



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:45 AM UTC

PDB ID : 8XSD / pdb_00008xsd
EMDB ID : EMD-38616
Title : BA.5 Spike complex with CR9
Authors : Feng, L.L.
Deposited on : 2024-01-09
Resolution : 3.55 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

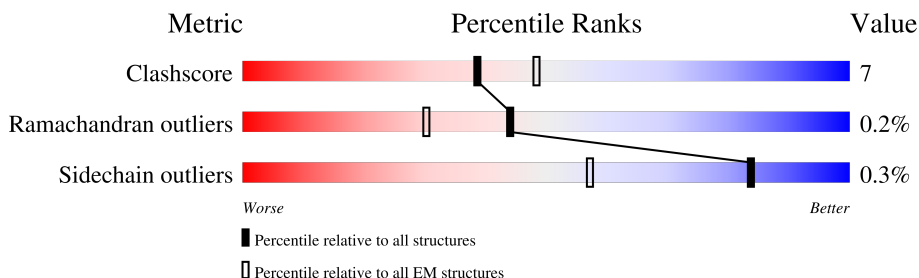
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1289	
1	B	1289	
1	C	1289	
2	G	115	
2	H	115	
2	I	115	
3	J	107	
3	K	107	

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Mol	Chain	Length	Quality of chain
3	L	107	96% 78% 22%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 29708 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	1048	Total	C	N	O	S	0	0
			8201	5249	1363	1551	38		
1	B	1055	Total	C	N	O	S	0	0
			8255	5280	1373	1564	38		
1	C	1050	Total	C	N	O	S	0	0
			8215	5254	1367	1557	37		

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	211	GLY	VAL	variant	UNP P0DTC2
A	337	ASP	GLY	variant	UNP P0DTC2
A	369	PHE	SER	variant	UNP P0DTC2
A	371	PRO	SER	variant	UNP P0DTC2
A	373	PHE	SER	variant	UNP P0DTC2
A	374	ALA	THR	variant	UNP P0DTC2
A	403	ASN	ASP	variant	UNP P0DTC2
A	406	SER	ARG	variant	UNP P0DTC2
A	415	ASN	LYS	variant	UNP P0DTC2
A	438	LYS	ASN	variant	UNP P0DTC2
A	450	ARG	LEU	variant	UNP P0DTC2
A	475	ASN	SER	variant	UNP P0DTC2
A	476	LYS	THR	variant	UNP P0DTC2
A	482	ALA	GLU	variant	UNP P0DTC2
A	484	VAL	PHE	variant	UNP P0DTC2
A	496	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	499	TYR	ASN	variant	UNP P0DTC2
A	503	HIS	TYR	variant	UNP P0DTC2
A	612	GLY	ASP	variant	UNP P0DTC2
A	653	TYR	HIS	variant	UNP P0DTC2
A	656	SER	ASN	variant	UNP P0DTC2
A	677	LYS	ASN	variant	UNP P0DTC2
A	679	HIS	PRO	variant	UNP P0DTC2
A	681	ALA	ARG	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	762	LYS	ASN	variant	UNP P0DTC2
A	794	TYR	ASP	variant	UNP P0DTC2
A	815	PRO	PHE	variant	UNP P0DTC2
A	890	PRO	ALA	variant	UNP P0DTC2
A	897	PRO	ALA	variant	UNP P0DTC2
A	940	PRO	ALA	variant	UNP P0DTC2
A	952	HIS	GLN	variant	UNP P0DTC2
A	967	LYS	ASN	variant	UNP P0DTC2
A	984	PRO	LYS	variant	UNP P0DTC2
A	985	PRO	VAL	variant	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	GLY	-	expression tag	UNP P0DTC2
A	1217	SER	-	expression tag	UNP P0DTC2
A	1218	TYR	-	expression tag	UNP P0DTC2
A	1219	ILE	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLU	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLN	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	TYR	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	ARG	-	expression tag	UNP P0DTC2
A	1232	LYS	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	GLU	-	expression tag	UNP P0DTC2
A	1236	TRP	-	expression tag	UNP P0DTC2
A	1237	VAL	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ARG	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	GLU	-	expression tag	UNP P0DTC2
A	1249	VAL	-	expression tag	UNP P0DTC2
A	1250	LEU	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	GLN	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	PRO	-	expression tag	UNP P0DTC2
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	TRP	-	expression tag	UNP P0DTC2
A	1257	SER	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	PRO	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	PHE	-	expression tag	UNP P0DTC2
A	1262	GLU	-	expression tag	UNP P0DTC2
A	1263	LYS	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	SER	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
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	SER	-	expression tag	UNP P0DTC2
A	1275	SER	-	expression tag	UNP P0DTC2
A	1276	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	TRP	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	PRO	-	expression tag	UNP P0DTC2
A	1281	GLN	-	expression tag	UNP P0DTC2
A	1282	PHE	-	expression tag	UNP P0DTC2
A	1283	GLU	-	expression tag	UNP P0DTC2
A	1284	LYS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
A	1289	HIS	-	expression tag	UNP P0DTC2
A	1290	HIS	-	expression tag	UNP P0DTC2
A	1291	HIS	-	expression tag	UNP P0DTC2
A	1292	HIS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	140	ASP	GLY	variant	UNP P0DTC2
B	211	GLY	VAL	variant	UNP P0DTC2
B	337	ASP	GLY	variant	UNP P0DTC2
B	369	PHE	SER	variant	UNP P0DTC2
B	371	PRO	SER	variant	UNP P0DTC2
B	373	PHE	SER	variant	UNP P0DTC2
B	374	ALA	THR	variant	UNP P0DTC2
B	403	ASN	ASP	variant	UNP P0DTC2
B	406	SER	ARG	variant	UNP P0DTC2
B	415	ASN	LYS	variant	UNP P0DTC2
B	438	LYS	ASN	variant	UNP P0DTC2
B	450	ARG	LEU	variant	UNP P0DTC2
B	475	ASN	SER	variant	UNP P0DTC2
B	476	LYS	THR	variant	UNP P0DTC2
B	482	ALA	GLU	variant	UNP P0DTC2
B	484	VAL	PHE	variant	UNP P0DTC2
B	496	ARG	GLN	variant	UNP P0DTC2
B	499	TYR	ASN	variant	UNP P0DTC2
B	503	HIS	TYR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	612	GLY	ASP	variant	UNP P0DTC2
B	653	TYR	HIS	variant	UNP P0DTC2
B	656	SER	ASN	variant	UNP P0DTC2
B	677	LYS	ASN	variant	UNP P0DTC2
B	679	HIS	PRO	variant	UNP P0DTC2
B	681	ALA	ARG	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	762	LYS	ASN	variant	UNP P0DTC2
B	794	TYR	ASP	variant	UNP P0DTC2
B	815	PRO	PHE	variant	UNP P0DTC2
B	890	PRO	ALA	variant	UNP P0DTC2
B	897	PRO	ALA	variant	UNP P0DTC2
B	940	PRO	ALA	variant	UNP P0DTC2
B	952	HIS	GLN	variant	UNP P0DTC2
B	967	LYS	ASN	variant	UNP P0DTC2
B	984	PRO	LYS	variant	UNP P0DTC2
B	985	PRO	VAL	variant	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	GLY	-	expression tag	UNP P0DTC2
B	1217	SER	-	expression tag	UNP P0DTC2
B	1218	TYR	-	expression tag	UNP P0DTC2
B	1219	ILE	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	GLU	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLN	-	expression tag	UNP P0DTC2
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	TYR	-	expression tag	UNP P0DTC2
B	1230	VAL	-	expression tag	UNP P0DTC2
B	1231	ARG	-	expression tag	UNP P0DTC2
B	1232	LYS	-	expression tag	UNP P0DTC2
B	1233	ASP	-	expression tag	UNP P0DTC2
B	1234	GLY	-	expression tag	UNP P0DTC2
B	1235	GLU	-	expression tag	UNP P0DTC2
B	1236	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1237	VAL	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ARG	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	GLU	-	expression tag	UNP P0DTC2
B	1249	VAL	-	expression tag	UNP P0DTC2
B	1250	LEU	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	GLN	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	PRO	-	expression tag	UNP P0DTC2
B	1255	GLY	-	expression tag	UNP P0DTC2
B	1256	TRP	-	expression tag	UNP P0DTC2
B	1257	SER	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	PRO	-	expression tag	UNP P0DTC2
B	1260	GLN	-	expression tag	UNP P0DTC2
B	1261	PHE	-	expression tag	UNP P0DTC2
B	1262	GLU	-	expression tag	UNP P0DTC2
B	1263	LYS	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	GLY	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	SER	-	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	SER	-	expression tag	UNP P0DTC2
B	1275	SER	-	expression tag	UNP P0DTC2
B	1276	ALA	-	expression tag	UNP P0DTC2
B	1277	TRP	-	expression tag	UNP P0DTC2
B	1278	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	PRO	-	expression tag	UNP P0DTC2
B	1281	GLN	-	expression tag	UNP P0DTC2
B	1282	PHE	-	expression tag	UNP P0DTC2
B	1283	GLU	-	expression tag	UNP P0DTC2
B	1284	LYS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
B	1289	HIS	-	expression tag	UNP P0DTC2
B	1290	HIS	-	expression tag	UNP P0DTC2
B	1291	HIS	-	expression tag	UNP P0DTC2
B	1292	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	140	ASP	GLY	variant	UNP P0DTC2
C	211	GLY	VAL	variant	UNP P0DTC2
C	337	ASP	GLY	variant	UNP P0DTC2
C	369	PHE	SER	variant	UNP P0DTC2
C	371	PRO	SER	variant	UNP P0DTC2
C	373	PHE	SER	variant	UNP P0DTC2
C	374	ALA	THR	variant	UNP P0DTC2
C	403	ASN	ASP	variant	UNP P0DTC2
C	406	SER	ARG	variant	UNP P0DTC2
C	415	ASN	LYS	variant	UNP P0DTC2
C	438	LYS	ASN	variant	UNP P0DTC2
C	450	ARG	LEU	variant	UNP P0DTC2
C	475	ASN	SER	variant	UNP P0DTC2
C	476	LYS	THR	variant	UNP P0DTC2
C	482	ALA	GLU	variant	UNP P0DTC2
C	484	VAL	PHE	variant	UNP P0DTC2
C	496	ARG	GLN	variant	UNP P0DTC2
C	499	TYR	ASN	variant	UNP P0DTC2
C	503	HIS	TYR	variant	UNP P0DTC2
C	612	GLY	ASP	variant	UNP P0DTC2
C	653	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	656	SER	ASN	variant	UNP P0DTC2
C	677	LYS	ASN	variant	UNP P0DTC2
C	679	HIS	PRO	variant	UNP P0DTC2
C	681	ALA	ARG	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	762	LYS	ASN	variant	UNP P0DTC2
C	794	TYR	ASP	variant	UNP P0DTC2
C	815	PRO	PHE	variant	UNP P0DTC2
C	890	PRO	ALA	variant	UNP P0DTC2
C	897	PRO	ALA	variant	UNP P0DTC2
C	940	PRO	ALA	variant	UNP P0DTC2
C	952	HIS	GLN	variant	UNP P0DTC2
C	967	LYS	ASN	variant	UNP P0DTC2
C	984	PRO	LYS	variant	UNP P0DTC2
C	985	PRO	VAL	variant	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	GLY	-	expression tag	UNP P0DTC2
C	1217	SER	-	expression tag	UNP P0DTC2
C	1218	TYR	-	expression tag	UNP P0DTC2
C	1219	ILE	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	GLU	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	ARG	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLN	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	TYR	-	expression tag	UNP P0DTC2
C	1230	VAL	-	expression tag	UNP P0DTC2
C	1231	ARG	-	expression tag	UNP P0DTC2
C	1232	LYS	-	expression tag	UNP P0DTC2
C	1233	ASP	-	expression tag	UNP P0DTC2
C	1234	GLY	-	expression tag	UNP P0DTC2
C	1235	GLU	-	expression tag	UNP P0DTC2
C	1236	TRP	-	expression tag	UNP P0DTC2
C	1237	VAL	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	ARG	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	GLU	-	expression tag	UNP P0DTC2
C	1249	VAL	-	expression tag	UNP P0DTC2
C	1250	LEU	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	GLN	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	PRO	-	expression tag	UNP P0DTC2
C	1255	GLY	-	expression tag	UNP P0DTC2
C	1256	TRP	-	expression tag	UNP P0DTC2
C	1257	SER	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	PRO	-	expression tag	UNP P0DTC2
C	1260	GLN	-	expression tag	UNP P0DTC2
C	1261	PHE	-	expression tag	UNP P0DTC2
C	1262	GLU	-	expression tag	UNP P0DTC2
C	1263	LYS	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	SER	-	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	SER	-	expression tag	UNP P0DTC2
C	1275	SER	-	expression tag	UNP P0DTC2
C	1276	ALA	-	expression tag	UNP P0DTC2
C	1277	TRP	-	expression tag	UNP P0DTC2
C	1278	SER	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1281	GLN	-	expression tag	UNP P0DTC2
C	1282	PHE	-	expression tag	UNP P0DTC2
C	1283	GLU	-	expression tag	UNP P0DTC2
C	1284	LYS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2
C	1289	HIS	-	expression tag	UNP P0DTC2
C	1290	HIS	-	expression tag	UNP P0DTC2
C	1291	HIS	-	expression tag	UNP P0DTC2
C	1292	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CR9 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	115	Total 863	C 540	N 152	O 165	S 6	0	0
2	G	115	Total 863	C 540	N 152	O 165	S 6	0	0
2	I	115	Total 863	C 540	N 152	O 165	S 6	0	0

