



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:20 PM UTC

PDB ID : 7XD2 / pdb_00007xd2
EMDB ID : EMD-33133
Title : SARS-CoV-2 S ectodomain trimer in complex with neutralizing antibody 10-5B
Authors : Wang, X.; Wang, Z.
Deposited on : 2022-03-26
Resolution : 3.30 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:

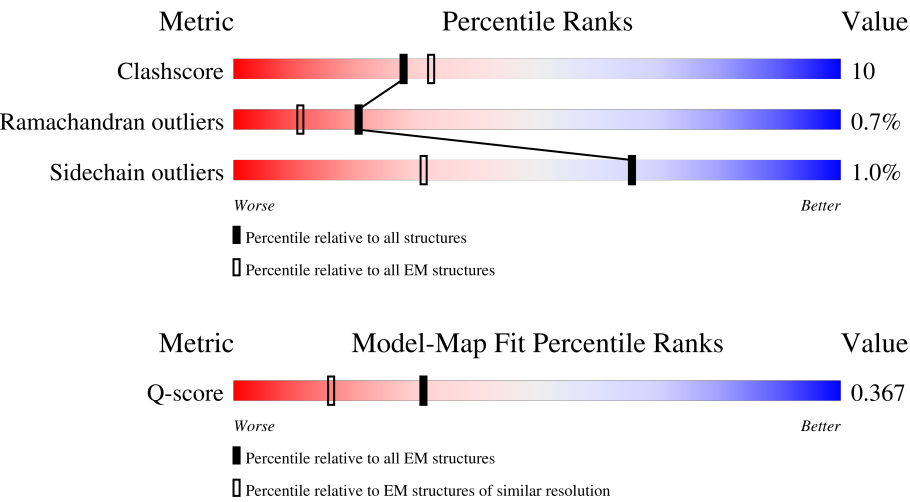
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1298	8% 63% 17% • 19%
1	B	1298	• 62% 17% • 19%
1	C	1298	11% 59% 16% • 24%
2	D	117	99% 61% 38% ••

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Mol	Chain	Length	Quality of chain
2	E	117	88% 60%38% ..
2	I	117	95% 59%39% ..
3	H	107	94% 69%29% .
3	J	107	97% 68%29% .
3	L	107	97% 67%31% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28084 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	1056	Total	C	N	O	S	0	0
			7969	5048	1340	1548	33		
1	B	1048	Total	C	N	O	S	0	0
			7943	5039	1334	1534	36		
1	C	987	Total	C	N	O	S	0	0
			7462	4751	1247	1432	32		

There are 285 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	SER	-	expression tag	UNP P0DTC2
A	1291	ASP	-	expression tag	UNP P0DTC2
A	1292	TYR	-	expression tag	UNP P0DTC2
A	1293	LYS	-	expression tag	UNP P0DTC2
A	1294	ASP	-	expression tag	UNP P0DTC2
A	1295	ASP	-	expression tag	UNP P0DTC2
A	1296	ASP	-	expression tag	UNP P0DTC2
A	1297	ASP	-	expression tag	UNP P0DTC2
A	1298	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	SER	-	expression tag	UNP P0DTC2
B	1291	ASP	-	expression tag	UNP P0DTC2
B	1292	TYR	-	expression tag	UNP P0DTC2
B	1293	LYS	-	expression tag	UNP P0DTC2
B	1294	ASP	-	expression tag	UNP P0DTC2
B	1295	ASP	-	expression tag	UNP P0DTC2
B	1296	ASP	-	expression tag	UNP P0DTC2
B	1297	ASP	-	expression tag	UNP P0DTC2
B	1298	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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
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	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1290	SER	-	expression tag	UNP P0DTC2
C	1291	ASP	-	expression tag	UNP P0DTC2
C	1292	TYR	-	expression tag	UNP P0DTC2
C	1293	LYS	-	expression tag	UNP P0DTC2
C	1294	ASP	-	expression tag	UNP P0DTC2
C	1295	ASP	-	expression tag	UNP P0DTC2
C	1296	ASP	-	expression tag	UNP P0DTC2
C	1297	ASP	-	expression tag	UNP P0DTC2
C	1298	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called H chain of antibody 10-5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	116	Total	C	N	O	S	0	0
			831	510	149	168	4		
2	E	116	Total	C	N	O	S	0	0
			831	510	149	168	4		
2	I	116	Total	C	N	O	S	0	0
			831	510	149	168	4		

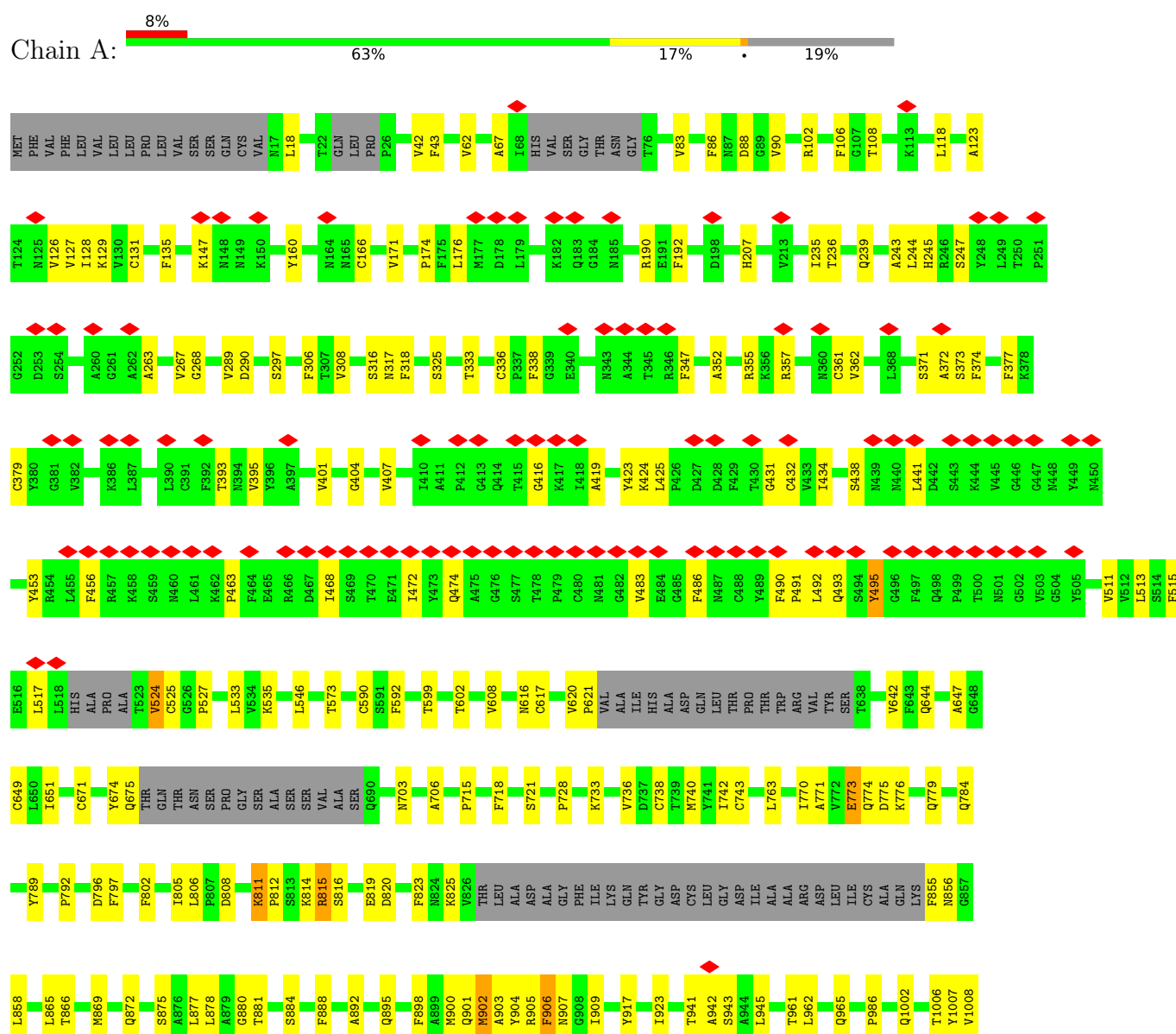
- Molecule 3 is a protein called L chain of antibody 10-5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	104	Total	C	N	O	S	0	0
			733	456	129	146	2		
3	H	105	Total	C	N	O	S	0	0
			742	461	130	149	2		
3	L	105	Total	C	N	O	S	0	0
			742	461	130	149	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: Spike glycoprotein

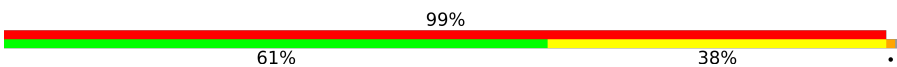






ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	GLY	LEU	ASP	GLY	ASP	ILE	SER	SER	GLY	ILE	ASN	ALA	SER	SER	THR	ASP	VAL	VAL	ASN	ILE	GLN	LYS	GLU	ILE	VAL	GLY	ASP	ARG	LEU	ASN	GLU	VAL	ALA	LYS	ASN	HIS	HIS	ASN	LEU	GLU	SER	SER	ILE	ASP	LEU	GLN	GLY	LYS	TYR	GLN	GLY	GLY	SER	GLY	TYR	ILE	PRO	GLY	ALA	SER	PRO	GLY		
ARG	ASP	GLN	ALA	TYR	VAL	ARG	ASP	GLY	GLY	GLU	TRP	VAL	LEU	LEU	LEU	GLY	ARG	SER	LEU	GLY	THR	PHE	LEU	VAL	GLY	ARG	SER	LEU	GLU	VAL	LEU	ASP	PHE	GLN	GLY	ASN	VAL	ALA	LYS	HIS	HIS	HIS	HIS	ASN	LEU	HIS	HIS	ASN	TRP	ASP	ALA	SER	TYR	GLY	GLN	GLY	GLY	SER	GLY	TYR	ILE	PRO	GLY	ALA	SER	PRO	GLY				
GLY	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	ASP	GLY	LYS	GLY	SER	ASP	TYR	TRP	LEU	ASN	LYS	ASP	PHE	LEU	VAL	ASP	GLY	ARG	SER	GLN	LYS	GLU	VAL	LEU	ASP	PHE	GLN	GLY	ASN	PRO	GLY	HIS	HIS	HIS	ASN	GLU	SER	HIS	ILE	ASP	ALA	TRP	SER	HIS	PRO	GLN	GLU	GLY	TYR	GLU	GLN	GLY	GLY	GLY	TYR	ILE	PRO	GLY	ALA	SER	PRO	GLY

- Molecule 2: H chain of antibody 10-5B

Chain D: 

GLU	V2	Q3	L4	V5	E6	S7	G8	Q9	G10	G11	I12	Q13	P14	G15	G16	S17	L18	R19	L20	S21	C22	A23	V24	S25	G26	F27	T28	V29	S30	R31	K32	S33	W34	V35	R36	Q37	A38	P39	G40	K41	G42	L43	E44	C45	V46	S47	V48	Y49	Y50	T51	G52	G53	N54	T55	D56	Y57	A58	D59	S60
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V61	K62	G63	R64	F65	T66	I67	S68	R69	D70	N71	S72	K73	N74	T75	L76	Y77	L78	Q79	M80	N81	S82	L83	R84	A85	E86	D87	T88	A89	L90	Y91	Y92	C93	Q94	R95	G96	S97	G98	P99	I100	H101	D102	A103	F104	D105	I106	S107	G108	Q109	G110	T111	M112	V113	T114	V115	S116	S117
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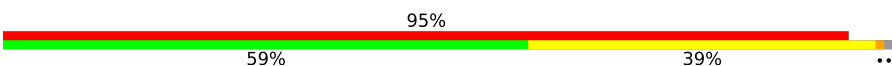
- Molecule 2: H chain of antibody 10-5B

Chain E: 

GLU	V2	Q3	L4	V5	E6	S7	G8	Q9	G10	G11	I12	Q13	P14	G15	G16	S17	L18	R19	L20	S21	C22	A23	V24	S25	G26	F27	T28	V29	S30	R31	K32	S33	W34	V35	R36	Q37	A38	P39	G40	K41	G42	L43	E44	C45	V46	S47	V48	Y49	Y50	T51	G52	G53	N54	T55	D56	Y57	A58	D59	S60
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V61	K62	G63	R64	F65	T66	I67	S68	R69	D70	N71	S72	K73	N74	T75	L76	Y77	L78	Q79	M80	N81	S82	L83	R84	A85	E86	D87	T88	A89	L90	Y91	R95	G96	S97	G98	G99	I100	H101	F104	D105	I106	W107	G108	Q109	G110	T111	M112	V113	V115	S116	S117
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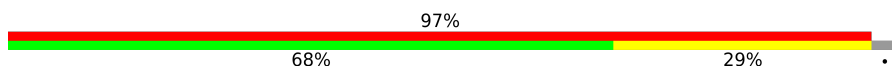
- Molecule 2: H chain of antibody 10-5B

Chain I: 

GLU	V2	Q3	L4	V5	E6	S7	G8	Q9	G10	G11	I12	Q13	P14	G15	G16	S17	L18	R19	L20	S21	C22	A23	V24	S25	G26	F27	T28	V29	S30	R31	K32	S33	W34	V35	R36	Q37	A38	P39	G40	K41	G42	L43	E44	C45	V46	S47	V48	Y49	Y50	T51	G52	G53	N54	T55	D56	Y57	A58	D59	S60
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V61	K62	G63	R64	F65	T66	I67	S68	R69	D70	N71	S72	K73	N74	T75	L76	Y77	L78	Q79	M80	N81	S82	L83	R84	A85	E86	D87	T88	A89	L90	Y91	Y92	C93	V94	R95	G96	S97	G98	G99	I100	H101	D102	A103	F104	D105	I106	W107	G108	Q109	G110	T111	M112	V113	T114	V115	S116	S117
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- Molecule 3: L chain of antibody 10-5B

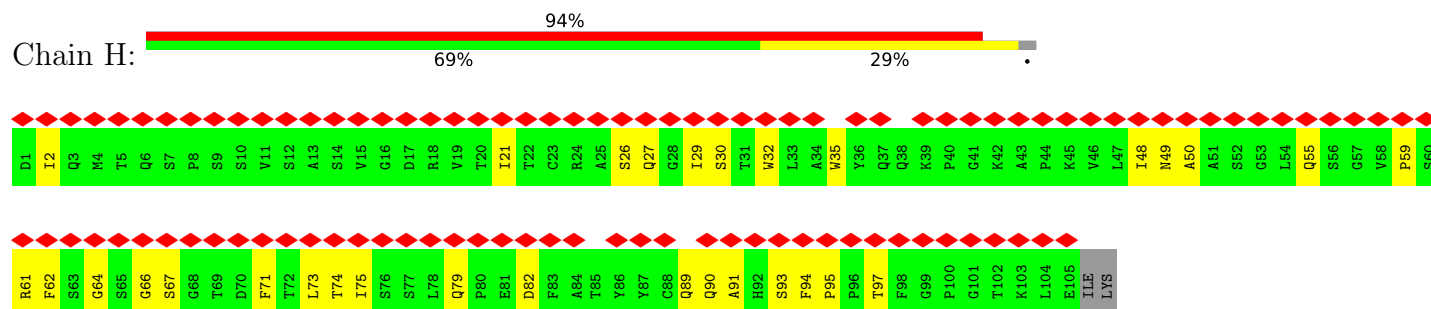
Chain J: 

