



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:10 PM UTC

PDB ID : 7YCZ / pdb_00007ycz
EMDB ID : EMD-33743
Title : SARS-CoV-2 Omicron 2-RBD up Spike trimer complexed with three XG005 molecules
Authors : Zhan, W.Q.; Zhang, X.; Chen, Z.G.; Sun, L.
Deposited on : 2022-07-02
Resolution : 3.24 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

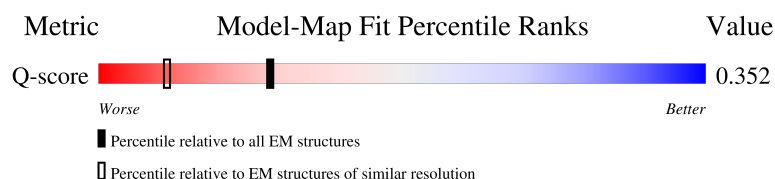
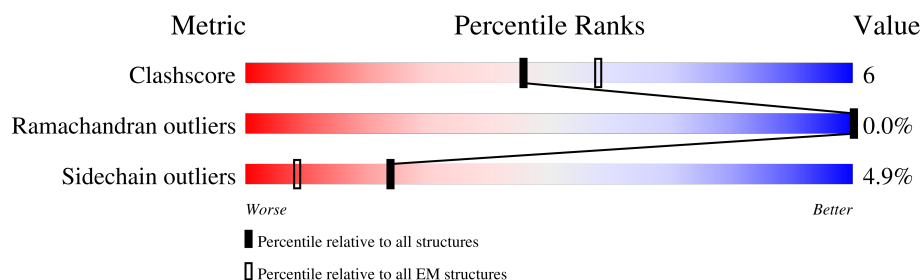
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.24 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14594 (2.74 - 3.74)

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

Mol	Chain	Length	Quality of chain
1	A	1285	
1	B	1285	
1	C	1285	
2	D	223	

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Mol	Chain	Length	Quality of chain
2	F	223	35% 77% 22%
2	H	223	5% 43% 11% 46%
3	E	205	20% 76% 21%
3	G	205	47% 78% 19%
3	I	205	45% 6% 48%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32113 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	1026	Total	C	N	O	S	0	0
			7989	5124	1326	1502	37		
1	B	1033	Total	C	N	O	S	0	0
			8043	5158	1338	1510	37		
1	C	1032	Total	C	N	O	S	0	0
			8035	5152	1337	1509	37		

There are 387 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	145	ASP	TYR	variant	UNP P0DTC2
A	209	ILE	-	insertion	UNP P0DTC2
A	210	VAL	-	insertion	UNP P0DTC2
A	211	ARG	ASN	variant	UNP P0DTC2
A	212	GLU	LEU	variant	UNP P0DTC2
A	213	PRO	VAL	variant	UNP P0DTC2
A	214	GLU	ARG	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	145	ASP	TYR	variant	UNP P0DTC2
B	209	ILE	-	insertion	UNP P0DTC2
B	210	VAL	-	insertion	UNP P0DTC2
B	211	ARG	ASN	variant	UNP P0DTC2
B	212	GLU	LEU	variant	UNP P0DTC2
B	213	PRO	VAL	variant	UNP P0DTC2
B	214	GLU	ARG	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	145	ASP	TYR	variant	UNP P0DTC2
C	209	ILE	-	insertion	UNP P0DTC2
C	210	VAL	-	insertion	UNP P0DTC2
C	211	ARG	ASN	variant	UNP P0DTC2
C	212	GLU	LEU	variant	UNP P0DTC2
C	213	PRO	VAL	variant	UNP P0DTC2
C	214	GLU	ARG	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called XG005-VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	223	Total	C	N	O	S	0	0
			1665	1053	274	330	8		
2	F	223	Total	C	N	O	S	0	0
			1665	1053	274	330	8		
2	H	121	Total	C	N	O	S	0	0
			926	588	151	181	6		

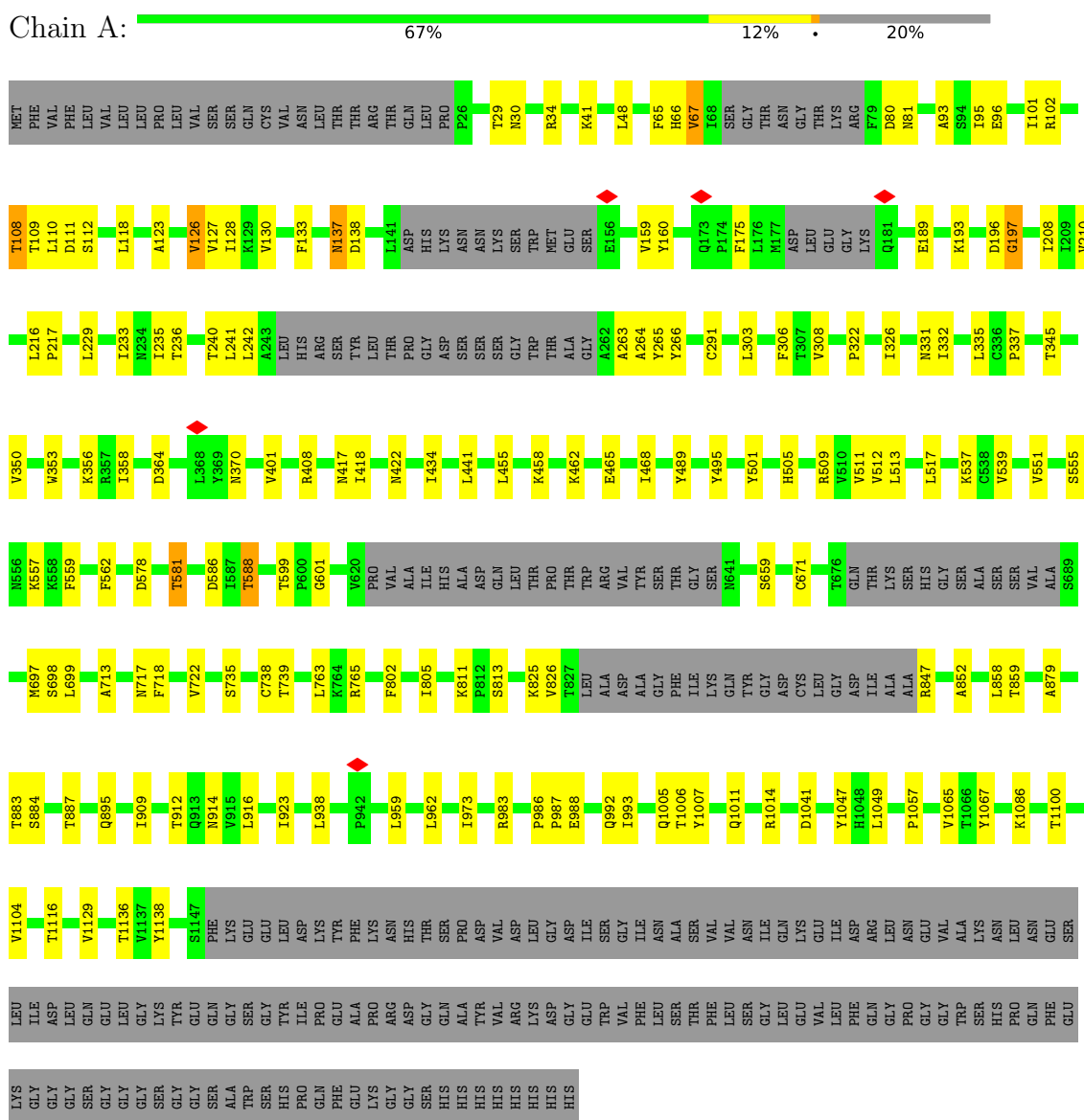
- Molecule 3 is a protein called XG005-VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	203	Total	C	N	O	S	0	0
			1504	940	248	311	5		
3	G	203	Total	C	N	O	S	0	0
			1504	940	248	311	5		
3	I	107	Total	C	N	O	S	0	0
			782	487	128	164	3		

3 Residue-property plots [i](#)

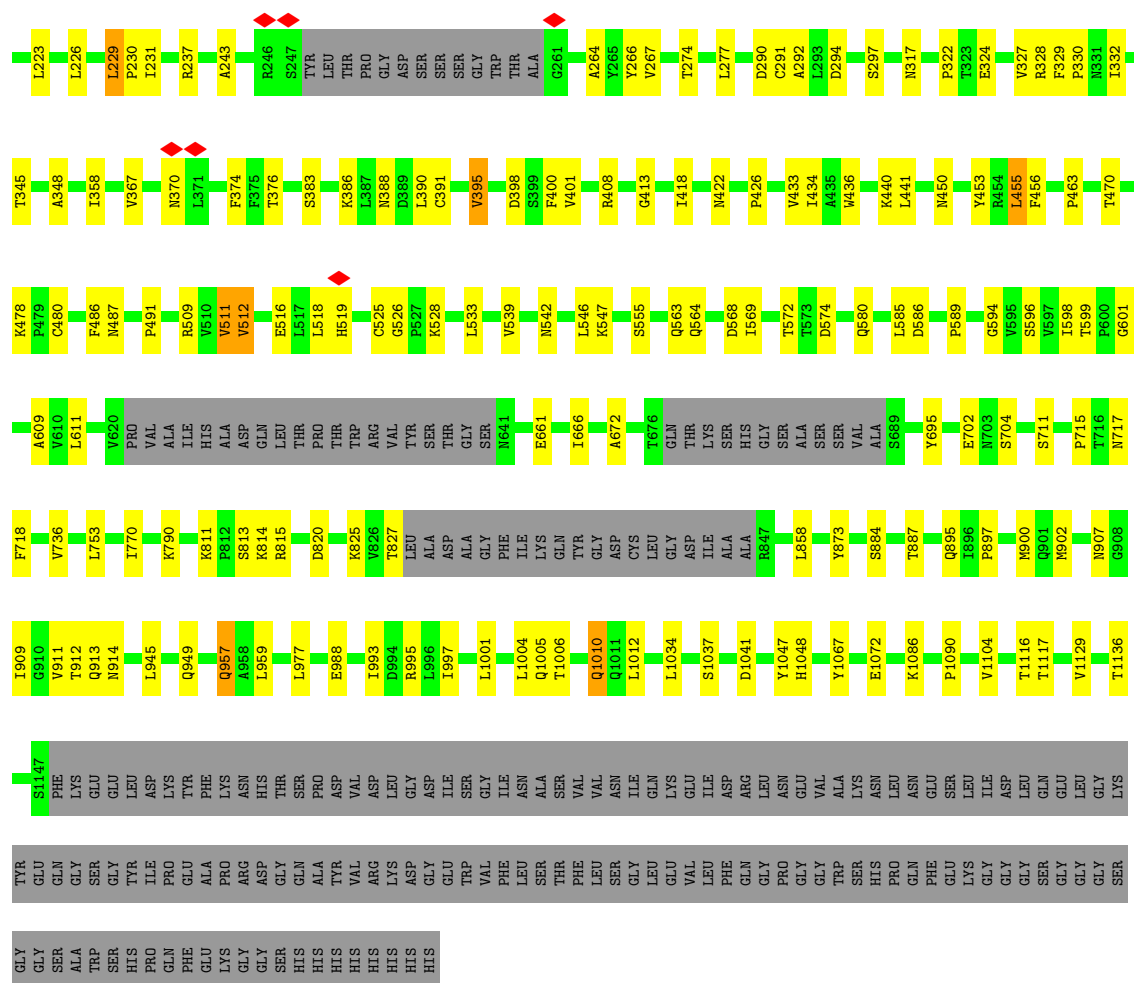
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