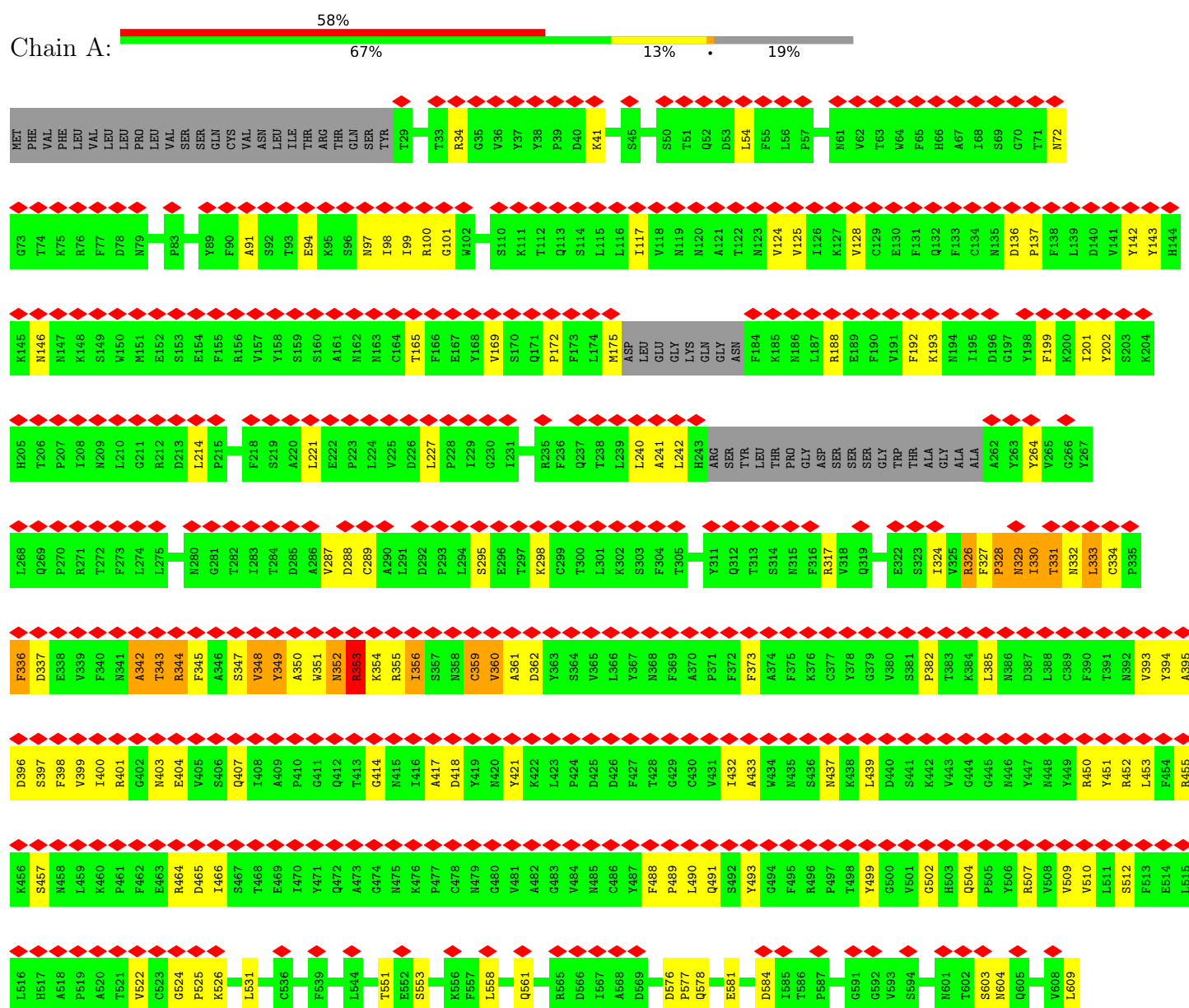
- Molecule 3 is a protein called CR9 light chain.

