



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 06:42 AM JST

PDB ID : 7WCH  
EMDB ID : EMD-32422  
Title : CryoEM structure of the SARS-CoV-2 S6P(B.1.617.2) in complex with SWA9 Fab  
Authors : Du, S.; Xiao, J.Y.  
Deposited on : 2021-12-20  
Resolution : 3.19 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>.

---

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

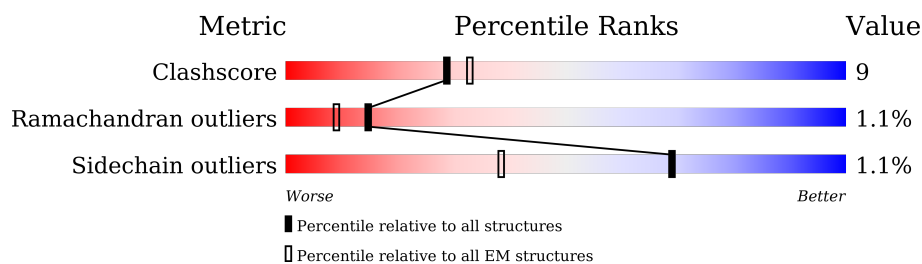
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.19 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	1286	
1	B	1286	
1	G	1286	
2	D	228	
2	H	228	
2	M	228	
3	E	111	
3	L	111	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	N	111	<div><div></div><div>54%</div><div></div><div>70%</div><div></div><div>21%</div><div></div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28319 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 Surface glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	999	Total	C	N	O	S	0	0
			7683	4902	1276	1470	35		
1	B	1002	Total	C	N	O	S	0	0
			7736	4933	1295	1473	35		
1	G	991	Total	C	N	O	S	0	0
			7653	4881	1271	1466	35		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP A0A8B1VBI1
A	683	SER	ARG	conflict	UNP A0A8B1VBI1
A	685	SER	ARG	conflict	UNP A0A8B1VBI1
A	817	PRO	PHE	conflict	UNP A0A8B1VBI1
A	892	PRO	ALA	conflict	UNP A0A8B1VBI1
A	899	PRO	ALA	conflict	UNP A0A8B1VBI1
A	942	PRO	ALA	conflict	UNP A0A8B1VBI1
A	986	PRO	LYS	conflict	UNP A0A8B1VBI1
A	987	PRO	VAL	conflict	UNP A0A8B1VBI1
A	1209	GLY	-	expression tag	UNP A0A8B1VBI1
A	1210	SER	-	expression tag	UNP A0A8B1VBI1
A	1211	GLY	-	expression tag	UNP A0A8B1VBI1
A	1212	TYR	-	expression tag	UNP A0A8B1VBI1
A	1213	ILE	-	expression tag	UNP A0A8B1VBI1
A	1214	PRO	-	expression tag	UNP A0A8B1VBI1
A	1215	GLU	-	expression tag	UNP A0A8B1VBI1
A	1216	ALA	-	expression tag	UNP A0A8B1VBI1
A	1217	PRO	-	expression tag	UNP A0A8B1VBI1
A	1218	ARG	-	expression tag	UNP A0A8B1VBI1
A	1219	ASP	-	expression tag	UNP A0A8B1VBI1
A	1220	GLY	-	expression tag	UNP A0A8B1VBI1
A	1221	GLN	-	expression tag	UNP A0A8B1VBI1
A	1222	ALA	-	expression tag	UNP A0A8B1VBI1
A	1223	TYR	-	expression tag	UNP A0A8B1VBI1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	VAL	-	expression tag	UNP A0A8B1VBI1
A	1225	ARG	-	expression tag	UNP A0A8B1VBI1
A	1226	LYS	-	expression tag	UNP A0A8B1VBI1
A	1227	ASP	-	expression tag	UNP A0A8B1VBI1
A	1228	GLY	-	expression tag	UNP A0A8B1VBI1
A	1229	GLU	-	expression tag	UNP A0A8B1VBI1
A	1230	TRP	-	expression tag	UNP A0A8B1VBI1
A	1231	VAL	-	expression tag	UNP A0A8B1VBI1
A	1232	LEU	-	expression tag	UNP A0A8B1VBI1
A	1233	LEU	-	expression tag	UNP A0A8B1VBI1
A	1234	SER	-	expression tag	UNP A0A8B1VBI1
A	1235	THR	-	expression tag	UNP A0A8B1VBI1
A	1236	PHE	-	expression tag	UNP A0A8B1VBI1
A	1237	LEU	-	expression tag	UNP A0A8B1VBI1
A	1238	GLY	-	expression tag	UNP A0A8B1VBI1
A	1239	ARG	-	expression tag	UNP A0A8B1VBI1
A	1240	SER	-	expression tag	UNP A0A8B1VBI1
A	1241	LEU	-	expression tag	UNP A0A8B1VBI1
A	1242	GLU	-	expression tag	UNP A0A8B1VBI1
A	1243	VAL	-	expression tag	UNP A0A8B1VBI1
A	1244	LEU	-	expression tag	UNP A0A8B1VBI1
A	1245	PHE	-	expression tag	UNP A0A8B1VBI1
A	1246	GLN	-	expression tag	UNP A0A8B1VBI1
A	1247	GLY	-	expression tag	UNP A0A8B1VBI1
A	1248	PRO	-	expression tag	UNP A0A8B1VBI1
A	1249	GLY	-	expression tag	UNP A0A8B1VBI1
A	1250	HIS	-	expression tag	UNP A0A8B1VBI1
A	1251	HIS	-	expression tag	UNP A0A8B1VBI1
A	1252	HIS	-	expression tag	UNP A0A8B1VBI1
A	1253	HIS	-	expression tag	UNP A0A8B1VBI1
A	1254	HIS	-	expression tag	UNP A0A8B1VBI1
A	1255	HIS	-	expression tag	UNP A0A8B1VBI1
A	1256	HIS	-	expression tag	UNP A0A8B1VBI1
A	1257	HIS	-	expression tag	UNP A0A8B1VBI1
A	1258	SER	-	expression tag	UNP A0A8B1VBI1
A	1259	ALA	-	expression tag	UNP A0A8B1VBI1
A	1260	TRP	-	expression tag	UNP A0A8B1VBI1
A	1261	SER	-	expression tag	UNP A0A8B1VBI1
A	1262	HIS	-	expression tag	UNP A0A8B1VBI1
A	1263	PRO	-	expression tag	UNP A0A8B1VBI1
A	1264	GLN	-	expression tag	UNP A0A8B1VBI1
A	1265	PHE	-	expression tag	UNP A0A8B1VBI1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	GLU	-	expression tag	UNP A0A8B1VBI1
A	1267	LYS	-	expression tag	UNP A0A8B1VBI1
A	1268	GLY	-	expression tag	UNP A0A8B1VBI1
A	1269	GLY	-	expression tag	UNP A0A8B1VBI1
A	1270	GLY	-	expression tag	UNP A0A8B1VBI1
A	1271	SER	-	expression tag	UNP A0A8B1VBI1
A	1272	GLY	-	expression tag	UNP A0A8B1VBI1
A	1273	GLY	-	expression tag	UNP A0A8B1VBI1
A	1274	GLY	-	expression tag	UNP A0A8B1VBI1
A	1275	GLY	-	expression tag	UNP A0A8B1VBI1
A	1276	SER	-	expression tag	UNP A0A8B1VBI1
A	1277	GLY	-	expression tag	UNP A0A8B1VBI1
A	1278	GLY	-	expression tag	UNP A0A8B1VBI1
A	1279	SER	-	expression tag	UNP A0A8B1VBI1
A	1280	ALA	-	expression tag	UNP A0A8B1VBI1
A	1281	TRP	-	expression tag	UNP A0A8B1VBI1
A	1282	SER	-	expression tag	UNP A0A8B1VBI1
A	1283	HIS	-	expression tag	UNP A0A8B1VBI1
A	1284	PRO	-	expression tag	UNP A0A8B1VBI1
A	1285	GLN	-	expression tag	UNP A0A8B1VBI1
A	1286	PHE	-	expression tag	UNP A0A8B1VBI1
A	1287	GLU	-	expression tag	UNP A0A8B1VBI1
A	1288	LYS	-	expression tag	UNP A0A8B1VBI1
B	682	GLY	ARG	conflict	UNP A0A8B1VBI1
B	683	SER	ARG	conflict	UNP A0A8B1VBI1
B	685	SER	ARG	conflict	UNP A0A8B1VBI1
B	817	PRO	PHE	conflict	UNP A0A8B1VBI1
B	892	PRO	ALA	conflict	UNP A0A8B1VBI1
B	899	PRO	ALA	conflict	UNP A0A8B1VBI1
B	942	PRO	ALA	conflict	UNP A0A8B1VBI1
B	986	PRO	LYS	conflict	UNP A0A8B1VBI1
B	987	PRO	VAL	conflict	UNP A0A8B1VBI1
B	1209	GLY	-	expression tag	UNP A0A8B1VBI1
B	1210	SER	-	expression tag	UNP A0A8B1VBI1
B	1211	GLY	-	expression tag	UNP A0A8B1VBI1
B	1212	TYR	-	expression tag	UNP A0A8B1VBI1
B	1213	ILE	-	expression tag	UNP A0A8B1VBI1
B	1214	PRO	-	expression tag	UNP A0A8B1VBI1
B	1215	GLU	-	expression tag	UNP A0A8B1VBI1
B	1216	ALA	-	expression tag	UNP A0A8B1VBI1
B	1217	PRO	-	expression tag	UNP A0A8B1VBI1
B	1218	ARG	-	expression tag	UNP A0A8B1VBI1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1219	ASP	-	expression tag	UNP A0A8B1VBI1
B	1220	GLY	-	expression tag	UNP A0A8B1VBI1
B	1221	GLN	-	expression tag	UNP A0A8B1VBI1
B	1222	ALA	-	expression tag	UNP A0A8B1VBI1
B	1223	TYR	-	expression tag	UNP A0A8B1VBI1
B	1224	VAL	-	expression tag	UNP A0A8B1VBI1
B	1225	ARG	-	expression tag	UNP A0A8B1VBI1
B	1226	LYS	-	expression tag	UNP A0A8B1VBI1
B	1227	ASP	-	expression tag	UNP A0A8B1VBI1
B	1228	GLY	-	expression tag	UNP A0A8B1VBI1
B	1229	GLU	-	expression tag	UNP A0A8B1VBI1
B	1230	TRP	-	expression tag	UNP A0A8B1VBI1
B	1231	VAL	-	expression tag	UNP A0A8B1VBI1
B	1232	LEU	-	expression tag	UNP A0A8B1VBI1
B	1233	LEU	-	expression tag	UNP A0A8B1VBI1
B	1234	SER	-	expression tag	UNP A0A8B1VBI1
B	1235	THR	-	expression tag	UNP A0A8B1VBI1
B	1236	PHE	-	expression tag	UNP A0A8B1VBI1
B	1237	LEU	-	expression tag	UNP A0A8B1VBI1
B	1238	GLY	-	expression tag	UNP A0A8B1VBI1
B	1239	ARG	-	expression tag	UNP A0A8B1VBI1
B	1240	SER	-	expression tag	UNP A0A8B1VBI1
B	1241	LEU	-	expression tag	UNP A0A8B1VBI1
B	1242	GLU	-	expression tag	UNP A0A8B1VBI1
B	1243	VAL	-	expression tag	UNP A0A8B1VBI1
B	1244	LEU	-	expression tag	UNP A0A8B1VBI1
B	1245	PHE	-	expression tag	UNP A0A8B1VBI1
B	1246	GLN	-	expression tag	UNP A0A8B1VBI1
B	1247	GLY	-	expression tag	UNP A0A8B1VBI1
B	1248	PRO	-	expression tag	UNP A0A8B1VBI1
B	1249	GLY	-	expression tag	UNP A0A8B1VBI1
B	1250	HIS	-	expression tag	UNP A0A8B1VBI1
B	1251	HIS	-	expression tag	UNP A0A8B1VBI1
B	1252	HIS	-	expression tag	UNP A0A8B1VBI1
B	1253	HIS	-	expression tag	UNP A0A8B1VBI1
B	1254	HIS	-	expression tag	UNP A0A8B1VBI1
B	1255	HIS	-	expression tag	UNP A0A8B1VBI1
B	1256	HIS	-	expression tag	UNP A0A8B1VBI1
B	1257	HIS	-	expression tag	UNP A0A8B1VBI1
B	1258	SER	-	expression tag	UNP A0A8B1VBI1
B	1259	ALA	-	expression tag	UNP A0A8B1VBI1
B	1260	TRP	-	expression tag	UNP A0A8B1VBI1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1261	SER	-	expression tag	UNP A0A8B1VBI1
B	1262	HIS	-	expression tag	UNP A0A8B1VBI1
B	1263	PRO	-	expression tag	UNP A0A8B1VBI1
B	1264	GLN	-	expression tag	UNP A0A8B1VBI1
B	1265	PHE	-	expression tag	UNP A0A8B1VBI1
B	1266	GLU	-	expression tag	UNP A0A8B1VBI1
B	1267	LYS	-	expression tag	UNP A0A8B1VBI1
B	1268	GLY	-	expression tag	UNP A0A8B1VBI1
B	1269	GLY	-	expression tag	UNP A0A8B1VBI1
B	1270	GLY	-	expression tag	UNP A0A8B1VBI1
B	1271	SER	-	expression tag	UNP A0A8B1VBI1
B	1272	GLY	-	expression tag	UNP A0A8B1VBI1
B	1273	GLY	-	expression tag	UNP A0A8B1VBI1
B	1274	GLY	-	expression tag	UNP A0A8B1VBI1
B	1275	GLY	-	expression tag	UNP A0A8B1VBI1
B	1276	SER	-	expression tag	UNP A0A8B1VBI1
B	1277	GLY	-	expression tag	UNP A0A8B1VBI1
B	1278	GLY	-	expression tag	UNP A0A8B1VBI1
B	1279	SER	-	expression tag	UNP A0A8B1VBI1
B	1280	ALA	-	expression tag	UNP A0A8B1VBI1
B	1281	TRP	-	expression tag	UNP A0A8B1VBI1
B	1282	SER	-	expression tag	UNP A0A8B1VBI1
B	1283	HIS	-	expression tag	UNP A0A8B1VBI1
B	1284	PRO	-	expression tag	UNP A0A8B1VBI1
B	1285	GLN	-	expression tag	UNP A0A8B1VBI1
B	1286	PHE	-	expression tag	UNP A0A8B1VBI1
B	1287	GLU	-	expression tag	UNP A0A8B1VBI1
B	1288	LYS	-	expression tag	UNP A0A8B1VBI1
G	682	GLY	ARG	conflict	UNP A0A8B1VBI1
G	683	SER	ARG	conflict	UNP A0A8B1VBI1
G	685	SER	ARG	conflict	UNP A0A8B1VBI1
G	817	PRO	PHE	conflict	UNP A0A8B1VBI1
G	892	PRO	ALA	conflict	UNP A0A8B1VBI1
G	899	PRO	ALA	conflict	UNP A0A8B1VBI1
G	942	PRO	ALA	conflict	UNP A0A8B1VBI1
G	986	PRO	LYS	conflict	UNP A0A8B1VBI1
G	987	PRO	VAL	conflict	UNP A0A8B1VBI1
G	1209	GLY	-	expression tag	UNP A0A8B1VBI1
G	1210	SER	-	expression tag	UNP A0A8B1VBI1
G	1211	GLY	-	expression tag	UNP A0A8B1VBI1
G	1212	TYR	-	expression tag	UNP A0A8B1VBI1
G	1213	ILE	-	expression tag	UNP A0A8B1VBI1