D1	I2	Q3	M4	T5	Q6	S7	P8	S9	S10	V11	S12	A13	S14	V15	G16	D17	R18	V19	T20	I21	T22	C23	R24	A25	S26	Q27	G28	I29	Q30	A31	T32	L33	A34	W35	Y36	Q37	Q38	K39	P40	G41	G42	A43	P44	K45	V46	L47	I48	N49	A50	A51	S52	G53	L54	Q55	S56	G57	V58	P59	S60
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R61	F62	S63	G64	S65	G66	S67	G68	T69	D70	F71	T72	L73	T74	I75	S76	S77	L78	Q79	P80	E81	D82	F83	A84	T85	Y86	Y87	C88	Q89	Q90	A91	H92	S93	F94	P95	P96	T97	F98	G99	P100	G101	T102	K103	L104	GLU	ILE	LYS
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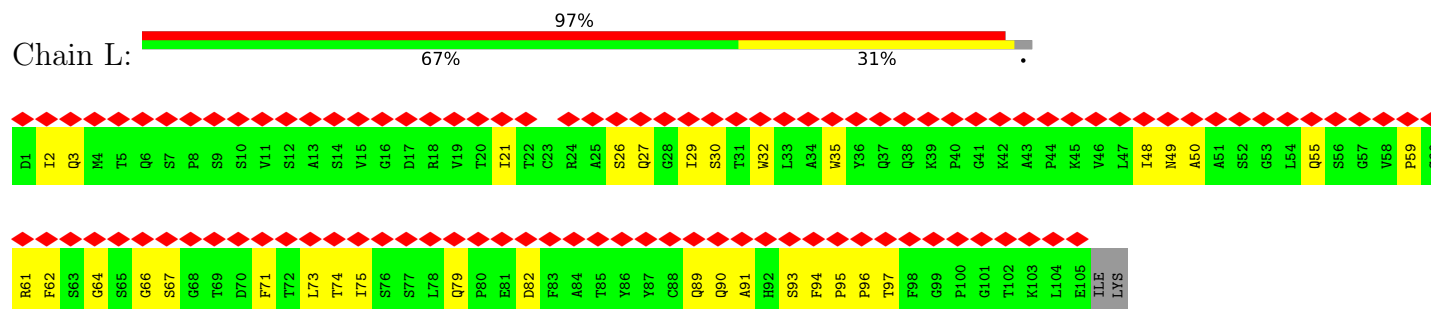
● Molecule 3: L chain of antibody 10-5B

Chain H:



● Molecule 3: L chain of antibody 10-5B

Chain L:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	368416	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.893	Depositor
Minimum map value	-1.885	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.22	Depositor
Map size ($\text{\AA}$)	310.40002, 310.40002, 310.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9700001, 0.9700001, 0.9700001	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	1.07	10/8147 (0.1%)	1.45	46/11109 (0.4%)
1	B	1.09	13/8122 (0.2%)	1.45	46/11078 (0.4%)
1	C	1.07	11/7629 (0.1%)	1.45	42/10393 (0.4%)
2	D	1.00	0/843	1.24	0/1142
2	E	0.99	0/843	1.24	0/1142
2	I	1.00	0/843	1.24	0/1142
3	H	1.03	0/761	1.29	0/1038
3	J	1.03	0/752	1.30	0/1026
3	L	1.03	0/761	1.29	0/1038
All	All	1.07	34/28701 (0.1%)	1.42	134/39108 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	PRO	C-O	-6.87	1.19	1.25
1	A	1021	SER	CA-CB	-6.49	1.43	1.53
1	A	816	SER	CA-CB	-6.45	1.43	1.53
1	C	715	PRO	C-O	-6.41	1.15	1.23
1	A	715	PRO	C-O	-6.27	1.16	1.23
1	C	816	SER	CA-CB	-6.20	1.44	1.53
1	C	897	PRO	C-O	-6.15	1.16	1.23
1	B	816	SER	CA-CB	-6.11	1.43	1.53
1	B	1078	ALA	CA-CB	-6.11	1.45	1.54
1	C	1021	SER	CA-CB	-6.05	1.43	1.53
1	C	721	SER	CA-CB	-5.91	1.44	1.53
1	B	1021	SER	CA-CB	-5.80	1.44	1.53
1	B	728	PRO	C-O	-5.80	1.17	1.23
1	B	715	PRO	C-O	-5.76	1.16	1.23
1	B	1051	SER	CA-CB	-5.72	1.44	1.53
1	B	711	SER	CA-CB	-5.70	1.44	1.53
1	A	1080	ALA	CA-CB	-5.69	1.46	1.53
1	C	1069	PRO	C-O	-5.61	1.17	1.23
1	A	728	PRO	C-O	-5.47	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	875	SER	CA-CB	-5.47	1.44	1.53
1	B	1053	PRO	C-O	-5.42	1.18	1.23
1	C	884	SER	CA-CB	-5.40	1.45	1.53
1	B	884	SER	CA-CB	-5.33	1.45	1.54
1	A	721	SER	CA-CB	-5.33	1.45	1.53
1	B	875	SER	CA-CB	-5.31	1.44	1.53
1	A	1053	PRO	C-O	-5.30	1.18	1.23
1	A	1066	THR	C-O	-5.25	1.17	1.23
1	C	728	PRO	C-O	-5.23	1.17	1.24
1	C	803	SER	CA-CB	-5.22	1.45	1.53
1	B	1050	MET	C-O	-5.20	1.17	1.23
1	B	1066	THR	C-O	-5.17	1.17	1.23
1	C	746	SER	CA-CB	-5.15	1.45	1.53
1	C	792	PRO	C-O	-5.13	1.20	1.25
1	B	730	SER	CA-CB	-5.05	1.45	1.53

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	ASN	CB-CA-C	-14.53	86.82	111.23
1	A	943	SER	N-CA-C	-11.83	98.37	112.92
1	B	1067	TYR	CB-CA-C	-10.59	92.53	110.22
1	B	812	PRO	N-CA-C	-9.73	99.55	113.47
1	B	759	PHE	N-CA-C	-9.50	101.89	112.72
1	A	855	PHE	CB-CA-C	-8.97	93.06	110.10
1	A	796	ASP	CB-CA-C	-8.95	98.69	111.85
1	A	1121	PHE	CA-CB-CG	8.86	122.66	113.80
1	A	904	TYR	N-CA-C	-8.80	102.95	114.31
1	B	1121	PHE	CA-CB-CG	8.76	122.56	113.80
1	C	856	ASN	CB-CA-C	-8.74	96.28	111.05
1	C	815	ARG	CB-CA-C	8.72	123.51	109.90
1	A	872	GLN	N-CA-C	-8.51	103.04	113.50
1	A	901	GLN	N-CA-C	-8.42	101.12	111.40
1	A	808	ASP	CB-CA-C	-8.29	100.61	110.15
1	B	760	CYS	CB-CA-C	-8.20	96.92	110.37
1	C	760	CYS	CB-CA-C	8.11	121.79	109.13
1	A	776	LYS	N-CA-C	-7.80	103.89	113.41
1	B	813	SER	N-CA-C	-7.64	102.52	113.21
1	A	1042	PHE	N-CA-C	-7.62	103.05	111.36
1	B	774	GLN	N-CA-C	-7.58	103.77	113.16
1	B	710	ASN	CB-CA-C	-7.31	101.10	111.85
1	B	796	ASP	CB-CA-C	-7.25	100.00	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	940	SER	N-CA-C	-7.20	104.37	113.01
1	C	796	ASP	CB-CA-C	-7.19	101.29	111.85
1	A	902	MET	CA-C-O	-7.07	113.34	121.47
1	B	86	PHE	CA-CB-CG	7.01	120.81	113.80
1	A	902	MET	N-CA-C	-6.98	100.15	110.48
1	C	776	LYS	N-CA-C	-6.85	105.05	113.41
1	B	620	VAL	N-CA-CB	6.74	114.75	110.50
1	B	888	PHE	CA-CB-CG	6.73	120.53	113.80
1	B	909	ILE	N-CA-C	-6.68	106.21	112.83
1	A	1044	GLY	CA-C-O	-6.60	117.67	122.23
1	B	324	GLU	N-CA-C	6.60	118.47	111.28
1	A	814	LYS	N-CA-C	-6.59	103.73	113.61
1	A	888	PHE	CA-CB-CG	6.57	120.37	113.80
1	C	888	PHE	CA-CB-CG	6.54	120.34	113.80
1	B	901	GLN	N-CA-C	-6.54	104.24	111.36
1	C	901	GLN	N-CA-C	-6.47	104.22	111.28
1	C	324	GLU	CB-CA-C	-6.43	106.37	114.40
1	C	950	ASP	N-CA-C	-6.43	105.59	113.50
1	C	86	PHE	CA-CB-CG	6.36	120.16	113.80
1	B	942	ALA	N-CA-C	-6.28	98.75	108.42
1	A	907	ASN	N-CA-C	-6.25	104.81	112.88
1	C	966	LEU	N-CA-C	-6.20	105.47	113.16
1	A	1126	CYS	CB-CA-C	-6.15	101.99	111.83
1	B	1044	GLY	CA-C-O	-6.13	118.00	122.23
1	C	729	VAL	N-CA-C	6.05	116.83	110.72
1	C	338	PHE	N-CA-C	-6.04	105.77	113.02
1	B	338	PHE	N-CA-C	-6.04	105.78	113.02
1	A	338	PHE	N-CA-C	-6.03	105.78	113.02
1	B	810	SER	N-CA-C	-6.03	106.01	113.19
1	B	892	ALA	CA-C-O	-6.03	114.99	121.56
1	B	814	LYS	N-CA-C	-6.02	105.24	112.58
1	B	219	GLY	CA-C-O	-5.99	118.00	122.37
1	C	308	VAL	CA-C-O	-5.98	116.95	121.68
1	A	909	ILE	N-CA-C	-5.93	106.96	112.83
1	C	665	PRO	CB-CA-C	-5.91	101.81	111.56
1	C	856	ASN	N-CA-C	5.91	118.39	108.23
1	B	1057	PRO	N-CD-CG	-5.90	94.34	103.20
1	A	892	ALA	CA-C-O	-5.89	115.03	121.87
1	C	899	ALA	CA-C-O	-5.85	114.34	120.55
1	B	1103	PHE	CA-C-O	-5.84	115.03	121.33
1	A	1038	LYS	N-CA-C	-5.83	105.36	112.88
1	B	784	GLN	N-CA-C	-5.81	106.04	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	616	ASN	N-CA-C	-5.81	101.81	110.23
1	A	1115	ILE	CA-C-O	-5.81	117.58	122.63
1	C	618	THR	N-CA-C	-5.75	106.05	114.39
1	C	759	PHE	N-CA-C	-5.70	106.10	113.16
1	B	1014	ARG	CB-CA-C	-5.70	101.17	110.85
1	C	616	ASN	N-CA-C	-5.68	102.00	110.23
1	A	814	LYS	CA-C-N	-5.67	115.17	123.00
1	A	814	LYS	C-N-CA	-5.67	115.17	123.00
1	C	1121	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	621	PRO	CA-C-N	-5.63	111.83	121.97
1	B	621	PRO	C-N-CA	-5.63	111.83	121.97
1	B	915	VAL	CA-C-O	-5.54	115.19	120.95
1	A	1103	PHE	CA-C-O	-5.51	115.34	121.51
1	C	667	GLY	CA-C-O	-5.51	116.81	121.66
1	A	941	THR	CB-CA-C	-5.50	103.97	111.95
1	C	965	GLN	N-CA-C	-5.46	106.21	112.92
1	C	761	THR	N-CA-C	-5.45	105.42	111.36
1	A	773	GLU	CB-CA-C	-5.45	98.92	110.31
1	A	86	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	872	GLN	N-CA-C	-5.44	105.77	112.90
1	C	1067	TYR	CB-CA-C	-5.42	101.95	110.79
1	C	942	ALA	N-CA-C	-5.39	99.31	110.80
1	A	1067	TYR	CB-CA-C	-5.39	102.15	110.78
1	C	728	PRO	N-CA-CB	-5.38	97.60	103.25
1	A	1035	GLY	CA-C-O	-5.38	116.30	121.41
1	C	1064	HIS	CA-C-O	-5.38	115.32	120.92
1	B	773	GLU	N-CA-C	-5.38	106.39	113.17
1	C	569	ILE	CA-C-O	-5.38	116.20	121.58
1	B	1022	ALA	CA-C-O	-5.38	114.72	120.42
1	B	905	ARG	CA-C-O	-5.36	114.74	120.42
1	B	1042	PHE	N-CA-C	-5.36	105.52	111.36
1	A	905	ARG	N-CA-C	-5.36	106.79	113.38
1	A	906	PHE	CB-CA-C	-5.31	101.22	110.09
1	A	797	PHE	CB-CA-C	5.29	119.80	110.37
1	B	743	CYS	CB-CA-C	-5.26	105.01	114.52
1	C	1042	PHE	N-CA-C	-5.25	105.63	111.36
1	B	217	PRO	N-CA-C	5.24	119.72	111.38
1	C	213	VAL	N-CA-C	-5.22	105.44	110.72
1	C	802	PHE	N-CA-C	-5.22	106.22	112.59
1	A	784	GLN	N-CA-C	-5.21	106.95	113.72
1	B	55	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	1047	TYR	CA-C-O	-5.19	115.68	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1044	GLY	CA-C-O	-5.19	118.08	122.29
1	C	915	VAL	CA-C-O	-5.19	115.55	120.95
1	B	42	VAL	CA-C-O	-5.17	116.76	121.72
1	C	945	LEU	CA-C-O	-5.16	115.40	120.82
1	B	648	GLY	CA-C-N	-5.16	114.79	122.74
1	B	648	GLY	C-N-CA	-5.16	114.79	122.74
1	A	671	CYS	CA-C-O	-5.14	115.61	121.58
1	A	743	CYS	CB-CA-C	-5.14	104.95	115.28
1	C	649	CYS	CB-CA-C	-5.13	100.32	109.71
1	A	986	PRO	N-CA-C	5.12	116.95	110.70
1	A	815	ARG	CB-CA-C	5.12	118.58	109.72
1	C	712	ILE	CA-C-O	-5.12	115.34	121.28
1	C	675	GLN	CB-CA-C	-5.11	100.39	110.10
1	B	322	PRO	CB-CA-C	-5.11	103.14	111.56
1	C	1065	VAL	CA-C-O	-5.09	115.79	121.23
1	B	941	THR	N-CA-C	5.08	116.79	108.76
1	A	706	ALA	CA-C-O	-5.08	116.29	122.64
1	C	1069	PRO	N-CA-CB	-5.08	98.61	103.33
1	B	1048	HIS	CB-CA-C	-5.07	101.31	109.72
1	A	895	GLN	CA-C-O	-5.05	116.19	121.55
1	B	161	SER	N-CA-C	-5.05	107.17	113.38
1	A	945	LEU	N-CA-C	-5.04	107.19	113.19
1	B	569	ILE	CA-C-O	-5.04	115.82	121.36
1	C	591	SER	N-CA-C	5.03	117.53	110.23
1	B	792	PRO	CB-CA-C	-5.03	104.79	110.92
1	A	1114	ILE	CA-C-O	-5.02	116.42	121.59
1	A	590	CYS	N-CA-CB	5.00	117.60	110.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	7969	0	7457	126	0
1	B	7943	0	7464	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7462	0	7017	123	0
2	D	831	0	779	29	0
2	E	831	0	779	30	0
2	I	831	0	779	31	0
3	H	742	0	676	25	0
3	J	733	0	670	25	0
3	L	742	0	676	27	0
All	All	28084	0	26297	523	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 10.

