

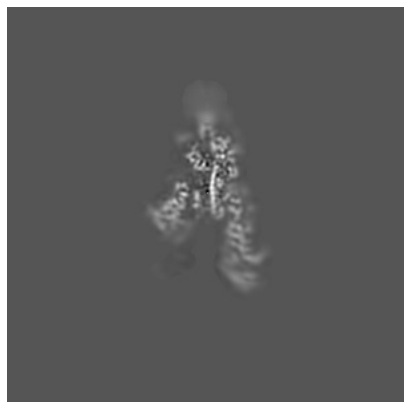


Z

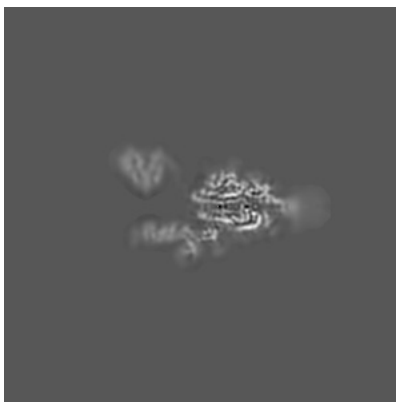
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

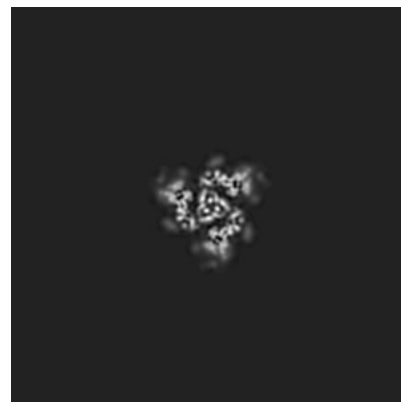
### 6.2.1 Primary map



X Index: 256

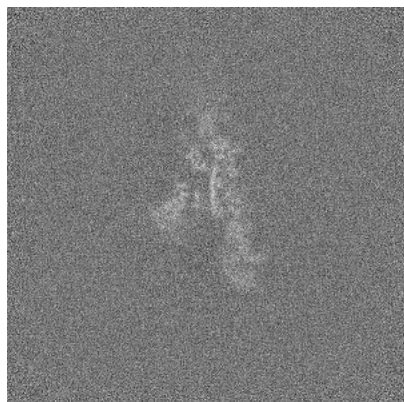


Y Index: 256

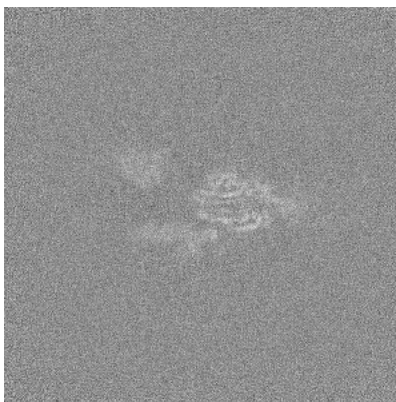


Z Index: 256

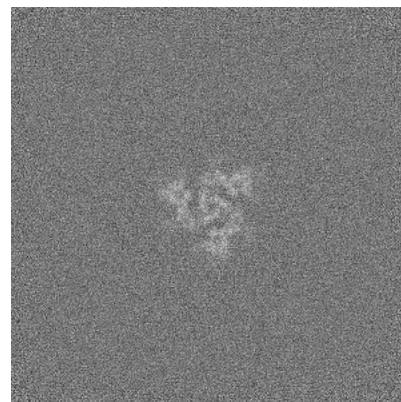
### 6.2.2 Raw map



X Index: 256



Y Index: 256

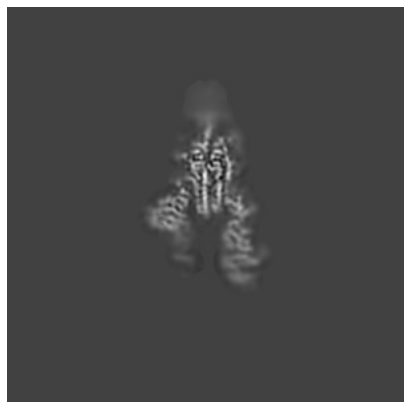


Z Index: 256

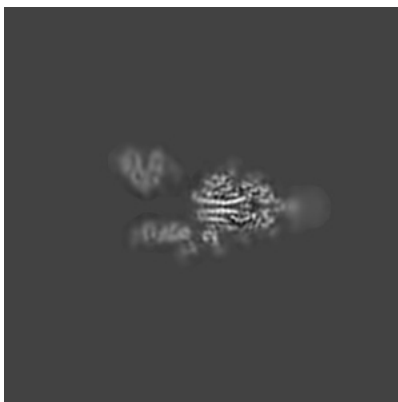
The images above show central slices of the map in three orthogonal directions.