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	1214	PRO	-	expression tag	UNP A0A8B1VBI1
G	1215	GLU	-	expression tag	UNP A0A8B1VBI1
G	1216	ALA	-	expression tag	UNP A0A8B1VBI1
G	1217	PRO	-	expression tag	UNP A0A8B1VBI1
G	1218	ARG	-	expression tag	UNP A0A8B1VBI1
G	1219	ASP	-	expression tag	UNP A0A8B1VBI1
G	1220	GLY	-	expression tag	UNP A0A8B1VBI1
G	1221	GLN	-	expression tag	UNP A0A8B1VBI1
G	1222	ALA	-	expression tag	UNP A0A8B1VBI1
G	1223	TYR	-	expression tag	UNP A0A8B1VBI1
G	1224	VAL	-	expression tag	UNP A0A8B1VBI1
G	1225	ARG	-	expression tag	UNP A0A8B1VBI1
G	1226	LYS	-	expression tag	UNP A0A8B1VBI1
G	1227	ASP	-	expression tag	UNP A0A8B1VBI1
G	1228	GLY	-	expression tag	UNP A0A8B1VBI1
G	1229	GLU	-	expression tag	UNP A0A8B1VBI1
G	1230	TRP	-	expression tag	UNP A0A8B1VBI1
G	1231	VAL	-	expression tag	UNP A0A8B1VBI1
G	1232	LEU	-	expression tag	UNP A0A8B1VBI1
G	1233	LEU	-	expression tag	UNP A0A8B1VBI1
G	1234	SER	-	expression tag	UNP A0A8B1VBI1
G	1235	THR	-	expression tag	UNP A0A8B1VBI1
G	1236	PHE	-	expression tag	UNP A0A8B1VBI1
G	1237	LEU	-	expression tag	UNP A0A8B1VBI1
G	1238	GLY	-	expression tag	UNP A0A8B1VBI1
G	1239	ARG	-	expression tag	UNP A0A8B1VBI1
G	1240	SER	-	expression tag	UNP A0A8B1VBI1
G	1241	LEU	-	expression tag	UNP A0A8B1VBI1
G	1242	GLU	-	expression tag	UNP A0A8B1VBI1
G	1243	VAL	-	expression tag	UNP A0A8B1VBI1
G	1244	LEU	-	expression tag	UNP A0A8B1VBI1
G	1245	PHE	-	expression tag	UNP A0A8B1VBI1
G	1246	GLN	-	expression tag	UNP A0A8B1VBI1
G	1247	GLY	-	expression tag	UNP A0A8B1VBI1
G	1248	PRO	-	expression tag	UNP A0A8B1VBI1
G	1249	GLY	-	expression tag	UNP A0A8B1VBI1
G	1250	HIS	-	expression tag	UNP A0A8B1VBI1
G	1251	HIS	-	expression tag	UNP A0A8B1VBI1
G	1252	HIS	-	expression tag	UNP A0A8B1VBI1
G	1253	HIS	-	expression tag	UNP A0A8B1VBI1
G	1254	HIS	-	expression tag	UNP A0A8B1VBI1
G	1255	HIS	-	expression tag	UNP A0A8B1VBI1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	1256	HIS	-	expression tag	UNP A0A8B1VBI1
G	1257	HIS	-	expression tag	UNP A0A8B1VBI1
G	1258	SER	-	expression tag	UNP A0A8B1VBI1
G	1259	ALA	-	expression tag	UNP A0A8B1VBI1
G	1260	TRP	-	expression tag	UNP A0A8B1VBI1
G	1261	SER	-	expression tag	UNP A0A8B1VBI1
G	1262	HIS	-	expression tag	UNP A0A8B1VBI1
G	1263	PRO	-	expression tag	UNP A0A8B1VBI1
G	1264	GLN	-	expression tag	UNP A0A8B1VBI1
G	1265	PHE	-	expression tag	UNP A0A8B1VBI1
G	1266	GLU	-	expression tag	UNP A0A8B1VBI1
G	1267	LYS	-	expression tag	UNP A0A8B1VBI1
G	1268	GLY	-	expression tag	UNP A0A8B1VBI1
G	1269	GLY	-	expression tag	UNP A0A8B1VBI1
G	1270	GLY	-	expression tag	UNP A0A8B1VBI1
G	1271	SER	-	expression tag	UNP A0A8B1VBI1
G	1272	GLY	-	expression tag	UNP A0A8B1VBI1
G	1273	GLY	-	expression tag	UNP A0A8B1VBI1
G	1274	GLY	-	expression tag	UNP A0A8B1VBI1
G	1275	GLY	-	expression tag	UNP A0A8B1VBI1
G	1276	SER	-	expression tag	UNP A0A8B1VBI1
G	1277	GLY	-	expression tag	UNP A0A8B1VBI1
G	1278	GLY	-	expression tag	UNP A0A8B1VBI1
G	1279	SER	-	expression tag	UNP A0A8B1VBI1
G	1280	ALA	-	expression tag	UNP A0A8B1VBI1
G	1281	TRP	-	expression tag	UNP A0A8B1VBI1
G	1282	SER	-	expression tag	UNP A0A8B1VBI1
G	1283	HIS	-	expression tag	UNP A0A8B1VBI1
G	1284	PRO	-	expression tag	UNP A0A8B1VBI1
G	1285	GLN	-	expression tag	UNP A0A8B1VBI1
G	1286	PHE	-	expression tag	UNP A0A8B1VBI1
G	1287	GLU	-	expression tag	UNP A0A8B1VBI1
G	1288	LYS	-	expression tag	UNP A0A8B1VBI1

- Molecule 2 is a protein called SWA9H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	121	Total	C	N	O	S	0	0
			927	574	165	180	8		
2	H	121	Total	C	N	O	S	0	0
			927	574	165	180	8		
2	M	121	Total	C	N	O	S	0	0
			927	574	165	180	8		

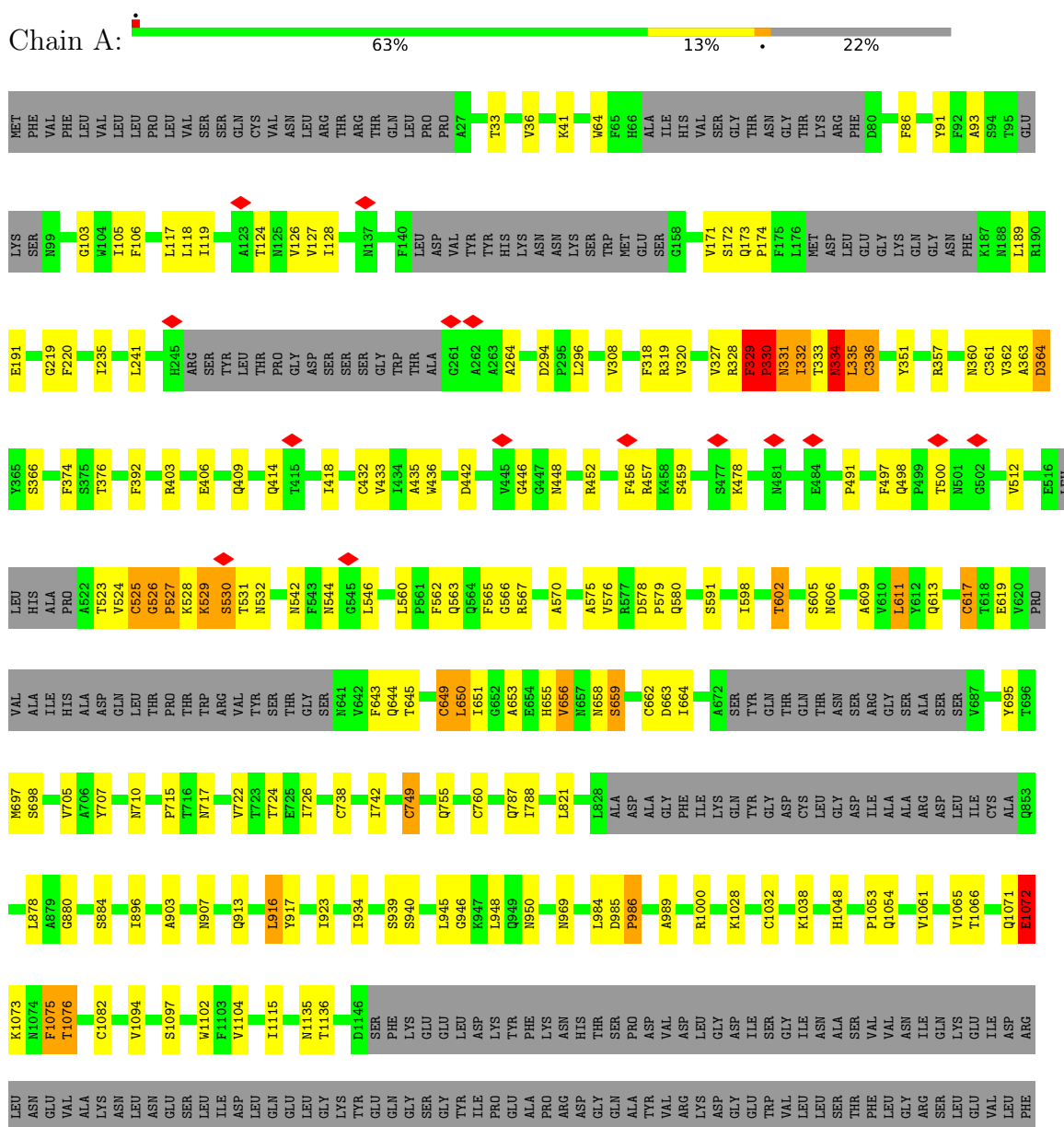
- Molecule 3 is a protein called SWA9L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	107	Total	C	N	O	S	0	0
			822	519	143	158	2		
3	L	107	Total	C	N	O	S	0	0
			822	519	143	158	2		
3	N	107	Total	C	N	O	S	0	0
			822	519	143	158	2		