All (523) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:GLN:HA	2:D:43:LEU:HA	1.67	0.77
2:E:37:GLN:HA	2:E:43:LEU:HA	1.67	0.76
2:I:37:GLN:HA	2:I:43:LEU:HA	1.67	0.75
2:E:38:ALA:HB3	2:E:41:LYS:HB3	1.70	0.73
3:L:29:ILE:HG23	3:L:32:TRP:HB2	1.71	0.72
2:I:38:ALA:HB3	2:I:41:LYS:HB3	1.70	0.71
3:H:29:ILE:HG23	3:H:32:TRP:HB2	1.71	0.71
2:D:38:ALA:HB3	2:D:41:LYS:HB3	1.70	0.71
3:J:29:ILE:HG23	3:J:32:TRP:HB2	1.71	0.71
2:E:90:LEU:HA	2:E:112:MET:HA	1.73	0.70
2:I:90:LEU:HA	2:I:112:MET:HA	1.73	0.70
2:I:33:SER:HB2	2:I:96:GLY:HA2	1.73	0.70
2:D:33:SER:HB2	2:D:96:GLY:HA2	1.73	0.69
2:D:12:ILE:HG21	2:D:18:LEU:HD11	1.75	0.69
2:D:90:LEU:HA	2:D:112:MET:HA	1.73	0.69
2:E:33:SER:HB2	2:E:96:GLY:HA2	1.73	0.69
2:E:12:ILE:HG21	2:E:18:LEU:HD11	1.75	0.68
2:I:12:ILE:HG21	2:I:18:LEU:HD11	1.75	0.68
1:A:617:CYS:SG	1:A:644:GLN:HB2	2.34	0.68
2:D:61:VAL:HA	2:D:64:ARG:HE	1.59	0.68
2:I:61:VAL:HA	2:I:64:ARG:HE	1.59	0.68
2:E:61:VAL:HA	2:E:64:ARG:HE	1.59	0.68
1:A:135:PHE:HA	1:A:160:TYR:HA	1.77	0.67
1:A:357:ARG:NH1	1:B:168:PHE:CE1	2.65	0.64
1:A:456:PHE:HD2	1:A:491:PRO:HA	1.62	0.64
1:C:456:PHE:HD2	1:C:491:PRO:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:PHE:HD2	1:B:491:PRO:HA	1.62	0.64
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.80	0.63
1:B:570:ALA:HB1	1:C:963:VAL:HG12	1.80	0.63
1:B:770:ILE:O	1:B:774:GLN:HG2	1.99	0.62
1:B:570:ALA:HB1	1:C:963:VAL:CG1	2.30	0.62
1:C:326:ILE:HG21	1:C:534:VAL:HG12	1.82	0.61
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.81	0.61
1:C:945:LEU:O	1:C:947:LYS:N	2.33	0.61
1:B:216:LEU:O	1:B:216:LEU:HD12	2.00	0.61
1:B:483:VAL:HG23	2:E:54:ASN:HB3	1.83	0.61
1:C:90:VAL:HG13	1:C:267:VAL:HG13	1.83	0.61
3:L:48:ILE:HG23	3:L:50:ALA:H	1.66	0.61
1:C:483:VAL:HG23	2:D:54:ASN:HB3	1.83	0.61
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.66	0.60
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.83	0.60
1:B:560:LEU:HB2	1:B:563:GLN:NE2	2.16	0.60
1:C:811:LYS:HB3	1:C:812:PRO:HD2	1.84	0.60
2:E:2:VAL:N	2:E:25:SER:HG	1.99	0.60
3:H:48:ILE:HG23	3:H:50:ALA:H	1.66	0.60
1:B:909:ILE:HD13	1:B:1049:LEU:HD21	1.83	0.60
2:D:2:VAL:N	2:D:25:SER:HG	2.00	0.60
2:D:46:VAL:HG22	2:D:61:VAL:HG22	1.84	0.59
1:A:483:VAL:HG23	2:I:54:ASN:HB3	1.83	0.59
1:C:886:TRP:H	1:C:886:TRP:HE3	1.50	0.59
2:E:20:LEU:HD13	2:E:78:LEU:HD23	1.84	0.59
2:I:46:VAL:HG22	2:I:61:VAL:HG22	1.84	0.59
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.32	0.59
3:J:48:ILE:HG23	3:J:50:ALA:H	1.66	0.59
1:B:139:PRO:HG2	1:B:239:GLN:HE22	1.68	0.59
2:D:20:LEU:HD13	2:D:78:LEU:HD23	1.84	0.59
2:I:20:LEU:HD13	2:I:78:LEU:HD23	1.84	0.59
1:C:826:VAL:HG23	1:C:945:LEU:HG	1.83	0.59
2:I:2:VAL:N	2:I:25:SER:HG	2.01	0.59
1:C:82:PRO:HD2	1:C:84:LEU:HD11	1.84	0.58
1:A:123:ALA:HA	1:A:176:LEU:HA	1.85	0.58
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.83	0.58
1:B:320:VAL:HA	1:B:623:ALA:HB1	1.83	0.58
1:B:791:THR:HG23	1:B:879:ALA:CB	2.33	0.58
1:C:723:THR:O	1:C:724:THR:HG23	2.03	0.58
1:B:736:VAL:HG23	1:B:767:LEU:HD13	1.86	0.58
3:J:90:GLN:CB	3:J:97:THR:H	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.86	0.58
3:H:90:GLN:CB	3:H:97:THR:H	2.17	0.58
1:B:32:PHE:HD1	1:B:59:PHE:CE1	2.22	0.58
1:A:419:ALA:HA	1:A:423:TYR:O	2.04	0.57
1:B:825:LYS:HB3	1:B:945:LEU:HD12	1.86	0.57
2:E:31:ARG:HD3	2:E:50:TYR:HD1	1.70	0.57
3:L:90:GLN:CB	3:L:97:THR:H	2.17	0.57
1:C:643:PHE:CE2	1:C:645:THR:HG22	2.39	0.57
2:E:46:VAL:HG22	2:E:61:VAL:HG22	1.84	0.57
1:A:1056:ALA:HB1	1:A:1057:PRO:HD2	1.86	0.57
1:B:419:ALA:HA	1:B:423:TYR:O	2.04	0.57
2:D:31:ARG:HD3	2:D:50:TYR:HD1	1.70	0.57
3:J:79:GLN:H	3:J:82:ASP:HB3	1.69	0.57
1:B:665:PRO:HB3	1:C:864:LEU:HD11	1.86	0.57
3:L:79:GLN:H	3:L:82:ASP:HB3	1.69	0.57
1:A:1086:LYS:HB3	1:A:1122:VAL:HG13	1.86	0.57
1:A:770:ILE:O	1:A:774:GLN:HG2	2.05	0.57
1:C:741:TYR:CE2	1:C:962:LEU:HG	2.40	0.57
1:A:811:LYS:HB3	1:A:812:PRO:CD	2.35	0.56
1:C:419:ALA:HA	1:C:423:TYR:O	2.04	0.56
1:C:812:PRO:O	1:C:813:SER:C	2.48	0.56
3:H:79:GLN:H	3:H:82:ASP:HB3	1.69	0.56
1:A:102:ARG:HG2	1:A:243:ALA:HB2	1.88	0.56
1:C:83:VAL:HA	1:C:237:ARG:NE	2.21	0.56
1:C:821:LEU:HD11	1:C:939:SER:HB2	1.87	0.56
1:A:308:VAL:HB	1:A:602:THR:HG23	1.88	0.56
1:A:416:GLY:H	1:A:419:ALA:HB3	1.71	0.56
1:A:869:MET:HE1	1:C:669:GLY:HA2	1.87	0.56
1:B:102:ARG:HH22	1:B:154:GLU:HG2	1.71	0.56
1:B:142:GLY:HA3	1:B:156:GLU:HB2	1.86	0.56
1:B:1115:ILE:HG23	1:B:1120:THR:HG21	1.88	0.56
1:C:416:GLY:H	1:C:419:ALA:HB3	1.71	0.56
2:I:31:ARG:HD3	2:I:50:TYR:HD1	1.70	0.56
1:A:83:VAL:HG22	1:A:239:GLN:CD	2.30	0.56
1:B:416:GLY:H	1:B:419:ALA:HB3	1.71	0.56
1:B:128:ILE:HG21	1:B:229:LEU:HD13	1.87	0.56
1:C:328:ARG:HD2	1:C:533:LEU:HB3	1.88	0.55
1:A:546:LEU:HD21	1:A:573:THR:HG21	1.88	0.55
1:A:395:VAL:HG23	1:A:524:VAL:HG21	1.89	0.55
1:C:128:ILE:O	1:C:169:GLU:HA	2.06	0.55
2:D:9:GLY:HA3	2:D:111:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.89	0.55
1:A:1095:PHE:CE1	1:A:1104:VAL:HG22	2.42	0.55
1:B:742:ILE:HD13	1:B:1001:LEU:HG	1.89	0.55
3:J:21:ILE:HG22	3:J:73:LEU:HB3	1.89	0.55
1:A:453:TYR:CE1	1:A:493:GLN:HB3	2.43	0.54
2:I:9:GLY:HA3	2:I:111:THR:HB	1.89	0.54
1:B:453:TYR:CE1	1:B:493:GLN:HB3	2.43	0.54
1:B:486:PHE:HB3	2:E:101:HIS:CE1	2.42	0.54
2:E:9:GLY:HA3	2:E:111:THR:HB	1.89	0.54
1:A:289:VAL:HG23	1:A:306:PHE:CE2	2.42	0.54
1:A:703:ASN:O	1:B:789:TYR:HA	2.08	0.54
1:B:31:SER:HA	1:B:216:LEU:HD11	1.89	0.54
1:C:486:PHE:HB3	2:D:101:HIS:CE1	2.43	0.54
3:J:89:GLN:HE22	3:J:91:ALA:HB2	1.73	0.54
3:H:89:GLN:HE22	3:H:91:ALA:HB2	1.73	0.54
1:A:811:LYS:HB3	1:A:812:PRO:HD3	1.89	0.54
1:C:456:PHE:HB3	1:C:474:GLN:HG2	1.89	0.54
1:A:486:PHE:HB3	2:I:101:HIS:CE1	2.43	0.54
1:C:1028:LYS:O	1:C:1032:CYS:HB2	2.08	0.54
3:H:21:ILE:HG22	3:H:73:LEU:HB3	1.89	0.54
3:L:21:ILE:HG22	3:L:73:LEU:HB3	1.89	0.54
1:C:453:TYR:CE1	1:C:493:GLN:HB3	2.43	0.53
1:B:577:ARG:HH21	1:B:582:LEU:HB3	1.74	0.53
1:B:646:ARG:HD3	1:B:668:ALA:HB1	1.89	0.53
1:C:100:ILE:HG23	1:C:243:ALA:HB3	1.90	0.53
1:C:144:TYR:H	1:C:152:TRP:HA	1.73	0.53
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.90	0.53
3:J:62:PHE:HB3	3:J:73:LEU:HD21	1.91	0.53
1:C:200:TYR:HB3	1:C:228:ASP:OD1	2.08	0.53
1:A:1082:CYS:HB2	1:A:1132:ILE:CG2	2.39	0.53
3:H:62:PHE:HB3	3:H:73:LEU:HD21	1.91	0.53
1:B:92:PHE:HE2	1:B:240:THR:CG2	2.21	0.53
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	1.90	0.53
1:C:438:SER:HB2	1:C:441:LEU:HB2	1.91	0.53
2:I:116:SER:OG	2:I:117:SER:N	2.42	0.53
1:B:456:PHE:HB3	1:B:474:GLN:HG2	1.89	0.53
1:A:438:SER:HB2	1:A:441:LEU:HB2	1.91	0.53
1:C:791:THR:HG23	1:C:879:ALA:HB2	1.90	0.53
1:A:1039:ARG:NH2	1:B:1031:GLU:OE2	2.43	0.52
1:C:141:LEU:HA	1:C:156:GLU:HG3	1.90	0.52
1:C:324:GLU:OE1	1:C:539:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:HG13	3:L:26:SER:HB3	1.91	0.52
1:A:371:SER:C	1:A:373:SER:H	2.17	0.52
1:B:81:ASN:N	1:B:82:PRO:HD3	2.25	0.52
1:B:210:ILE:HG13	1:B:212:LEU:H	1.74	0.52
3:J:2:ILE:HG13	3:J:26:SER:HB3	1.91	0.52
1:A:118:LEU:O	1:A:128:ILE:HA	2.10	0.52
1:A:456:PHE:CD2	1:A:491:PRO:HA	2.45	0.52
1:A:190:ARG:HB3	1:A:192:PHE:HE1	1.74	0.52
1:B:69:HIS:HA	1:B:76:THR:O	2.09	0.52
1:B:189:LEU:HD21	1:B:191:GLU:OE2	2.08	0.52
3:H:2:ILE:HG13	3:H:26:SER:HB3	1.91	0.52
1:A:456:PHE:HB3	1:A:474:GLN:HG2	1.89	0.52
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.45	0.52
1:B:1115:ILE:CG2	1:B:1120:THR:HG21	2.39	0.52
2:D:116:SER:OG	2:D:117:SER:N	2.42	0.52
2:E:116:SER:OG	2:E:117:SER:N	2.42	0.52
1:B:438:SER:HB2	1:B:441:LEU:HB2	1.91	0.52
1:C:237:ARG:HG2	1:C:238:PHE:N	2.25	0.52
1:C:770:ILE:O	1:C:774:GLN:HG2	2.10	0.52
3:L:59:PRO:HB2	3:L:61:ARG:HG2	1.92	0.52
3:H:59:PRO:HB2	3:H:61:ARG:HG2	1.92	0.51
1:C:37:TYR:HA	1:C:223:LEU:H	1.75	0.51
2:E:36:ARG:NH2	2:E:46:VAL:HB	2.26	0.51
3:L:62:PHE:HB3	3:L:73:LEU:HD21	1.91	0.51
1:C:374:PHE:CE2	1:C:377:PHE:HB2	2.46	0.51
3:J:21:ILE:CG2	3:J:73:LEU:HB3	2.41	0.51
1:A:131:CYS:CB	1:A:166:CYS:HA	2.40	0.51
1:A:533:LEU:HD12	1:A:533:LEU:O	2.11	0.51
1:C:119:ILE:HA	1:C:128:ILE:HG13	1.93	0.51
2:D:36:ARG:NH2	2:D:46:VAL:HB	2.26	0.51