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

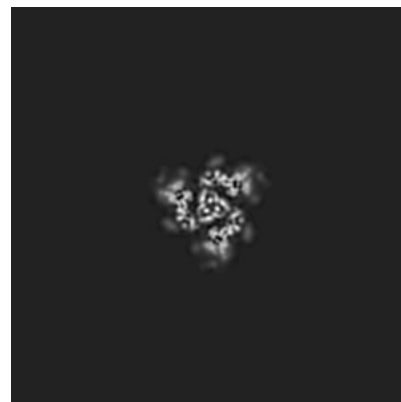
### 6.3.1 Primary map



X Index: 263

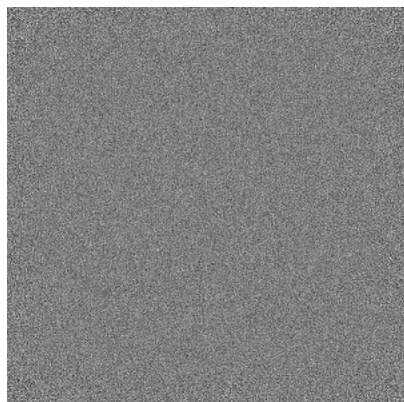


Y Index: 253

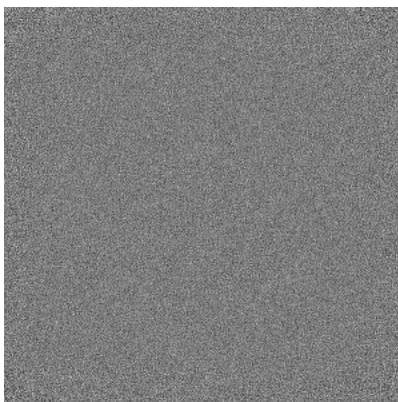


Z Index: 256

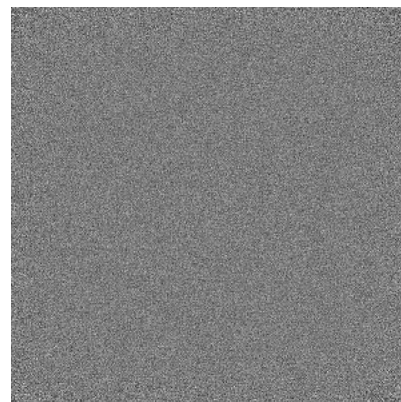
### 6.3.2 Raw map



X Index: 0



Y Index: 0

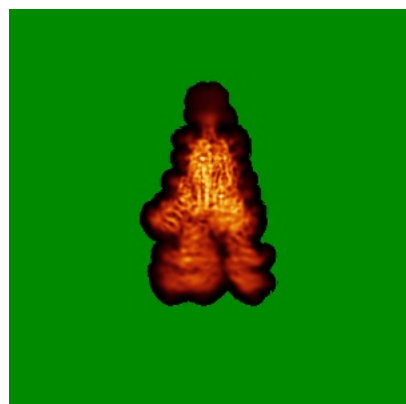


Z Index: 0

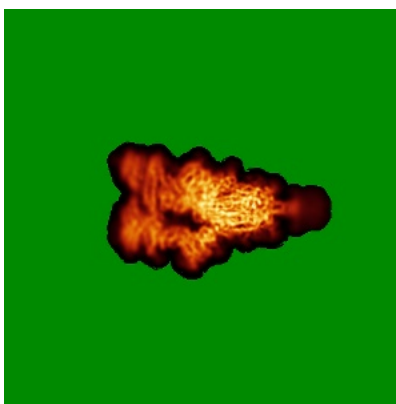
The images above show the largest variance slices of the map in three orthogonal directions.