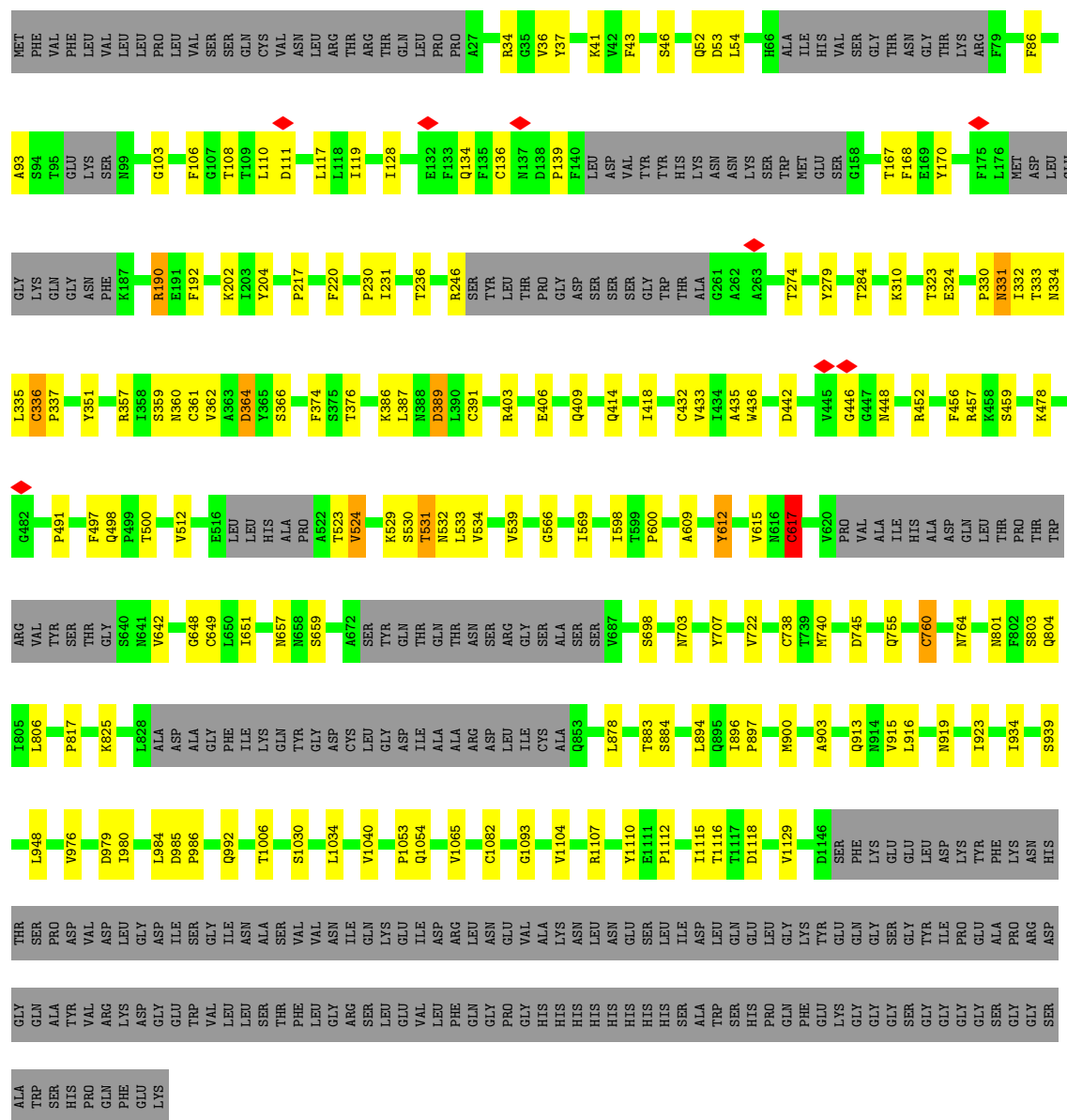
### 3 Residue-property plots

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

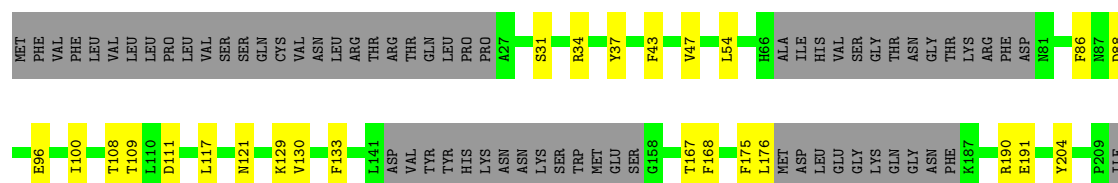
#### • Molecule 1: Surface glycoprotein

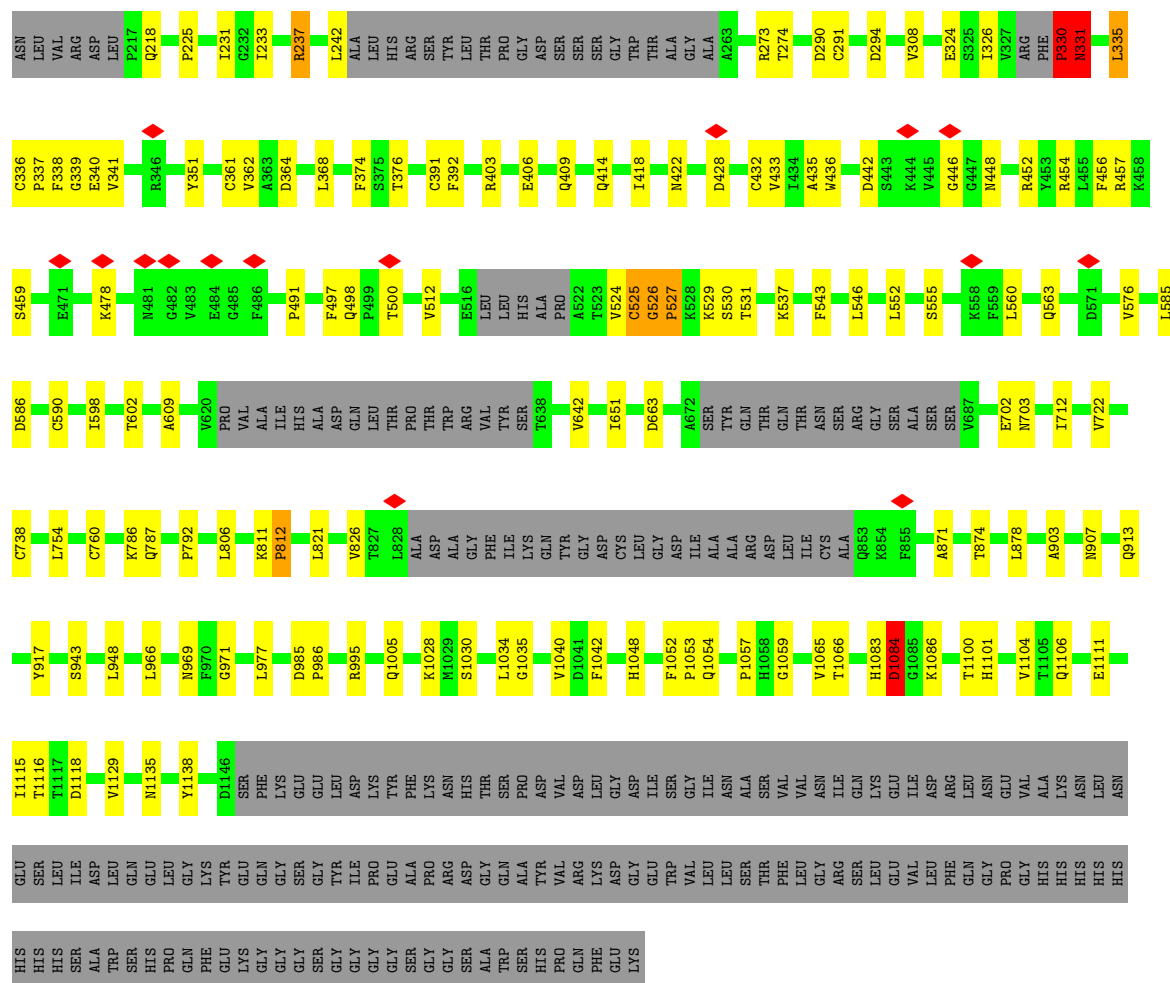


Chain B:

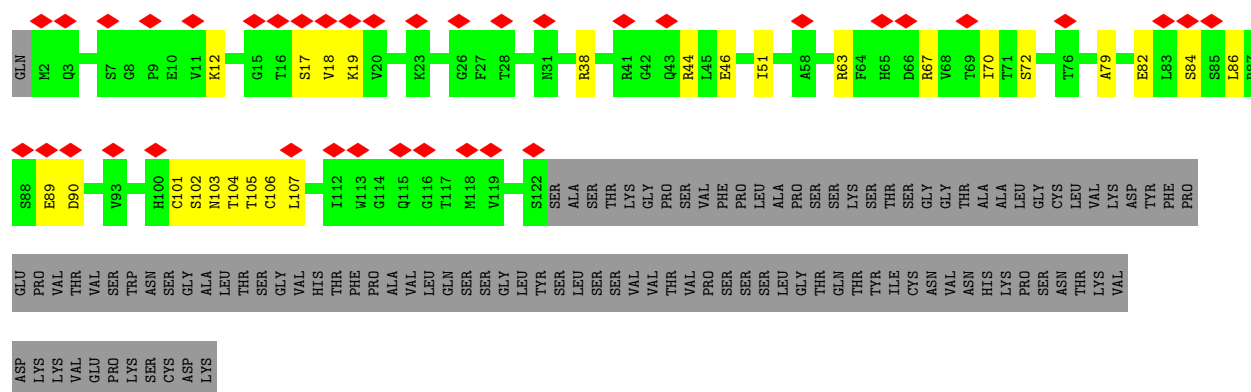


## Chain G:





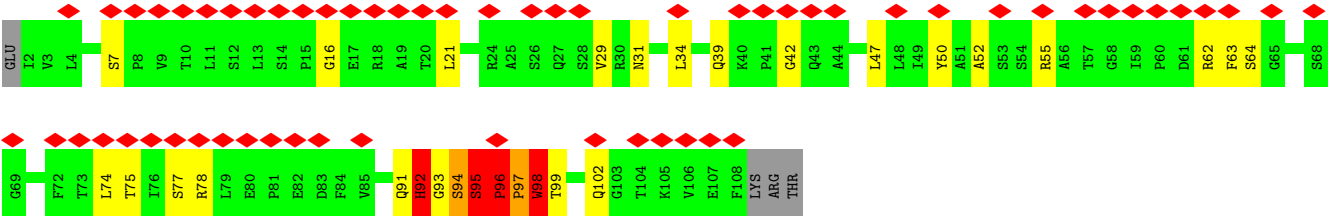
- Molecule 2: SWA9H



- Molecule 2: SWA9H









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	324843	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.180	Depositor
Minimum map value	-1.492	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.304	Depositor
Map size ( $\text{\AA}$ )	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.74	9/7855 (0.1%)	0.81	14/10702 (0.1%)
1	B	0.69	4/7908 (0.1%)	0.71	12/10767 (0.1%)
1	G	0.70	2/7822 (0.0%)	0.71	10/10648 (0.1%)
2	D	0.35	0/945	0.67	1/1281 (0.1%)
2	H	0.35	0/945	0.67	1/1281 (0.1%)
2	M	0.35	0/945	0.67	1/1281 (0.1%)
3	E	0.69	5/843 (0.6%)	1.01	1/1148 (0.1%)
3	L	0.69	5/843 (0.6%)	1.01	1/1148 (0.1%)
3	N	0.69	5/843 (0.6%)	1.01	1/1148 (0.1%)
All	All	0.68	30/28949 (0.1%)	0.76	42/39404 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
1	G	0	6
3	E	0	1
3	L	0	1
3	N	0	1
All	All	0	19

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	738	CYS	CB-SG	-6.88	1.70	1.82
1	A	617	CYS	CB-SG	6.30	1.93	1.82
1	A	1072	GLU	C-O	-6.04	1.11	1.23
1	G	738	CYS	CB-SG	-5.94	1.72	1.81
1	A	1072	GLU	CG-CD	-5.82	1.43	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1094	VAL	CB-CG1	-5.81	1.40	1.52
3	L	92	HIS	CA-C	-5.74	1.38	1.52
1	A	1082	CYS	CB-SG	-5.74	1.72	1.81
3	N	92	HIS	CA-C	-5.73	1.38	1.52
1	B	760	CYS	CB-SG	-5.71	1.72	1.81
3	E	92	HIS	CA-C	-5.71	1.38	1.52
1	A	1076	THR	C-O	-5.65	1.12	1.23
1	A	1094	VAL	CB-CG2	-5.64	1.41	1.52
3	E	98	TRP	CB-CG	-5.49	1.40	1.50
3	N	98	TRP	CB-CG	-5.46	1.40	1.50
3	L	98	TRP	CB-CG	-5.42	1.40	1.50
3	L	92	HIS	N-CA	-5.40	1.35	1.46
3	E	98	TRP	CD2-CE2	-5.38	1.34	1.41
3	N	92	HIS	N-CA	-5.33	1.35	1.46
3	E	92	HIS	N-CA	-5.33	1.35	1.46
3	N	98	TRP	CD2-CE2	-5.30	1.34	1.41
3	L	98	TRP	CD2-CE2	-5.30	1.34	1.41
3	L	98	TRP	CG-CD1	-5.18	1.29	1.36
1	A	1072	GLU	CA-CB	-5.16	1.42	1.53
1	A	1075	PHE	C-O	-5.11	1.13	1.23
1	B	615	VAL	C-O	-5.08	1.13	1.23
1	G	1040	VAL	CB-CG1	-5.08	1.42	1.52
3	N	98	TRP	CG-CD1	-5.03	1.29	1.36
3	E	98	TRP	CG-CD1	-5.03	1.29	1.36
1	B	617	CYS	CB-SG	-5.03	1.73	1.81

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	PHE	C-N-CD	-25.38	64.77	120.60
1	A	526	GLY	C-N-CD	-24.77	66.10	120.60
3	L	96	PRO	C-N-CD	-18.99	78.82	120.60
3	N	96	PRO	C-N-CD	-18.98	78.83	120.60
3	E	96	PRO	C-N-CD	-18.93	78.95	120.60
1	G	526	GLY	C-N-CD	-12.40	93.32	120.60
1	B	738	CYS	CA-CB-SG	8.84	129.92	114.00
1	B	760	CYS	CA-CB-SG	-7.75	100.05	114.00
1	B	617	CYS	CA-CB-SG	-7.63	100.26	114.00
1	A	749	CYS	CA-CB-SG	7.49	127.49	114.00
1	A	334	ASN	C-N-CA	-7.14	103.86	121.70
1	A	546	LEU	CA-CB-CG	6.91	131.18	115.30
1	A	649	CYS	CB-CA-C	-6.78	96.84	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1072	GLU	CB-CA-C	-6.60	97.20	110.40
1	G	432	CYS	CA-CB-SG	6.54	125.77	114.00
1	A	432	CYS	CA-CB-SG	6.54	125.77	114.00
1	B	432	CYS	CA-CB-SG	6.53	125.75	114.00
1	G	760	CYS	CA-CB-SG	-6.50	102.30	114.00
1	G	330	PRO	CA-C-N	-6.31	103.31	117.20
1	B	190	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	G	364	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	364	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	364	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	948	LEU	CB-CG-CD1	-5.96	100.88	111.00
1	B	333	THR	N-CA-C	5.83	126.73	111.00
1	G	821	LEU	CB-CG-CD1	5.73	120.74	111.00
1	A	41	LYS	CA-CB-CG	5.72	125.99	113.40
1	G	754	LEU	CA-CB-CG	5.69	128.39	115.30
1	G	331	ASN	N-CA-C	-5.69	95.64	111.00
1	A	878	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	B	336	CYS	CB-CA-C	5.57	121.55	110.40
1	A	611	LEU	CB-CG-CD1	-5.44	101.76	111.00
1	B	745	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	1082	CYS	CA-CB-SG	5.39	123.69	114.00
1	A	916	LEU	CA-CB-CG	-5.26	103.20	115.30
1	A	330	PRO	N-CA-C	5.24	125.73	112.10
2	D	107	LEU	CA-CB-CG	5.17	127.19	115.30
2	H	107	LEU	CA-CB-CG	5.16	127.17	115.30
2	M	107	LEU	CA-CB-CG	5.14	127.12	115.30
1	G	812	PRO	CA-N-CD	-5.13	104.32	111.50
1	B	533	LEU	CA-CB-CG	5.07	126.95	115.30
1	G	428	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	PRO	Mainchain
1	A	570	ALA	Peptide
1	A	749	CYS	Peptide
1	A	86	PHE	Peptide
1	A	940	SER	Peptide
1	A	986	PRO	Peptide
1	B	110	LEU	Peptide
1	B	612	TYR	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	657	ASN	Peptide
1	B	86	PHE	Peptide
3	E	7	SER	Peptide
1	G	1084	ASP	Peptide
1	G	31	SER	Peptide
1	G	330	PRO	Mainchain
1	G	590	CYS	Peptide
1	G	86	PHE	Peptide
1	G	986	PRO	Peptide
3	L	7	SER	Peptide
3	N	7	SER	Peptide

## 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	7683	0	7408	154	0
1	B	7736	0	7498	116	0
1	G	7653	0	7425	116	0
2	D	927	0	894	15	0
2	H	927	0	894	13	0
2	M	927	0	894	13	0
3	E	822	0	802	42	0
3	L	822	0	802	43	0
3	N	822	0	802	41	0
All	All	28319	0	27419	512	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 9.