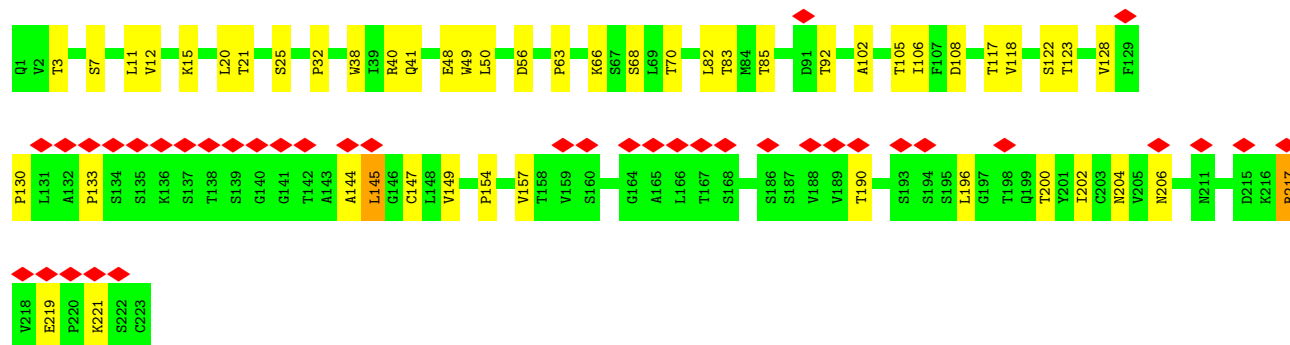
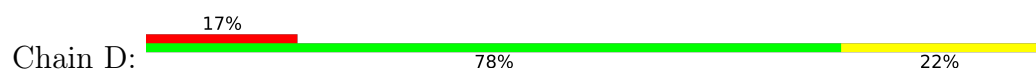


• Molecule 1: Spike glycoprotein

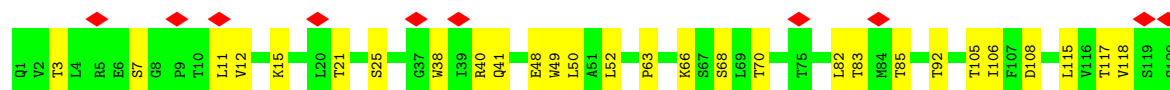
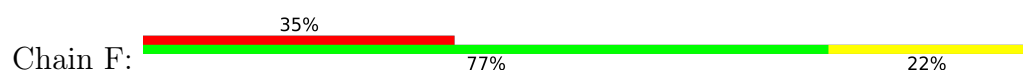


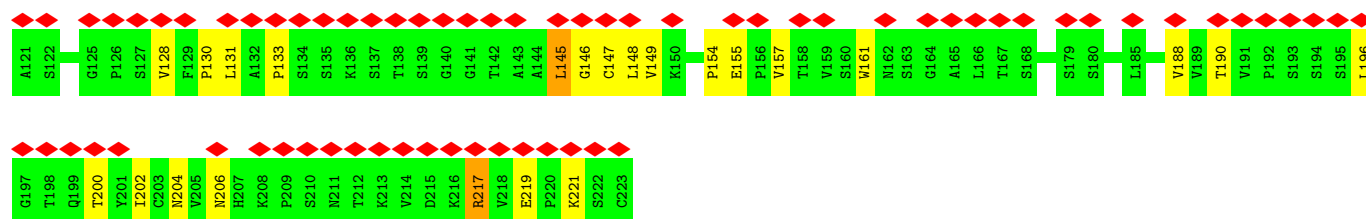


• Molecule 2: XG005-VH

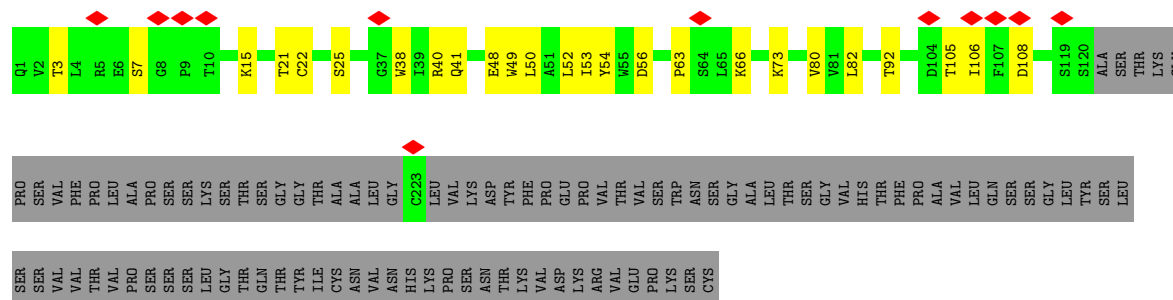
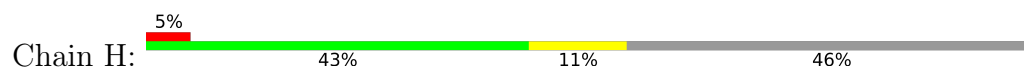


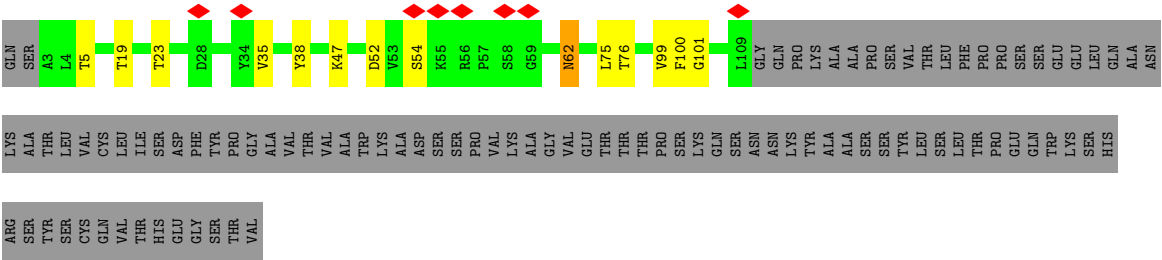
• Molecule 2: XG005-VH





• Molecule 2: XG005-VH





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	616627	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 ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.888	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0452	Depositor
Map size ($\text{\AA}$)	340.48, 340.48, 340.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.064, 1.064, 1.064	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	0.13	0/8179	0.36	0/11137
1	B	0.14	0/8235	0.34	0/11214
1	C	0.14	0/8227	0.36	1/11202 (0.0%)
2	D	0.11	0/1705	0.29	0/2331
2	F	0.11	0/1705	0.29	0/2331
2	H	0.09	0/946	0.25	0/1291
3	E	0.10	0/1540	0.27	0/2103
3	G	0.10	0/1540	0.28	0/2103
3	I	0.11	0/798	0.27	0/1088
All	All	0.13	0/32875	0.33	1/44800 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	329	PHE	N-CA-C	-5.20	101.09	109.82