1:A:374:PHE:CE2	1:A:377:PHE:HB2	2.46	0.51
1:B:456:PHE:CD2	1:B:491:PRO:HA	2.45	0.51
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.46	0.51
1:B:825:LYS:HB3	1:B:945:LEU:CD1	2.40	0.51
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.46	0.51
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.92	0.51
2:I:36:ARG:NH2	2:I:46:VAL:HB	2.26	0.51
3:L:89:GLN:HE22	3:L:91:ALA:HB2	1.73	0.51
1:B:914:ASN:OD1	1:B:915:VAL:N	2.44	0.51
1:C:1081:ILE:HD12	1:C:1095:PHE:CE1	2.46	0.51
3:J:59:PRO:HB2	3:J:61:ARG:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:GLU:HA	2:E:21:SER:O	2.11	0.51
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.46	0.50
1:C:896:ILE:HD11	1:C:904:TYR:CZ	2.46	0.50
3:H:21:ILE:CG2	3:H:73:LEU:HB3	2.41	0.50
1:A:866:THR:H	1:A:869:MET:HE3	1.76	0.50
1:C:289:VAL:HG23	1:C:306:PHE:CE2	2.47	0.50
1:A:1081:ILE:CD1	1:A:1133:VAL:HG23	2.41	0.50
1:B:374:PHE:CE2	1:B:377:PHE:HB2	2.46	0.50
1:A:533:LEU:HD12	1:A:533:LEU:C	2.36	0.50
1:C:456:PHE:CD2	1:C:491:PRO:HA	2.44	0.50
3:J:64:GLY:HA3	3:J:73:LEU:HA	1.94	0.50
3:L:21:ILE:CG2	3:L:73:LEU:HB3	2.41	0.50
3:L:64:GLY:HA3	3:L:73:LEU:HA	1.94	0.50
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.77	0.50
1:B:374:PHE:HE2	1:B:377:PHE:HB2	1.77	0.50
1:B:673:SER:OG	1:B:695:TYR:HE2	1.95	0.49
1:A:374:PHE:HE2	1:A:377:PHE:HB2	1.77	0.49
1:A:789:TYR:HA	1:C:703:ASN:O	2.11	0.49
1:B:791:THR:CG2	1:B:879:ALA:CB	2.90	0.49
1:C:374:PHE:HE2	1:C:377:PHE:HB2	1.77	0.49
2:I:6:GLU:HA	2:I:21:SER:O	2.11	0.49
1:B:117:LEU:HD11	1:B:128:ILE:HG22	1.94	0.49
1:B:791:THR:HG23	1:B:879:ALA:HB2	1.94	0.49
1:C:1086:LYS:HB3	1:C:1122:VAL:HG13	1.94	0.49
1:B:193:VAL:HG13	1:B:270:LEU:HD11	1.93	0.49
1:C:431:GLY:HA3	1:C:513:LEU:O	2.13	0.49
1:C:962:LEU:HD13	1:C:1007:TYR:HB2	1.94	0.49
3:H:64:GLY:HA3	3:H:73:LEU:HA	1.94	0.49
1:B:30:ASN:ND2	1:B:32:PHE:CE1	2.79	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.13	0.49
1:A:424:LYS:HE2	1:A:463:PRO:HG3	1.95	0.49
2:D:6:GLU:HA	2:D:21:SER:O	2.11	0.49
2:I:33:SER:CB	2:I:96:GLY:HA2	2.42	0.49
1:A:961:THR:O	1:A:965:GLN:HG2	2.12	0.49
1:B:424:LYS:HE2	1:B:463:PRO:HG3	1.95	0.49
1:B:560:LEU:HB2	1:B:563:GLN:CD	2.38	0.49
1:C:811:LYS:HB3	1:C:812:PRO:CD	2.42	0.49
1:B:18:LEU:HD23	1:B:21:ARG:HD3	1.94	0.49
1:C:369:TYR:HB3	1:C:377:PHE:CE2	2.47	0.49
1:A:42:VAL:HG12	1:A:43:PHE:N	2.27	0.48
1:A:865:LEU:HA	1:A:869:MET:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:HA3	1:A:513:LEU:O	2.13	0.48
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.13	0.48
1:B:318:PHE:CZ	1:B:623:ALA:HB3	2.48	0.48
3:H:30:SER:HA	3:H:67:SER:HA	1.95	0.48
1:A:336:CYS:HA	1:A:361:CYS:HB2	1.94	0.48
1:A:486:PHE:HB3	2:I:101:HIS:NE2	2.29	0.48
1:A:878:LEU:HD21	1:A:1052:PHE:HB3	1.96	0.48
1:C:322:PRO:HA	1:C:538:CYS:O	2.13	0.48
1:C:424:LYS:HE2	1:C:463:PRO:HG3	1.95	0.48
1:C:486:PHE:HB3	2:D:101:HIS:NE2	2.28	0.48
1:C:620:VAL:HG23	1:C:621:PRO:HD3	1.95	0.48
1:C:822:LEU:HD23	1:C:1056:ALA:CB	2.43	0.48
2:I:20:LEU:HB2	2:I:78:LEU:HB3	1.95	0.48
1:B:785:VAL:CG1	1:B:787:GLN:O	2.61	0.48
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.14	0.48
1:A:825:LYS:NZ	1:A:942:ALA:HB3	2.29	0.48
1:C:330:PRO:HA	1:C:579:PRO:HB2	1.96	0.48
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.49	0.48
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.95	0.48
1:C:770:ILE:HD12	1:C:1015:ALA:CB	2.44	0.48
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.49	0.47
1:B:486:PHE:HB3	2:E:101:HIS:NE2	2.29	0.47
1:C:328:ARG:HH21	1:C:580:GLN:HB3	1.79	0.47
1:A:308:VAL:H	1:A:602:THR:CG2	2.25	0.47
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.95	0.47
1:C:318:PHE:O	1:C:592:PHE:HA	2.14	0.47
1:C:721:SER:OG	1:C:1066:THR:OG1	2.31	0.47
1:C:738:CYS:O	1:C:742:ILE:HG13	2.15	0.47
2:D:20:LEU:HB2	2:D:78:LEU:HB3	1.95	0.47
2:D:33:SER:CB	2:D:96:GLY:HA2	2.42	0.47
3:H:35:TRP:CD1	3:H:73:LEU:HD13	2.50	0.47
3:H:94:PHE:CD1	3:H:95:PRO:HA	2.49	0.47
3:L:35:TRP:CD1	3:L:73:LEU:HD13	2.49	0.47
1:B:308:VAL:CG1	1:B:599:THR:HG21	2.44	0.47
3:L:30:SER:HA	3:L:67:SER:HA	1.95	0.47
1:A:126:VAL:H	1:A:174:PRO:HA	1.78	0.47
1:C:961:THR:O	1:C:965:GLN:HG3	2.14	0.47
1:B:395:VAL:HG23	1:B:524:VAL:HG21	1.96	0.47
1:C:822:LEU:CD2	1:C:1056:ALA:HB2	2.45	0.47
3:J:30:SER:HA	3:J:67:SER:HA	1.95	0.47
2:E:20:LEU:HB2	2:E:78:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:PHE:CD1	3:J:95:PRO:HA	2.49	0.47
1:A:90:VAL:HG13	1:A:267:VAL:HG13	1.96	0.47
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.50	0.47
1:B:134:GLN:HB3	1:B:162:SER:HB3	1.97	0.47
1:C:576:VAL:HG23	1:C:587:ILE:HD13	1.95	0.47
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.97	0.47
1:C:822:LEU:HD23	1:C:1056:ALA:HB2	1.96	0.47
1:C:965:GLN:OE1	1:C:1003:SER:HB2	2.14	0.47
1:B:994:ASP:O	1:B:998:THR:HG23	2.15	0.47
1:C:723:THR:C	1:C:724:THR:HG23	2.40	0.47
3:J:35:TRP:CD1	3:J:73:LEU:HD13	2.50	0.47
1:A:674:TYR:O	1:A:675:GLN:C	2.58	0.47
1:A:1115:ILE:CG2	1:A:1120:THR:HG21	2.45	0.47
1:C:541:PHE:CZ	1:C:587:ILE:HG12	2.50	0.47
2:E:33:SER:CB	2:E:96:GLY:HA2	2.42	0.47
1:A:599:THR:HG22	1:A:608:VAL:HG12	1.96	0.46
1:C:723:THR:O	1:C:724:THR:CG2	2.62	0.46
1:A:1024:LEU:HD11	1:A:1042:PHE:HE1	1.80	0.46
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.96	0.46
3:L:94:PHE:CD1	3:L:95:PRO:HA	2.49	0.46
1:A:642:VAL:HG13	1:A:649:CYS:SG	2.55	0.46
1:B:393:THR:HB	1:B:517:LEU:HA	1.98	0.46
1:B:666:ILE:CD1	1:B:672:ALA:HB2	2.46	0.46
1:B:785:VAL:HG12	1:B:787:GLN:O	2.15	0.46
1:A:1080:ALA:O	1:A:1081:ILE:HD13	2.15	0.46
1:A:1116:THR:HG22	1:A:1138:TYR:HD2	1.81	0.46
1:B:328:ARG:HH22	1:B:581:THR:HG23	1.80	0.46
1:B:932:GLY:O	1:B:935:GLN:HG2	2.16	0.46
1:C:909:ILE:HD13	1:C:1049:LEU:HD21	1.98	0.46
3:J:29:ILE:HB	3:J:71:PHE:CZ	2.51	0.46
1:A:869:MET:SD	1:C:697:MET:HE3	2.56	0.46
1:B:905:ARG:HD3	1:B:1049:LEU:O	2.16	0.46
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.81	0.46
3:L:29:ILE:HB	3:L:71:PHE:CZ	2.51	0.46
1:A:393:THR:HB	1:A:517:LEU:HA	1.98	0.46
2:D:47:SER:CB	2:D:61:VAL:HG21	2.45	0.46
3:J:49:ASN:OD1	3:J:55:GLN:HA	2.16	0.46
3:H:29:ILE:HB	3:H:71:PHE:CZ	2.51	0.46
1:A:108:THR:HA	1:A:236:THR:H	1.81	0.46
1:B:984:LEU:HD12	1:B:984:LEU:HA	1.78	0.46
2:I:47:SER:CB	2:I:61:VAL:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:VAL:CG2	1:B:877:LEU:HG	2.47	0.45
2:E:47:SER:CB	2:E:61:VAL:HG21	2.46	0.45
1:B:546:LEU:HD11	1:B:576:VAL:HG21	1.99	0.45
3:L:49:ASN:OD1	3:L:55:GLN:HA	2.16	0.45
1:B:92:PHE:CE2	1:B:240:THR:HG22	2.51	0.45
1:B:96:GLU:HG3	1:B:99:ASN:H	1.80	0.45
1:B:395:VAL:HG22	1:B:515:PHE:HD1	1.81	0.45
3:J:32:TRP:HB3	3:J:91:ALA:HB3	1.99	0.45
1:A:18:LEU:HD21	1:A:244:LEU:HD21	1.99	0.45
1:C:791:THR:HG23	1:C:879:ALA:CB	2.46	0.45
1:A:815:ARG:HD2	1:A:820:ASP:OD1	2.17	0.45
1:B:570:ALA:HA	1:C:964:LYS:HG3	1.99	0.45
3:H:32:TRP:HB3	3:H:91:ALA:HB3	1.98	0.45
1:C:83:VAL:HA	1:C:237:ARG:HE	1.80	0.45
1:C:1056:ALA:O	1:C:1057:PRO:C	2.59	0.45
3:H:49:ASN:OD1	3:H:55:GLN:HA	2.16	0.45
1:A:620:VAL:HG21	1:A:651:ILE:HD11	1.99	0.45
1:B:742:ILE:CD1	1:B:1001:LEU:HG	2.46	0.45
1:A:404:GLY:O	1:A:407:VAL:HG22	2.17	0.45
1:B:90:VAL:HG13	1:B:267:VAL:HG13	1.99	0.45
1:C:393:THR:HB	1:C:517:LEU:HA	1.98	0.45
1:A:880:GLY:O	1:A:884:SER:HB2	2.17	0.44
1:C:822:LEU:HD12	1:C:945:LEU:HD21	1.99	0.44
1:B:111:ASP:O	1:B:112:SER:HB2	2.16	0.44
1:C:289:VAL:HG23	1:C:306:PHE:CZ	2.52	0.44
1:A:62:VAL:HG12	1:A:268:GLY:HA3	2.00	0.44
1:C:502:GLY:O	1:C:506:GLN:N	2.49	0.44
1:A:106:PHE:HB3	1:A:235:ILE:CG2	2.48	0.44
1:C:643:PHE:CE2	1:C:645:THR:CG2	3.00	0.44
1:A:533:LEU:CD1	1:A:535:LYS:HE3	2.47	0.44
1:B:643:PHE:CE2	1:B:670:ILE:HD13	2.53	0.44
1:C:1116:THR:HG22	1:C:1138:TYR:HD2	1.83	0.44
3:H:2:ILE:HG22	3:H:97:THR:HB	2.00	0.44
1:A:83:VAL:HG22	1:A:239:GLN:OE1	2.17	0.44
1:C:38:TYR:CE1	1:C:224:GLU:HG2	2.53	0.44
3:L:32:TRP:HB3	3:L:91:ALA:HB3	1.99	0.44
1:A:773:GLU:OE2	1:A:1019:ARG:HD3	2.18	0.44
1:A:815:ARG:HA	1:A:819:GLU:OE1	2.18	0.44
1:B:193:VAL:HG23	1:B:223:LEU:HD12	2.00	0.44
1:B:736:VAL:HG13	1:B:858:LEU:HD23	2.00	0.44