All (512) 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)
3:E:96:PRO:HB2	3:E:97:PRO:CD	1.58	1.33
3:L:96:PRO:HB2	3:L:97:PRO:CD	1.58	1.33
3:N:96:PRO:HB2	3:N:97:PRO:CD	1.58	1.32

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:95:SER:CB	3:N:96:PRO:HD3	1.61	1.29
3:E:96:PRO:CB	3:E:97:PRO:HD3	1.59	1.29
3:L:95:SER:CB	3:L:96:PRO:HD3	1.61	1.28
1:A:392:PHE:O	1:A:524:VAL:CG2	1.78	1.28
1:B:530:SER:O	1:B:531:THR:CG2	1.80	1.27
1:A:392:PHE:O	1:A:524:VAL:HG22	1.13	1.26
3:N:96:PRO:CB	3:N:97:PRO:HD3	1.58	1.25
1:B:530:SER:O	1:B:531:THR:HG22	1.34	1.23
3:L:96:PRO:CB	3:L:97:PRO:HD3	1.58	1.22
3:L:96:PRO:CB	3:L:97:PRO:CD	2.17	1.21
3:E:95:SER:CB	3:E:96:PRO:HD3	1.61	1.20
1:A:392:PHE:C	1:A:524:VAL:CG2	2.12	1.19
3:E:95:SER:OG	3:E:96:PRO:HD3	1.42	1.17
1:A:362:VAL:HG13	1:A:526:GLY:O	1.40	1.15
3:L:95:SER:OG	3:L:96:PRO:HD3	1.42	1.15
1:A:362:VAL:CG1	1:A:526:GLY:O	1.95	1.15
3:N:95:SER:OG	3:N:96:PRO:HD3	1.42	1.14
3:N:91:GLN:HE22	3:N:94:SER:HB3	1.07	1.14
1:A:357:ARG:CZ	1:B:167:THR:O	1.97	1.12
3:L:91:GLN:HE22	3:L:94:SER:HB3	1.07	1.11
1:A:330:PRO:CD	1:A:580:GLN:HG2	1.58	1.10
1:A:336:CYS:SG	1:A:363:ALA:HA	1.92	1.09
3:E:91:GLN:HE22	3:E:94:SER:HB3	1.07	1.08
1:A:330:PRO:HD3	1:A:580:GLN:HG2	1.20	1.08
3:E:96:PRO:CB	3:E:97:PRO:CD	2.17	1.07
3:N:96:PRO:CB	3:N:97:PRO:CD	2.17	1.06
1:A:643:PHE:CZ	1:A:655:HIS:CE1	2.43	1.05
3:E:95:SER:CB	3:E:96:PRO:CD	2.36	1.03
3:L:95:SER:CB	3:L:96:PRO:CD	2.35	1.03
3:N:95:SER:CB	3:N:96:PRO:CD	2.36	1.02
1:B:360:ASN:ND2	1:G:168:PHE:CD1	2.28	1.02
3:L:95:SER:HB2	3:L:96:PRO:HD3	1.41	1.02
3:L:95:SER:OG	3:L:96:PRO:CD	2.08	1.02
3:N:95:SER:OG	3:N:96:PRO:CD	2.08	1.01
1:B:360:ASN:ND2	1:G:168:PHE:CE1	2.28	1.00
3:E:95:SER:OG	3:E:96:PRO:CD	2.08	1.00
3:N:91:GLN:HE22	3:N:94:SER:CB	1.75	1.00
3:L:91:GLN:HE22	3:L:94:SER:CB	1.75	1.00
3:N:91:GLN:NE2	3:N:94:SER:HB3	1.77	0.99
3:E:95:SER:HB2	3:E:96:PRO:HD3	1.42	0.99
3:E:91:GLN:NE2	3:E:94:SER:HB3	1.76	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:91:GLN:NE2	3:L:94:SER:HB3	1.76	0.98
3:E:91:GLN:HE22	3:E:94:SER:CB	1.75	0.98
1:B:617:CYS:HA	1:B:649:CYS:SG	2.05	0.97
3:N:95:SER:HB2	3:N:96:PRO:HD3	1.42	0.96
1:B:360:ASN:HD21	1:G:168:PHE:HD1	1.14	0.95
3:N:91:GLN:NE2	3:N:94:SER:CB	2.31	0.94
1:A:330:PRO:CD	1:A:580:GLN:CG	2.41	0.91
1:B:530:SER:O	1:B:531:THR:HG23	1.70	0.91
3:E:91:GLN:NE2	3:E:94:SER:CB	2.30	0.91
1:A:392:PHE:C	1:A:524:VAL:HG22	1.84	0.91
3:L:91:GLN:NE2	3:L:94:SER:CB	2.30	0.91
1:A:336:CYS:SG	1:A:363:ALA:CA	2.56	0.90
3:E:92:HIS:O	3:E:92:HIS:ND1	2.06	0.89
1:B:334:ASN:CG	1:B:360:ASN:O	2.11	0.88
3:N:92:HIS:O	3:N:92:HIS:ND1	2.06	0.88
3:L:92:HIS:O	3:L:92:HIS:ND1	2.06	0.88
1:A:357:ARG:NH1	1:B:167:THR:O	2.07	0.86
1:G:335:LEU:HD22	1:G:335:LEU:H	1.40	0.86
1:A:643:PHE:CZ	1:A:655:HIS:ND1	2.44	0.85
1:B:334:ASN:OD1	1:B:360:ASN:O	1.92	0.85
3:L:96:PRO:CB	3:L:97:PRO:HD2	2.06	0.85
3:N:97:PRO:O	3:N:99:THR:N	2.11	0.84
3:L:97:PRO:O	3:L:99:THR:N	2.11	0.83
3:N:96:PRO:CB	3:N:97:PRO:HD2	2.05	0.83
3:E:97:PRO:O	3:E:99:THR:N	2.11	0.83
3:N:96:PRO:CG	3:N:97:PRO:HD2	2.09	0.83
3:L:96:PRO:CG	3:L:97:PRO:HD2	2.09	0.82
3:E:96:PRO:CB	3:E:97:PRO:HD2	2.05	0.81
1:G:391:CYS:HG	1:G:525:CYS:HG	1.27	0.81
3:E:96:PRO:CG	3:E:97:PRO:HD2	2.09	0.81
3:N:96:PRO:HG2	3:N:97:PRO:HD2	1.63	0.81
1:A:330:PRO:HD3	1:A:580:GLN:CG	2.07	0.81
3:L:96:PRO:HG2	3:L:97:PRO:HD2	1.63	0.81
3:E:96:PRO:HG2	3:E:97:PRO:HD2	1.63	0.79
1:A:363:ALA:N	1:A:525:CYS:O	2.16	0.79
1:G:335:LEU:HA	1:G:362:VAL:O	1.83	0.79
1:G:391:CYS:SG	1:G:524:VAL:O	2.41	0.79
3:E:95:SER:HG	3:E:96:PRO:HD3	1.49	0.78
1:B:334:ASN:ND2	1:B:360:ASN:O	2.17	0.77
1:B:530:SER:C	1:B:531:THR:HG23	2.05	0.76
1:B:360:ASN:ND2	1:G:168:PHE:HE1	1.82	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PHE:C	1:A:524:VAL:HG21	2.07	0.75
1:G:335:LEU:H	1:G:335:LEU:CD2	1.99	0.75
1:B:330:PRO:O	1:B:331:ASN:O	2.06	0.74
1:B:530:SER:C	1:B:531:THR:CG2	2.50	0.74
1:A:392:PHE:O	1:A:524:VAL:HG23	1.86	0.73
1:B:617:CYS:HG	1:B:649:CYS:HG	1.21	0.72
1:A:296:LEU:HD21	1:A:606:ASN:HD22	1.55	0.72
1:G:338:PHE:O	1:G:341:VAL:N	2.21	0.71
1:A:523:THR:CG2	1:B:230:PRO:HG2	2.21	0.71
3:N:91:GLN:NE2	3:N:94:SER:HB2	2.05	0.70
3:E:91:GLN:NE2	3:E:94:SER:HB2	2.05	0.70
1:A:334:ASN:OD1	1:A:361:CYS:HB3	1.91	0.70
1:A:643:PHE:CE2	1:A:655:HIS:ND1	2.59	0.70
1:B:334:ASN:O	1:B:362:VAL:N	2.18	0.70
3:L:91:GLN:NE2	3:L:94:SER:HB2	2.05	0.69
1:A:529:LYS:O	1:A:530:SER:HB3	1.92	0.69
1:A:327:VAL:HA	1:A:542:ASN:HB3	1.75	0.69
1:B:612:TYR:O	1:B:648:GLY:HA3	1.93	0.69
1:B:357:ARG:NH1	1:G:167:THR:O	2.26	0.68
1:A:328:ARG:HD2	1:A:531:THR:H	1.59	0.67
1:B:360:ASN:ND2	1:G:168:PHE:HD1	1.81	0.67
1:A:821:LEU:HD11	1:A:939:SER:HB2	1.78	0.66
1:G:555:SER:HB2	1:G:586:ASP:HB2	1.78	0.65
1:G:336:CYS:HB3	1:G:337:PRO:CD	2.26	0.65
1:A:643:PHE:CE2	1:A:655:HIS:CE1	2.84	0.65
1:A:392:PHE:C	1:A:524:VAL:HG23	2.13	0.65
3:N:96:PRO:HB2	3:N:97:PRO:HD3	0.74	0.65
3:E:96:PRO:HB2	3:E:97:PRO:HD3	0.74	0.65
1:G:336:CYS:N	1:G:362:VAL:O	2.26	0.65
1:A:296:LEU:CD2	1:A:606:ASN:HD22	2.09	0.64
3:N:64:SER:HB3	3:N:75:THR:HB	1.80	0.64
1:B:330:PRO:C	1:B:331:ASN:O	2.34	0.64
1:A:392:PHE:H	1:A:524:VAL:HG23	1.61	0.64
3:E:64:SER:HB3	3:E:75:THR:HB	1.80	0.64
3:L:95:SER:HB2	3:L:96:PRO:CD	2.19	0.63
1:A:724:THR:HB	1:A:934:ILE:HD11	1.81	0.63
1:A:524:VAL:HG23	1:A:524:VAL:O	1.98	0.63
3:L:64:SER:HB3	3:L:75:THR:HB	1.80	0.63
1:G:335:LEU:CA	1:G:362:VAL:O	2.47	0.62
1:G:1030:SER:HA	1:G:1034:LEU:HD12	1.81	0.62
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.63	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:CYS:HB3	1:A:361:CYS:SG	2.39	0.62
1:G:391:CYS:HG	1:G:525:CYS:CB	2.10	0.62
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.65	0.62
3:E:95:SER:OG	3:E:96:PRO:HD2	1.99	0.62
1:B:760:CYS:O	1:B:764:ASN:ND2	2.33	0.61
3:N:95:SER:OG	3:N:96:PRO:HD2	1.99	0.61
1:A:392:PHE:N	1:A:524:VAL:HG23	2.15	0.61
1:A:330:PRO:HG2	1:A:579:PRO:O	1.92	0.61
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.34	0.60
1:G:811:LYS:NZ	1:G:812:PRO:O	2.31	0.60
1:B:659:SER:HB3	1:B:698:SER:HB2	1.83	0.60
1:B:1006:THR:OG1	1:G:1005:GLN:NE2	2.34	0.60
1:B:117:LEU:HD21	1:B:231:ILE:HG21	1.84	0.60
1:G:1028:LYS:NZ	1:G:1042:PHE:O	2.34	0.60
1:A:357:ARG:NH1	1:B:168:PHE:HA	2.17	0.60
3:L:96:PRO:HB2	3:L:97:PRO:HD3	0.74	0.60
1:G:326:ILE:O	1:G:531:THR:OG1	2.19	0.59
1:A:392:PHE:CA	1:A:524:VAL:CG2	2.80	0.59
1:B:617:CYS:HA	1:B:649:CYS:HG	1.67	0.59
1:A:656:VAL:HG12	1:A:695:TYR:HB3	1.84	0.59
1:A:392:PHE:CA	1:A:524:VAL:HG23	2.33	0.59
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.36	0.58
3:N:95:SER:HB2	3:N:96:PRO:CD	2.19	0.58
1:B:531:THR:OG1	1:B:532:ASN:N	2.34	0.58
1:A:916:LEU:HD12	1:A:923:ILE:HD13	1.84	0.58
1:A:566:GLY:HA2	1:B:43:PHE:HB3	1.85	0.58
1:A:334:ASN:ND2	1:A:360:ASN:O	2.31	0.58
1:A:357:ARG:NE	1:B:167:THR:O	2.36	0.58
1:B:976:VAL:HG12	1:B:979:ASP:H	1.68	0.58
1:A:127:VAL:HG22	1:A:171:VAL:HG22	1.85	0.57
3:E:96:PRO:CG	3:E:97:PRO:CD	2.74	0.57
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.21	0.57
3:N:95:SER:HG	3:N:96:PRO:HD3	1.67	0.57
1:A:329:PHE:N	1:A:329:PHE:CD1	2.72	0.56
1:G:391:CYS:CB	1:G:525:CYS:HB3	2.35	0.56
1:A:446:GLY:H	1:A:498:GLN:HE22	1.54	0.56
3:L:95:SER:OG	3:L:96:PRO:HD2	1.99	0.56
1:G:478:LYS:NZ	3:N:31:ASN:O	2.39	0.56
1:A:478:LYS:NZ	3:E:31:ASN:O	2.39	0.56
2:M:38:ARG:HH11	2:M:90:ASP:HA	1.71	0.56
1:B:446:GLY:H	1:B:498:GLN:HE22	1.54	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:446:GLY:H	1:G:498:GLN:HE22	1.54	0.56
1:G:130:VAL:HB	1:G:168:PHE:HB3	1.88	0.55
2:H:102:SER:O	2:H:102:SER:OG	2.23	0.55
1:G:338:PHE:O	1:G:340:GLU:N	2.39	0.55
1:A:362:VAL:HG11	1:A:526:GLY:O	2.01	0.55
2:D:38:ARG:HH11	2:D:90:ASP:HA	1.71	0.55
1:A:118:LEU:O	1:A:128:ILE:HA	2.06	0.55
1:G:560:LEU:HB3	1:G:563:GLN:HG3	1.88	0.55
3:E:95:SER:HB2	3:E:96:PRO:CD	2.19	0.55
3:E:97:PRO:O	3:E:99:THR:OG1	2.13	0.55
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.89	0.55
2:H:38:ARG:HH11	2:H:90:ASP:HA	1.71	0.55
3:L:96:PRO:CG	3:L:97:PRO:CD	2.74	0.55
3:N:98:TRP:CD1	3:N:98:TRP:N	2.70	0.55
1:G:273:ARG:NH2	1:G:290:ASP:OD2	2.40	0.55
1:A:172:SER:OG	1:A:173:GLN:N	2.39	0.54
1:G:392:PHE:O	1:G:524:VAL:CG2	2.55	0.54
1:B:478:LYS:NZ	3:L:31:ASN:O	2.39	0.54
1:G:722:VAL:HG22	1:G:1065:VAL:HG22	1.89	0.54
1:B:111:ASP:HA	1:B:134:GLN:HA	1.88	0.54
1:A:329:PHE:HD2	1:A:544:ASN:HA	1.73	0.54
1:G:1053:PRO:O	1:G:1054:GLN:NE2	2.41	0.54
3:E:98:TRP:CD1	3:E:98:TRP:N	2.70	0.54
1:A:562:PHE:O	1:B:41:LYS:NZ	2.37	0.54
2:D:38:ARG:NH1	2:D:89:GLU:O	2.41	0.54
1:G:1106:GLN:HE21	1:G:1111:GLU:HG2	1.73	0.54
1:B:336:CYS:SG	1:B:362:VAL:N	2.75	0.53
1:G:335:LEU:HA	1:G:362:VAL:HB	1.91	0.53
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.90	0.53
2:M:38:ARG:NH1	2:M:89:GLU:O	2.41	0.53
1:B:1030:SER:HA	1:B:1034:LEU:HD12	1.90	0.53
1:G:338:PHE:O	1:G:339:GLY:C	2.46	0.53
1:G:391:CYS:SG	1:G:525:CYS:HB3	2.48	0.53
1:A:308:VAL:N	1:A:602:THR:OG1	2.41	0.53
1:A:106:PHE:HB3	1:A:235:ILE:HD11	1.90	0.53
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.27	0.52
1:A:563:GLN:HE21	1:B:43:PHE:HD1	1.56	0.52
1:G:338:PHE:CD2	1:G:368:LEU:HD11	2.45	0.52
2:H:38:ARG:NH1	2:H:89:GLU:O	2.41	0.52
1:A:896:ILE:HA	1:G:712:ILE:HG22	1.91	0.52
1:A:946:GLY:O	1:A:950:ASN:HB2	2.08	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:O	1:B:361:CYS:HB2	2.10	0.52
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.92	0.52
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.91	0.52
1:A:565:PHE:HE1	1:A:567:ARG:HH21	1.58	0.52
1:A:650:LEU:HG	1:A:653:ALA:HB3	1.92	0.51
2:M:38:ARG:NH2	2:M:46:GLU:OE1	2.44	0.51
1:A:334:ASN:OD1	1:A:361:CYS:CB	2.49	0.51
1:A:456:PHE:HD2	1:A:491:PRO:HA	1.76	0.51
2:H:38:ARG:NH2	2:H:46:GLU:OE1	2.44	0.51
1:A:578:ASP:OD1	1:A:578:ASP:N	2.43	0.51
1:A:330:PRO:HG2	1:A:330:PRO:O	2.11	0.51
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.93	0.51
1:G:336:CYS:HB3	1:G:337:PRO:HD2	1.92	0.51
1:G:529:LYS:O	1:G:531:THR:HG23	2.11	0.51
1:A:715:PRO:HD3	1:B:894:LEU:HD21	1.91	0.51
1:B:330:PRO:O	1:B:331:ASN:C	2.45	0.51
1:G:456:PHE:HD2	1:G:491:PRO:HA	1.76	0.51
2:D:38:ARG:NH2	2:D:46:GLU:OE1	2.44	0.51
1:A:351:TYR:OH	1:A:452:ARG:NH2	2.44	0.50
1:G:330:PRO:O	1:G:331:ASN:HB2	2.11	0.50
3:E:62:ARG:HG3	3:E:78:ARG:HB2	1.94	0.50
1:G:34:ARG:NH1	1:G:191:GLU:OE2	2.42	0.50
3:L:62:ARG:HG3	3:L:78:ARG:HB2	1.94	0.50
1:B:1129:VAL:HG13	1:G:917:TYR:HB3	1.93	0.50
2:M:18:VAL:HB	2:M:86:LEU:HD11	1.94	0.50
3:N:97:PRO:O	3:N:99:THR:OG1	2.13	0.50
2:D:51:ILE:HD11	2:D:70:ILE:HG22	1.94	0.50
2:M:51:ILE:HD11	2:M:70:ILE:HG22	1.94	0.50
3:N:91:GLN:HE21	3:N:94:SER:H	1.60	0.50
2:D:18:VAL:HB	2:D:86:LEU:HD11	1.94	0.50
1:B:456:PHE:HD2	1:B:491:PRO:HA	1.76	0.50
2:D:102:SER:O	2:D:102:SER:OG	2.23	0.50
2:M:67:ARG:HB2	2:M:84:SER:HB3	1.94	0.50
1:G:351:TYR:OH	1:G:452:ARG:NH2	2.45	0.50
1:B:351:TYR:OH	1:B:452:ARG:NH2	2.45	0.50
2:H:18:VAL:HB	2:H:86:LEU:HD11	1.94	0.50
1:A:294:ASP:OD1	1:A:294:ASP:N	2.43	0.49
1:A:392:PHE:HB2	1:A:524:VAL:HG21	1.93	0.49
1:B:915:VAL:O	1:B:919:ASN:ND2	2.45	0.49
3:N:62:ARG:HG3	3:N:78:ARG:HB2	1.94	0.49
1:A:105:ILE:HD11	1:A:241:LEU:HD21	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:ASP:N	1:G:294:ASP:OD1	2.45	0.49
2:H:67:ARG:HB2	2:H:84:SER:HB3	1.94	0.49
1:A:33:THR:OG1	1:A:219:GLY:O	2.30	0.49
1:B:939:SER:O	1:B:939:SER:OG	2.28	0.49
1:G:374:PHE:HA	1:G:436:TRP:HB3	1.95	0.49
2:M:101:CYS:HA	2:M:106:CYS:HA	1.94	0.49
1:A:376:THR:HB	1:A:435:ALA:HB3	1.95	0.49
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.95	0.49
3:E:91:GLN:HE21	3:E:94:SER:H	1.59	0.49
2:D:67:ARG:HB2	2:D:84:SER:HB3	1.94	0.49
1:G:108:THR:O	1:G:237:ARG:NE	2.45	0.49
2:D:101:CYS:HA	2:D:106:CYS:HA	1.94	0.49
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.95	0.48
1:A:457:ARG:NH1	1:A:459:SER:O	2.44	0.48