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	7989	0	7780	74	0
1	B	8043	0	7836	122	0
1	C	8035	0	7826	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1665	0	1665	29	0
2	F	1665	0	1665	30	0
2	H	926	0	925	16	0
3	E	1504	0	1454	28	0
3	G	1504	0	1454	22	0
3	I	782	0	753	7	0
All	All	32113	0	31358	393	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 (393) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.72	0.72
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.75	0.69
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.74	0.69
2:H:63:PRO:HA	2:H:66:LYS:HE2	1.76	0.68
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.75	0.68
1:C:897:PRO:HD2	1:C:900:MET:HE2	1.76	0.67
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.75	0.67
1:A:95:ILE:H	1:A:264:ALA:HB3	1.58	0.67
1:A:67:VAL:HG13	1:A:80:ASP:H	1.59	0.66
2:F:63:PRO:HA	2:F:66:LYS:HE2	1.76	0.66
1:C:542:ASN:HD22	1:C:547:LYS:HG2	1.61	0.65
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.62	0.65
2:D:63:PRO:HA	2:D:66:LYS:HE2	1.78	0.65
3:E:170:GLN:HE22	3:E:172:ASN:HB3	1.62	0.65
1:A:895:GLN:NE2	1:B:706:ALA:O	2.29	0.64
1:A:65:PHE:HB2	1:A:265:TYR:HB3	1.78	0.64
1:B:790:LYS:HE3	1:C:702:GLU:HB3	1.80	0.64
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.80	0.64
1:A:137:ASN:ND2	1:A:138:ASP:OD1	2.31	0.63
3:G:170:GLN:HE22	3:G:172:ASN:HB3	1.63	0.63
1:A:599:THR:HG22	1:A:601:GLY:H	1.64	0.63
1:C:327:VAL:HG22	1:C:542:ASN:HB3	1.81	0.63
2:F:130:PRO:HA	2:F:147:CYS:HA	1.79	0.62
1:B:123:ALA:O	1:B:125:ASN:ND2	2.31	0.62
2:D:130:PRO:HA	2:D:147:CYS:HA	1.80	0.62
1:A:962:LEU:HD11	1:A:1007:TYR:HB2	1.82	0.62
1:C:123:ALA:O	1:C:125:ASN:ND2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:994:ASP:HB3	1:C:995:ARG:HH22	1.64	0.62
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.81	0.62
1:A:825:LYS:NZ	1:A:938:LEU:O	2.33	0.61
1:B:52:GLN:NE2	1:B:274:THR:OG1	2.33	0.61
1:C:811:LYS:NZ	1:C:820:ASP:OD1	2.34	0.61
1:A:988:GLU:O	1:A:992:GLN:NE2	2.34	0.61
2:D:128:VAL:HG22	2:D:149:VAL:HG22	1.83	0.61
1:B:913:GLN:NE2	1:C:1090:PRO:O	2.35	0.59
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.84	0.59
1:B:599:THR:HG22	1:B:601:GLY:H	1.67	0.59
1:A:739:THR:OG1	1:B:319:ARG:NH2	2.36	0.58
1:C:1006:THR:O	1:C:1010:GLN:NE2	2.37	0.58
2:F:128:VAL:HG22	2:F:149:VAL:HG22	1.85	0.58
1:B:562:PHE:O	1:B:564:GLN:NE2	2.36	0.57
2:D:204:ASN:O	2:D:206:ASN:ND2	2.37	0.57
1:B:367:VAL:O	1:B:370:ASN:ND2	2.38	0.57
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.69	0.57
3:E:42:PRO:HD2	3:E:169:LYS:HZ2	1.70	0.57
1:B:326:ILE:HD11	1:B:534:VAL:HG22	1.85	0.57
2:F:204:ASN:O	2:F:206:ASN:ND2	2.38	0.57
1:A:659:SER:HB3	1:A:698:SER:HB2	1.87	0.56
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.38	0.56
1:B:790:LYS:NZ	1:C:704:SER:OG	2.39	0.56
1:C:83:VAL:HB	1:C:237:ARG:HD3	1.86	0.56
1:B:880:GLY:O	1:B:884:SER:OG	2.21	0.56
1:B:1086:LYS:HD3	1:B:1122:VAL:HG11	1.88	0.56
2:D:219:GLU:O	2:D:221:LYS:NZ	2.35	0.56
3:E:164:THR:HG21	3:E:178:SER:HB2	1.88	0.56
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.70	0.56
1:C:102:ARG:HD3	1:C:243:ALA:HB2	1.87	0.56
1:B:324:GLU:H	1:B:539:VAL:HG12	1.71	0.55
1:B:191:VAL:HB	1:B:202:TYR:HB2	1.89	0.55
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.88	0.55
1:B:765:ARG:NH2	1:C:957:GLN:OE1	2.35	0.55
2:F:49:TRP:HB2	3:G:100:PHE:HE1	1.72	0.55
1:B:195:ILE:HD11	1:B:198:TYR:HB2	1.89	0.55
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.39	0.55
3:G:162:VAL:HG13	3:G:179:SER:HA	1.88	0.55
1:B:141:LEU:HB2	1:B:243:ALA:HA	1.89	0.54
2:D:217:ARG:NH1	2:D:219:GLU:OE2	2.41	0.54
3:E:162:VAL:HG13	3:E:179:SER:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:LYS:HE2	1:B:813:SER:HB2	1.88	0.54
1:B:444:LYS:HG2	1:B:448:ASN:HB2	1.90	0.54
1:C:825:LYS:HD2	1:C:945:LEU:HD23	1.89	0.54
2:F:11:LEU:HD22	2:F:154:PRO:HG3	1.90	0.54
1:B:847:ARG:NH1	1:C:574:ASP:OD1	2.40	0.54
2:D:12:VAL:HG12	2:D:118:VAL:HG21	1.90	0.54
2:D:106:ILE:O	3:E:38:TYR:OH	2.25	0.54
2:F:3:THR:OG1	2:F:25:SER:OG	2.26	0.54
2:H:49:TRP:HB2	3:I:100:PHE:HE1	1.72	0.54
1:B:43:PHE:HD1	1:C:563:GLN:HE22	1.54	0.54
1:B:384:PRO:HD2	1:C:456:PHE:HE1	1.72	0.54
3:E:123:PRO:HD3	3:E:135:LEU:HG	1.90	0.54
2:F:202:ILE:O	2:F:204:ASN:ND2	2.41	0.54
2:F:106:ILE:O	3:G:38:TYR:OH	2.24	0.54
3:E:118:VAL:HA	3:E:139:ILE:HG22	1.89	0.53
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.91	0.53
1:A:811:LYS:HD3	1:A:813:SER:HB2	1.90	0.53
3:G:118:VAL:HA	3:G:139:ILE:HG22	1.90	0.53
2:D:202:ILE:O	2:D:204:ASN:ND2	2.42	0.53
2:D:200:THR:HG23	2:D:217:ARG:HG2	1.91	0.52
2:F:7:SER:OG	2:F:21:THR:OG1	2.27	0.52
1:B:856:LYS:HE3	1:C:572:THR:HG21	1.91	0.52
1:C:108:THR:O	1:C:237:ARG:NH2	2.42	0.52
1:C:398:ASP:HB2	1:C:512:VAL:HG13	1.91	0.52
1:A:551:VAL:HB	1:A:588:THR:HG23	1.91	0.52
1:A:765:ARG:NH2	1:B:957:GLN:OE1	2.42	0.52
1:C:478:LYS:O	1:C:487:ASN:ND2	2.37	0.52
1:A:434:ILE:HD13	1:A:513:LEU:HD13	1.91	0.52
2:F:217:ARG:NH1	2:F:219:GLU:OE2	2.41	0.52
1:B:191:VAL:HG23	1:B:223:LEU:HD22	1.91	0.52
1:B:984:LEU:HD13	1:B:989:ALA:HA	1.91	0.52
1:C:907:ASN:HD21	1:C:913:GLN:HE21	1.57	0.52
1:C:478:LYS:NZ	1:C:480:CYS:SG	2.83	0.52
2:F:40:ARG:HE	2:F:50:LEU:HD11	1.75	0.52
2:H:7:SER:OG	2:H:21:THR:OG1	2.27	0.52
1:B:193:LYS:HE2	1:B:202:TYR:HE2	1.75	0.52
1:B:62:VAL:HG11	1:B:266:TYR:HB3	1.90	0.52
1:C:884:SER:OG	1:C:887:THR:OG1	2.27	0.52
2:D:11:LEU:HD22	2:D:154:PRO:HG3	1.91	0.52
2:F:217:ARG:H	2:F:217:ARG:HE	1.58	0.51
1:C:450:ASN:ND2	2:D:56:ASP:OD2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:ARG:H	2:D:217:ARG:HE	1.58	0.51
1:B:912:THR:OG1	1:B:1106:GLN:NE2	2.42	0.51
1:A:159:VAL:HG11	1:A:241:LEU:HD13	1.91	0.51
2:D:49:TRP:HB2	3:E:100:PHE:HE1	1.75	0.51
3:E:5:THR:OG1	3:E:23:THR:OG1	2.28	0.51
1:B:105:ILE:HG12	1:B:241:LEU:HD11	1.91	0.51
2:D:40:ARG:HB3	2:D:48:GLU:HG3	1.93	0.51
1:B:374:PHE:H	1:C:486:PHE:HZ	1.59	0.51
2:H:3:THR:OG1	2:H:25:SER:OG	2.27	0.51
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.43	0.51
1:C:177:MET:SD	1:C:177:MET:N	2.84	0.51
1:C:97:LYS:H	1:C:100:ILE:HD13	1.76	0.51
1:C:134:GLN:OE1	1:C:161:SER:OG	2.28	0.51
3:G:164:THR:HG21	3:G:178:SER:HB2	1.92	0.51
3:I:62:ASN:O	3:I:62:ASN:ND2	2.44	0.51
1:B:501:TYR:HB3	1:B:505:HIS:HB2	1.93	0.51
3:E:62:ASN:O	3:E:62:ASN:ND2	2.43	0.51
3:E:152:LYS:HB3	3:E:157:PRO:HA	1.93	0.51
2:H:106:ILE:O	3:I:38:TYR:OH	2.26	0.50
1:B:895:GLN:NE2	1:C:711:SER:OG	2.45	0.50
3:I:5:THR:OG1	3:I:23:THR:OG1	2.29	0.50
3:G:62:ASN:O	3:G:62:ASN:ND2	2.44	0.50
2:D:7:SER:OG	2:D:21:THR:OG1	2.30	0.50
1:B:984:LEU:HB3	1:B:989:ALA:HB2	1.93	0.50
1:C:811:LYS:HE2	1:C:813:SER:HB2	1.93	0.50
3:G:5:THR:OG1	3:G:23:THR:OG1	2.29	0.50
3:G:65:SER:HG	3:G:76:THR:HG1	1.53	0.50
1:B:130:VAL:HG21	1:B:231:ILE:HG12	1.93	0.50
1:B:472:ILE:HD13	1:B:472:ILE:H	1.77	0.50
2:H:40:ARG:HB2	2:H:50:LEU:HD11	1.93	0.50
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.44	0.49
3:G:152:LYS:HB3	3:G:157:PRO:HA	1.94	0.49
2:F:200:THR:HG23	2:F:217:ARG:HG2	1.94	0.49
2:F:219:GLU:O	2:F:221:LYS:NZ	2.35	0.49
3:G:123:PRO:HD3	3:G:135:LEU:HG	1.94	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.95	0.49
1:C:367:VAL:HA	1:C:370:ASN:HD21	1.76	0.49
1:C:456:PHE:HD2	1:C:491:PRO:HA	1.78	0.49
1:B:102:ARG:NH1	1:B:121:ASN:O	2.43	0.49
2:D:40:ARG:HB2	2:D:50:LEU:HD11	1.94	0.49
1:C:434:ILE:HB	1:C:511:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:SER:HB3	2:F:85:THR:H	1.77	0.49
2:F:108:ASP:OD1	2:F:108:ASP:N	2.46	0.49
3:I:99:VAL:HG22	3:I:101:GLY:H	1.78	0.49
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.77	0.49
2:H:108:ASP:OD1	2:H:108:ASP:N	2.46	0.49
1:A:337:PRO:HG2	1:A:358:ILE:HD12	1.95	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.95	0.49
1:B:104:TRP:HE3	1:B:119:ILE:HB	1.78	0.49
1:B:978:ASN:O	1:C:547:LYS:NZ	2.46	0.49
2:D:3:THR:OG1	2:D:25:SER:OG	2.31	0.49
1:B:201:ILE:HB	1:B:227:VAL:HG23	1.95	0.48
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.95	0.48
1:C:132:GLU:HB2	1:C:164:ASN:HB2	1.94	0.48
1:C:596:SER:HB2	1:C:611:LEU:HB3	1.94	0.48
1:A:858:LEU:HD13	1:A:959:LEU:HD22	1.95	0.48
1:B:107:GLY:H	1:B:235:ILE:HG23	1.78	0.48
1:C:229:LEU:H	1:C:229:LEU:HD22	1.79	0.48
3:G:139:ILE:HG21	3:G:198:VAL:HG21	1.94	0.48
2:H:40:ARG:HE	2:H:50:LEU:HD11	1.78	0.48
1:B:742:ILE:HG21	1:B:997:ILE:HG13	1.95	0.48
2:F:70:THR:HG1	2:F:83:THR:HG1	1.58	0.48
1:C:717:ASN:OD1	1:C:718:PHE:N	2.45	0.48
2:F:40:ARG:HB2	2:F:50:LEU:HD11	1.95	0.48
1:B:659:SER:HB3	1:B:698:SER:HB2	1.96	0.48
1:C:328:ARG:HH21	1:C:580:GLN:HB2	1.78	0.48
1:C:1037:SER:H	1:C:1048:HIS:HD2	1.62	0.48
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	1.96	0.48
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.95	0.48
1:B:244:LEU:HG	1:B:246:ARG:HG2	1.95	0.48
1:B:553:THR:O	1:B:586:ASP:N	2.46	0.48
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.96	0.48
1:B:1037:SER:H	1:B:1048:HIS:HD2	1.61	0.48
1:C:330:PRO:HD2	1:C:525:CYS:SG	2.54	0.48
2:H:49:TRP:HE1	2:H:52:LEU:HB2	1.78	0.47
2:D:70:THR:OG1	2:D:83:THR:OG1	2.29	0.47
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.47	0.47
1:A:717:ASN:OD1	1:A:718:PHE:N	2.45	0.47
1:B:181:GLN:OE1	1:B:182:GLY:N	2.47	0.47
1:B:229:LEU:HD22	1:B:229:LEU:H	1.79	0.47
1:B:170:TYR:CE2	1:B:172:SER:HB3	2.50	0.47
3:G:20:ILE:HD12	3:G:104:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:HD12	1:A:983:ARG:HD2	1.96	0.47
1:C:96:GLU:HB2	1:C:100:ILE:HD13	1.97	0.47
1:B:188:ARG:HG2	1:B:205:HIS:HD2	1.80	0.47
1:A:138:ASP:OD1	1:A:138:ASP:N	2.48	0.47
1:A:501:TYR:HB3	1:A:505:HIS:HB2	1.96	0.47
1:B:676:THR:OG1	1:B:690:GLN:OE1	2.28	0.47
1:A:987:PRO:HD3	1:C:413:GLY:HA3	1.97	0.46
2:F:12:VAL:HG12	2:F:118:VAL:HG21	1.96	0.46
1:A:81:ASN:HD22	1:A:240:THR:HG23	1.80	0.46
1:B:331:ASN:HD22	1:B:331:ASN:HA	1.59	0.46
1:B:661:GLU:O	1:B:695:TYR:OH	2.27	0.46