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:ASP:HA	2:D:62:LYS:HE2	2.00	0.44
3:L:2:ILE:HG22	3:L:97:THR:HB	2.00	0.44
1:C:212:LEU:O	1:C:212:LEU:HG	2.17	0.44
1:B:112:SER:HB3	1:B:164:ASN:HB2	2.00	0.44
1:B:533:LEU:HD23	1:B:533:LEU:H	1.83	0.44
1:C:495:TYR:HD1	1:C:495:TYR:HA	1.72	0.44
3:J:27:GLN:H	3:J:29:ILE:HD12	1.83	0.44
3:H:27:GLN:H	3:H:29:ILE:HD12	1.83	0.44
1:A:775:ASP:O	1:A:779:GLN:HG3	2.18	0.43
1:B:898:PHE:O	1:B:899:ALA:C	2.60	0.43
1:C:404:GLY:O	1:C:407:VAL:HG22	2.17	0.43
1:C:939:SER:C	1:C:941:THR:N	2.73	0.43
2:D:64:ARG:HB3	2:D:82:SER:OG	2.18	0.43
2:D:80:MET:HE3	2:D:83:LEU:HA	1.99	0.43
2:I:59:ASP:HA	2:I:62:LYS:HE2	2.00	0.43
1:A:740:MET:HE2	1:A:740:MET:HB3	1.91	0.43
3:J:79:GLN:HB2	3:J:82:ASP:HB2	2.00	0.43
1:A:147:LYS:HD3	1:A:147:LYS:HA	1.84	0.43
1:A:617:CYS:O	1:A:620:VAL:HG12	2.18	0.43
1:B:159:VAL:HG13	1:B:160:TYR:HD1	1.82	0.43
2:D:69:ARG:HA	2:D:76:LEU:HA	2.01	0.43
3:J:2:ILE:HG22	3:J:97:THR:HB	2.00	0.43
1:B:331:ASN:O	1:B:332:ILE:HG12	2.18	0.43
1:C:95:THR:HG22	1:C:189:LEU:HA	2.00	0.43
2:I:80:MET:HE3	2:I:83:LEU:HA	1.99	0.43
1:B:98:SER:HB2	1:B:100:ILE:HG13	2.00	0.43
1:B:434:ILE:HB	1:B:511:VAL:HG12	2.01	0.43
1:C:120:VAL:HG21	1:C:129:LYS:HE3	2.01	0.43
1:C:391:CYS:HA	1:C:525:CYS:HB3	2.00	0.43
2:E:80:MET:HE3	2:E:83:LEU:HA	1.99	0.43
1:A:434:ILE:HB	1:A:511:VAL:HG12	2.01	0.43
1:A:902:MET:O	1:A:903:ALA:HB3	2.19	0.43
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.18	0.43
1:B:909:ILE:HG13	1:B:911:VAL:HG23	2.00	0.43
1:C:368:LEU:HB3	1:C:377:PHE:CE1	2.54	0.43
3:H:89:GLN:NE2	3:H:91:ALA:HB2	2.34	0.43
3:L:79:GLN:HB2	3:L:82:ASP:HB2	2.00	0.43
1:B:404:GLY:O	1:B:407:VAL:HG22	2.17	0.43
2:E:69:ARG:HA	2:E:76:LEU:HA	2.01	0.43
1:A:647:ALA:HA	1:B:862:PRO:HG3	1.99	0.43
1:C:67:ALA:HB1	1:C:260:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ASP:C	1:C:82:PRO:HD3	2.44	0.43
2:D:4:LEU:HB3	2:D:22:CYS:SG	2.59	0.43
2:D:106:ILE:C	2:D:107:TRP:HD1	2.27	0.43
2:E:64:ARG:HB3	2:E:82:SER:OG	2.18	0.43
1:B:231:ILE:HG22	1:B:233:ILE:HG23	2.00	0.43
1:B:495:TYR:HD1	1:B:495:TYR:HA	1.72	0.43
1:C:434:ILE:HB	1:C:511:VAL:HG12	2.01	0.43
2:E:4:LEU:HB3	2:E:22:CYS:SG	2.59	0.43
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.80	0.42
1:B:129:LYS:HA	1:B:170:TYR:O	2.18	0.42
2:I:64:ARG:HB3	2:I:82:SER:OG	2.18	0.42
1:A:898:PHE:C	1:A:900:MET:H	2.26	0.42
1:B:324:GLU:HB2	1:B:539:VAL:HG23	2.01	0.42
1:B:551:VAL:HG23	1:B:590:CYS:HB3	2.02	0.42
1:C:805:ILE:HD12	1:C:878:LEU:HD21	2.00	0.42
2:E:59:ASP:HA	2:E:62:LYS:HE2	2.00	0.42
1:A:123:ALA:HB1	1:A:176:LEU:HD12	2.01	0.42
1:A:352:ALA:HA	1:A:468:ILE:HG12	2.01	0.42
1:B:308:VAL:HG12	1:B:599:THR:HG21	2.01	0.42
1:B:1081:ILE:HD13	1:B:1115:ILE:HD13	2.00	0.42
1:C:721:SER:OG	1:C:721:SER:O	2.31	0.42
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.84	0.42
1:B:32:PHE:HD1	1:B:59:PHE:HE1	1.65	0.42
2:I:88:THR:HG21	2:I:115:VAL:HB	2.02	0.42
1:B:34:ARG:NE	1:B:191:GLU:OE2	2.52	0.42
1:B:142:GLY:CA	1:B:156:GLU:HB2	2.49	0.42
1:B:379:CYS:HA	1:B:432:CYS:HA	2.02	0.42
1:B:776:LYS:HE2	1:B:776:LYS:HB3	1.85	0.42
1:C:368:LEU:HB3	1:C:377:PHE:HE1	1.85	0.42
3:J:89:GLN:NE2	3:J:91:ALA:HB2	2.34	0.42
2:I:4:LEU:HB3	2:I:22:CYS:SG	2.59	0.42
2:I:83:LEU:HD12	2:I:83:LEU:H	1.85	0.42
1:A:1095:PHE:CD1	1:A:1104:VAL:HG22	2.55	0.42
2:I:69:ARG:HA	2:I:76:LEU:HA	2.01	0.42
3:L:27:GLN:H	3:L:29:ILE:HD12	1.83	0.42
1:A:1115:ILE:HG22	1:A:1120:THR:HG21	2.01	0.42
2:E:106:ILE:C	2:E:107:TRP:HD1	2.27	0.42
3:H:79:GLN:HB2	3:H:82:ASP:HB2	2.00	0.42
3:L:66:GLY:HA2	3:L:71:PHE:HA	2.01	0.42
1:A:190:ARG:HG3	1:A:207:HIS:CD2	2.54	0.42
1:A:733:LYS:HE3	1:A:771:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ALA:HA	1:B:468:ILE:HG12	2.01	0.42
2:E:88:THR:HG21	2:E:115:VAL:HB	2.02	0.42
2:I:106:ILE:C	2:I:107:TRP:HD1	2.27	0.42
3:L:89:GLN:NE2	3:L:91:ALA:HB2	2.34	0.42
1:B:366:SER:HA	1:B:369:TYR:CE1	2.54	0.42
1:B:746:SER:OG	1:B:749:CYS:HB3	2.19	0.42
1:B:906:PHE:O	1:B:909:ILE:HG12	2.19	0.42
1:A:379:CYS:HA	1:A:432:CYS:HA	2.02	0.42
1:C:352:ALA:HA	1:C:468:ILE:HG12	2.01	0.42
2:E:83:LEU:HD12	2:E:83:LEU:H	1.85	0.42
3:H:62:PHE:HA	3:H:74:THR:O	2.20	0.42
3:H:66:GLY:HA2	3:H:71:PHE:HA	2.01	0.42
1:A:289:VAL:HG23	1:A:306:PHE:CZ	2.54	0.41
1:A:318:PHE:O	1:A:592:PHE:HA	2.20	0.41
1:A:371:SER:C	1:A:373:SER:N	2.75	0.41
1:B:18:LEU:HA	1:B:18:LEU:HD12	1.82	0.41
2:D:83:LEU:HD12	2:D:83:LEU:H	1.85	0.41
1:B:621:PRO:HG2	1:B:622:VAL:HG23	2.03	0.41
1:C:128:ILE:HD13	1:C:170:TYR:HB3	2.03	0.41
1:A:962:LEU:HD13	1:A:1007:TYR:HB2	2.02	0.41
1:C:939:SER:C	1:C:941:THR:H	2.29	0.41
1:C:1086:LYS:HB3	1:C:1122:VAL:CG1	2.49	0.41
3:J:62:PHE:HA	3:J:74:THR:O	2.20	0.41
3:J:66:GLY:HA2	3:J:71:PHE:HA	2.01	0.41
2:I:48:VAL:HB	2:I:56:ASP:OD1	2.20	0.41
1:A:738:CYS:O	1:A:742:ILE:HG12	2.21	0.41
1:A:898:PHE:C	1:A:900:MET:N	2.77	0.41
1:C:534:VAL:CG1	1:C:539:VAL:HG21	2.51	0.41
3:L:62:PHE:HA	3:L:74:THR:O	2.20	0.41
1:A:18:LEU:HD21	1:A:244:LEU:CD2	2.50	0.41
1:A:127:VAL:HG13	1:A:171:VAL:HG23	2.01	0.41
1:A:900:MET:HG3	1:A:917:TYR:OH	2.21	0.41
1:A:1038:LYS:HB3	1:A:1038:LYS:HE2	1.87	0.41
1:B:216:LEU:HD12	1:B:216:LEU:C	2.45	0.41
1:C:911:VAL:HG13	1:C:1106:GLN:HE22	1.85	0.41
1:B:229:LEU:HA	1:B:230:PRO:HD3	1.94	0.41
1:B:756:TYR:OH	1:B:998:THR:HG22	2.20	0.41
1:C:666:ILE:HD11	1:C:672:ALA:HB2	2.03	0.41
2:D:88:THR:HG21	2:D:115:VAL:HB	2.02	0.41
2:E:48:VAL:HB	2:E:56:ASP:OD1	2.20	0.41
2:E:64:ARG:O	2:E:81:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:TYR:HD1	1:A:495:TYR:HA	1.72	0.41
1:B:724:THR:HG22	1:B:1063:LEU:CD2	2.51	0.41
3:H:27:GLN:OE1	3:H:93:SER:HB3	2.21	0.41
2:I:64:ARG:O	2:I:81:ASN:HB2	2.21	0.41
1:C:416:GLY:N	1:C:419:ALA:HB3	2.36	0.41
2:D:48:VAL:HB	2:D:56:ASP:OD1	2.20	0.41
1:A:245:HIS:CE1	1:A:247:SER:HB2	2.56	0.41
1:A:362:VAL:HG11	1:A:527:PRO:HB3	2.02	0.41
1:A:620:VAL:N	1:A:621:PRO:HD2	2.36	0.41
1:B:290:ASP:O	1:B:297:SER:HB3	2.21	0.41
1:B:425:LEU:HD12	1:B:425:LEU:HA	1.80	0.41
1:B:541:PHE:O	1:B:547:THR:HA	2.21	0.41
1:B:552:LEU:HD23	1:B:587:ILE:HG13	2.03	0.41
1:B:569:ILE:O	1:B:570:ALA:HB3	2.20	0.41
1:B:1029:MET:HE2	1:B:1029:MET:HB2	1.86	0.41
1:C:355:ARG:HH21	1:C:355:ARG:HG3	1.86	0.41
1:C:379:CYS:HA	1:C:432:CYS:HA	2.02	0.41
3:L:94:PHE:CD1	3:L:96:PRO:HD3	2.56	0.41
1:A:118:LEU:HD23	1:A:129:LYS:HE3	2.03	0.41
1:B:555:SER:OG	1:B:557:LYS:HG2	2.21	0.41
1:C:1027:THR:HG22	1:C:1042:PHE:CZ	2.56	0.41
3:J:62:PHE:HD1	3:J:75:ILE:HG12	1.86	0.41
1:A:42:VAL:CG1	1:A:43:PHE:N	2.84	0.40
1:A:823:PHE:CE1	1:A:1057:PRO:HA	2.57	0.40
1:A:1081:ILE:HD13	1:A:1133:VAL:HG23	2.03	0.40
1:B:1084:ASP:HB3	1:B:1086:LYS:HE2	2.03	0.40
1:C:814:LYS:O	1:C:815:ARG:C	2.62	0.40
3:H:62:PHE:HD1	3:H:75:ILE:HG12	1.86	0.40
2:I:6:GLU:OE2	2:I:93:CYS:SG	2.79	0.40
3:L:62:PHE:HD1	3:L:75:ILE:HG12	1.86	0.40
1:A:877:LEU:O	1:A:881:THR:HG22	2.21	0.40
3:L:27:GLN:OE1	3:L:93:SER:HB3	2.21	0.40
1:A:355:ARG:HH21	1:A:355:ARG:HG3	1.86	0.40
1:C:38:TYR:HE1	1:C:224:GLU:HG2	1.86	0.40
1:C:336:CYS:HA	1:C:361:CYS:HB2	2.03	0.40
1:A:290:ASP:O	1:A:297:SER:HB3	2.21	0.40
1:A:1027:THR:HG22	1:A:1042:PHE:CZ	2.57	0.40
1:C:805:ILE:HD12	1:C:878:LEU:HD11	2.03	0.40
1:C:994:ASP:OD1	1:C:994:ASP:O	2.39	0.40
1:A:316:SER:HB3	1:A:317:ASN:H	1.64	0.40
1:A:718:PHE:CE1	1:A:923:ILE:HG12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.92	0.40
1:B:416:GLY:N	1:B:419:ALA:HB3	2.36	0.40
1:C:65:PHE:CE1	1:C:84:LEU:HD21	2.57	0.40
3:J:94:PHE:CD1	3:J:96:PRO:HD3	2.56	0.40
3:L:3:GLN:O	3:L:26:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1042/1298 (80%)	988 (95%)	48 (5%)	6 (1%)	21	52
1	B	1032/1298 (80%)	969 (94%)	59 (6%)	4 (0%)	30	60
1	C	963/1298 (74%)	904 (94%)	48 (5%)	11 (1%)	11	39
2	D	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	43
2	E	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	43
2	I	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	43
3	H	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
3	J	102/107 (95%)	97 (95%)	5 (5%)	0	100	100
3	L	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
All	All	3687/4566 (81%)	3481 (94%)	182 (5%)	24 (1%)	20	49