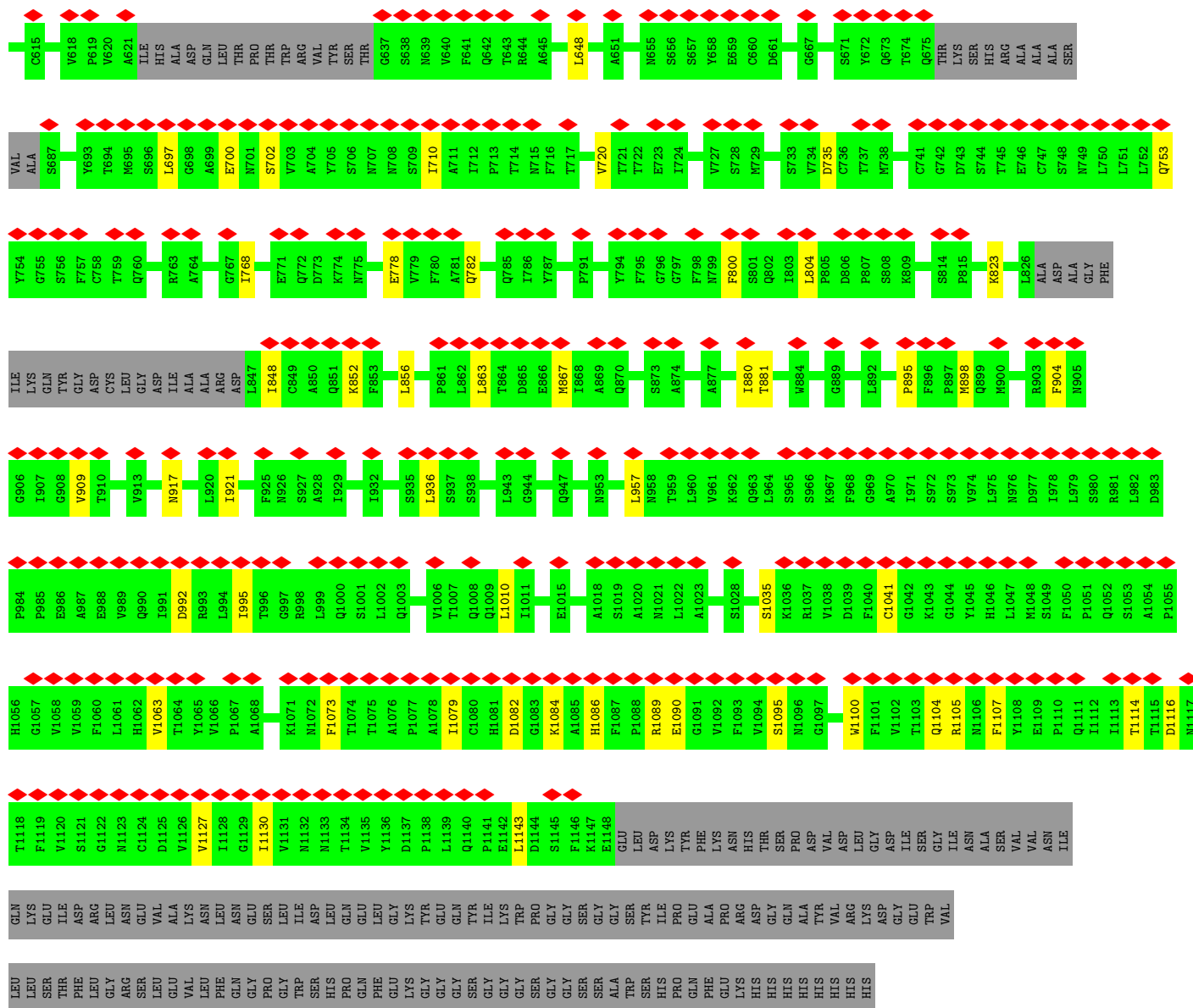
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total 816	C 510	N 139	O 165	S 2	0	0
3	J	107	Total 816	C 510	N 139	O 165	S 2	0	0
3	K	107	Total 816	C 510	N 139	O 165	S 2	0	0

3 Residue-property plots

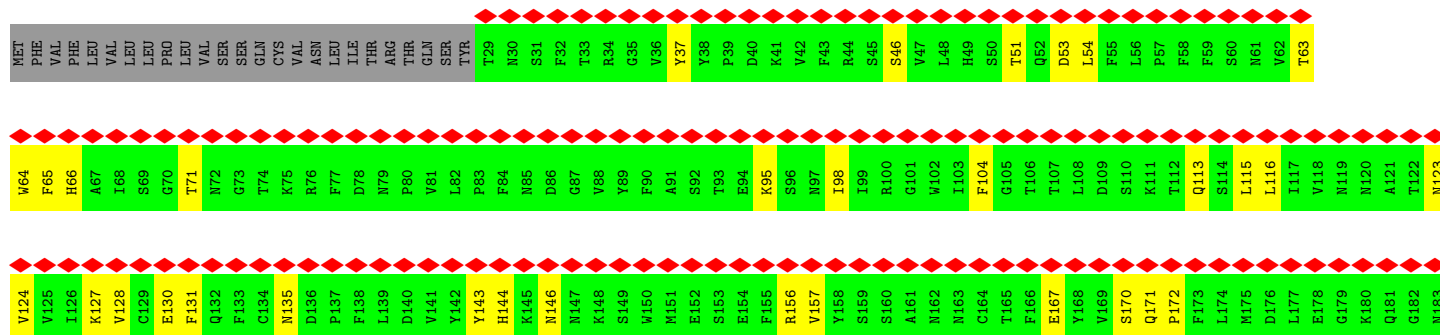
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