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.97	0.46
1:A:417:ASN:HD21	1:A:455:LEU:HD23	1.80	0.46
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.98	0.46
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.96	0.46
1:B:437:ASN:ND2	1:B:506:GLN:OE1	2.39	0.46
1:A:326:ILE:HD13	1:A:539:VAL:HG21	1.98	0.46
3:E:27:SER:HB2	3:E:29:VAL:HG12	1.97	0.46
1:A:102:ARG:HH12	1:A:123:ALA:H	1.63	0.46
1:B:329:PHE:O	1:B:580:GLN:NE2	2.47	0.46
3:G:119:THR:OG1	3:G:138:LEU:O	2.33	0.46
1:C:391:CYS:HA	1:C:525:CYS:HA	1.97	0.46
1:A:34:ARG:NH1	1:A:189:GLU:OE2	2.48	0.46
1:A:557:LYS:HE3	1:A:559:PHE:HE1	1.81	0.46
1:A:763:LEU:HD21	1:A:1005:GLN:HG2	1.97	0.46
1:B:965:GLN:NE2	1:B:1003:SER:HB3	2.31	0.46
1:B:1005:GLN:NE2	1:C:1006:THR:OG1	2.47	0.46
1:A:1011:GLN:OE1	1:A:1014:ARG:NH2	2.49	0.46
1:B:374:PHE:HD1	1:B:436:TRP:HB3	1.80	0.46
1:A:735:SER:OG	1:A:859:THR:OG1	2.33	0.45
1:B:410:ILE:HG23	1:B:425:LEU:HD11	1.98	0.45
1:A:699:LEU:HD22	1:C:873:TYR:CZ	2.51	0.45
1:A:879:ALA:O	1:A:883:THR:OG1	2.29	0.45
3:E:119:THR:OG1	3:E:138:LEU:O	2.32	0.45
3:E:135:LEU:HD22	3:E:151:TRP:HH2	1.81	0.45
1:B:95:ILE:HG12	1:B:187:LEU:HD13	1.98	0.45
2:D:68:SER:HB3	2:D:85:THR:H	1.81	0.45
2:F:40:ARG:HB3	2:F:48:GLU:HG3	1.99	0.45
1:B:560:LEU:HB2	1:B:563:GLN:HG2	1.98	0.45
1:C:977:LEU:HD22	1:C:993:ILE:HD11	1.99	0.45
1:A:1116:THR:HG22	1:A:1138:TYR:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:SER:OG	1:C:386:LYS:O	2.33	0.45
1:C:827:THR:N	1:C:949:GLN:OE1	2.50	0.45
3:E:152:LYS:HD3	3:E:157:PRO:HB3	1.98	0.45
3:E:24:ALA:HB1	3:E:27:SER:HB3	1.97	0.45
1:A:128:ILE:HD13	1:A:229:LEU:HD11	1.98	0.45
1:A:126:VAL:HG12	1:A:128:ILE:HG13	1.99	0.45
1:B:294:ASP:N	1:B:294:ASP:OD1	2.49	0.45
1:B:994:ASP:HA	1:B:997:ILE:HG22	1.99	0.45
1:C:52:GLN:OE1	1:C:274:THR:OG1	2.25	0.45
1:B:126:VAL:HG21	1:B:176:LEU:HD13	1.99	0.45
1:B:847:ARG:HH21	1:B:852:ALA:HA	1.82	0.45
2:D:40:ARG:HE	2:D:50:LEU:HD11	1.82	0.45
3:G:121:PHE:HE2	3:G:138:LEU:HB3	1.81	0.45
1:B:81:ASN:HD22	1:B:239:GLN:HE21	1.65	0.44
2:D:38:TRP:CG	2:D:82:LEU:HD22	2.51	0.44
1:A:48:LEU:HD22	1:A:306:PHE:HE1	1.82	0.44
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.99	0.44
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.99	0.44
3:E:52:ASP:O	3:E:55:LYS:N	2.36	0.44
1:B:324:GLU:HG2	1:B:325:SER:H	1.83	0.44
1:B:444:LYS:HB2	2:H:54:TYR:CZ	2.53	0.44
1:C:327:VAL:HG11	1:C:528:LYS:HZ2	1.81	0.44
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.99	0.44
1:C:811:LYS:HG3	1:C:814:LYS:H	1.82	0.44
2:H:41:GLN:O	2:H:41:GLN:NE2	2.51	0.44
1:B:353:TRP:O	1:B:466:ARG:NH1	2.50	0.44
1:C:105:ILE:HB	1:C:135:PHE:HZ	1.83	0.44
3:E:137:CYS:HB2	3:E:151:TRP:CZ2	2.53	0.44
1:A:101:ILE:HD11	1:A:263:ALA:HB1	2.00	0.44
1:B:80:ASP:N	1:B:80:ASP:OD1	2.51	0.44
1:B:977:LEU:HD22	1:B:993:ILE:HD11	2.00	0.44
1:C:811:LYS:HD3	1:C:815:ARG:H	1.82	0.44
3:E:121:PHE:HE2	3:E:138:LEU:HB3	1.82	0.44
3:G:137:CYS:HB2	3:G:151:TRP:CZ2	2.52	0.44
1:B:307:THR:HG23	1:B:602:THR:HB	1.98	0.44
1:C:453:TYR:HE2	1:C:455:LEU:HD23	1.82	0.44
3:G:135:LEU:HD22	3:G:151:TRP:HH2	1.82	0.44
1:A:41:LYS:HD3	1:B:564:GLN:HE21	1.83	0.44
1:A:108:THR:HG23	1:A:109:THR:H	1.82	0.44
1:A:578:ASP:HB3	1:A:581:THR:O	2.18	0.44
1:A:916:LEU:HD12	1:A:923:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:GLN:O	2:D:41:GLN:NE2	2.51	0.44
3:E:19:THR:HG22	3:E:76:THR:HG22	2.00	0.44
1:A:216:LEU:HD12	1:A:217:PRO:HD2	2.00	0.44
1:B:110:LEU:HD23	1:B:237:ARG:HE	1.82	0.44
1:B:574:ASP:O	1:B:587:ILE:N	2.50	0.44
1:C:599:THR:HG22	1:C:601:GLY:H	1.82	0.44
2:F:38:TRP:CG	2:F:82:LEU:HD22	2.52	0.44
3:E:170:GLN:OE1	3:E:172:ASN:N	2.41	0.43
2:F:133:PRO:HG3	2:F:145:LEU:HD23	2.00	0.43
1:B:298:GLU:HG2	1:B:315:THR:HB	2.00	0.43
1:C:348:ALA:HB3	1:C:400:PHE:HA	2.00	0.43
3:E:48:LEU:HD21	3:E:51:TYR:HB3	2.00	0.43
1:B:656:VAL:HG22	1:B:658:ASN:H	1.83	0.43
1:C:290:ASP:O	1:C:297:SER:HB3	2.18	0.43
1:C:294:ASP:OD1	1:C:297:SER:OG	2.28	0.43
3:E:52:ASP:O	3:E:54:SER:N	2.51	0.43
1:C:191:VAL:HG23	1:C:223:LEU:HD22	2.01	0.43
2:D:133:PRO:HG3	2:D:145:LEU:HD23	2.00	0.43
1:A:118:LEU:HD11	1:A:133:PHE:CE1	2.54	0.43
1:A:303:LEU:HD22	1:A:308:VAL:HG23	2.01	0.43
1:B:374:PHE:CD1	1:B:436:TRP:HB3	2.54	0.43
1:C:358:ILE:HG13	1:C:395:VAL:HG13	2.01	0.43
2:F:49:TRP:HE1	2:F:52:LEU:HB2	1.84	0.43
1:A:111:ASP:OD1	1:A:112:SER:N	2.49	0.43
1:C:441:LEU:HD12	2:D:32:PRO:HB2	2.01	0.43
1:B:84:LEU:O	1:B:238:PHE:N	2.50	0.43
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.84	0.43
1:C:274:THR:HB	1:C:291:CYS:HB3	2.00	0.42
2:H:38:TRP:CG	2:H:82:LEU:HD22	2.54	0.42
1:C:401:VAL:HG22	1:C:509:ARG:HG2	2.01	0.42
1:C:542:ASN:ND2	1:C:547:LYS:HG2	2.33	0.42
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.54	0.42
1:B:615:VAL:HG13	1:B:619:GLU:HB2	2.01	0.42
1:B:666:ILE:HD12	1:B:670:ILE:HG22	2.01	0.42
3:G:99:VAL:HG22	3:G:101:GLY:H	1.84	0.42
1:A:847:ARG:HH12	1:A:852:ALA:HA	1.85	0.42
1:C:126:VAL:HG23	1:C:175:PHE:HA	2.00	0.42
2:H:22:CYS:N	2:H:80:VAL:O	2.52	0.42
1:B:92:PHE:O	1:B:190:PHE:N	2.43	0.42
1:B:97:LYS:HB2	1:B:185:LYS:HD2	2.02	0.42
1:C:661:GLU:O	1:C:695:TYR:OH	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:THR:OG1	2:F:83:THR:OG1	2.32	0.42
3:E:99:VAL:HG22	3:E:101:GLY:H	1.84	0.42
2:F:41:GLN:O	2:F:41:GLN:NE2	2.53	0.42
3:G:68:LYS:HE3	3:G:68:LYS:HB3	1.93	0.42
1:B:358:ILE:HB	1:B:395:VAL:HG13	2.01	0.42
1:B:1086:LYS:HG3	1:B:1088:HIS:CE1	2.54	0.42
1:C:440:LYS:HG2	2:D:102:ALA:HB1	2.02	0.42
1:C:374:PHE:HD1	1:C:436:TRP:HB3	1.85	0.42
2:D:108:ASP:OD1	2:D:108:ASP:N	2.47	0.42
1:A:895:GLN:HG2	1:B:713:ALA:HB2	2.02	0.42
1:A:1006:THR:OG1	1:C:1005:GLN:NE2	2.52	0.42
1:B:392:PHE:N	1:B:524:VAL:O	2.40	0.42
3:E:139:ILE:HG21	3:E:198:VAL:HG21	2.01	0.42
1:C:317:ASN:HD22	1:C:594:GLY:HA2	1.84	0.41
2:D:122:SER:OG	2:D:123:THR:N	2.53	0.41
2:F:115:LEU:HD23	2:F:155:GLU:HB3	2.02	0.41
1:A:562:PHE:HD2	1:C:41:LYS:HZ2	1.69	0.41
1:A:986:PRO:N	1:A:987:PRO:HD2	2.36	0.41
1:B:444:LYS:NZ	2:H:56:ASP:OD1	2.53	0.41
1:C:80:ASP:OD1	1:C:80:ASP:N	2.53	0.41
1:C:291:CYS:SG	1:C:292:ALA:N	2.93	0.41
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	2.02	0.41
2:D:144:ALA:HB3	3:E:121:PHE:HE1	1.85	0.41
3:G:152:LYS:HD3	3:G:157:PRO:HB3	2.01	0.41
1:A:196:ASP:OD1	1:A:197:GLY:N	2.53	0.41
1:B:353:TRP:CD1	1:B:353:TRP:H	2.38	0.41
2:H:40:ARG:HB3	2:H:48:GLU:HG3	2.03	0.41
1:B:158:ARG:HD2	1:B:158:ARG:HA	1.94	0.41
1:B:409:GLN:HE22	1:B:417:ASN:H	1.69	0.41
1:B:584:ILE:H	1:B:584:ILE:HG12	1.62	0.41
1:B:671:CYS:SG	1:B:697:MET:HB3	2.61	0.41
1:C:568:ASP:OD1	1:C:569:ILE:N	2.44	0.41
1:C:753:LEU:HA	1:C:997:ILE:HD11	2.02	0.41
2:F:146:GLY:HA3	2:F:188:VAL:HG12	2.02	0.41
1:B:67:VAL:HB	1:B:263:ALA:HB3	2.01	0.41
1:B:855:PHE:CG	1:C:589:PRO:HG2	2.56	0.41
1:C:324:GLU:H	1:C:539:VAL:HG12	1.86	0.41
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.85	0.41
1:B:708:SER:HB3	1:B:711:SER:HB3	2.01	0.41
1:B:886:TRP:HZ3	1:B:905:ARG:HG2	1.85	0.41
1:C:388:ASN:O	1:C:526:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:858:LEU:HD13	1:C:959:LEU:HD22	2.02	0.41
1:A:335:LEU:HD11	1:A:364:ASP:HB2	2.02	0.41
1:B:408:ARG:H	1:B:408:ARG:HG3	1.65	0.41
1:C:130:VAL:HG21	1:C:231:ILE:HG12	2.02	0.41
1:C:198:TYR:CE1	1:C:230:PRO:HB3	2.55	0.41
1:C:909:ILE:HG13	1:C:911:VAL:HG22	2.03	0.41
1:A:29:THR:OG1	1:A:30:ASN:N	2.54	0.41
1:A:462:LYS:HG2	1:A:465:GLU:OE1	2.21	0.41
1:A:671:CYS:SG	1:A:697:MET:HB2	2.60	0.41
1:A:713:ALA:HB2	1:C:895:GLN:HG2	2.02	0.41
1:A:826:VAL:HB	1:A:1057:PRO:HG2	2.02	0.41
1:B:290:ASP:O	1:B:297:SER:HB3	2.21	0.41
1:C:322:PRO:HB3	1:C:539:VAL:HA	2.03	0.41
3:I:52:ASP:O	3:I:54:SER:N	2.54	0.41
1:A:101:ILE:HA	1:A:242:LEU:HG	2.02	0.41
1:A:884:SER:OG	1:A:887:THR:OG1	2.39	0.41
1:B:192:PHE:HE1	1:B:201:ILE:HG23	1.86	0.41
1:B:242:LEU:HD23	1:B:242:LEU:H	1.86	0.41
1:C:736:VAL:HG21	1:C:1004:LEU:HD11	2.02	0.41
1:A:264:ALA:HB1	1:A:266:TYR:CE2	2.56	0.40
1:B:357:ARG:NH2	1:B:396:TYR:OH	2.52	0.40
1:B:1082:CYS:HB2	1:B:1132:ILE:HD11	2.03	0.40
2:F:131:LEU:HD21	2:F:148:LEU:HD22	2.04	0.40
2:F:146:GLY:HA2	2:F:161:TRP:HZ2	1.87	0.40
3:I:19:THR:HG22	3:I:76:THR:HG22	2.03	0.40
1:B:290:ASP:OD1	1:B:291:CYS:N	2.43	0.40
1:C:119:ILE:HG12	1:C:128:ILE:HG23	2.03	0.40
3:G:42:PRO:HD2	3:G:169:LYS:NZ	2.36	0.40
3:G:52:ASP:O	3:G:54:SER:N	2.55	0.40
2:H:53:ILE:HD13	2:H:73:LYS:HB3	2.03	0.40
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	2.04	0.40
3:E:20:ILE:HD12	3:E:104:THR:HG21	2.03	0.40
3:E:192:ARG:H	3:E:192:ARG:HG3	1.74	0.40
1:A:353:TRP:CD1	1:A:353:TRP:H	2.40	0.40
1:A:441:LEU:HD23	1:A:441:LEU:H	1.86	0.40
1:B:1116:THR:H	1:B:1119:ASN:HD21	1.69	0.40
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.03	0.40
1:C:790:LYS:HE2	1:C:790:LYS:HB2	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1010/1285 (79%)	977 (97%)	32 (3%)	1 (0%)	48	77
1	B	1017/1285 (79%)	972 (96%)	44 (4%)	1 (0%)	48	77
1	C	1016/1285 (79%)	965 (95%)	51 (5%)	0	100	100
2	D	221/223 (99%)	201 (91%)	20 (9%)	0	100	100
2	F	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
2	H	118/223 (53%)	114 (97%)	4 (3%)	0	100	100
3	E	201/205 (98%)	178 (89%)	23 (11%)	0	100	100
3	G	201/205 (98%)	181 (90%)	20 (10%)	0	100	100
3	I	105/205 (51%)	95 (90%)	10 (10%)	0	100	100
All	All	4110/5139 (80%)	3882 (94%)	226 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	PRO
1	A	197	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	885/1115 (79%)	842 (95%)	43 (5%)	22	53
1	B	891/1115 (80%)	852 (96%)	39 (4%)	25	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	890/1115 (80%)	847 (95%)	43 (5%)	23	53
2	D	194/194 (100%)	184 (95%)	10 (5%)	21	51
2	F	194/194 (100%)	185 (95%)	9 (5%)	24	55
2	H	106/194 (55%)	103 (97%)	3 (3%)	38	64
3	E	170/172 (99%)	158 (93%)	12 (7%)	13	42
3	G	170/172 (99%)	157 (92%)	13 (8%)	12	39
3	I	88/172 (51%)	84 (96%)	4 (4%)	24	55
All	All	3588/4443 (81%)	3412 (95%)	176 (5%)	24	53