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	LYS
1	B	332	ILE
1	C	280	ASN

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Mol	Chain	Res	Type
1	C	707	TYR
1	C	813	SER
1	C	942	ALA
1	C	946	GLY
2	D	89	ALA
2	E	89	ALA
2	I	89	ALA
1	A	88	ASP
1	A	372	ALA
1	A	472	ILE
1	B	472	ILE
1	B	940	SER
1	C	332	ILE
1	C	472	ILE
1	B	330	PRO
1	C	525	CYS
1	C	82	PRO
1	C	1057	PRO
1	A	325	SER
1	A	1127	ASP
1	C	811	LYS

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	845/1122 (75%)	838 (99%)	7 (1%)	73	79
1	B	846/1122 (75%)	838 (99%)	8 (1%)	70	78
1	C	788/1122 (70%)	777 (99%)	11 (1%)	59	73
2	D	85/95 (90%)	84 (99%)	1 (1%)	63	75
2	E	85/95 (90%)	84 (99%)	1 (1%)	63	75
2	I	85/95 (90%)	84 (99%)	1 (1%)	63	75
3	H	74/89 (83%)	74 (100%)	0	100	100
3	J	73/89 (82%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	74/89 (83%)	74 (100%)	0	100	100
All	All	2955/3918 (75%)	2926 (99%)	29 (1%)	65	76

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	THR
1	A	347	PHE
1	A	401	VAL
1	A	495	TYR
1	A	524	VAL
1	A	525	CYS
1	A	906	PHE
1	B	66	HIS
1	B	215	ASP
1	B	332	ILE
1	B	347	PHE
1	B	401	VAL
1	B	495	TYR
1	B	524	VAL
1	B	886	TRP
1	C	47	VAL
1	C	108	THR
1	C	154	GLU
1	C	156	GLU
1	C	241	LEU
1	C	333	THR
1	C	347	PHE
1	C	401	VAL
1	C	495	TYR
1	C	515	PHE
1	C	524	VAL
2	D	111	THR
2	E	111	THR
2	I	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	66	HIS

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Mol	Chain	Res	Type
1	A	115	GLN
1	A	317	ASN
1	A	370	ASN
1	A	440	ASN
1	A	481	ASN
1	A	493	GLN
1	A	607	GLN
1	A	616	ASN
1	A	655	HIS
1	A	751	ASN
1	A	755	GLN
1	A	787	GLN
1	A	901	GLN
1	A	969	ASN
1	A	1002	GLN
1	A	1083	HIS
1	A	1108	ASN
1	B	121	ASN
1	B	134	GLN
1	B	188	ASN
1	B	370	ASN
1	B	440	ASN
1	B	481	ASN
1	B	493	GLN
1	B	536	ASN
1	B	613	GLN
1	B	703	ASN
1	B	751	ASN
1	B	762	GLN
1	B	787	GLN
1	B	1005	GLN
1	B	1011	GLN
1	B	1058	HIS
1	B	1088	HIS
1	B	1106	GLN
1	B	1108	ASN
1	C	81	ASN
1	C	196	ASN
1	C	370	ASN
1	C	388	ASN
1	C	440	ASN
1	C	481	ASN

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Mol	Chain	Res	Type
1	C	493	GLN
1	C	536	ASN
1	C	616	ASN
1	C	655	HIS
1	C	675	GLN
1	C	703	ASN
1	C	787	GLN
1	C	907	ASN
1	C	955	ASN
1	C	1005	GLN
1	C	1083	HIS
1	C	1106	GLN
1	C	1108	ASN
3	J	89	GLN
3	H	89	GLN
3	L	89	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 ⓘ

There are no chain breaks in this entry.

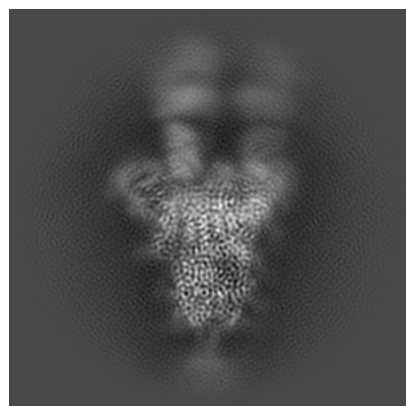
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33133. These allow visual inspection of the internal detail of the map and identification of artifacts.

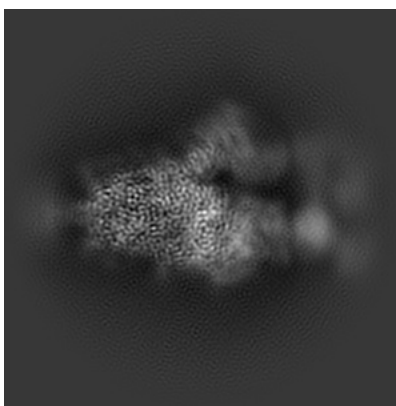
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

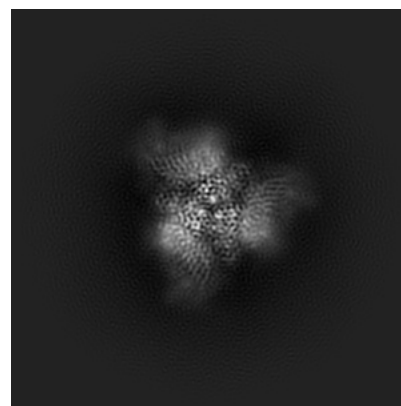
6.1.1 Primary map



X

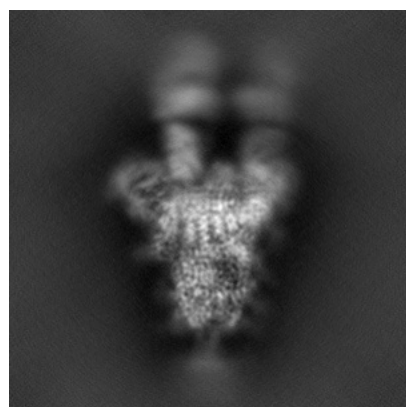


Y

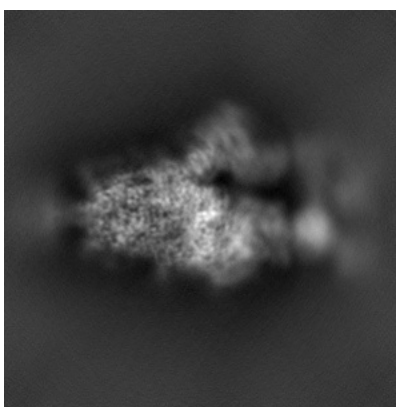


Z

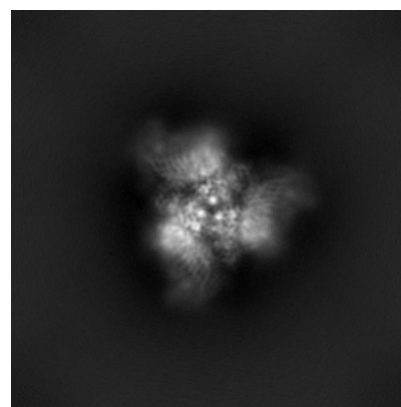
6.1.2 Raw map



X



Y

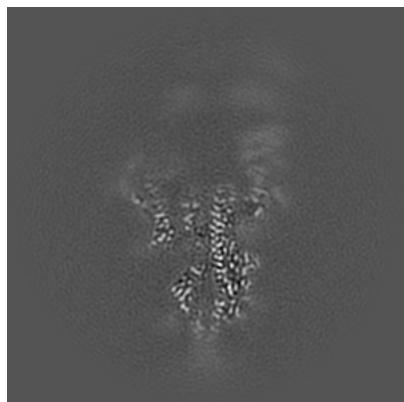


Z

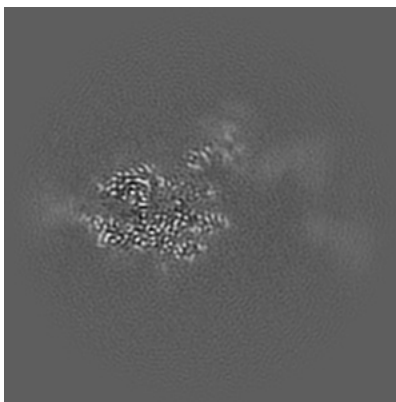
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

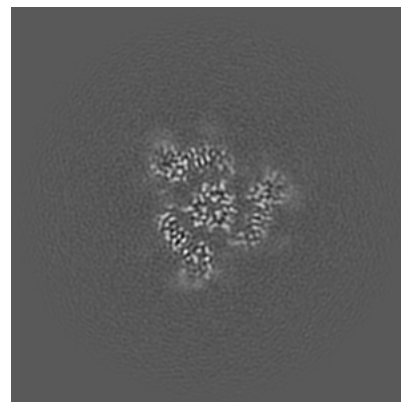
6.2.1 Primary map



X Index: 160

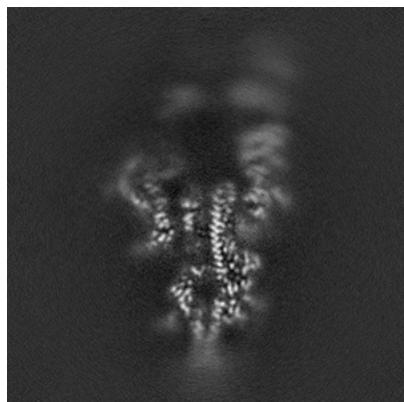


Y Index: 160

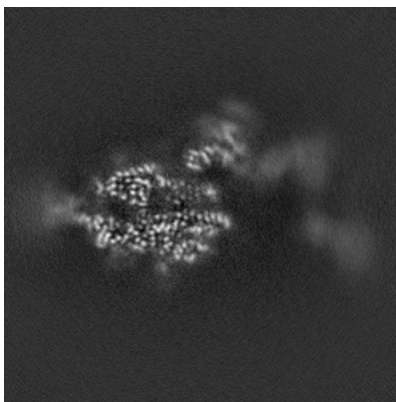


Z Index: 160

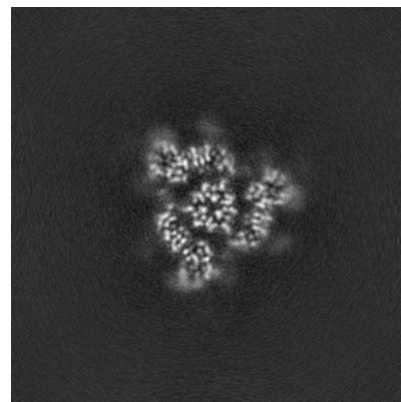
6.2.2 Raw map



X Index: 160



Y Index: 160

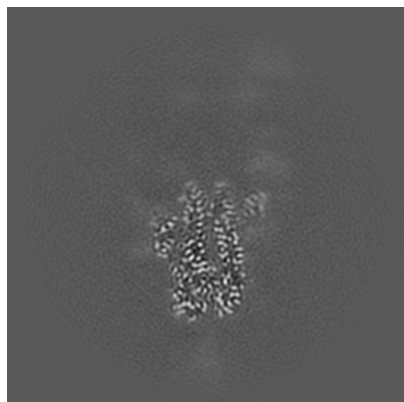


Z Index: 160

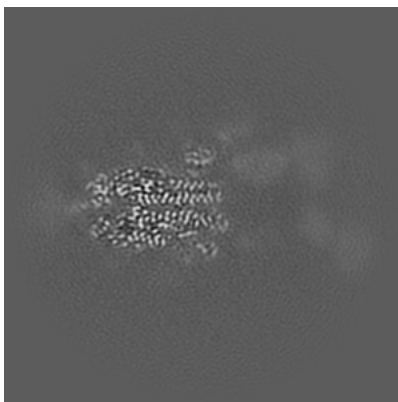
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

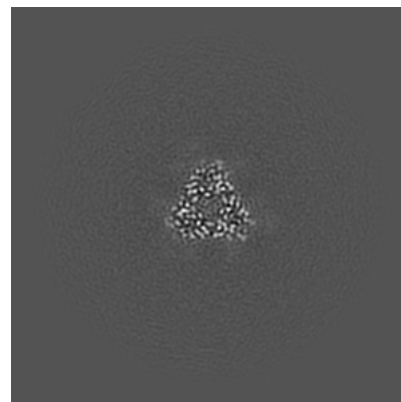
6.3.1 Primary map



X Index: 169

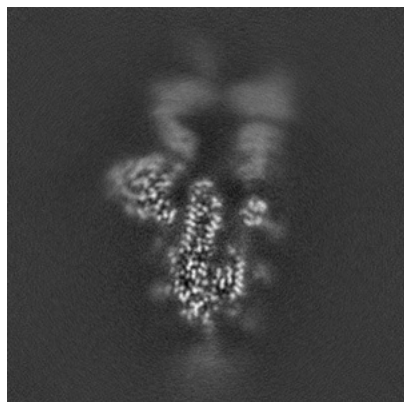


Y Index: 154

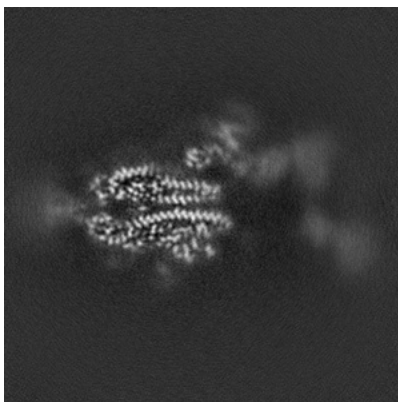


Z Index: 100

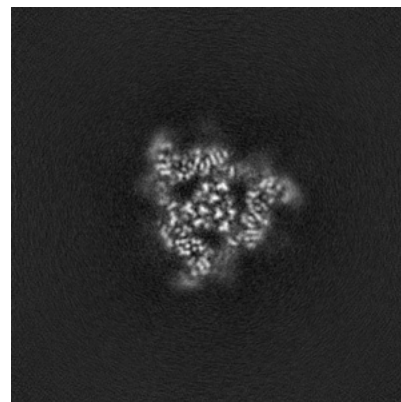
6.3.2 Raw map



X Index: 146



Y Index: 157

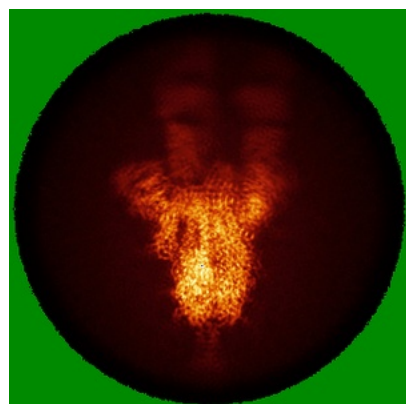


Z Index: 155

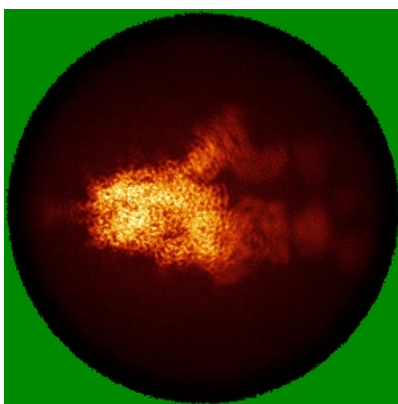
The images above show the largest variance slices of the map in three orthogonal directions.