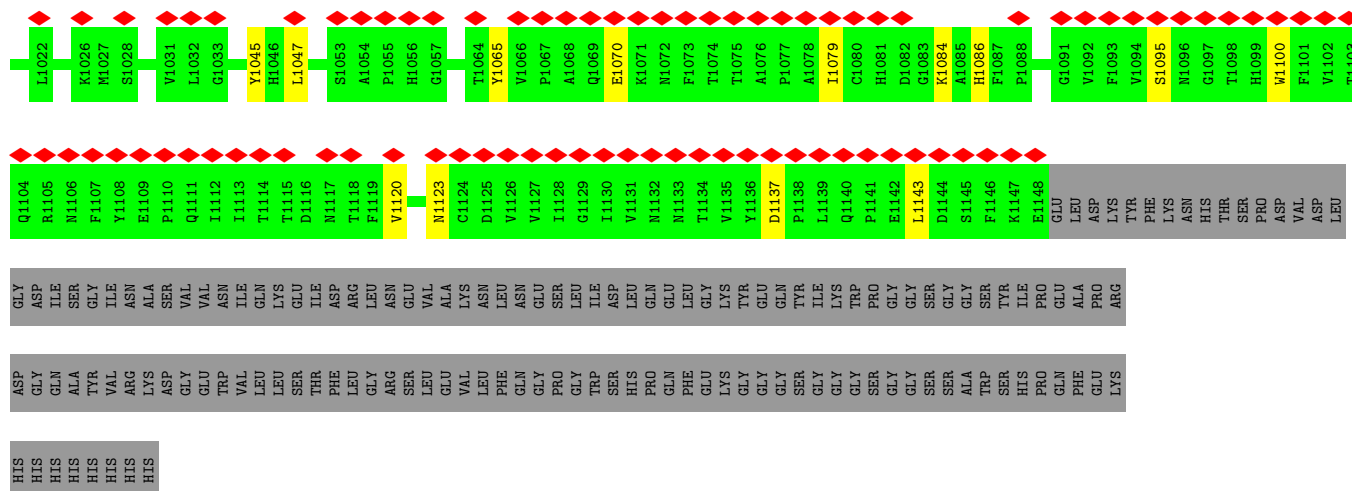




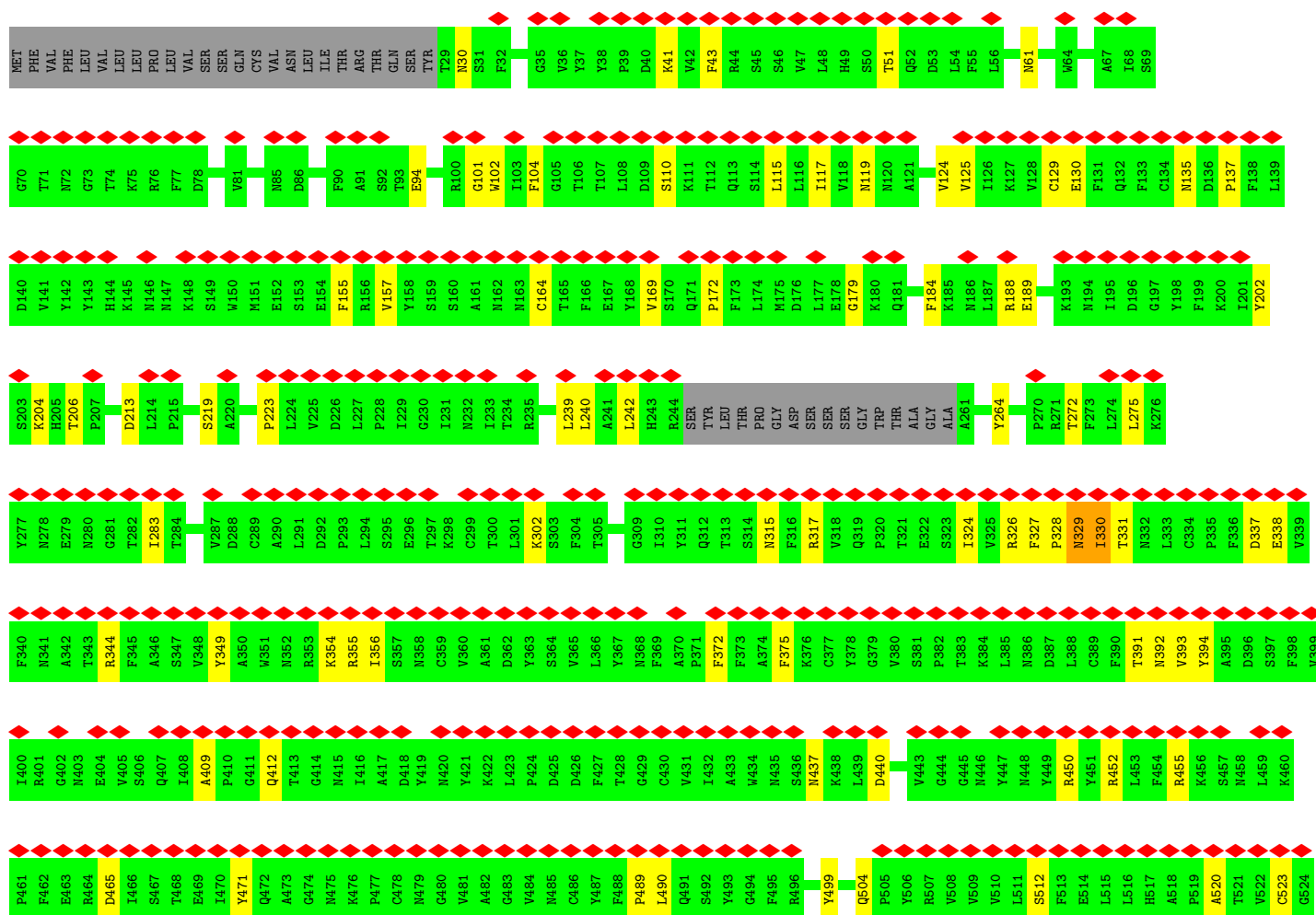
● Molecule 1: Spike glycoprotein

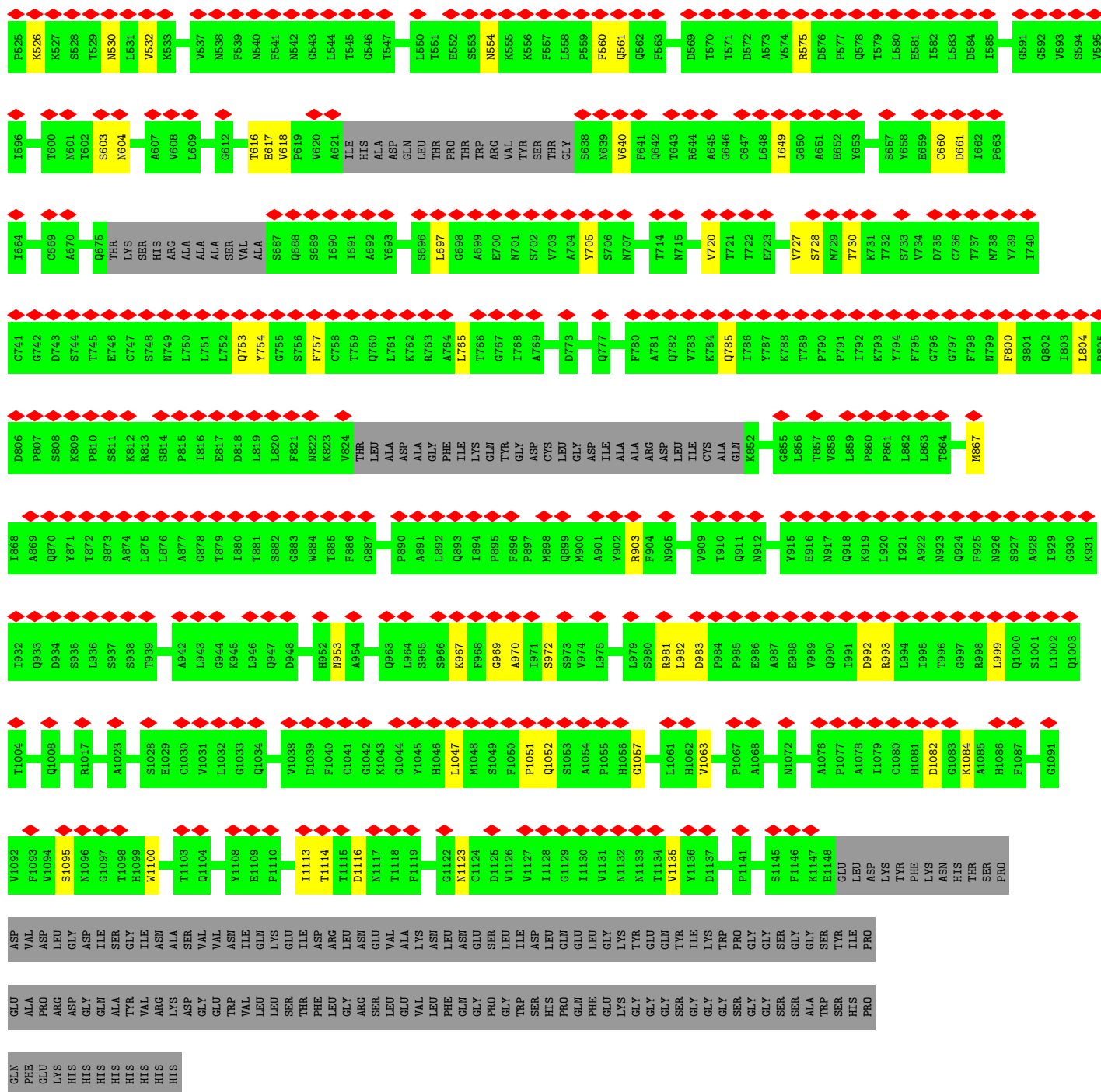


F184	K185	N186	L187	R188	E189	F190	V191	F192	K193	N194	I195	D196	G197	Y198	F199	K200	I201	Y202	S203	K204	H205	T206	P207	I208	N209	L210	G211	R212	D213	L214	P215	Q216	Q217	F218	S219	A220	L221	E222	P223	L224	V225	C226	L227	P228	I229	G230	N231	I232	T233	R234	R235	F236	Q237	T238	L239	A240	L241	H242	H243					
ARG	SER	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	GLY	TRP	THR	ALA	GLY	ALA	A262	Y263	Y264	Y265	G266	Y267	L268	Q269	P270	R271	T272	F273	S274	L275	K276	Y277	N278	E279	N280	G281	T282	I283	T284	D285	A286	V287	C288	A289	A290	L291	D292	P293	L294	S295	E296	T297	K298	C299	T300	L301	K302	S303							
F304	T305	V306	E307	K308	G309	I310	Y311	Q312	T313	S314	N315	F316	R317	V318	Q319	P320	T321	E322	S323	I324	V325	R326	F327	P328	N329	I330	S331	N332	L333	C334	F335	F336	D337	E338	Q339	F340	N341	R342	T343	R344	F345	A346	S347	V348	Y349	A350	W351	N352	R353	K354	R355	I356	S357	N358	C359	V360	A361	D362	Y363					
S364	V365	L366	Y367	N368	F369	A370	P371	F372	F373	A374	C377	Y378	S381	P382	T383	K384	L385	T391	N392	V393	Y394	A395	D396	S397	F398	V399	I400	R401	E404	V405	S406	Q407	I408	A409	Q412	N415	I416	A417	D418	Y419	N420	Y421	K422	L423	P424	D425	D426	F427	T428	G429	C430	A433												
Y434	N435	S436	N437	K438	L439	D440	S441	K442	V443	G444	G445	N446	Y447	N448	Y449	R450	Y451	R452	L453	F454	R455	K456	S457	N458	L459	K460	P461	F462	E463	R464	D465	I466	S467	T468	E469	I470	Y471	Q472	A473	G474	N475	K476	P477	C478	N479	G480	V481	A482	G483	V484	E485	C486	Y487	F488	P489	L490	Q491	S492	Y493					
G494	F495	R496	P497	T498	Y499	G500	V501	G502	H503	Q504	P505	Y506	R507	V508	S512	F513	E514	L515	L516	H517	A518	P519	A520	T521	V522	G523	G524	P525	K526	K527	S528	T529	N530	L531	V532	K533	N534	K535	C536	V537	N538	F539	N540	F541	L542	T547	G548	V549	L550	V551	E552	S553	N554	K555	K556	F557	L558							