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	67	VAL
1	A	96	GLU
1	A	108	THR
1	A	110	LEU
1	A	126	VAL
1	A	127	VAL
1	A	130	VAL
1	A	137	ASN
1	A	160	TYR
1	A	175	PHE
1	A	193	LYS
1	A	208	ILE
1	A	210	VAL
1	A	233	ILE
1	A	235	ILE
1	A	236	THR
1	A	291	CYS
1	A	331	ASN
1	A	332	ILE
1	A	345	THR
1	A	350	VAL
1	A	356	LYS
1	A	370	ASN
1	A	408	ARG
1	A	458	LYS
1	A	468	ILE
1	A	489	TYR

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Mol	Chain	Res	Type
1	A	495	TYR
1	A	511	VAL
1	A	512	VAL
1	A	517	LEU
1	A	537	LYS
1	A	581	THR
1	A	588	THR
1	A	738	CYS
1	A	993	ILE
1	A	1041	ASP
1	A	1086	LYS
1	A	1100	THR
1	A	1104	VAL
1	A	1129	VAL
1	A	1136	THR
1	B	33	THR
1	B	66	HIS
1	B	67	VAL
1	B	105	ILE
1	B	108	THR
1	B	117	LEU
1	B	126	VAL
1	B	135	PHE
1	B	158	ARG
1	B	159	VAL
1	B	224	GLU
1	B	226	LEU
1	B	227	VAL
1	B	327	VAL
1	B	331	ASN
1	B	395	VAL
1	B	408	ARG
1	B	449	TYR
1	B	456	PHE
1	B	458	LYS
1	B	468	ILE
1	B	470	THR
1	B	472	ILE
1	B	478	LYS
1	B	488	CYS
1	B	493	ARG
1	B	535	LYS

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Mol	Chain	Res	Type
1	B	538	CYS
1	B	542	ASN
1	B	546	LEU
1	B	584	ILE
1	B	756	TYR
1	B	790	LYS
1	B	957	GLN
1	B	984	LEU
1	B	1034	LEU
1	B	1041	ASP
1	B	1104	VAL
1	B	1129	VAL
1	C	66	HIS
1	C	67	VAL
1	C	83	VAL
1	C	105	ILE
1	C	108	THR
1	C	115	GLN
1	C	118	LEU
1	C	157	PHE
1	C	195	ILE
1	C	206	THR
1	C	226	LEU
1	C	229	LEU
1	C	267	VAL
1	C	277	LEU
1	C	332	ILE
1	C	345	THR
1	C	376	THR
1	C	390	LEU
1	C	395	VAL
1	C	408	ARG
1	C	433	VAL
1	C	455	LEU
1	C	470	THR
1	C	511	VAL
1	C	512	VAL
1	C	516	GLU
1	C	518	LEU
1	C	519	HIS
1	C	546	LEU
1	C	564	GLN

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Mol	Chain	Res	Type
1	C	902	MET
1	C	957	GLN
1	C	988	GLU
1	C	1001	LEU
1	C	1010	GLN
1	C	1034	LEU
1	C	1041	ASP
1	C	1086	LYS
1	C	1104	VAL
1	C	1116	THR
1	C	1117	THR
1	C	1129	VAL
1	C	1136	THR
2	D	15	LYS
2	D	20	LEU
2	D	92	THR
2	D	105	THR
2	D	117	THR
2	D	145	LEU
2	D	157	VAL
2	D	190	THR
2	D	196	LEU
2	D	217	ARG
3	E	35	VAL
3	E	47	LYS
3	E	62	ASN
3	E	75	LEU
3	E	120	LEU
3	E	135	LEU
3	E	139	ILE
3	E	159	LYS
3	E	163	GLU
3	E	169	LYS
3	E	189	LYS
3	E	194	TYR
2	F	15	LYS
2	F	92	THR
2	F	105	THR
2	F	117	THR
2	F	145	LEU
2	F	157	VAL
2	F	190	THR

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Mol	Chain	Res	Type
2	F	196	LEU
2	F	217	ARG
3	G	35	VAL
3	G	47	LYS
3	G	62	ASN
3	G	75	LEU
3	G	120	LEU
3	G	134	THR
3	G	135	LEU
3	G	139	ILE
3	G	159	LYS
3	G	163	GLU
3	G	169	LYS
3	G	189	LYS
3	G	194	TYR
2	H	15	LYS
2	H	92	THR
2	H	105	THR
3	I	35	VAL
3	I	47	LYS
3	I	62	ASN
3	I	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	87	ASN
1	A	99	ASN
1	A	122	ASN
1	A	218	GLN
1	A	271	GLN
1	A	321	GLN
1	A	331	ASN
1	A	360	ASN
1	A	409	GLN
1	A	417	ASN
1	A	450	ASN
1	A	460	ASN
1	A	487	ASN
1	A	540	ASN
1	A	542	ASN

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Mol	Chain	Res	Type
1	A	690	GLN
1	A	710	ASN
1	A	755	GLN
1	A	853	GLN
1	A	913	GLN
1	A	914	ASN
1	A	992	GLN
1	A	1005	GLN
1	A	1048	HIS
1	A	1058	HIS
1	A	1088	HIS
1	A	1108	ASN
1	B	52	GLN
1	B	81	ASN
1	B	121	ASN
1	B	164	ASN
1	B	165	ASN
1	B	173	GLN
1	B	186	ASN
1	B	205	HIS
1	B	317	ASN
1	B	331	ASN
1	B	370	ASN
1	B	394	ASN
1	B	409	GLN
1	B	417	ASN
1	B	460	ASN
1	B	481	ASN
1	B	540	ASN
1	B	564	GLN
1	B	613	GLN
1	B	644	GLN
1	B	762	GLN
1	B	784	GLN
1	B	853	GLN
1	B	895	GLN
1	B	901	GLN
1	B	913	GLN
1	B	935	GLN
1	B	965	GLN
1	B	992	GLN
1	B	1002	GLN

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Mol	Chain	Res	Type
1	B	1005	GLN
1	B	1011	GLN
1	B	1048	HIS
1	B	1119	ASN
1	C	81	ASN
1	C	115	GLN
1	C	121	ASN
1	C	165	ASN
1	C	173	GLN
1	C	181	GLN
1	C	271	GLN
1	C	317	ASN
1	C	354	ASN
1	C	370	ASN
1	C	394	ASN
1	C	409	GLN
1	C	417	ASN
1	C	540	ASN
1	C	563	GLN
1	C	710	ASN
1	C	762	GLN
1	C	784	GLN
1	C	853	GLN
1	C	872	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	1005	GLN
1	C	1011	GLN
1	C	1048	HIS
2	D	41	GLN
2	D	199	GLN
2	D	204	ASN
3	E	39	GLN
3	E	40	GLN
3	E	81	GLN
3	E	111	GLN
3	E	197	GLN
2	F	41	GLN
2	F	86	ASN
2	F	199	GLN
2	F	204	ASN

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Mol	Chain	Res	Type
3	G	39	GLN
3	G	40	GLN
3	G	71	ASN
3	G	81	GLN
3	G	111	GLN
3	G	197	GLN
2	H	41	GLN
3	I	39	GLN
3	I	81	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

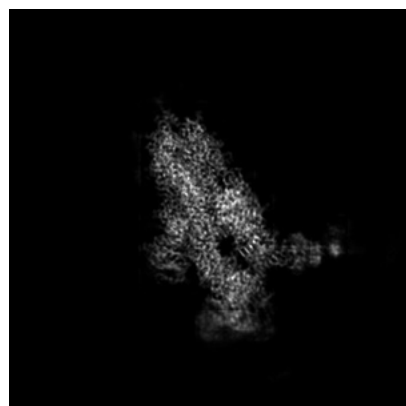
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33743. These allow visual inspection of the internal detail of the map and identification of artifacts.

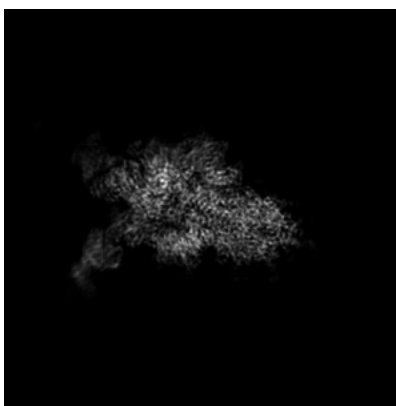
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