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

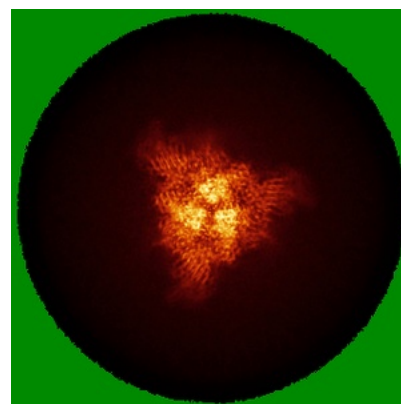
6.4.1 Primary map



X

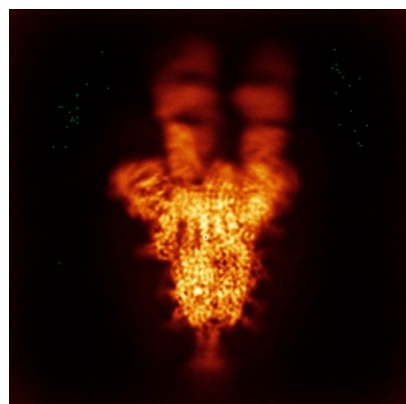


Y

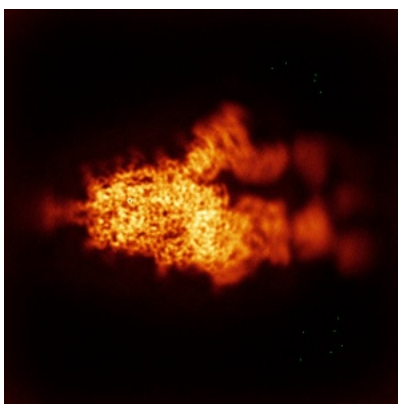


Z

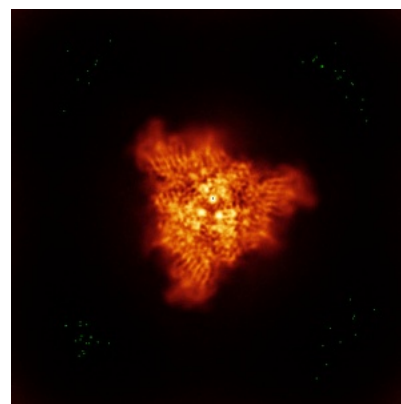
6.4.2 Raw map



X



Y

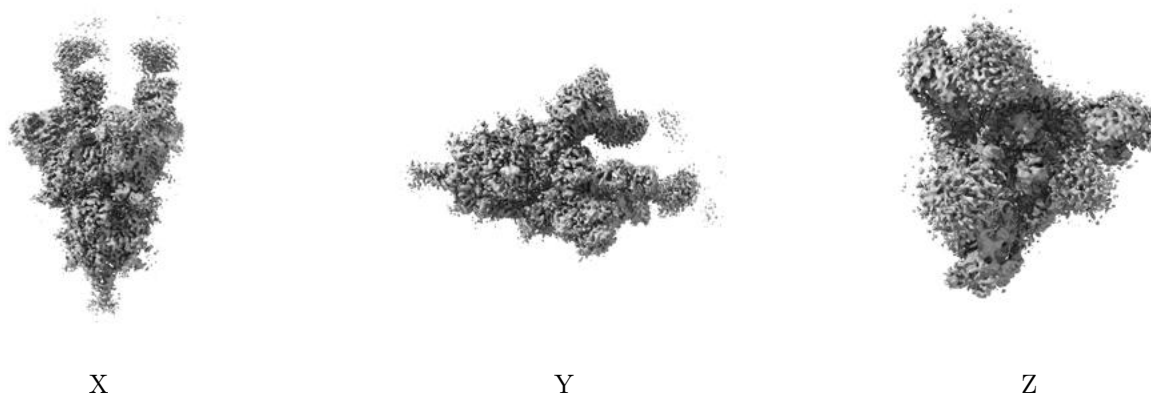


Z

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.

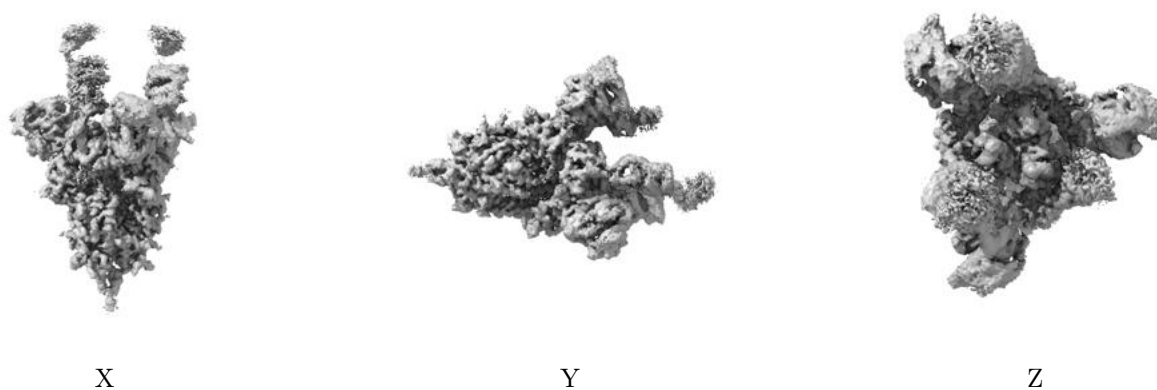
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

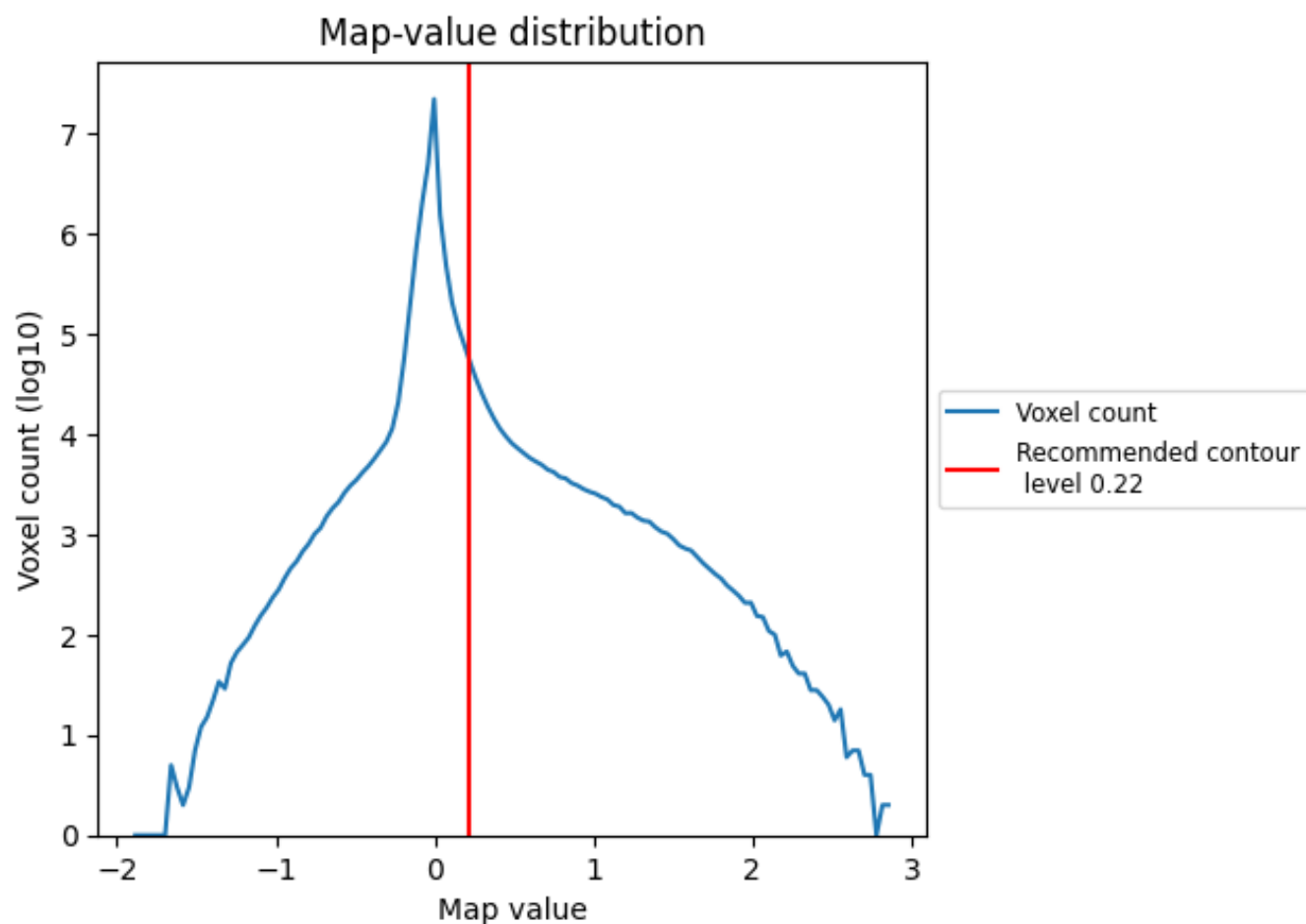
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

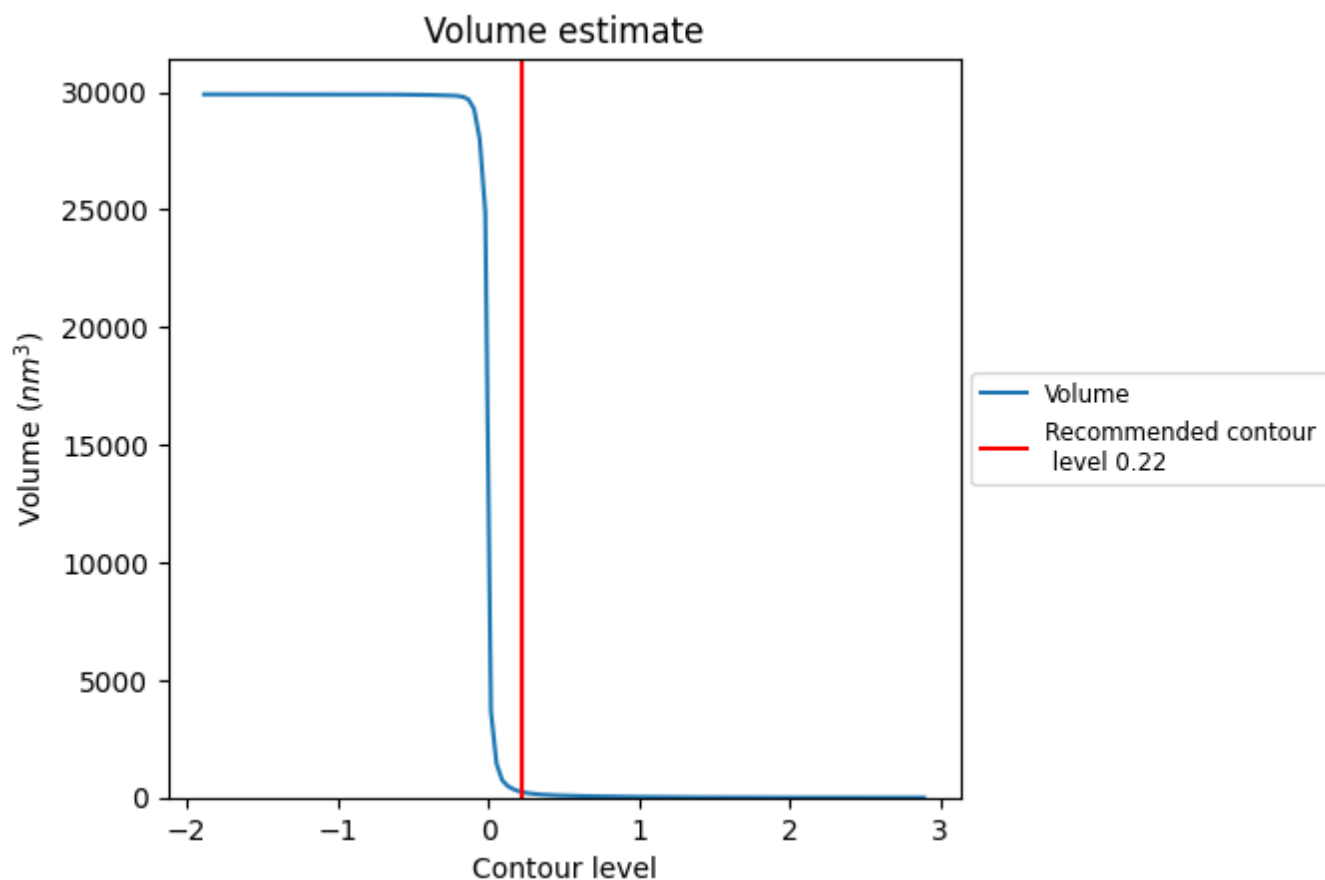
This section contains the results of statistical analysis of the map.

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.

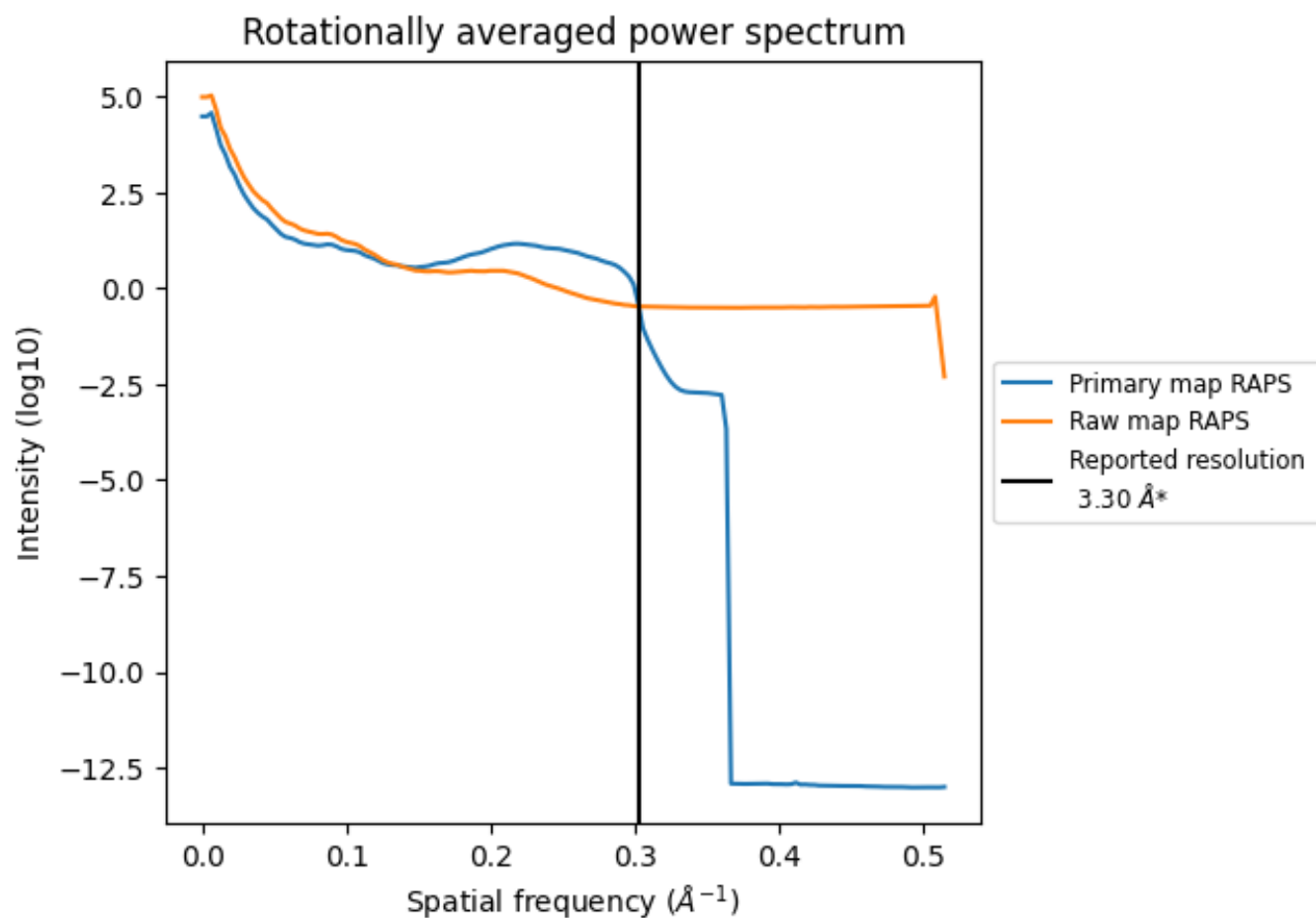
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 246 nm³; this corresponds to an approximate mass of 222 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 ⓘ