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

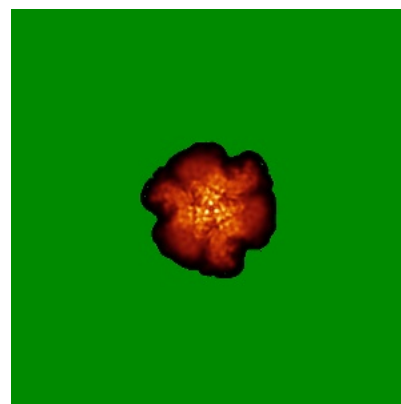
### 6.4.1 Primary map



X

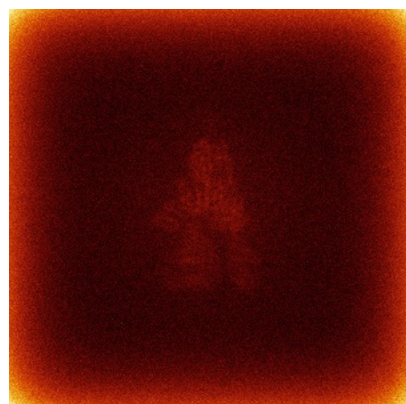


Y

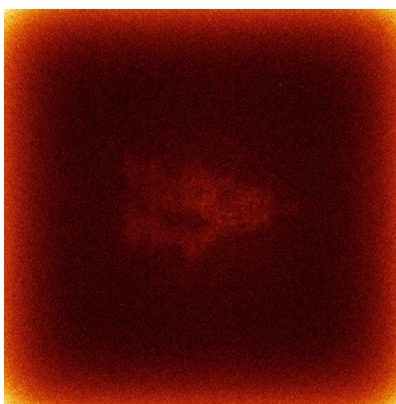


Z

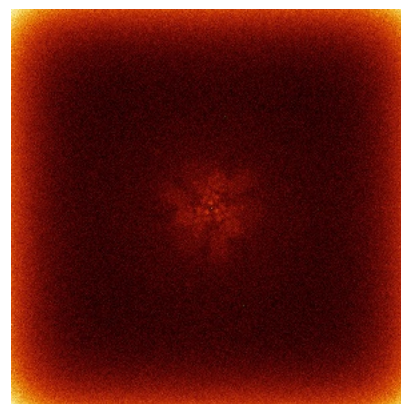
### 6.4.2 Raw map



X



Y



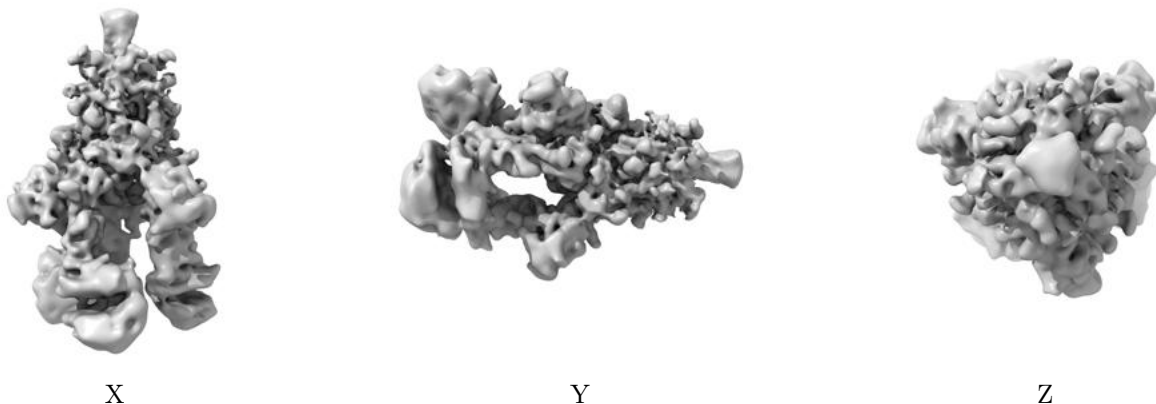
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



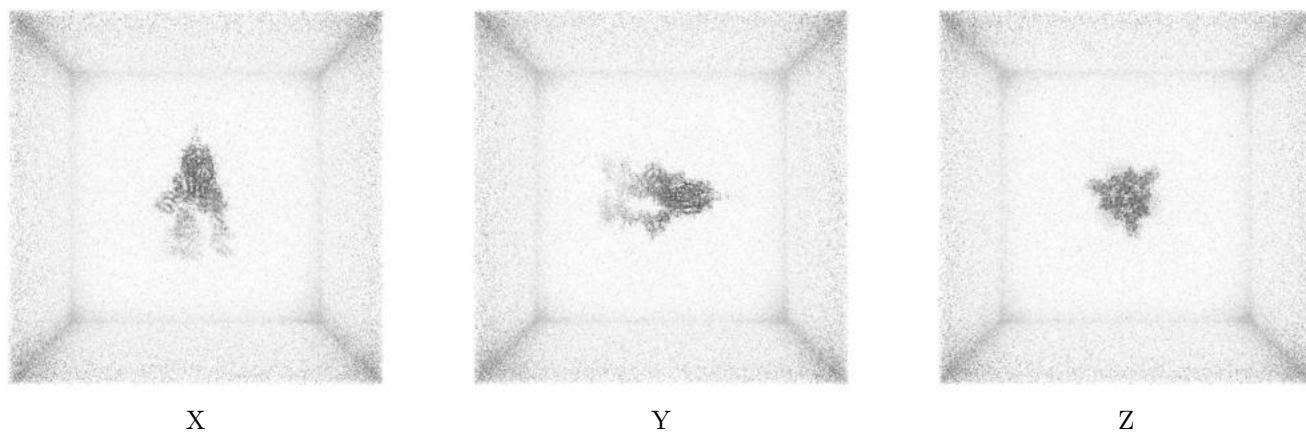
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

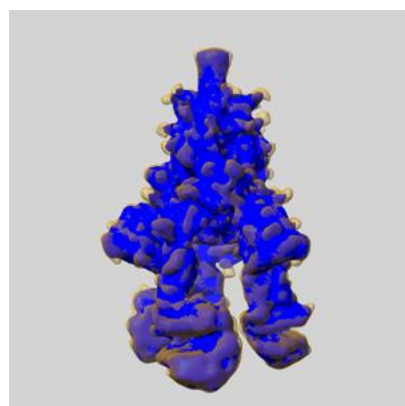
## 6.6 Mask visualisation [i](#)