P559	F560	Q561	Q562	F563	G564	R565	D566	T570	V574	R575	D576	P577	Q578	T579	E581	L582	L583	T586	P587	C588	S589	F590	G591	G592	G593	V594	S594	K527	S528	T529	N530	L531	V532	K533	N534	K535	C536	V537	N538	F539	N540	F541	L542	T547	G548	V549	L550	V551	E552	S553	N554	K555	K556	F557	L558									
ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	G637	S638	N639	V640	F641	Q642	T643	R644	A645	G646	C647	L648	I649	G650	A651	E652	F653	V654	N655	S656	G657	Y658	E659	C660	D661	L662	P663	T664	G665	A666	G667	I668	C669	A670	S671	Y672	Q673	T674	Q675	THR	LYS	SER	HIS	ARG	ALA	ALA	ALA					
SER	VAL	ALA	S687	Q688	S689	T690	I691	A692	Y693	T694	H695	S696	L697	G698	A699	E700	N701	S702	V703	A704	Y705	S706	N707	M708	S709	I710	A711	I712	P713	T714	N715	F716	T717	L718	S719	T722	E723	I724	D735	C736	T737	Y738	Y739	L740	C741	G742	D743	C747	S748	N749	L750	L751	L752	Q753	Y754	G755								
S756	F757	C758	T759	Q760	L761	K762	R763	A764	L765	T766	G767	I768	A769	V770	E771	Q772	V783	K784	Q785	L786	Y787	K788	T789	P790	F791	L792	K793	Y794	F795	G796	G797	F798	N799	F800	S801	Q802	I803	L804	P805	D806	P807	S808	R809	P810	S811	K812	R813	S814	P815	E816	D817	E818	L819	L820	F821	N822	K823	H824						
T825	L826	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	I847	T848	C849	A850	O851	K852	F853	N854	G855	P860	T864	D865	E866	N867	T868	A869	Q870	Y871	T872	S873	A874	L875	L876	A877	Q878	T879	I880	T881	S882	C883	W884	T885	F886	C887	A888													
A891	L892	Q893	T894	P895	F896	P897	M898	K899	M900	A901	R902	Y903	F904	N905	G906	S907	S908	Y909	T910	Q911	N912	V913	L914	Y915	E916	N917	Q918	K919	L920	I921	A922	N923	Q924	F925	N926	S927	G930	K931	I932	Q933	D934	S935	L936	S937	T938	T939	Y1000	V1001	T1002	Q1003	T1004	Y1005	V1006	T1007	Q1008	Q1009	L1010	I1011	H1012	A1013	A1014	E1015	Q1016	R1017
L957	N958	T959	L960	V961	K962	Q963	L964	S965	S966	K967	F968	G969	A970	I971	S972	S973	V974	D977	L978	L979	S980	N981	L982	D983	P984	P985	E986	A987	E988	Q989	Q990	I991	D992	R993	L994	I995	T996	G997	R998	L999	Q1000	S1001	L1002	Q1003	T1004	Y1005	V1006	T1007	Q1008	Q1009	L1010	I1011	H1012	A1013	A1014	E1015	I1016	R1017						