1:G:34:ARG:NH2	1:G:218:GLN:O	2.46	0.48
3:E:16:GLY:HA2	3:E:78:ARG:HH12	1.79	0.48
1:G:96:GLU:OE1	1:G:100:ILE:N	2.44	0.48
2:M:102:SER:O	2:M:102:SER:OG	2.23	0.48
1:A:705:VAL:HB	1:B:883:THR:HG21	1.95	0.48
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.95	0.48
2:H:101:CYS:HA	2:H:106:CYS:HA	1.95	0.48
3:N:16:GLY:HA2	3:N:78:ARG:HH12	1.79	0.48
1:A:333:THR:O	1:A:335:LEU:N	2.46	0.48
1:B:980:ILE:HD11	1:B:992:GLN:HB3	1.95	0.48
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.79	0.48
1:B:1110:TYR:CZ	1:B:1112:PRO:HG3	2.49	0.48
3:L:91:GLN:HE21	3:L:94:SER:H	1.60	0.48
3:N:96:PRO:CG	3:N:97:PRO:CD	2.74	0.48
1:B:376:THR:HB	1:B:435:ALA:HB3	1.95	0.48
1:G:442:ASP:O	1:G:448:ASN:ND2	2.47	0.48
3:L:98:TRP:CD1	3:L:98:TRP:N	2.70	0.48
1:A:643:PHE:CE1	1:A:655:HIS:ND1	2.82	0.48
1:A:1075:PHE:CD1	1:A:1075:PHE:N	2.81	0.48
1:B:442:ASP:O	1:B:448:ASN:ND2	2.47	0.48
1:A:332:ILE:HD13	1:A:527:PRO:HB3	1.96	0.48
1:A:442:ASP:O	1:A:448:ASN:ND2	2.47	0.48
1:A:659:SER:HB3	1:A:698:SER:HB3	1.96	0.48
1:A:787:GLN:OE1	1:G:703:ASN:ND2	2.46	0.48
1:B:357:ARG:NH1	1:G:167:THR:OG1	2.46	0.48
1:G:1048:HIS:HA	1:G:1066:THR:HG22	1.96	0.48
1:G:308:VAL:HG22	1:G:602:THR:HG23	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:376:THR:HB	1:G:435:ALA:HB3	1.95	0.48
3:L:16:GLY:HA2	3:L:78:ARG:HH12	1.78	0.48
1:A:332:ILE:CD1	1:A:527:PRO:CB	2.91	0.47
1:B:108:THR:HG23	1:B:236:THR:HG22	1.96	0.47
2:H:51:ILE:HD11	2:H:70:ILE:HG22	1.94	0.47
3:L:62:ARG:HG2	3:L:77:SER:HB3	1.97	0.47
1:G:663:ASP:OD1	1:G:663:ASP:N	2.42	0.47
1:A:124:THR:HG22	1:A:174:PRO:HG3	1.97	0.47
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.97	0.47
1:G:117:LEU:HG	1:G:130:VAL:HG22	1.96	0.47
1:G:392:PHE:O	1:G:524:VAL:HG23	2.15	0.47
1:G:552:LEU:HD13	1:G:585:LEU:HD13	1.96	0.47
1:B:387:LEU:C	1:B:389:ASP:H	2.18	0.47
1:A:332:ILE:CD1	1:A:527:PRO:HB3	2.44	0.47
1:G:903:ALA:HB1	1:G:913:GLN:HB2	1.96	0.47
1:A:329:PHE:CE1	1:A:528:LYS:CB	2.98	0.47
1:A:984:LEU:HB3	1:A:989:ALA:HB2	1.95	0.47
1:B:403:ARG:HG3	1:B:497:PHE:HE1	1.80	0.47
1:B:534:VAL:HG23	1:B:539:VAL:HG11	1.97	0.46
1:G:642:VAL:HG12	1:G:651:ILE:HG12	1.97	0.46
1:G:985:ASP:OD1	1:G:985:ASP:N	2.43	0.46
1:A:318:PHE:HE2	1:A:619:GLU:HB3	1.80	0.46
1:A:330:PRO:HB3	1:A:580:GLN:HB3	1.11	0.46
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.96	0.46
1:B:1040:VAL:HG21	1:G:1035:GLY:HA3	1.97	0.46
2:D:44:ARG:NH1	3:E:102:GLN:OE1	2.48	0.46
1:G:109:THR:OG1	1:G:111:ASP:OD1	2.30	0.46
1:A:93:ALA:HB1	1:A:189:LEU:HD11	1.97	0.46
1:A:329:PHE:HE1	1:A:528:LYS:CB	2.28	0.46
1:A:565:PHE:HB3	1:A:576:VAL:HG23	1.97	0.46
1:G:392:PHE:O	1:G:524:VAL:HG22	2.14	0.46
3:N:62:ARG:HG2	3:N:77:SER:HB3	1.97	0.46
1:A:362:VAL:CG1	1:A:527:PRO:HD3	2.46	0.46
1:A:403:ARG:HG3	1:A:497:PHE:HE1	1.81	0.46
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.45	0.46
1:G:88:ASP:OD1	1:G:88:ASP:N	2.47	0.46
1:G:403:ARG:HG3	1:G:497:PHE:HE1	1.81	0.46
1:B:93:ALA:HA	1:B:190:ARG:O	2.15	0.46
3:N:21:LEU:HD22	3:N:74:LEU:HD23	1.98	0.46
1:A:969:ASN:HB3	1:B:755:GLN:HB3	1.98	0.45
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.96	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:47:LEU:HD21	3:E:50:TYR:HB3	1.98	0.45
3:E:62:ARG:HG2	3:E:77:SER:HB3	1.97	0.45
1:A:560:LEU:HB2	1:A:563:GLN:HE22	1.81	0.45
1:A:643:PHE:HZ	1:A:655:HIS:CE1	2.25	0.45
2:H:44:ARG:NH1	3:L:102:GLN:OE1	2.48	0.45
1:A:103:GLY:HA3	1:A:119:ILE:O	2.17	0.45
1:A:611:LEU:HD23	1:A:613:GLN:HG3	1.98	0.45
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.98	0.45
1:G:1116:THR:OG1	1:G:1118:ASP:OD1	2.21	0.45
3:N:47:LEU:HD21	3:N:50:TYR:HB3	1.98	0.45
1:B:406:GLU:HG3	1:B:418:ILE:HG13	1.98	0.45
1:B:569:ILE:HD12	1:G:47:VAL:HG23	1.99	0.45
1:B:642:VAL:HG13	1:B:651:ILE:HG12	1.98	0.45
1:G:335:LEU:CD2	1:G:335:LEU:N	2.72	0.45
2:M:44:ARG:NH1	3:N:102:GLN:OE1	2.49	0.45
1:A:406:GLU:HG3	1:A:418:ILE:HG13	1.98	0.45
1:A:880:GLY:O	1:A:884:SER:OG	2.26	0.45
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.97	0.45
1:G:391:CYS:HB2	1:G:525:CYS:HB3	1.98	0.45
1:G:526:GLY:HA2	1:G:527:PRO:HD3	1.49	0.45
1:A:560:LEU:HD21	1:B:284:THR:HG22	1.99	0.45
1:A:755:GLN:OE1	1:G:969:ASN:ND2	2.43	0.45
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.98	0.45
3:E:21:LEU:HD22	3:E:74:LEU:HD23	1.99	0.45
3:N:39:GLN:HE22	3:N:42:GLY:H	1.64	0.45
1:A:524:VAL:C	1:A:525:CYS:SG	2.95	0.45
1:A:738:CYS:HB3	1:A:760:CYS:HB3	1.89	0.45
1:B:1093:GLY:HA2	1:B:1107:ARG:HG3	1.99	0.45
3:E:39:GLN:HE22	3:E:42:GLY:H	1.64	0.45
1:G:457:ARG:NH1	1:G:459:SER:O	2.44	0.45
1:G:598:ILE:HB	1:G:609:ALA:HB3	1.99	0.45
1:B:804:GLN:HB2	1:B:817:PRO:HB2	1.98	0.45
3:L:21:LEU:HD22	3:L:74:LEU:HD23	1.99	0.45
1:A:330:PRO:O	1:A:580:GLN:HA	2.17	0.44
1:B:409:GLN:HA	1:B:414:GLN:HG2	1.99	0.44
1:G:1104:VAL:HG23	1:G:1115:ILE:HG12	1.99	0.44
3:L:47:LEU:HD21	3:L:50:TYR:HB3	1.98	0.44
1:A:566:GLY:HA3	1:A:575:ALA:HB3	2.00	0.44
1:A:1072:GLU:O	1:A:1072:GLU:HG2	2.17	0.44
1:B:897:PRO:HG2	1:B:900:MET:HB2	1.99	0.44
2:D:19:LYS:HD2	2:D:82:GLU:HB3	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:274:THR:HG23	1:G:291:CYS:HB2	1.99	0.44
3:N:34:LEU:H	3:N:52:ALA:HB2	1.82	0.44
2:D:63:ARG:O	2:D:67:ARG:NH2	2.51	0.44
2:H:63:ARG:O	2:H:67:ARG:NH2	2.50	0.44
1:A:1038:LYS:HE3	1:A:1038:LYS:HB3	1.77	0.44
1:B:566:GLY:HA2	1:G:43:PHE:HB3	1.99	0.44
1:B:703:ASN:ND2	1:G:787:GLN:OE1	2.32	0.44
1:G:943:SER:O	1:G:943:SER:OG	2.35	0.44
1:G:100:ILE:HG22	1:G:242:LEU:HD11	2.00	0.44
3:L:95:SER:HG	3:L:96:PRO:CD	2.23	0.44
1:B:323:THR:OG1	1:B:324:GLU:N	2.50	0.44
1:A:662:CYS:HB2	1:A:697:MET:HG3	2.00	0.44
1:A:917:TYR:HB3	1:G:1129:VAL:HG13	1.99	0.44
1:G:121:ASN:HD21	1:G:175:PHE:HB2	1.81	0.44
3:N:55:ARG:NH1	3:N:63:PHE:O	2.51	0.44
1:B:128:ILE:HD12	1:B:170:TYR:HD2	1.81	0.44
1:B:192:PHE:HA	1:B:204:TYR:O	2.17	0.44
3:E:34:LEU:H	3:E:52:ALA:HB2	1.82	0.44
1:A:296:LEU:HD21	1:A:606:ASN:ND2	2.28	0.43
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.99	0.43
1:B:598:ILE:HB	1:B:609:ALA:HB3	2.00	0.43
1:G:406:GLU:HG3	1:G:418:ILE:HG13	1.99	0.43
2:M:63:ARG:O	2:M:67:ARG:NH2	2.51	0.43
1:A:644:GLN:NE2	1:A:645:THR:O	2.46	0.43
1:G:1084:ASP:HB2	1:G:1086:LYS:HE2	2.00	0.43
3:L:39:GLN:HE22	3:L:42:GLY:H	1.64	0.43
1:B:804:GLN:HA	1:B:817:PRO:HD2	2.00	0.43
1:G:176:LEU:HG	1:G:190:ARG:HD3	1.99	0.43
1:G:433:VAL:HG13	1:G:512:VAL:HG22	2.00	0.43
3:L:97:PRO:C	3:L:99:THR:N	2.72	0.43
1:B:433:VAL:HG13	1:B:512:VAL:HG22	2.00	0.43
1:B:457:ARG:NH1	1:B:459:SER:O	2.44	0.43
2:H:19:LYS:HD2	2:H:82:GLU:HB3	2.00	0.43
1:A:788:ILE:HB	1:G:702:GLU:HG2	2.01	0.43
1:A:903:ALA:HB1	1:A:913:GLN:HG3	1.99	0.43
1:B:136:CYS:HB2	1:B:139:PRO:HG3	2.00	0.43
1:G:1116:THR:HG22	1:G:1138:TYR:HD2	1.83	0.43
1:B:1107:ARG:HH22	1:G:907:ASN:HD22	1.65	0.43
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.53	0.43
1:A:360:ASN:OD1	1:B:168:PHE:HE1	2.00	0.43
1:B:806:LEU:HA	1:B:806:LEU:HD23	1.85	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:55:ARG:NH1	3:E:63:PHE:O	2.51	0.43
3:E:97:PRO:C	3:E:99:THR:N	2.72	0.43
1:G:409:GLN:HA	1:G:414:GLN:HG2	1.99	0.43
1:G:871:ALA:HA	1:G:874:THR:HG22	2.01	0.43
1:A:433:VAL:HG13	1:A:512:VAL:HG22	2.00	0.43
1:G:324:GLU:OE2	1:G:537:LYS:NZ	2.51	0.43
1:G:786:LYS:HG3	1:G:787:GLN:HG3	2.00	0.43
1:G:826:VAL:HB	1:G:1057:PRO:HG2	2.00	0.43
3:L:34:LEU:H	3:L:52:ALA:HB2	1.82	0.43
3:L:55:ARG:NH1	3:L:63:PHE:O	2.51	0.43
1:B:46:SER:HA	1:B:279:TYR:O	2.19	0.43
2:M:19:LYS:HD2	2:M:82:GLU:HB3	2.00	0.43
1:B:37:TYR:OH	1:B:54:LEU:O	2.24	0.42
1:G:878:LEU:HD21	1:G:1052:PHE:HB3	2.00	0.42
3:L:21:LEU:HB2	3:L:74:LEU:HB3	2.01	0.42
1:A:364:ASP:OD1	1:A:366:SER:OG	2.29	0.42
1:B:903:ALA:HB1	1:B:913:GLN:HG2	2.02	0.42
1:B:984:LEU:HB3	1:B:985:ASP:H	1.72	0.42
1:G:966:LEU:HA	1:G:966:LEU:HD23	1.79	0.42
2:M:104:THR:O	2:M:105:THR:HG23	2.20	0.42
1:B:103:GLY:HA3	1:B:119:ILE:O	2.20	0.42
1:A:319:ARG:HD3	1:B:740:MET:HE1	2.01	0.42
1:A:392:PHE:HB2	1:A:524:VAL:CG2	2.49	0.42
2:D:104:THR:O	2:D:105:THR:HG23	2.20	0.42
3:E:78:ARG:HA	3:E:78:ARG:HH11	1.85	0.42
1:A:320:VAL:HG12	1:A:591:SER:HB3	2.01	0.42
1:A:498:GLN:HG3	1:A:500:THR:H	1.85	0.42
1:A:717:ASN:HB3	1:A:1071:GLN:CG	2.49	0.42
1:B:52:GLN:OE1	1:B:274:THR:OG1	2.31	0.42
1:B:498:GLN:HG3	1:B:500:THR:H	1.85	0.42
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.52	0.42
1:B:530:SER:HB3	1:B:531:THR:H	1.75	0.42
1:B:707:TYR:HB3	1:G:792:PRO:HG3	2.01	0.42
1:B:801:ASN:ND2	1:B:803:SER:OG	2.52	0.42
3:E:40:LYS:HA	3:E:41:PRO:HD3	1.87	0.42
1:G:336:CYS:N	1:G:361:CYS:HB2	2.35	0.42
3:N:29:VAL:HG21	3:N:34:LEU:HD12	2.02	0.42
1:A:332:ILE:CD1	1:A:527:PRO:HB2	2.49	0.42
1:A:985:ASP:HA	1:A:986:PRO:HD3	1.87	0.42
1:G:1100:THR:OG1	1:G:1101:HIS:N	2.53	0.42
1:A:662:CYS:SG	1:A:663:ASP:N	2.92	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:TYR:OH	1:G:54:LEU:O	2.38	0.42
1:G:391:CYS:SG	1:G:525:CYS:CB	3.05	0.42
1:G:806:LEU:HD23	1:G:806:LEU:HA	1.87	0.42
1:A:945:LEU:HD12	1:A:948:LEU:HD12	2.01	0.42
1:G:1083:HIS:HB2	1:G:1135:ASN:O	2.20	0.42
3:L:40:LYS:HA	3:L:41:PRO:HD3	1.87	0.42
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.93	0.41
1:G:231:ILE:HD12	1:G:233:ILE:HG22	2.01	0.41
1:G:422:ASN:ND2	1:G:454:ARG:O	2.49	0.41
1:G:543:PHE:CG	1:G:576:VAL:HG11	2.55	0.41
1:G:977:LEU:HD23	1:G:977:LEU:HA	1.90	0.41
1:B:916:LEU:HD12	1:B:923:ILE:HD13	2.02	0.41
2:H:104:THR:O	2:H:105:THR:HG23	2.20	0.41
3:L:29:VAL:HG21	3:L:34:LEU:HD12	2.02	0.41
1:B:359:SER:HA	1:B:524:VAL:HG22	2.03	0.41
2:H:72:SER:HA	2:H:79:ALA:HA	2.02	0.41
3:N:21:LEU:HB2	3:N:74:LEU:HB3	2.02	0.41
3:N:78:ARG:HH11	3:N:78:ARG:HA	1.85	0.41
1:B:985:ASP:HA	1:B:986:PRO:HD3	1.94	0.41
1:A:710:ASN:OD1	1:A:710:ASN:N	2.54	0.41
3:E:24:ARG:HA	3:E:24:ARG:HD3	1.93	0.41
1:G:129:LYS:HB2	1:G:133:PHE:HZ	1.86	0.41
1:G:498:GLN:HG3	1:G:500:THR:H	1.85	0.41
1:G:971:GLY:HA3	1:G:995:ARG:HH21	1.86	0.41
1:B:36:VAL:HG11	1:B:220:PHE:CZ	2.56	0.41
2:D:12:LYS:NZ	2:D:17:SER:O	2.45	0.41
1:A:330:PRO:CD	1:A:579:PRO:HG2	2.50	0.41
1:A:392:PHE:CB	1:A:524:VAL:HG21	2.51	0.41
1:B:34:ARG:HH21	1:B:217:PRO:HG2	1.84	0.41
3:L:96:PRO:HG2	3:L:97:PRO:CD	2.41	0.41
3:N:96:PRO:HG2	3:N:97:PRO:CD	2.41	0.41
1:A:335:LEU:HD13	1:A:335:LEU:HA	1.49	0.41
1:A:524:VAL:CG2	1:A:524:VAL:O	2.68	0.41
1:A:598:ILE:HB	1:A:609:ALA:HB3	2.02	0.41
1:B:202:LYS:HE2	1:B:202:LYS:HB2	1.91	0.41
1:B:825:LYS:HD3	1:B:825:LYS:HA	1.87	0.41
2:D:72:SER:HA	2:D:79:ALA:HA	2.02	0.41
3:E:21:LEU:HB2	3:E:74:LEU:HB3	2.02	0.41
1:A:658:ASN:O	1:A:659:SER:C	2.59	0.41
1:B:806:LEU:HD23	1:B:878:LEU:HD23	2.03	0.41
1:G:948:LEU:HD21	1:G:1059:GLY:HA3	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:78:ARG:HA	3:L:78:ARG:HH11	1.85	0.41
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.31	0.41
1:B:364:ASP:OD1	1:B:366:SER:OG	2.29	0.41
2:D:86:LEU:HD23	2:D:86:LEU:HA	1.90	0.41
1:G:543:PHE:O	1:G:546:LEU:HB3	2.21	0.41
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.20	0.40
1:B:980:ILE:HG21	1:B:980:ILE:HD13	1.87	0.40
2:M:72:SER:HA	2:M:79:ALA:HA	2.02	0.40
1:A:106:PHE:HB2	1:A:117:LEU:HB3	2.03	0.40
1:A:613:GLN:HE21	1:A:613:GLN:HB2	1.63	0.40
1:B:884:SER:O	1:B:884:SER:OG	2.33	0.40
1:A:336:CYS:CB	1:A:361:CYS:SG	3.08	0.40
1:B:336:CYS:HA	1:B:337:PRO:HD3	1.76	0.40
1:G:204:TYR:HA	1:G:225:PRO:HA	2.03	0.40
1:G:971:GLY:HA3	1:G:995:ARG:HD3	2.04	0.40
1:A:531:THR:HB	1:A:532:ASN:H	1.79	0.40
3:L:95:SER:HG	3:L:96:PRO:HD2	1.81	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	979/1286 (76%)	899 (92%)	71 (7%)	9 (1%)	14	49
1	B	982/1286 (76%)	913 (93%)	65 (7%)	4 (0%)	30	64
1	G	969/1286 (75%)	897 (93%)	68 (7%)	4 (0%)	30	64
2	D	119/228 (52%)	105 (88%)	13 (11%)	1 (1%)	16	51
2	H	119/228 (52%)	105 (88%)	13 (11%)	1 (1%)	16	51
2	M	119/228 (52%)	105 (88%)	13 (11%)	1 (1%)	16	51
3	E	105/111 (95%)	86 (82%)	13 (12%)	6 (6%)	1	11