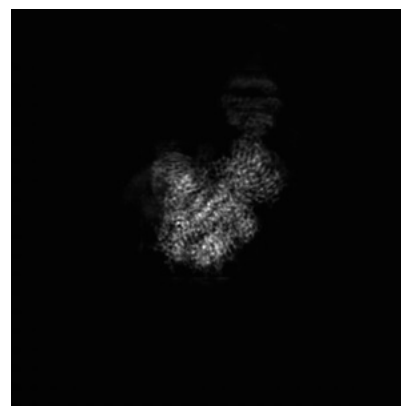
6.1.1 Primary map



X

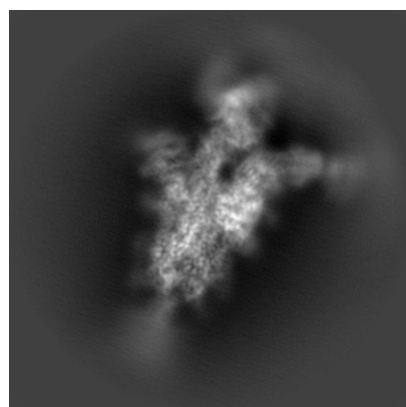


Y

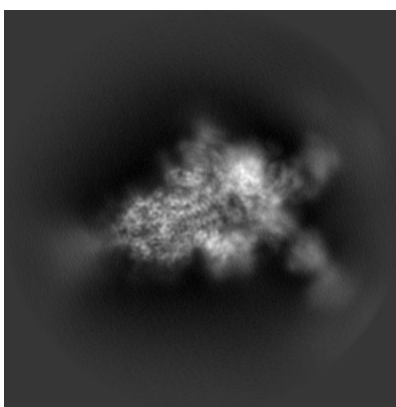


Z

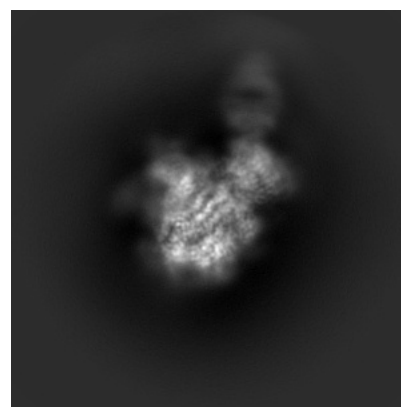
6.1.2 Raw map



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: 160

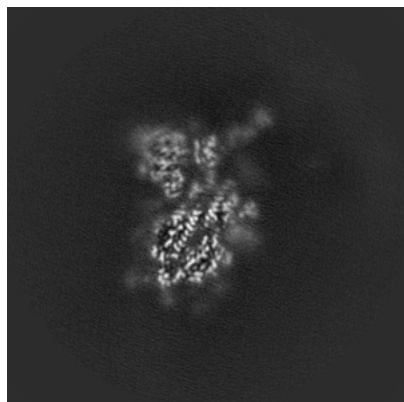


Y Index: 160

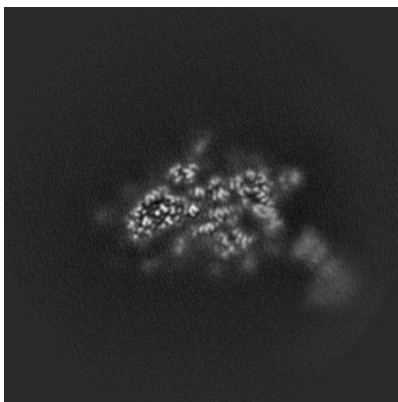


Z Index: 160

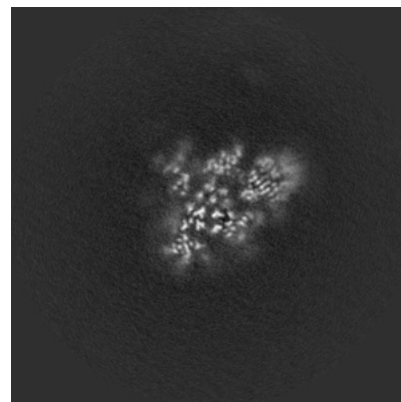
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 134

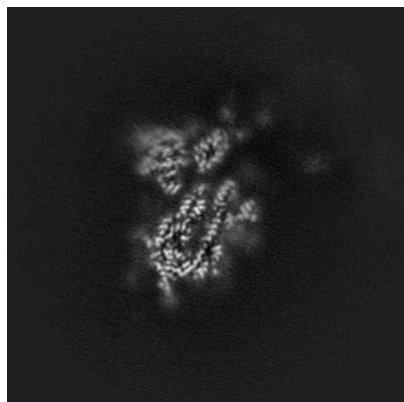


Y Index: 152

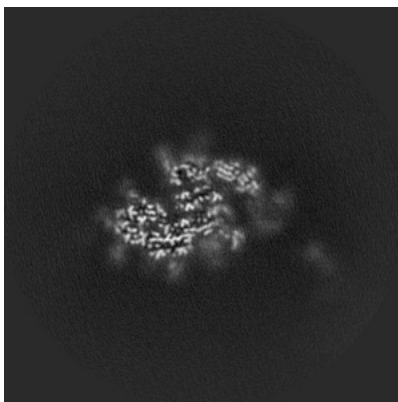


Z Index: 151

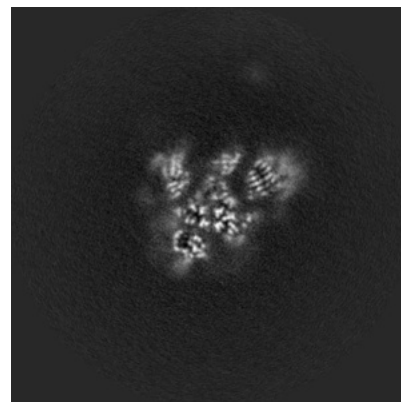
6.3.2 Raw map



X Index: 164



Y Index: 148

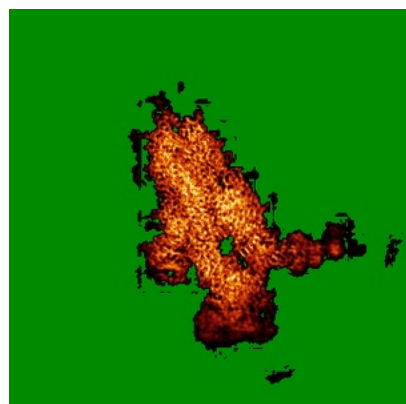


Z Index: 164

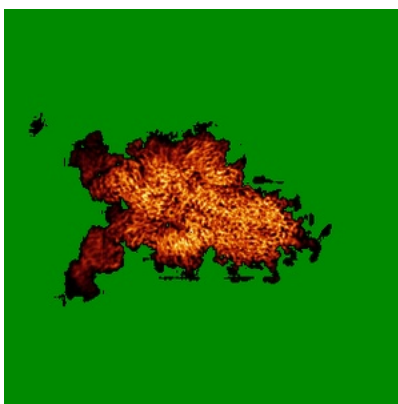
The images above show the largest variance slices of the map in three orthogonal directions.

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

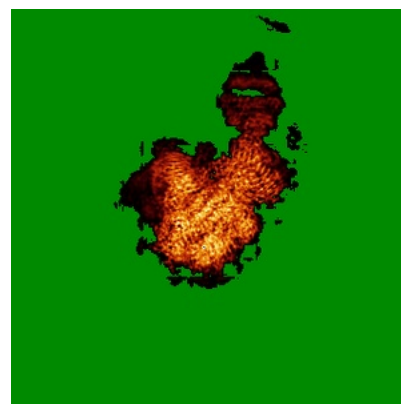
6.4.1 Primary map



X

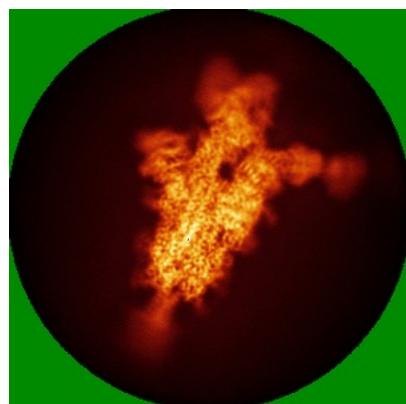


Y

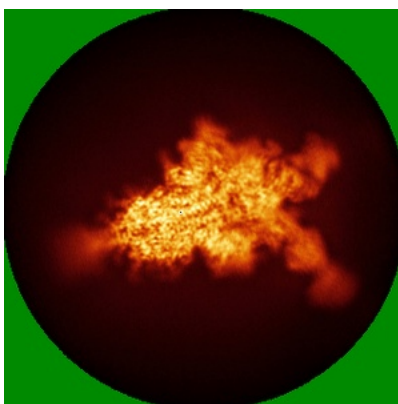


Z

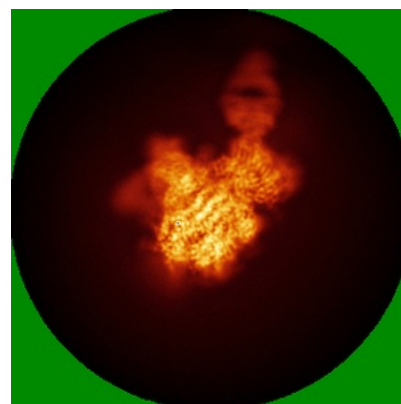
6.4.2 Raw map



X



Y

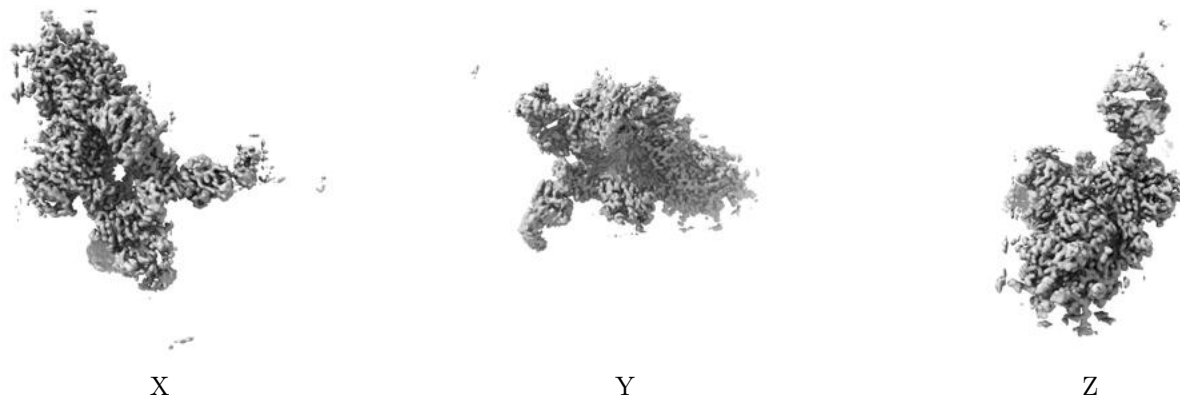


Z

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.

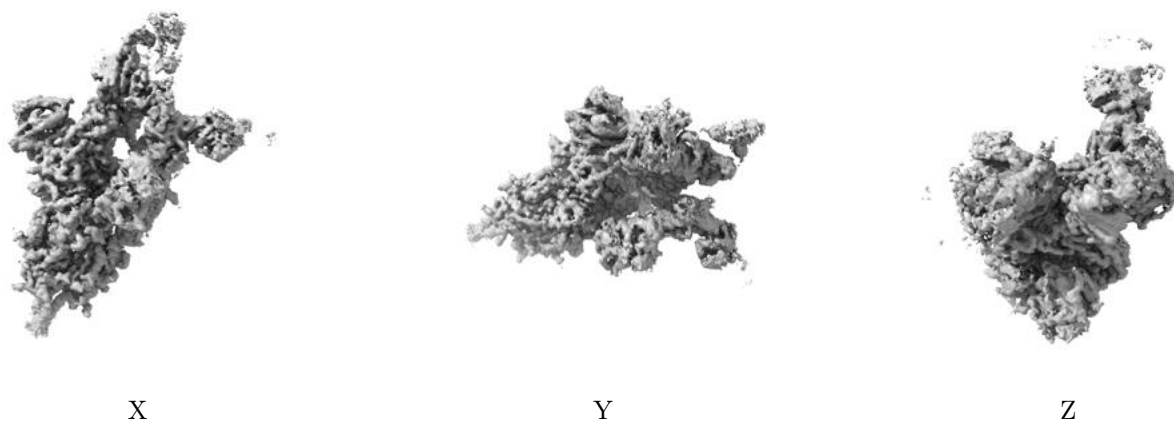
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0452. 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.