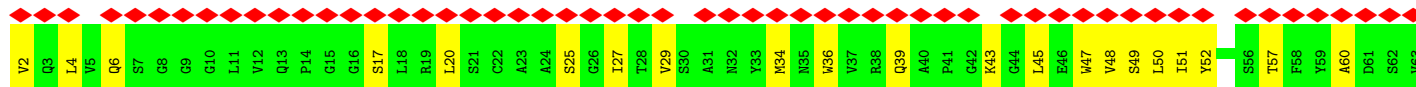


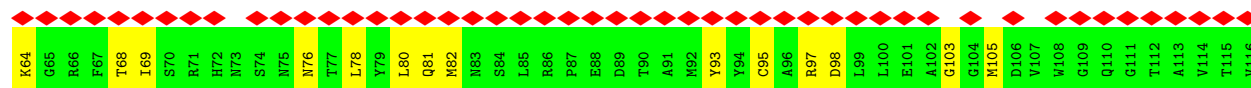
• Molecule 1: Spike glycoprotein



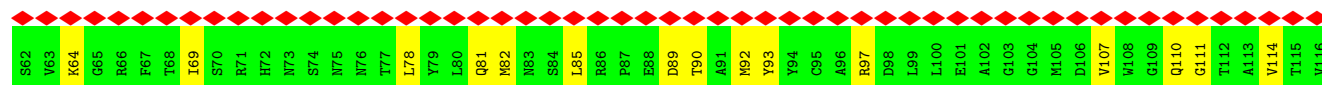


• Molecule 2: CR9 heavy chain

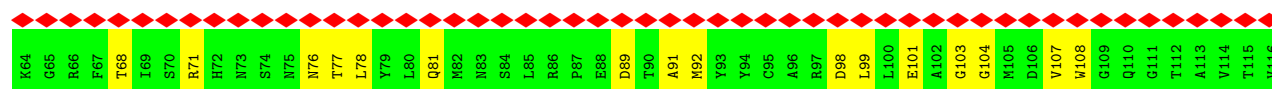




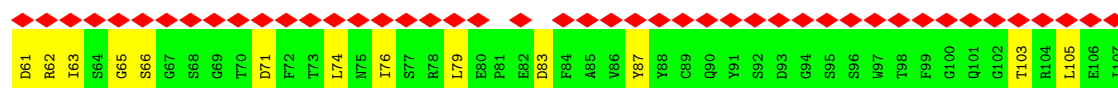
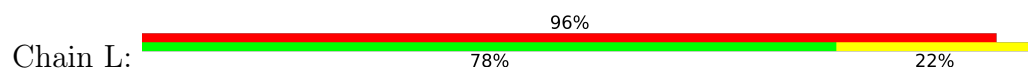
- Molecule 2: CR9 heavy chain



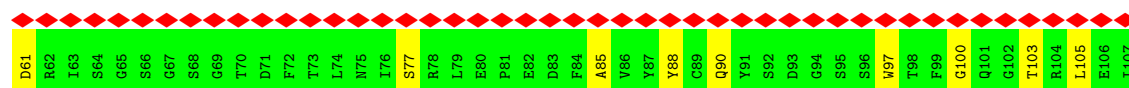
- Molecule 3: CR9 light chain



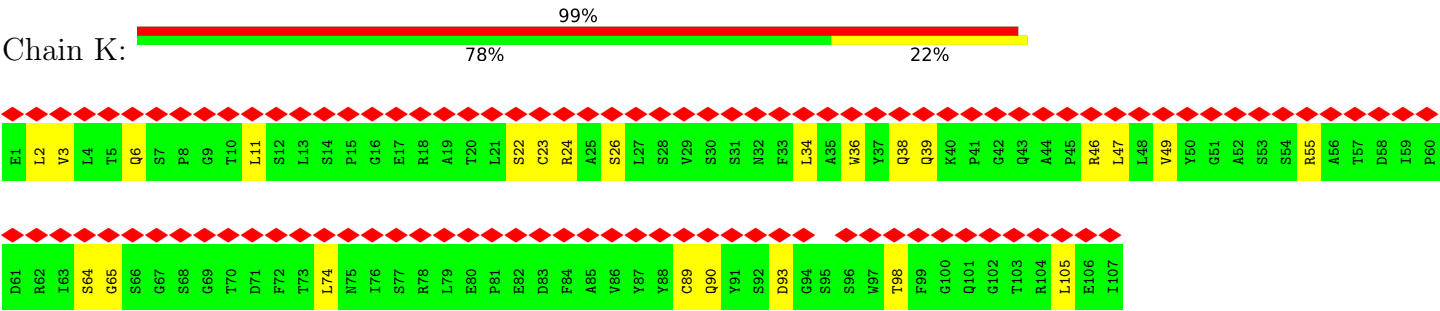
- Molecule 3: CR9 light chain



- Molecule 3: CR9 light chain



- Molecule 3: CR9 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	282590	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.716	Depositor
Minimum map value	-1.480	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.27	0/8397	0.50	2/11428 (0.0%)
1	B	0.20	0/8452	0.49	5/11502 (0.0%)
1	C	0.18	0/8412	0.44	1/11448 (0.0%)
2	G	0.16	0/880	0.44	0/1194
2	H	0.17	0/880	0.51	0/1194
2	I	0.14	0/880	0.41	0/1194
3	J	0.15	0/834	0.45	0/1134
3	K	0.15	0/834	0.45	0/1134
3	L	0.16	0/834	0.51	0/1134
All	All	0.21	0/30403	0.47	8/41362 (0.0%)

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	4
1	B	0	1
1	C	0	1
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	PRO	N-CA-C	6.98	123.42	111.77
1	B	327	PHE	N-CA-C	-6.54	101.83	110.40
1	A	349	TYR	N-CA-C	-6.38	105.25	113.16
1	B	327	PHE	CB-CA-C	5.72	117.72	109.09
1	A	330	ILE	N-CA-C	-5.62	104.38	110.23
1	C	728	SER	N-CA-C	5.20	117.63	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	ALA	CA-C-N	-5.12	114.97	122.19
1	B	361	ALA	C-N-CA	-5.12	114.97	122.19

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	ARG	Sidechain
1	A	329	ASN	Peptide
1	A	344	ARG	Sidechain
1	A	353	ARG	Sidechain
1	B	326	ARG	Sidechain
1	C	329	ASN	Peptide

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	8201	0	8008	149	0
1	B	8255	0	8060	107	0
1	C	8215	0	8009	87	0
2	G	863	0	838	23	0
2	H	863	0	838	22	0
2	I	863	0	838	21	0
3	J	816	0	785	18	0
3	K	816	0	785	16	0
3	L	816	0	785	13	0
All	All	29708	0	28946	430	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 7.