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	105/111 (95%)	86 (82%)	13 (12%)	6 (6%)	1	11
3	N	105/111 (95%)	86 (82%)	13 (12%)	6 (6%)	1	11
All	All	3602/4875 (74%)	3282 (91%)	282 (8%)	38 (1%)	15	44

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	PRO
1	A	527	PRO
1	A	529	LYS
1	A	530	SER
1	A	659	SER
1	B	331	ASN
2	D	103	ASN
3	E	94	SER
3	E	95	SER
3	E	97	PRO
3	E	98	TRP
1	G	1084	ASP
2	H	103	ASN
3	L	94	SER
3	L	95	SER
3	L	97	PRO
3	L	98	TRP
2	M	103	ASN
3	N	94	SER
3	N	95	SER
3	N	97	PRO
3	N	98	TRP
1	A	334	ASN
1	G	331	ASN
1	G	527	PRO
1	A	617	CYS
1	B	531	THR
1	A	331	ASN
1	B	896	ILE
1	A	329	PHE
1	B	529	LYS
1	G	530	SER
3	E	93	GLY
3	L	93	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	N	93	GLY
3	E	96	PRO
3	L	96	PRO
3	N	96	PRO

### 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	846/1113 (76%)	830 (98%)	16 (2%)	52	76
1	B	854/1113 (77%)	845 (99%)	9 (1%)	70	86
1	G	850/1113 (76%)	847 (100%)	3 (0%)	89	94
2	D	103/196 (53%)	103 (100%)	0	100	100
2	H	103/196 (53%)	103 (100%)	0	100	100
2	M	103/196 (53%)	103 (100%)	0	100	100
3	E	91/95 (96%)	89 (98%)	2 (2%)	47	73
3	L	91/95 (96%)	89 (98%)	2 (2%)	47	73
3	N	91/95 (96%)	89 (98%)	2 (2%)	47	73
All	All	3132/4212 (74%)	3098 (99%)	34 (1%)	69	86

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	PHE
1	A	330	PRO
1	A	331	ASN
1	A	332	ILE
1	A	335	LEU
1	A	336	CYS
1	A	525	CYS
1	A	602	THR
1	A	605	SER
1	A	649	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	650	LEU
1	A	651	ILE
1	A	656	VAL
1	A	907	ASN
1	A	1072	GLU
1	A	1073	LYS
1	B	246	ARG
1	B	332	ILE
1	B	335	LEU
1	B	386	LYS
1	B	389	ASP
1	B	391	CYS
1	B	523	THR
1	B	524	VAL
1	B	617	CYS
3	E	92	HIS
3	E	95	SER
1	G	237	ARG
1	G	335	LEU
1	G	525	CYS
3	L	92	HIS
3	L	95	SER
3	N	92	HIS
3	N	95	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	606	ASN
1	A	613	GLN
1	B	282	ASN
1	B	801	ASN
3	E	91	GLN
1	G	1071	GLN
3	L	91	GLN
3	N	91	GLN

### 5.3.3 RNA ⓘ

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.