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

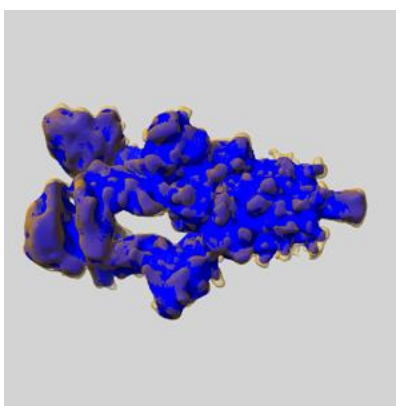
A mask typically either:

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

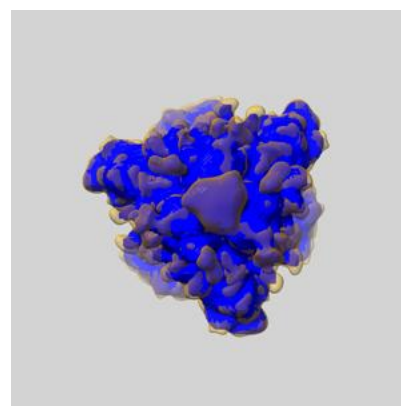
### 6.6.1 emd\_11688\_msk\_1.map [i](#)



X



Y

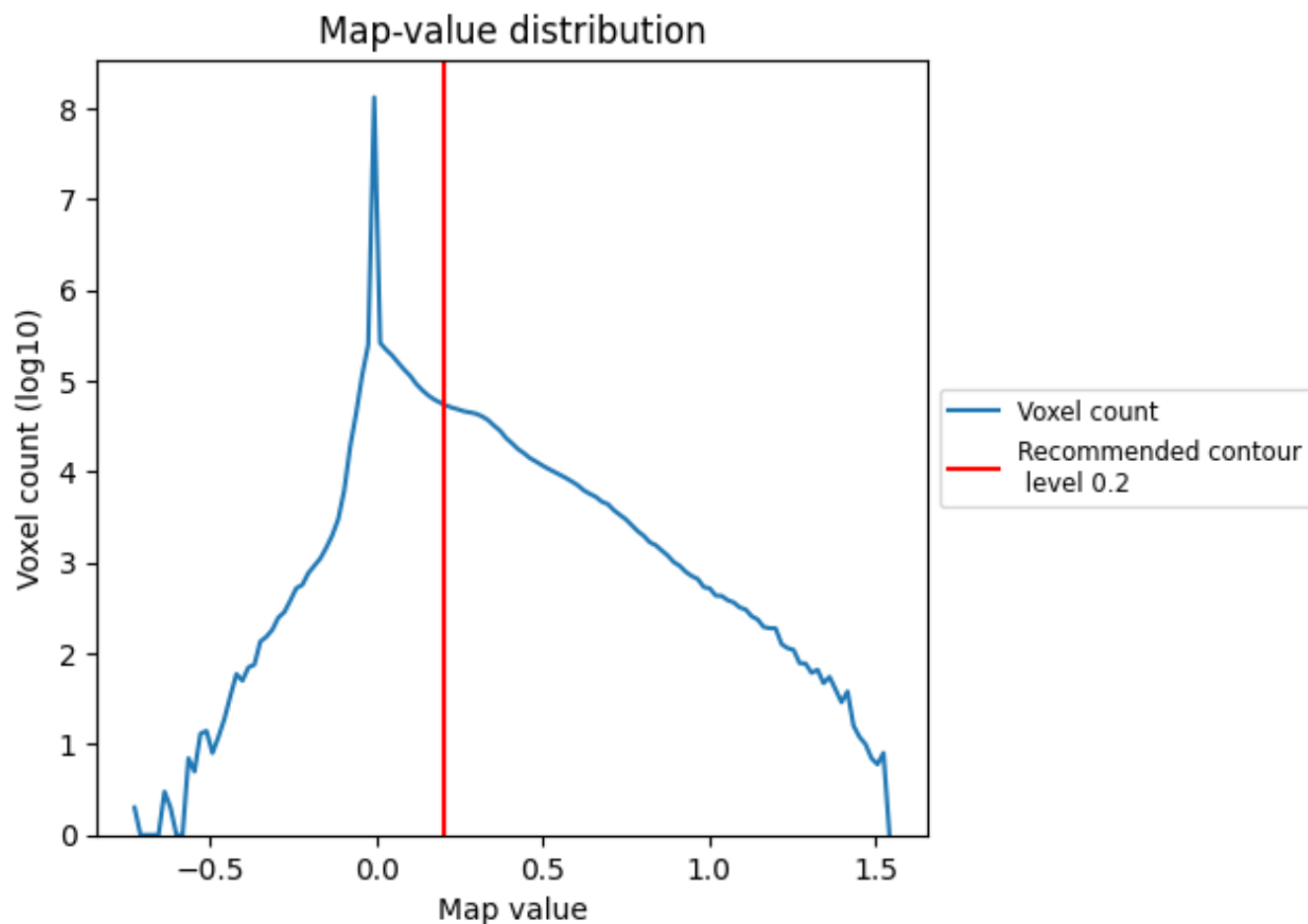


Z

## 7 Map analysis [i](#)

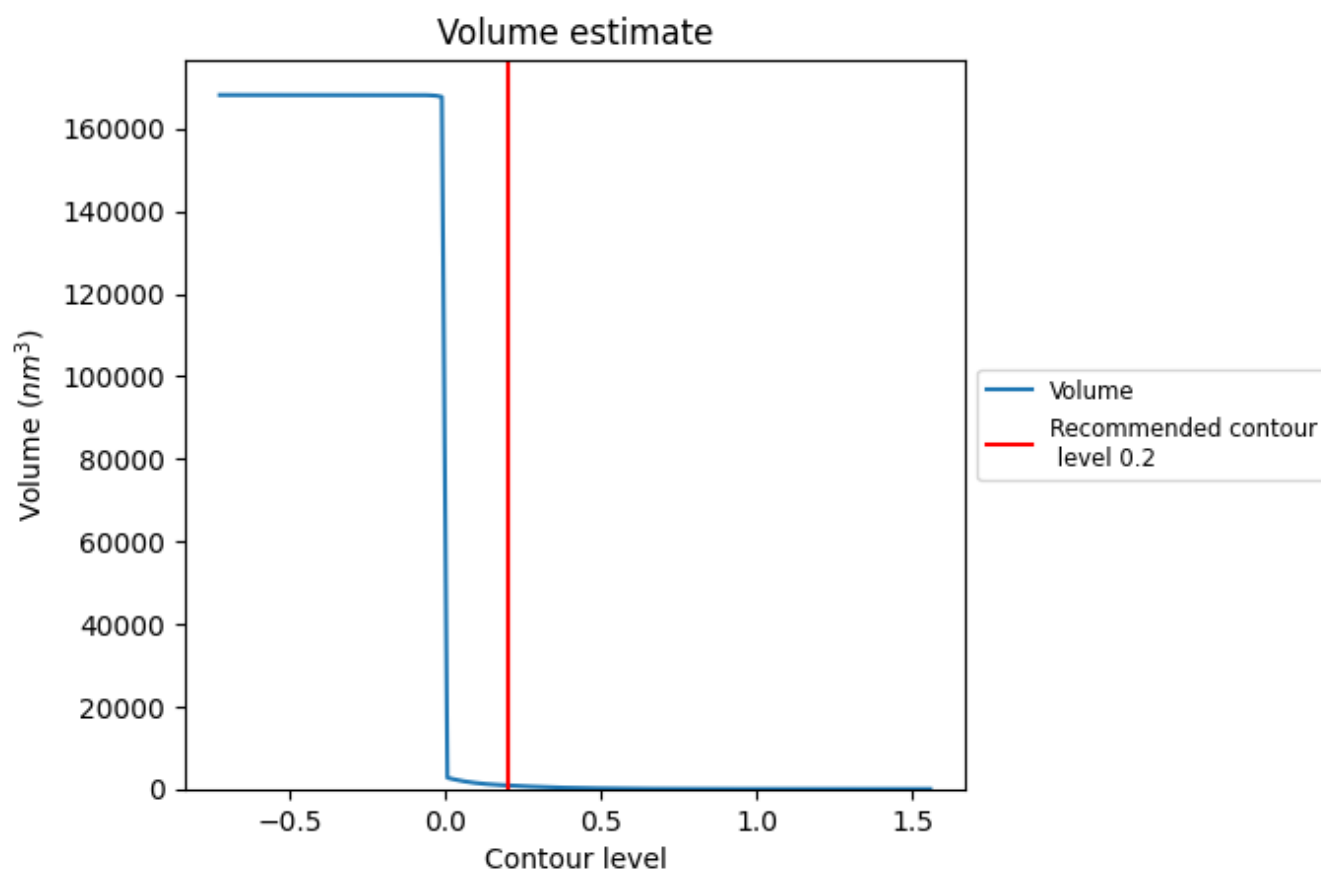
This section contains the results of statistical analysis of the map.