All (430) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:HG21	1:A:493:TYR:HE2	1.27	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HB2	1:A:578:GLN:HA	1.41	0.97
1:A:348:VAL:HB	1:A:451:TYR:HB3	1.45	0.96
1:B:331:THR:HG21	1:B:525:PRO:HG3	1.54	0.89
1:A:348:VAL:HB	1:A:451:TYR:CB	2.05	0.86
1:A:360:VAL:HA	1:A:522:VAL:HG12	1.56	0.83
3:L:4:LEU:HA	3:L:24:ARG:O	1.77	0.83
1:A:352:ASN:H	1:A:398:PHE:HB3	1.44	0.81
1:A:348:VAL:HG21	1:A:493:TYR:CE2	2.14	0.80
2:G:17:SER:HA	2:G:82:MET:O	1.81	0.79
2:H:17:SER:HA	2:H:82:MET:O	1.84	0.78
1:A:576:ASP:HB2	1:A:581:GLU:H	1.55	0.72
1:A:348:VAL:CB	1:A:451:TYR:HB3	2.20	0.71
1:A:394:TYR:HB2	1:A:512:SER:HB3	1.73	0.71
1:A:753:GLN:HE22	1:C:969:GLY:H	1.37	0.71
1:B:326:ARG:O	1:B:577:PRO:HG2	1.91	0.71
1:A:360:VAL:CA	1:A:522:VAL:HG12	2.21	0.70
1:A:344:ARG:HH22	1:A:439:LEU:HG	1.57	0.70
1:A:199:PHE:HB3	1:A:227:LEU:HB2	1.76	0.67
1:C:450:ARG:HE	1:C:490:LEU:HB3	1.56	0.67
1:A:334:CYS:SG	1:A:360:VAL:N	2.67	0.67
1:B:326:ARG:HE	1:B:578:GLN:HE21	1.43	0.67
1:C:135:ASN:HB2	1:C:157:VAL:HA	1.76	0.66
3:J:59:ILE:HG22	3:J:61:ASP:H	1.60	0.65
1:A:329:ASN:CB	1:A:578:GLN:HA	2.24	0.64
3:L:21:LEU:HD11	3:L:103:THR:HG21	1.80	0.64
1:A:326:ARG:HG3	1:A:531:LEU:HD12	1.79	0.63
1:B:331:THR:CG2	1:B:525:PRO:HG3	2.28	0.63
2:I:36:TRP:HB3	2:I:49:SER:HB2	1.81	0.63
2:I:39:GLN:HB3	2:I:92:MET:HB2	1.80	0.63
1:A:354:LYS:N	1:A:395:ALA:O	2.32	0.63
1:B:578:GLN:C	1:B:580:LEU:H	2.07	0.63
1:B:441:SER:HB2	1:B:497:PRO:HB3	1.79	0.63
1:B:326:ARG:HD3	1:B:528:SER:O	2.00	0.62
1:A:334:CYS:HA	1:A:359:CYS:HB2	1.82	0.62
1:B:326:ARG:HE	1:B:578:GLN:NE2	1.97	0.62
1:B:331:THR:HB	1:B:360:VAL:HG21	1.82	0.62
1:A:352:ASN:HB2	1:A:397:SER:O	2.00	0.62
3:L:8:PRO:O	3:L:103:THR:OG1	2.19	0.61
2:G:38:ARG:NH2	2:G:89:ASP:O	2.34	0.61
3:J:37:TYR:HB3	3:J:47:LEU:HD13	1.82	0.61
1:A:354:LYS:HB2	1:A:395:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HB	1:A:393:VAL:HB	1.82	0.60
1:A:351:TRP:CD1	1:A:421:TYR:HB2	2.36	0.60
1:A:404:GLU:HG3	1:A:407:GLN:HE21	1.67	0.60
1:B:576:ASP:HB3	1:B:578:GLN:O	2.01	0.60
1:A:137:PRO:HG3	1:A:241:ALA:HA	1.83	0.60
1:A:72:ASN:ND2	1:A:142:TYR:O	2.34	0.60
1:B:450:ARG:NH2	1:B:489:PRO:O	2.35	0.60
2:H:68:THR:HB	2:H:81:GLN:HB3	1.83	0.60
1:B:113:GLN:NE2	1:B:128:VAL:O	2.35	0.60
1:C:903:ARG:NH1	1:C:1047:LEU:O	2.35	0.60
1:A:1089:ARG:NH1	1:A:1116:ASP:O	2.35	0.60
1:A:551:THR:HG23	1:A:584:ASP:HB3	1.83	0.60
1:B:135:ASN:ND2	1:B:156:ARG:O	2.34	0.59
3:L:62:ARG:NH2	3:L:83:ASP:OD2	2.35	0.59
3:J:36:TRP:HB2	3:J:49:VAL:HG12	1.84	0.59
1:C:970:ALA:HB2	1:C:993:ARG:HD2	1.85	0.59
2:H:97:ARG:HD3	2:H:105:MET:HE1	1.84	0.59
1:A:326:ARG:O	1:A:577:PRO:HG2	2.03	0.59
2:H:27:ILE:O	2:H:76:ASN:ND2	2.35	0.59
2:H:36:TRP:HB3	2:H:49:SER:HB2	1.85	0.59
1:B:491:GLN:NE2	2:I:101:GLU:OE2	2.36	0.58
1:B:579:THR:O	1:B:581:GLU:HG3	2.03	0.58
2:G:92:MET:HG3	2:G:111:GLY:HA2	1.86	0.58
1:A:450:ARG:NH2	1:A:489:PRO:O	2.36	0.58
1:C:324:ILE:HD11	1:C:532:VAL:H	1.69	0.58
1:A:97:ASN:O	1:A:100:ARG:NH1	2.37	0.57
1:B:127:LYS:NZ	1:B:167:GLU:OE2	2.37	0.57
2:H:39:GLN:NE2	2:H:43:LYS:O	2.37	0.57
1:B:667:GLY:HA3	1:C:867:MET:HE1	1.85	0.57
1:B:800:PHE:HB3	1:B:804:LEU:HD23	1.87	0.57
1:B:417:ALA:HB1	1:B:422:LYS:HD3	1.86	0.57
1:B:124:VAL:HG13	1:B:172:PRO:HA	1.86	0.56
2:I:47:TRP:HE1	2:I:50:LEU:HG	1.71	0.56
1:C:101:GLY:HA3	1:C:239:LEU:HB3	1.88	0.56
1:C:104:PHE:HB2	1:C:115:LEU:HB2	1.87	0.56
3:L:48:LEU:HD11	3:L:87:TYR:HD2	1.71	0.56
1:B:328:PRO:HA	1:B:578:GLN:CD	2.30	0.56
1:C:327:PHE:HB3	1:C:328:PRO:HD2	1.86	0.56
1:B:199:PHE:HB3	1:B:227:LEU:HB2	1.88	0.56
3:L:59:ILE:HG22	3:L:61:ASP:H	1.71	0.56
1:C:355:ARG:HH12	1:C:392:ASN:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:TYR:HE1	3:J:29:VAL:HA	1.70	0.55
2:G:90:THR:HG23	2:G:114:VAL:H	1.70	0.55
1:B:412:GLN:O	1:B:422:LYS:NZ	2.38	0.55
3:J:18:ARG:HG2	3:J:77:SER:HA	1.89	0.55
1:A:333:LEU:C	1:A:359:CYS:HB2	2.32	0.55
1:B:864:THR:HG22	1:B:867:MET:HE3	1.88	0.55
1:B:847:LEU:HG	1:B:849:CYS:H	1.71	0.55
1:C:660:CYS:SG	1:C:661:ASP:N	2.80	0.55
2:G:35:ASN:HB3	2:G:50:LEU:HD23	1.88	0.55
1:C:523:CYS:O	1:C:526:LYS:NZ	2.40	0.54
3:L:76:ILE:HD13	3:L:79:LEU:HD23	1.89	0.54
1:A:136:ASP:N	1:A:136:ASP:OD1	2.41	0.54
1:A:1143:LEU:HD11	1:B:1143:LEU:HD12	1.89	0.54
1:A:332:ASN:HD21	1:A:360:VAL:HG23	1.73	0.54