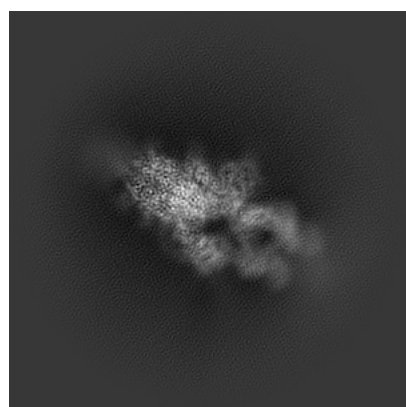
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32422. These allow visual inspection of the internal detail of the map and identification of artifacts.

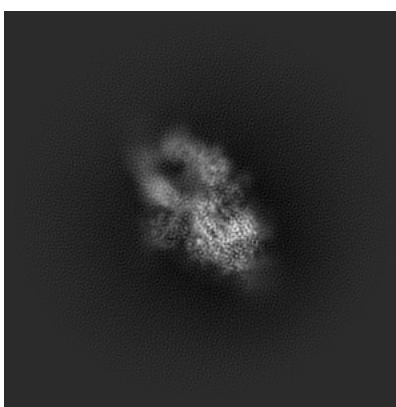
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

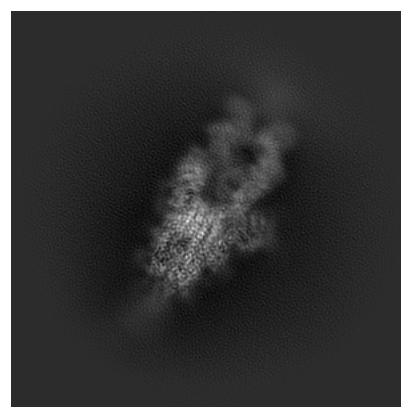
#### 6.1.1 Primary map



X



Y

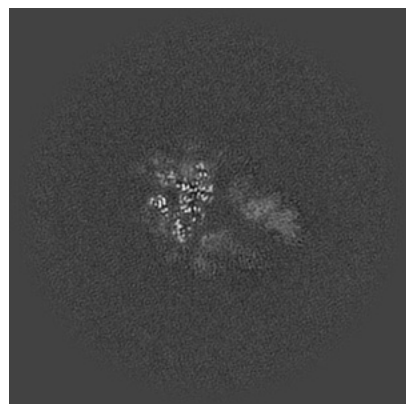


Z

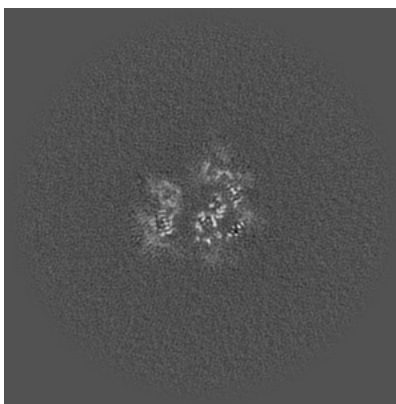
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

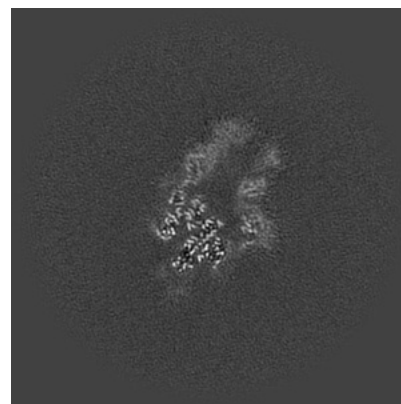
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

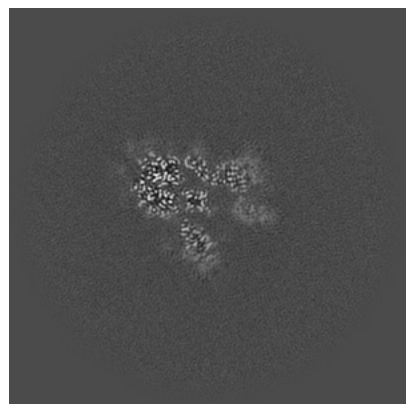


Z Index: 200

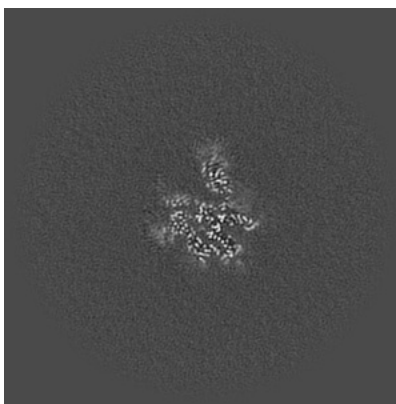
The images above show central slices of the map in three orthogonal directions.

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

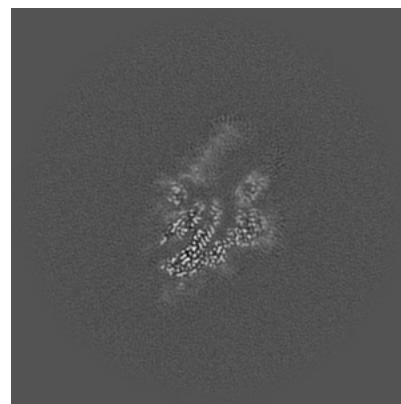
### 6.3.1 Primary map



X Index: 179



Y Index: 177

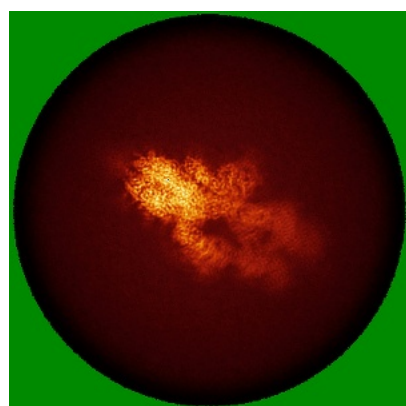


Z Index: 207

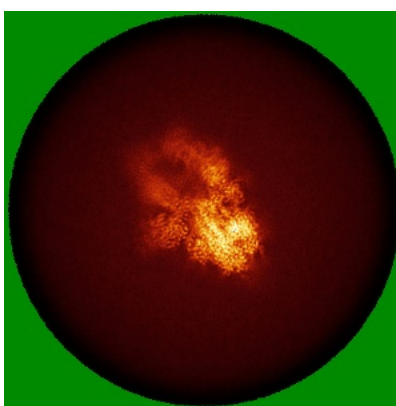
The images above show the largest variance slices of the map in three orthogonal directions.

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

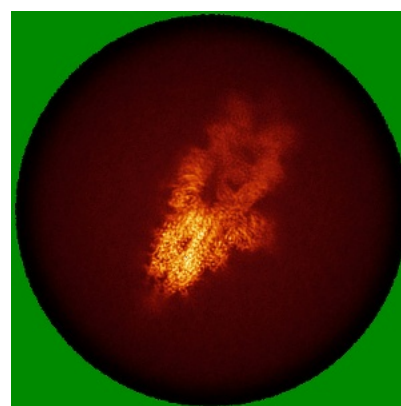
### 6.4.1 Primary map



X



Y



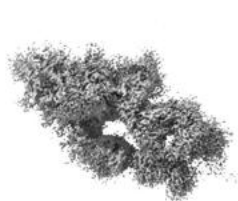
Z

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



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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.304. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

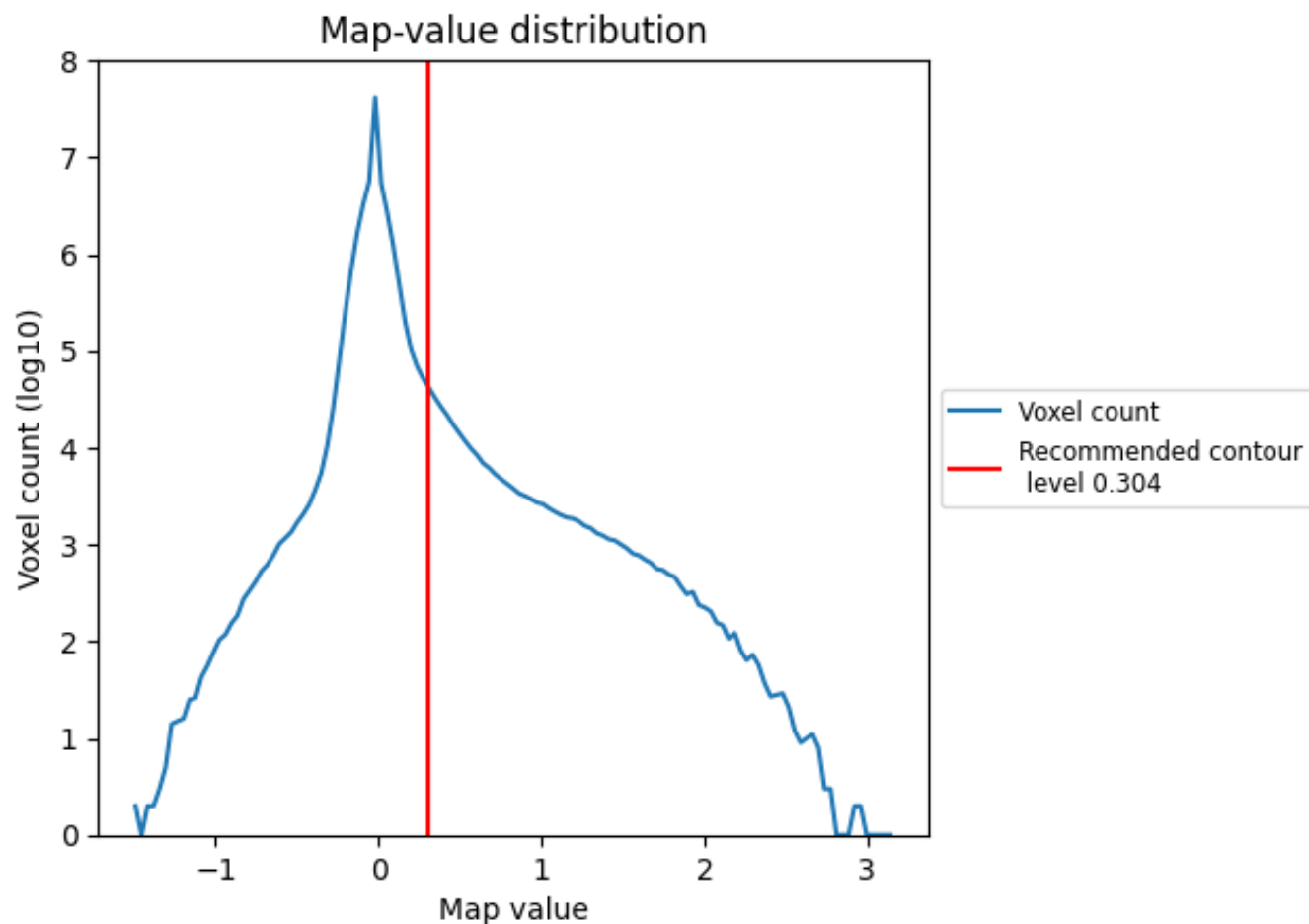
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

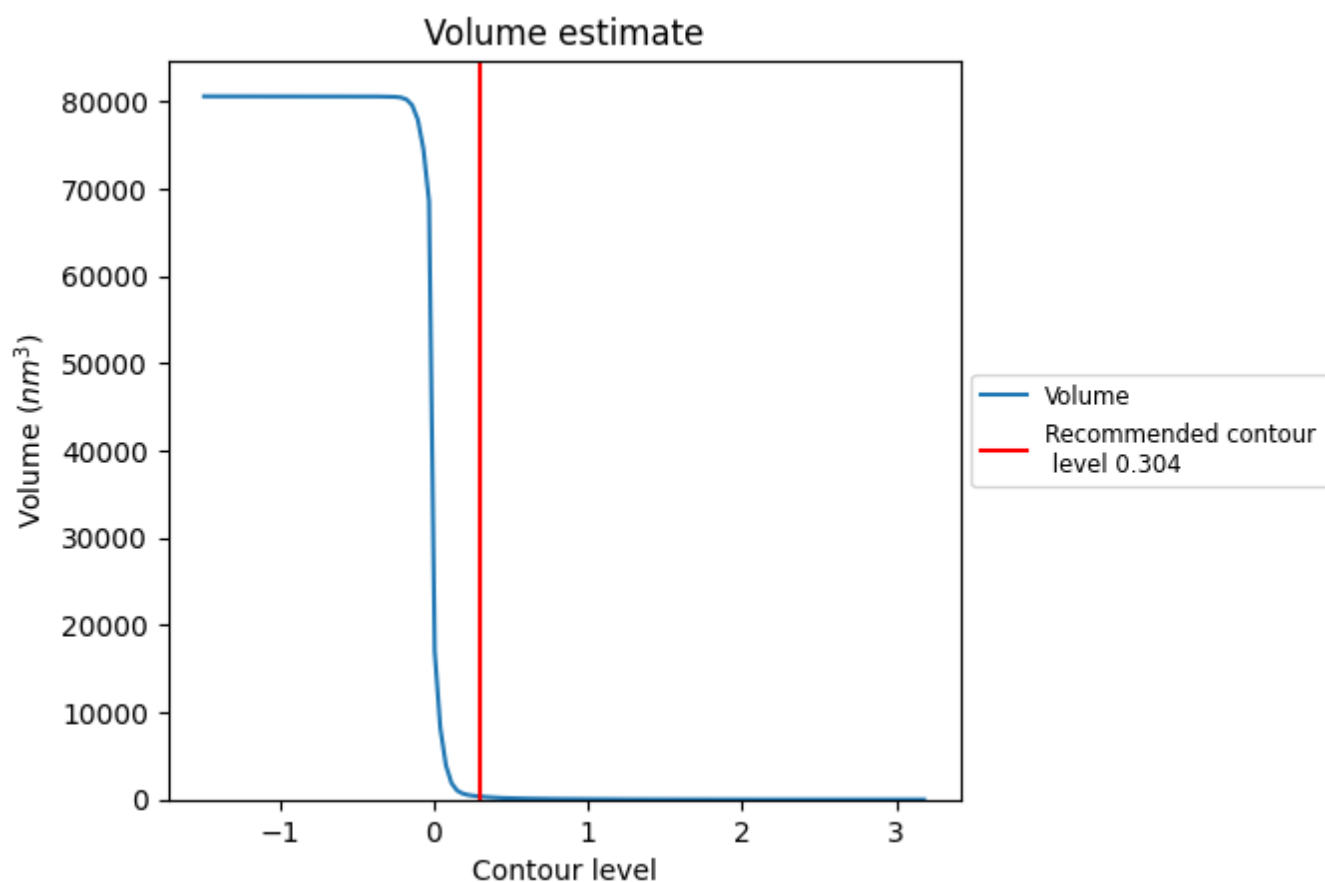
This section contains the results of statistical analysis of the map.