### 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](#)

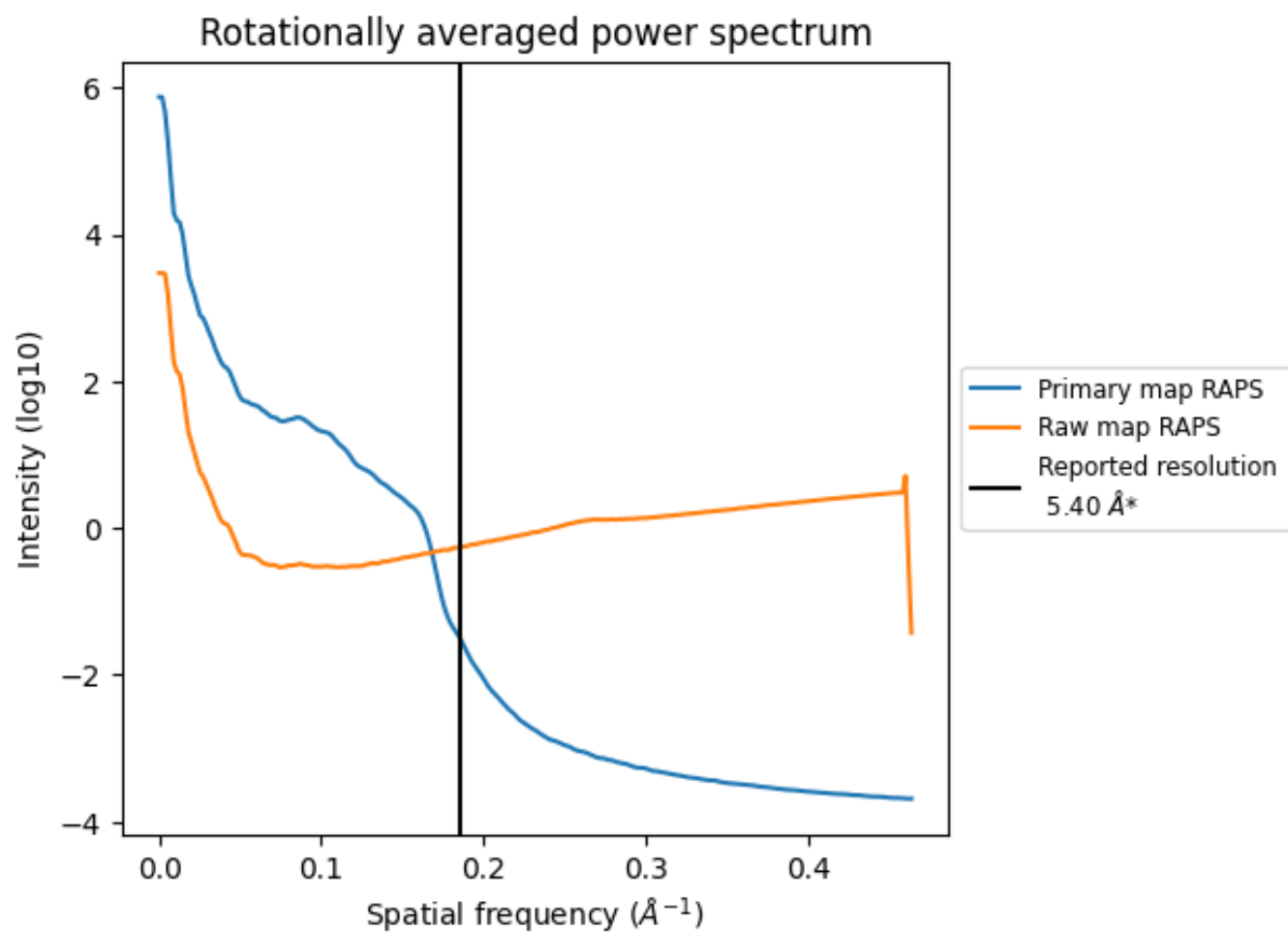


The volume at the recommended contour level is 852 nm<sup>3</sup>; this corresponds to an approximate mass of 770 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