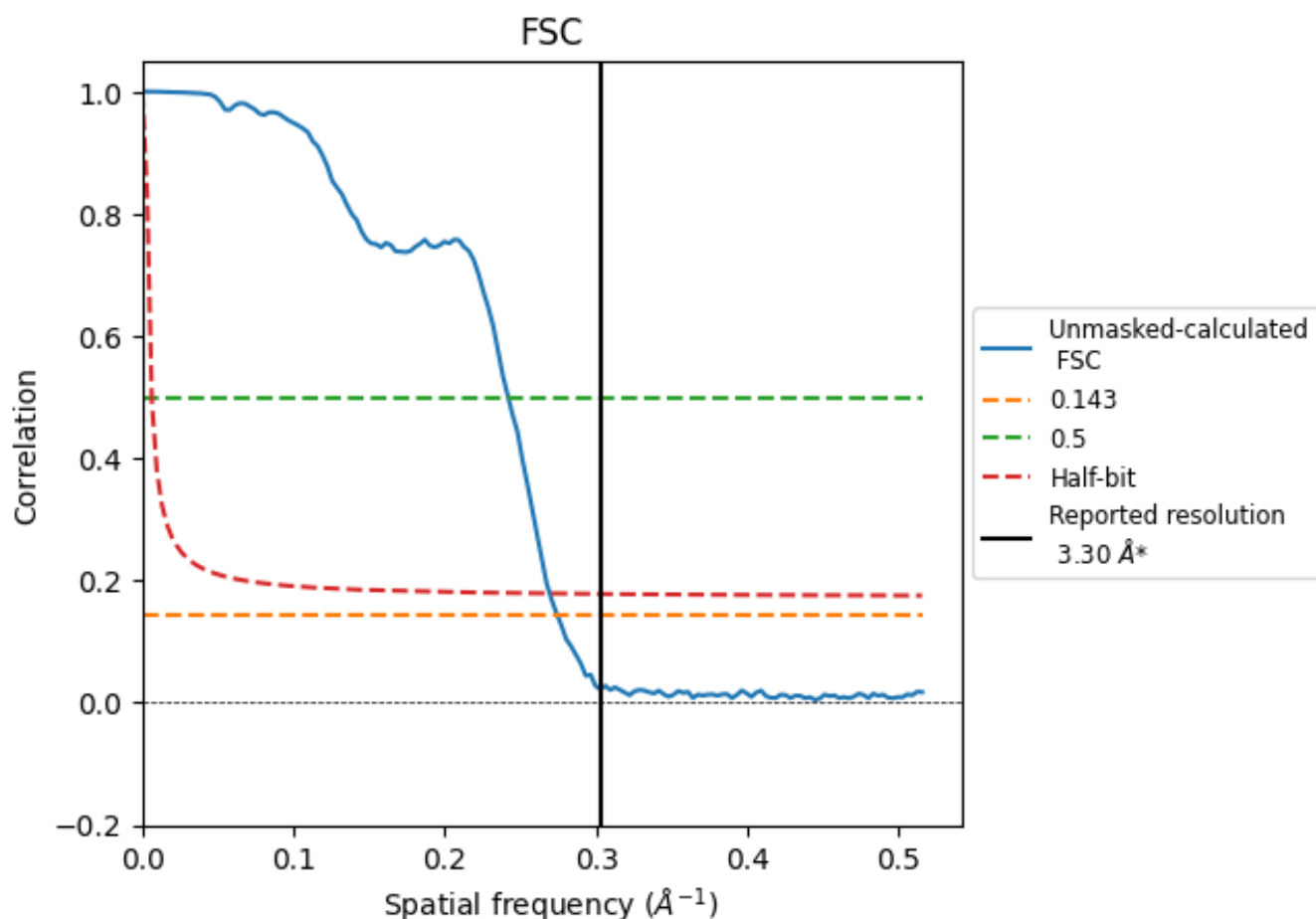


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

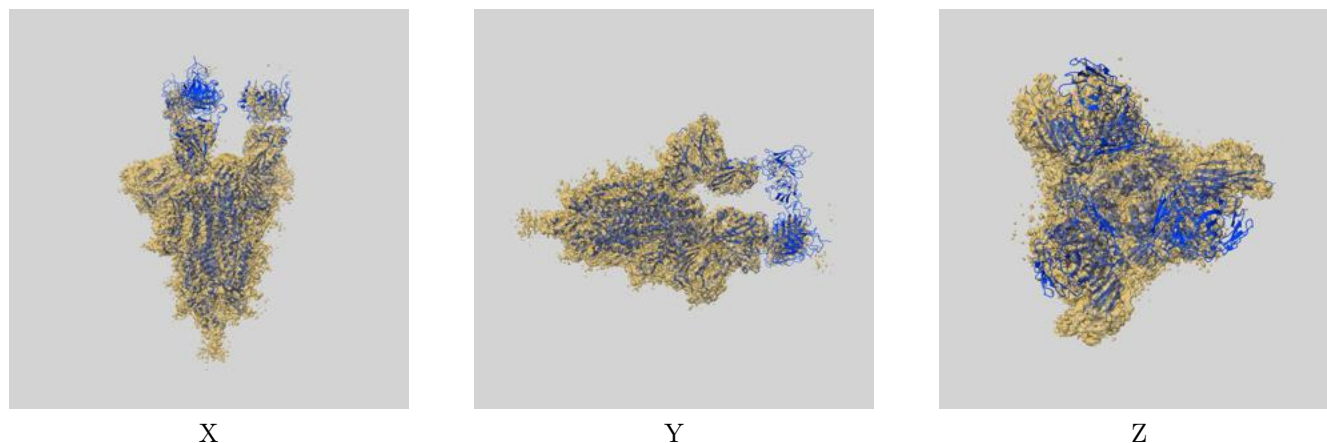
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	4.13	3.71

*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 3.64 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

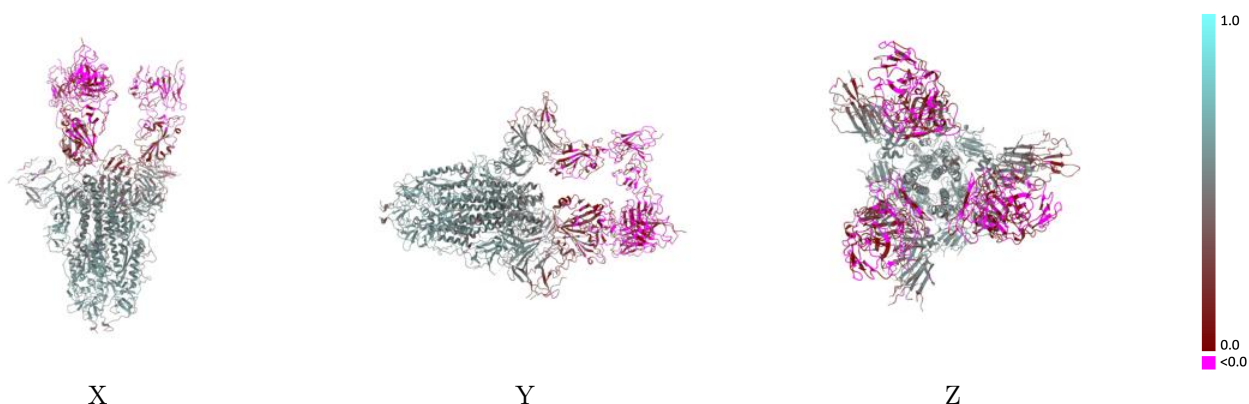
This section contains information regarding the fit between EMDB map EMD-33133 and PDB model 7XD2. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



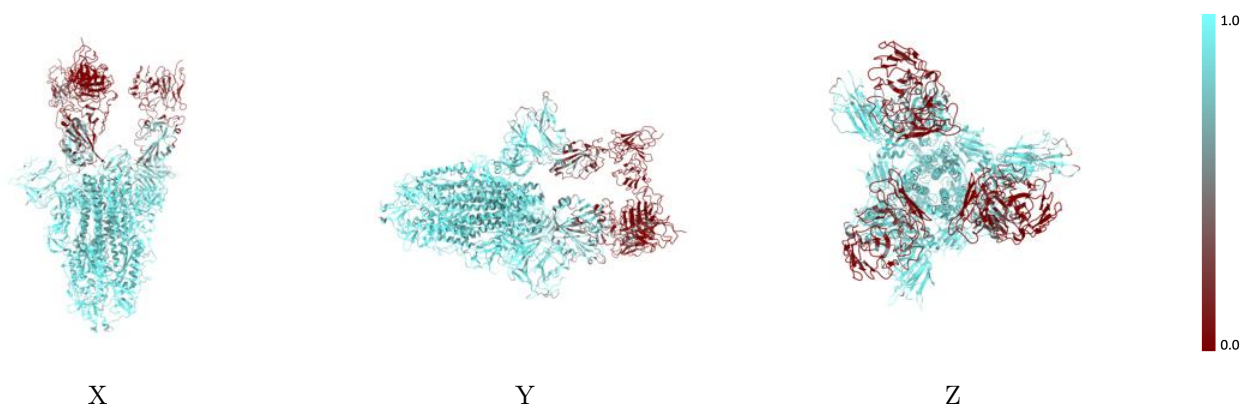
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



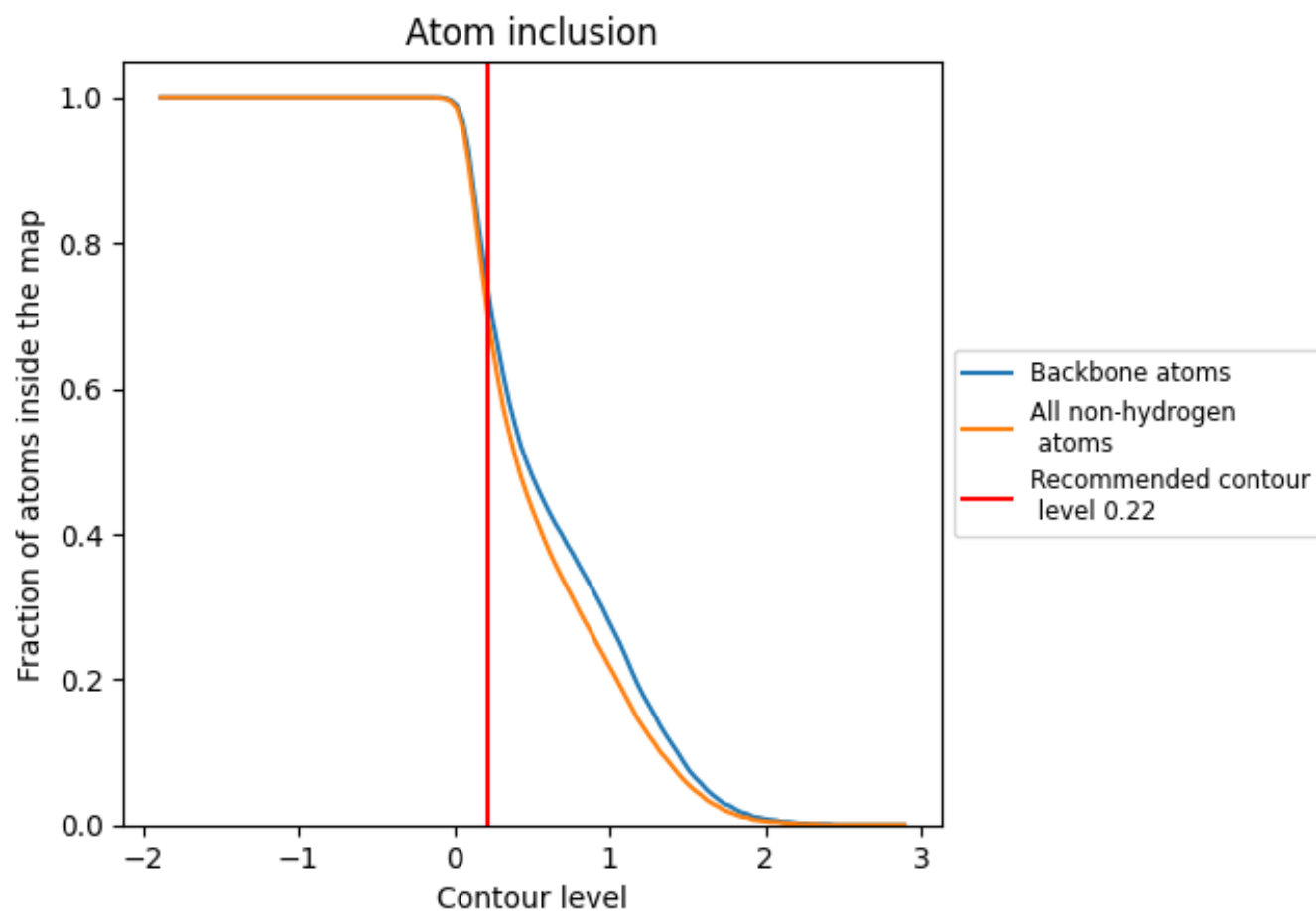
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 70% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.3670
A	0.8190	0.4300
B	0.8560	0.4470
C	0.7960	0.4390
D	0.0030	-0.0130
E	0.1120	0.0180
H	0.0880	0.0310
I	0.0680	0.0140
J	0.0050	0.0120
L	0.0520	0.0290

1.0

0.0

<0.0