### 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.

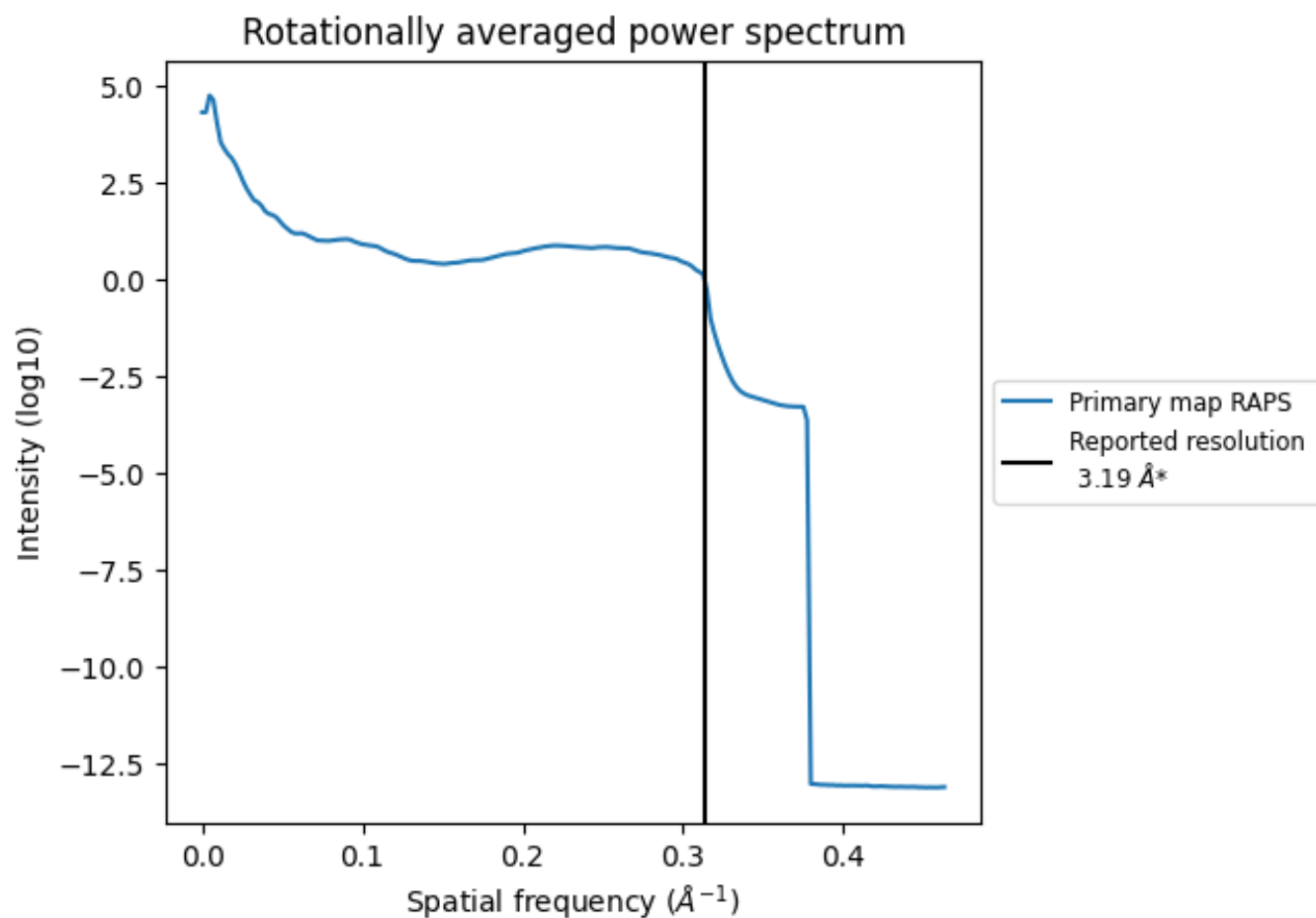
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm<sup>3</sup>; this corresponds to an approximate mass of 306 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 0.313 Å<sup>-1</sup>

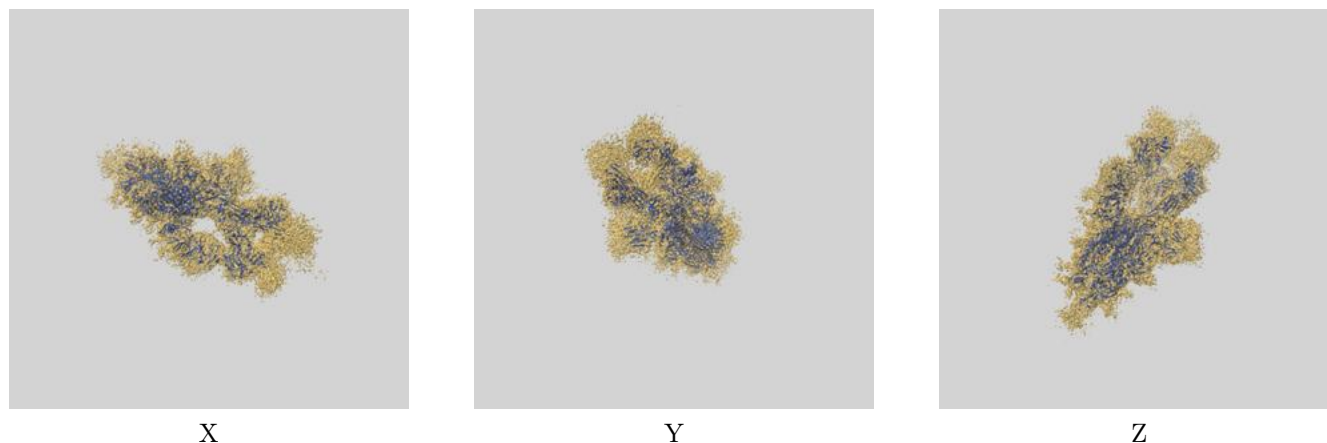
## 8 Fourier-Shell correlation

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

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

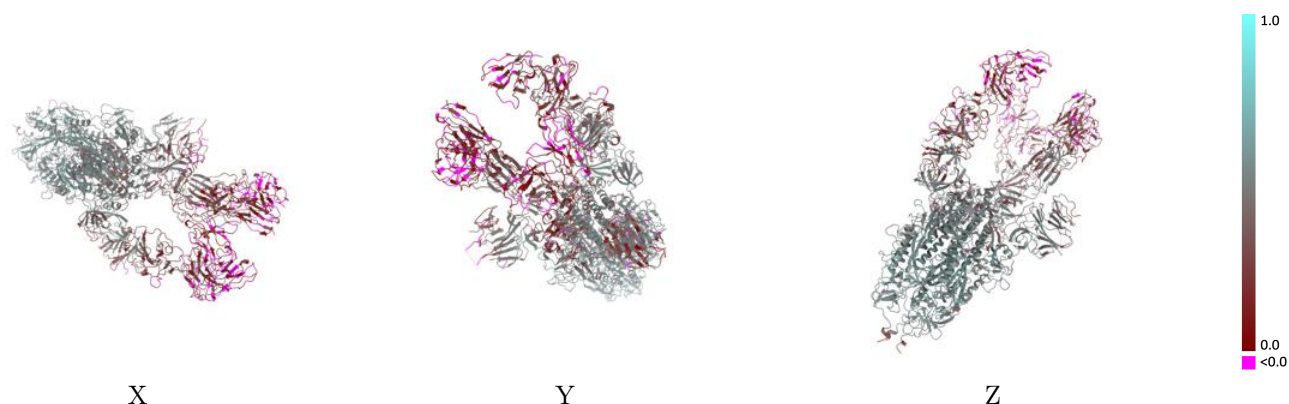
This section contains information regarding the fit between EMDB map EMD-32422 and PDB model 7WCH. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

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



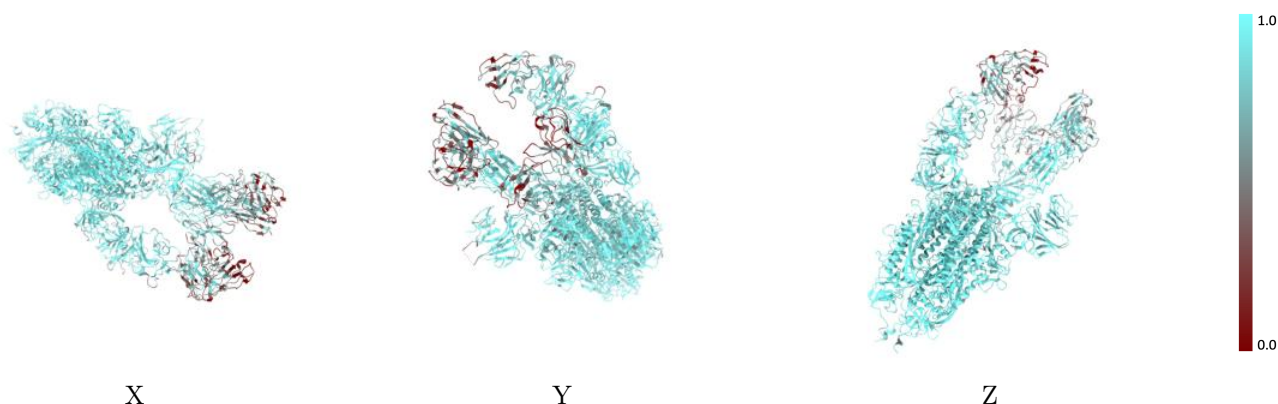
The images above show the 3D surface view of the map at the recommended contour level 0.304 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



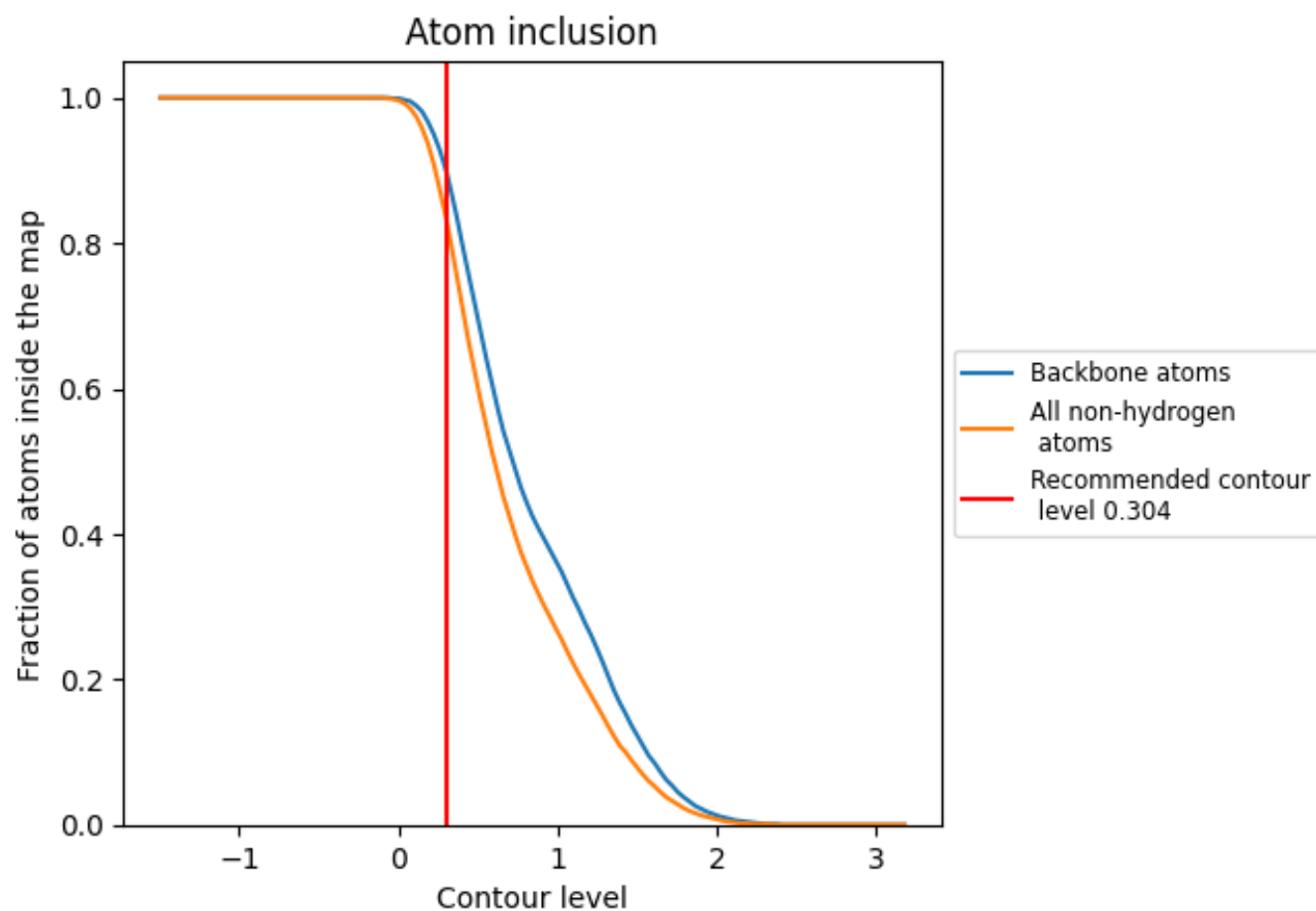
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.304).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.304) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8320	<div></div> 0.3900
A	<div></div> 0.8920	<div></div> 0.4400
B	<div></div> 0.9030	<div></div> 0.4510
D	<div></div> 0.5200	<div></div> 0.1180
E	<div></div> 0.3990	<div></div> 0.0740
G	<div></div> 0.9040	<div></div> 0.4580
H	<div></div> 0.7240	<div></div> 0.2130
L	<div></div> 0.5740	<div></div> 0.1340
M	<div></div> 0.5680	<div></div> 0.1460
N	<div></div> 0.3880	<div></div> 0.0510

1.0

0.0

<0.0