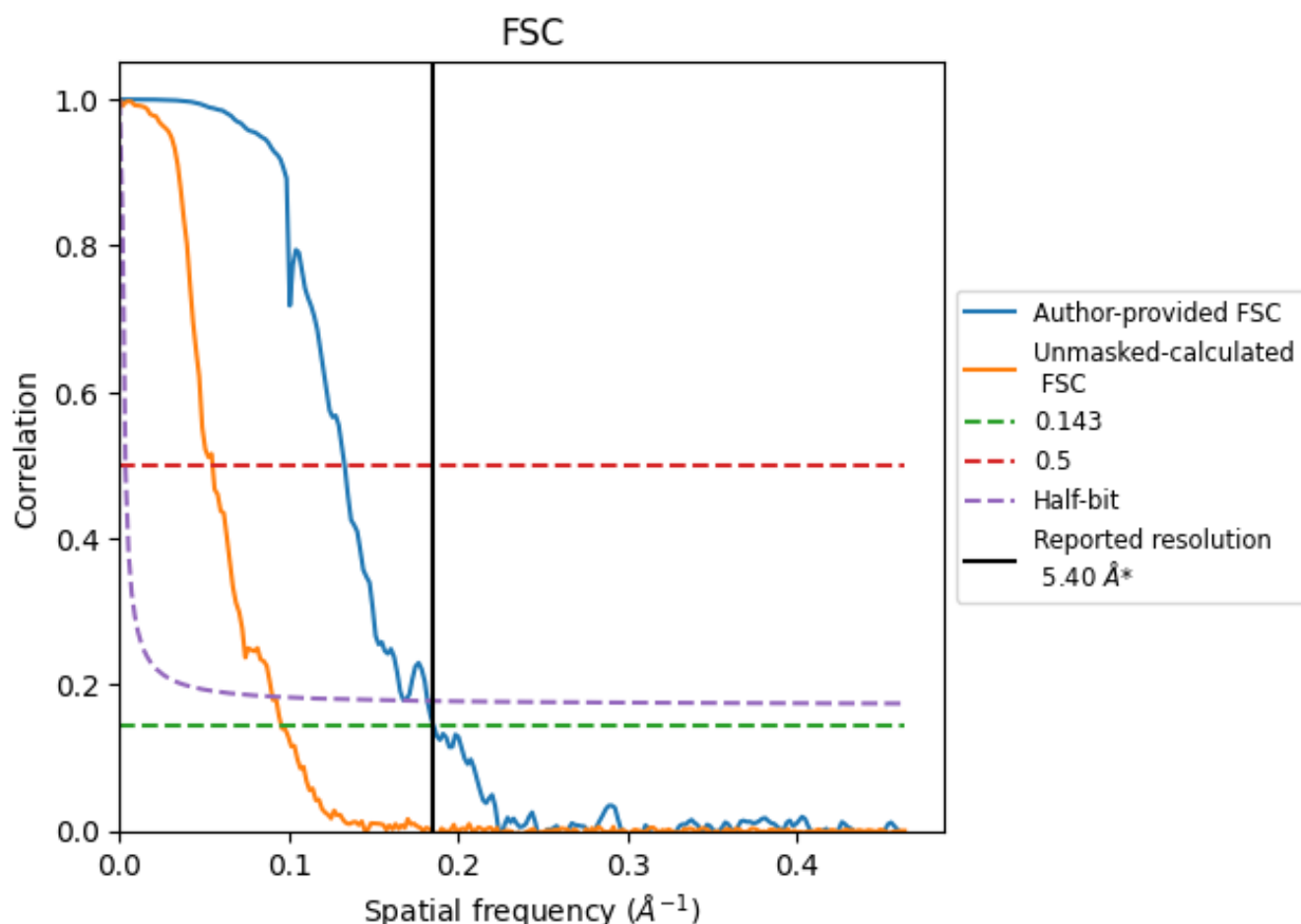


\*Reported resolution corresponds to spatial frequency of 0.185  $\text{\AA}^{-1}$

## 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 0.185 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

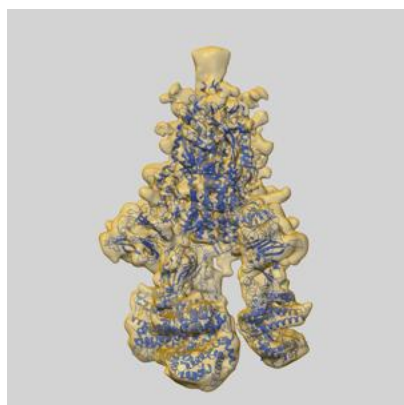
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	5.39	7.52	5.50
Unmasked-calculated*	10.45	18.21	11.07

\*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 10.45 differs from the reported value 5.4 by more than 10 %

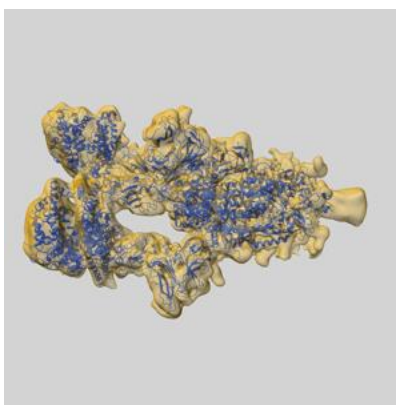
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11688 and PDB model 7A98. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

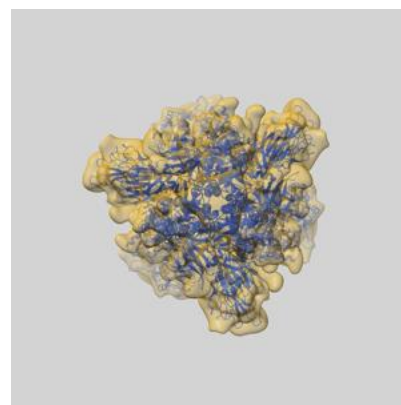
### 9.1 Map-model overlay [i](#)



X



Y



Z

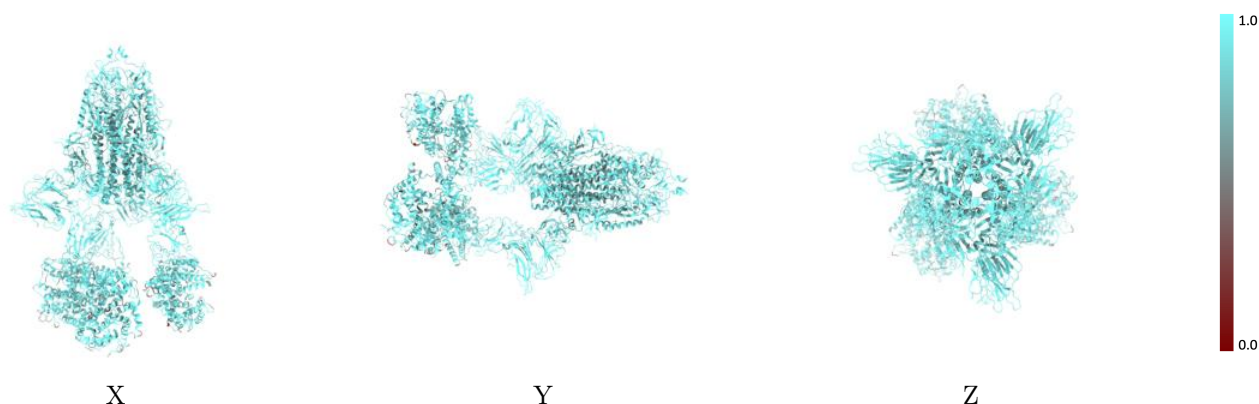
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