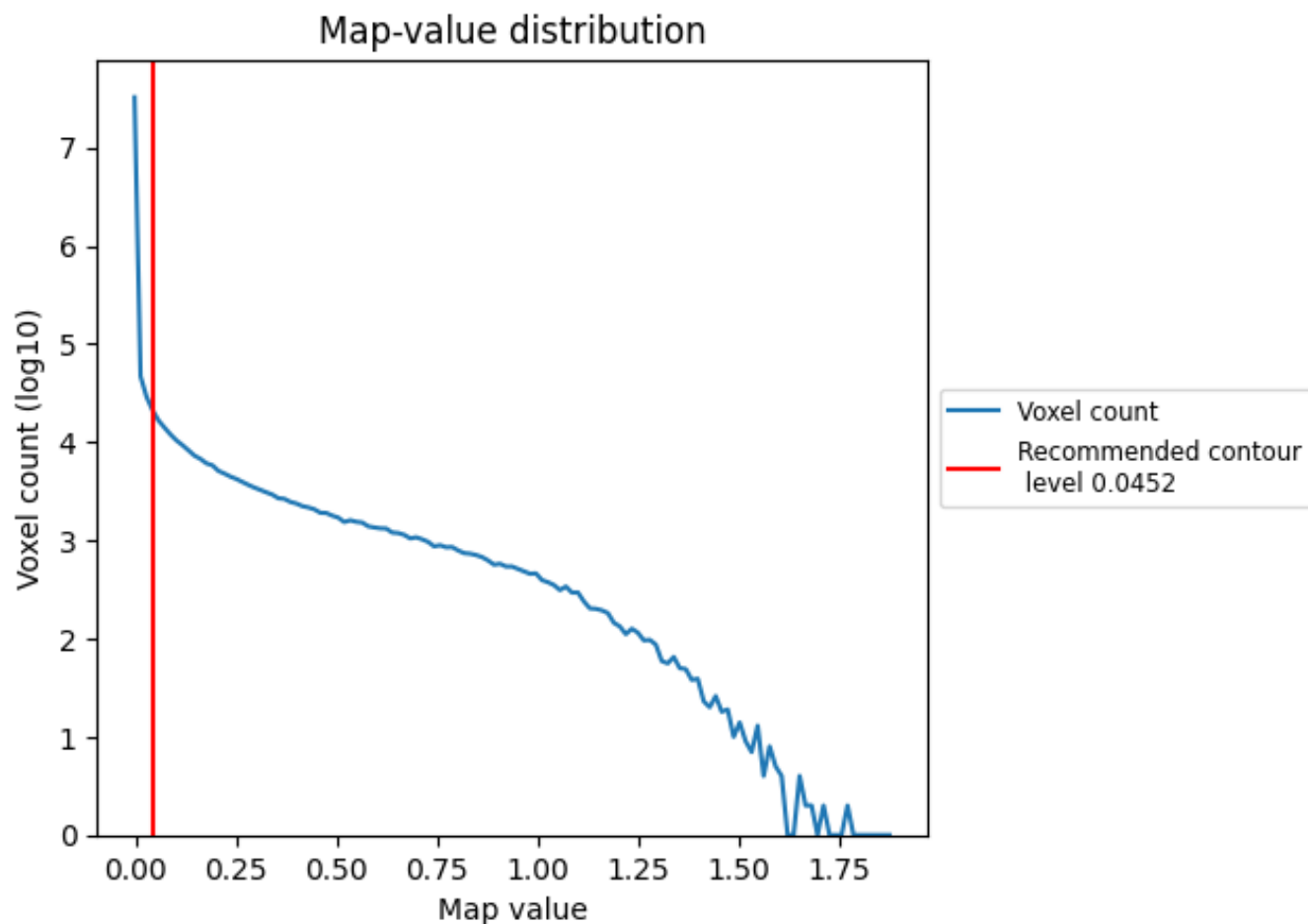
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

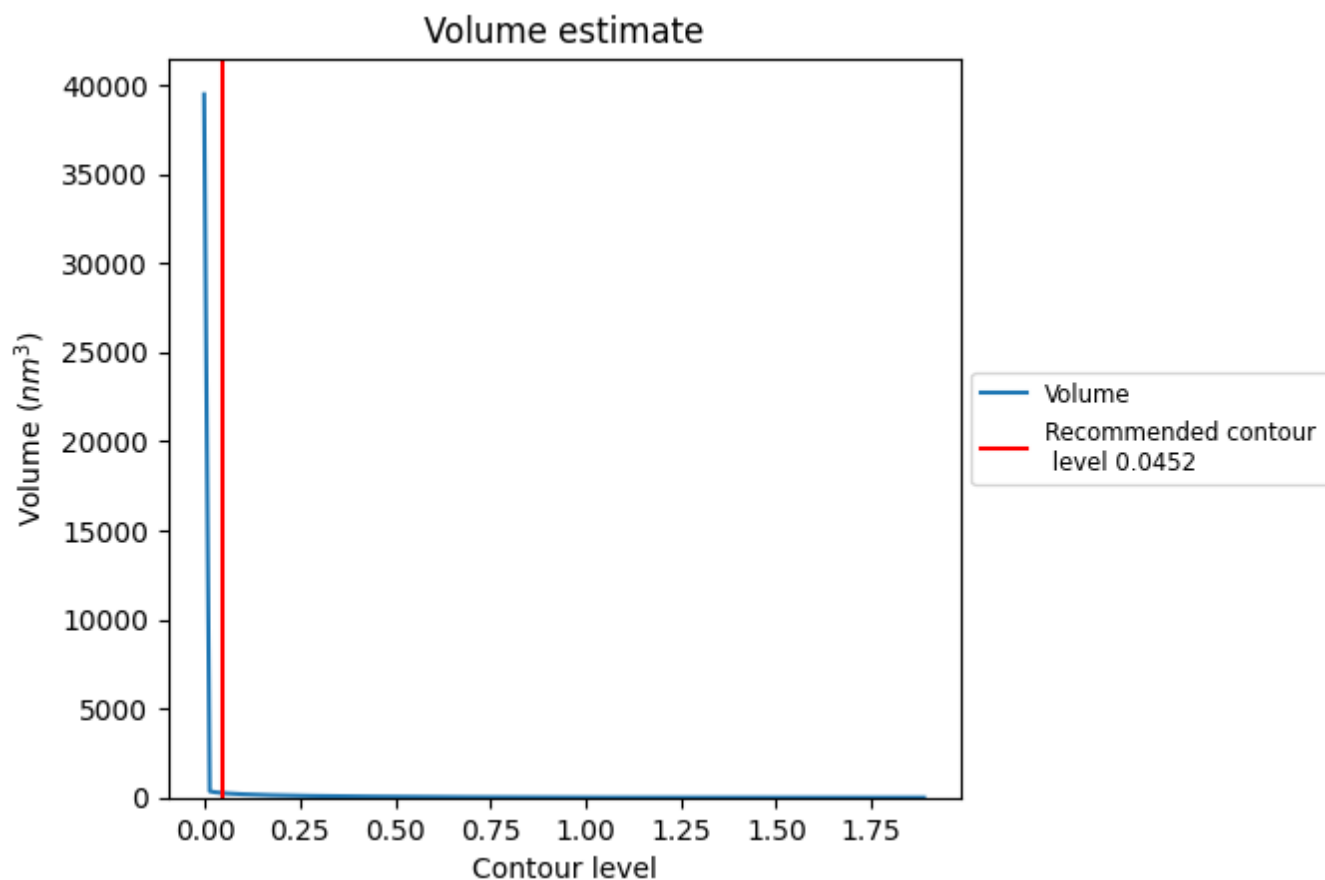
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

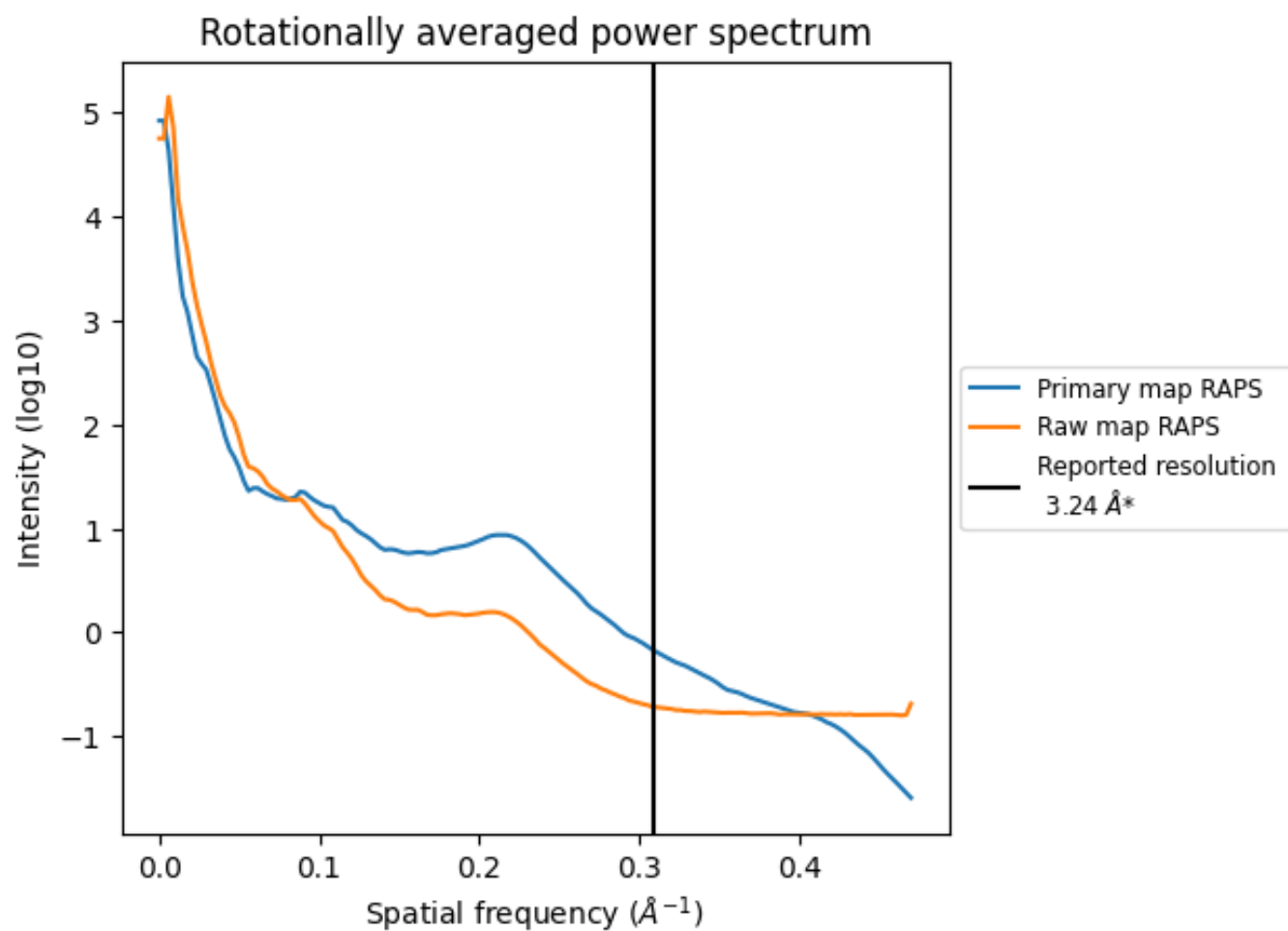
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm³; this corresponds to an approximate mass of 232 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 ⓘ