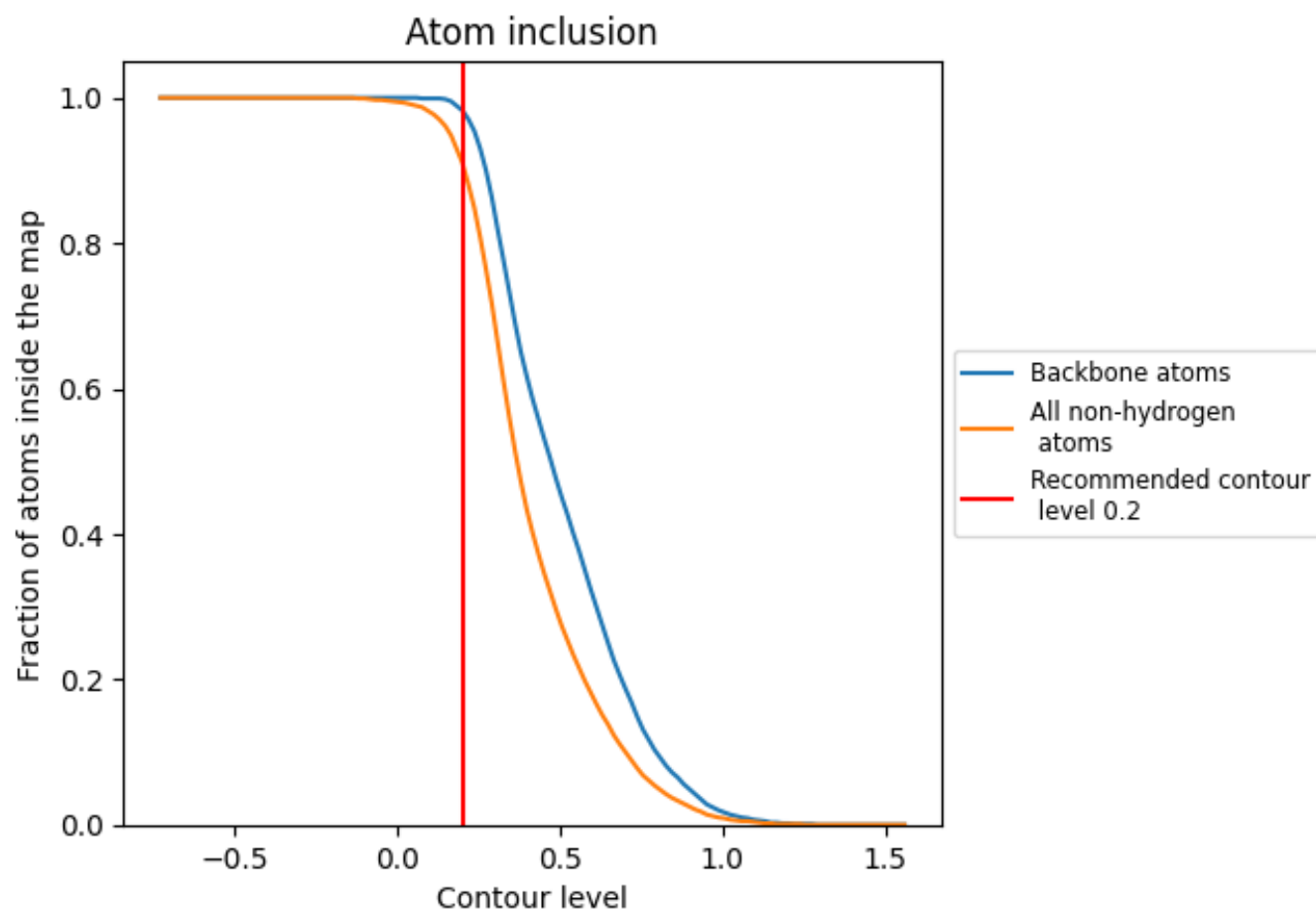
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9110</div>	<div><div></div>0.1490</div>
A	<div><div></div>0.9240</div>	<div><div></div>0.1740</div>
B	<div><div></div>0.9230</div>	<div><div></div>0.1740</div>
C	<div><div></div>0.9230</div>	<div><div></div>0.1730</div>
D	<div><div></div>0.8880</div>	<div><div></div>0.1050</div>
E	<div><div></div>0.8880</div>	<div><div></div>0.1050</div>
F	<div><div></div>0.8890</div>	<div><div></div>0.1060</div>

1.0

0.0

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