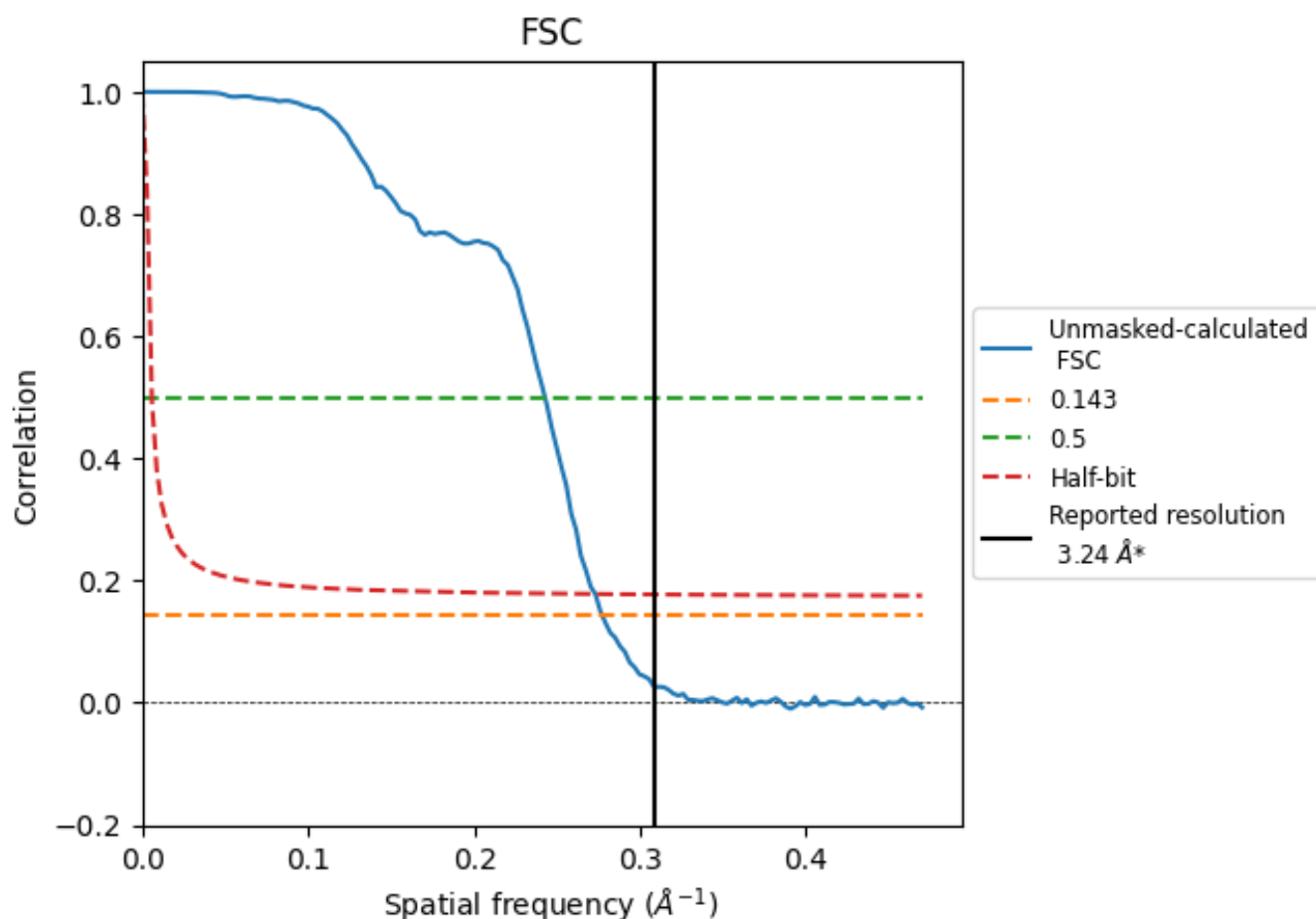


*Reported resolution corresponds to spatial frequency of 0.309 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.309 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

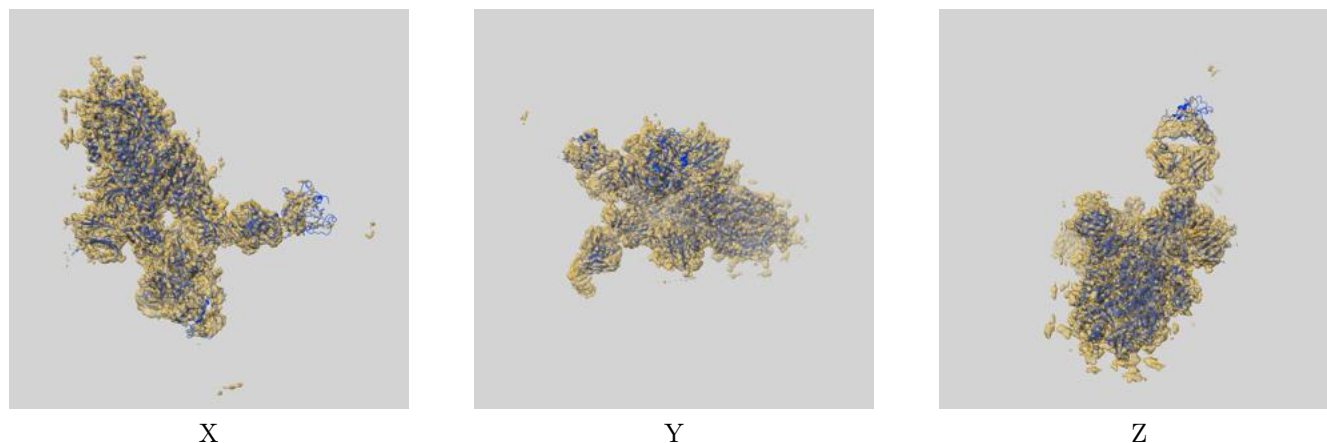
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.12	3.66

*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 3.61 differs from the reported value 3.24 by more than 10 %

9 Map-model fit [i](#)

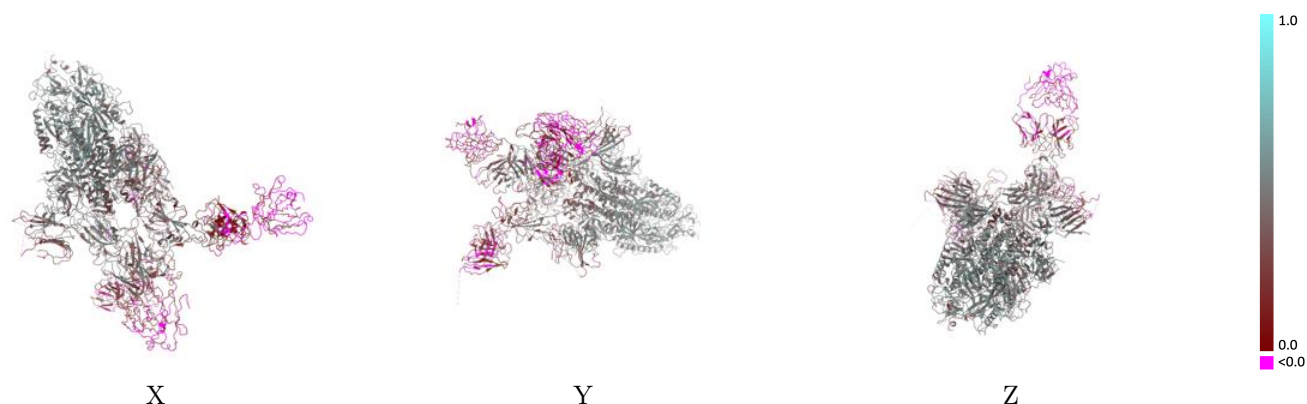
This section contains information regarding the fit between EMDB map EMD-33743 and PDB model 7YCZ. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



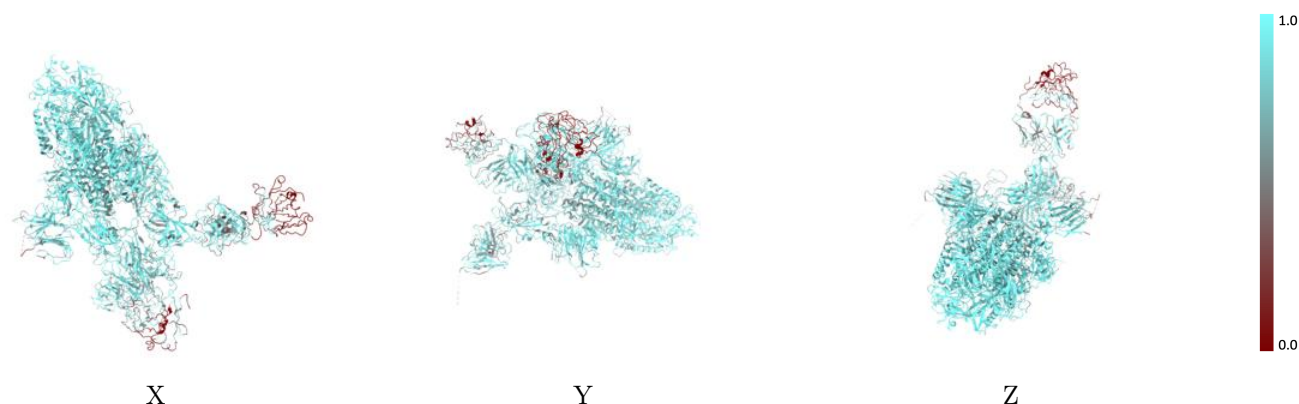
The images above show the 3D surface view of the map at the recommended contour level 0.0452 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



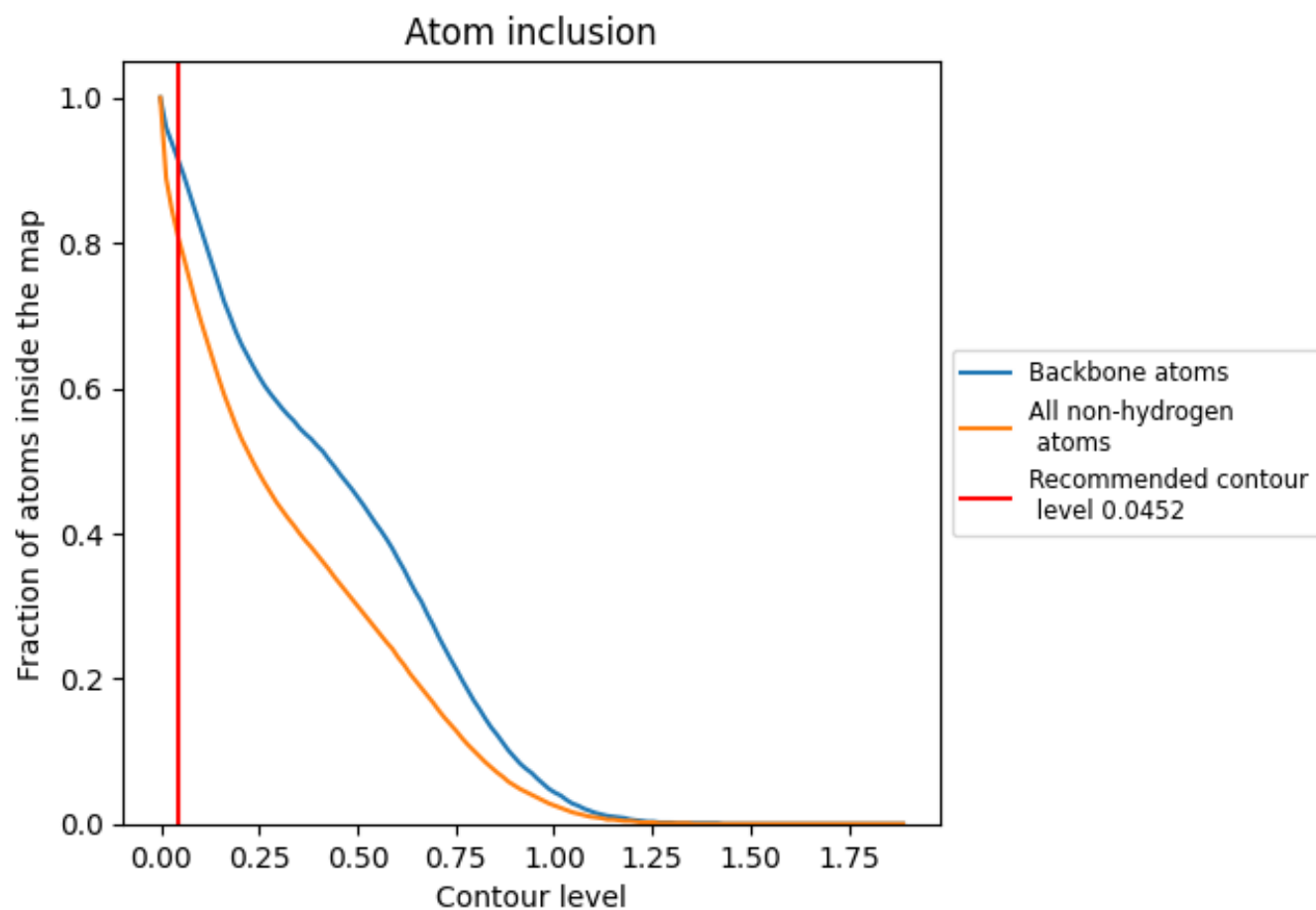
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0452).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.0452) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.3520
A	0.8720	0.4250
B	0.8620	0.4180
C	0.8760	0.4300
D	0.6670	0.2280
E	0.6680	0.2270
F	0.5390	0.0740
G	0.4240	0.0400
H	0.7280	0.1180
I	0.7400	0.0820