1:A:97:ASN:HB2	1:A:100:ARG:HH12	1.71	0.54
1:C:204:LYS:HE2	1:C:219:SER:HB3	1.90	0.54
1:A:333:LEU:O	1:A:359:CYS:HB2	2.08	0.54
3:L:11:LEU:HG	3:L:105:LEU:HG	1.88	0.54
3:K:3:VAL:H	3:K:26:SER:HB3	1.73	0.54
1:A:455:ARG:NH1	1:A:457:SER:O	2.41	0.53
1:B:360:VAL:HA	1:B:522:VAL:HG12	1.90	0.53
1:B:401:ARG:NH2	3:K:93:ASP:O	2.41	0.53
1:C:1082:ASP:HB2	1:C:1084:LYS:HE2	1.89	0.53
2:H:51:ILE:HD13	2:H:57:THR:HG22	1.90	0.53
1:A:336:PHE:HE1	1:A:361:ALA:HB1	1.73	0.53
1:B:394:TYR:HB2	1:B:512:SER:HB3	1.89	0.53
1:A:418:ASP:OD2	2:G:56:SER:OG	2.27	0.53
1:A:800:PHE:HB3	1:A:804:LEU:HD23	1.90	0.53
1:B:754:TYR:OH	1:B:992:ASP:OD1	2.26	0.53
1:B:1084:LYS:HE2	1:B:1120:VAL:HG11	1.90	0.53
1:B:46:SER:HA	1:B:277:TYR:O	2.08	0.53
1:C:800:PHE:HB3	1:C:804:LEU:HD23	1.91	0.53
1:B:851:GLN:HB2	1:B:852:LYS:HZ2	1.74	0.53
1:A:344:ARG:HE	1:A:507:ARG:HH22	1.56	0.53
1:A:353:ARG:HA	1:A:396:ASP:OD1	2.09	0.53
1:C:394:TYR:HB2	1:C:512:SER:HB3	1.91	0.53
1:A:351:TRP:CZ2	1:A:464:ARG:HB2	2.44	0.53
3:K:6:GLN:NE2	3:K:89:CYS:SG	2.80	0.53
1:B:127:LYS:HD3	1:B:131:PHE:HZ	1.73	0.52
1:B:104:PHE:HB2	1:B:115:LEU:HB2	1.90	0.52
2:I:68:THR:HB	2:I:81:GLN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:GLN:HE21	1:A:1107:PHE:HB3	1.75	0.52
2:I:38:ARG:NH2	2:I:89:ASP:O	2.43	0.52
1:A:895:PRO:HA	1:C:705:TYR:HE1	1.73	0.52
1:A:1079:ILE:O	1:A:1086:HIS:N	2.42	0.52
2:G:51:ILE:HG21	2:G:69:ILE:HG12	1.91	0.52
3:K:11:LEU:HG	3:K:105:LEU:HG	1.90	0.52
1:A:124:VAL:HG23	1:A:172:PRO:HA	1.92	0.52
1:A:349:TYR:HD1	1:A:451:TYR:HA	1.75	0.52
1:B:401:ARG:NH2	1:B:404:GLU:OE2	2.41	0.52
1:C:727:VAL:H	1:C:1057:GLY:HA2	1.73	0.52
2:H:47:TRP:HE1	2:H:50:LEU:HG	1.75	0.52
2:G:39:GLN:NE2	2:G:43:LYS:O	2.43	0.52
3:J:13:LEU:HD11	3:J:105:LEU:HB3	1.92	0.52
1:A:373:PHE:N	1:A:433:ALA:O	2.42	0.52
1:B:1084:LYS:HA	1:B:1123:ASN:HA	1.91	0.52
2:H:6:GLN:HE22	2:H:95:CYS:H	1.56	0.52
2:I:4:LEU:HD12	2:I:24:ALA:HB2	1.91	0.52
1:A:396:ASP:HB2	1:A:510:VAL:HB	1.90	0.51
1:A:493:TYR:O	3:J:32:ASN:ND2	2.43	0.51
1:A:1114:THR:OG1	1:A:1116:ASP:OD1	2.28	0.51
1:C:616:THR:OG1	1:C:617:GLU:OE1	2.24	0.51
1:A:348:VAL:HB	1:A:451:TYR:HB2	1.91	0.51
1:B:325:VAL:HG22	1:B:540:ASN:HB3	1.92	0.51
1:C:137:PRO:HA	1:C:155:PHE:HA	1.93	0.51
3:J:22:SER:OG	3:J:24:ARG:NH1	2.44	0.51
1:B:135:ASN:H	1:B:157:VAL:HA	1.76	0.51
1:B:123:ASN:HA	1:B:172:PRO:HD3	1.92	0.51
2:G:2:VAL:N	2:G:25:SER:O	2.44	0.51
2:I:53:ALA:O	2:I:71:ARG:NH2	2.44	0.51
1:C:179:GLY:HA3	1:C:184:PHE:HB3	1.92	0.51
1:C:455:ARG:NH2	1:C:465:ASP:OD2	2.43	0.51
3:K:11:LEU:HB2	3:K:105:LEU:HA	1.91	0.51
1:B:578:GLN:O	1:B:580:LEU:N	2.44	0.51
1:C:240:LEU:HD11	1:C:242:LEU:HD13	1.93	0.51
1:C:754:TYR:OH	1:C:992:ASP:OD2	2.25	0.51
1:B:578:GLN:C	1:B:580:LEU:N	2.66	0.50
2:I:45:LEU:HD11	3:K:39:GLN:HE22	1.76	0.50
1:A:334:CYS:HA	1:A:359:CYS:CB	2.39	0.50
1:C:344:ARG:NH2	1:C:440:ASP:OD2	2.44	0.50
2:H:29:VAL:HG22	2:H:76:ASN:HB2	1.92	0.50
3:K:22:SER:O	3:K:24:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:SER:OG	1:B:507:ARG:NH1	2.43	0.50
1:A:432:ILE:HG13	1:A:509:VAL:HB	1.92	0.50
1:A:465:ASP:OD1	1:A:465:ASP:N	2.44	0.50
2:I:34:MET:HE3	2:I:78:LEU:HD22	1.94	0.50
1:B:701:ASN:ND2	1:C:785:GLN:OE1	2.45	0.50
3:J:49:VAL:HG23	3:J:55:ARG:HA	1.93	0.50
2:I:99:LEU:HG	2:I:101:GLU:H	1.76	0.50
1:A:351:TRP:HZ3	1:A:353:ARG:HB3	1.77	0.50
1:C:157:VAL:HG11	1:C:239:LEU:HD11	1.93	0.50
1:A:317:ARG:HD3	1:B:738:MET:HE2	1.94	0.49
2:G:34:MET:SD	2:G:51:ILE:HG23	2.52	0.49
1:A:91:ALA:HB3	1:A:264:TYR:HB2	1.94	0.49
1:C:1114:THR:OG1	1:C:1116:ASP:OD1	2.29	0.49
1:B:525:PRO:HB2	1:B:527:LYS:HE3	1.95	0.49
3:K:2:LEU:HD22	3:K:98:THR:HG21	1.94	0.49
1:A:452:ARG:HH22	1:A:466:ILE:HA	1.77	0.49
1:A:700:GLU:OE2	1:B:788:LYS:NZ	2.41	0.49
1:C:640:VAL:HG12	1:C:649:ILE:HG12	1.94	0.49
2:G:4:LEU:HD22	2:G:107:VAL:HG11	1.95	0.49
2:H:39:GLN:HB2	2:H:45:LEU:HD13	1.95	0.49
1:B:381:SER:HB3	1:B:384:LYS:HG2	1.95	0.49
1:B:143:TYR:HB3	1:B:146:ASN:HB3	1.94	0.49
1:A:351:TRP:CD1	1:A:351:TRP:H	2.28	0.49
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.25	0.49
1:B:64:TRP:CD1	1:B:66:HIS:HB2	2.48	0.49
1:A:345:PHE:HD2	1:A:398:PHE:C	2.21	0.48
1:A:351:TRP:CZ3	1:A:353:ARG:HB3	2.47	0.48
1:A:437:ASN:HB3	1:A:504:GLN:HB3	1.94	0.48
1:B:864:THR:HG23	1:B:866:GLU:H	1.78	0.48
2:H:50:LEU:HD22	2:H:52:TYR:HE1	1.78	0.48
1:B:1095:SER:HB2	1:B:1100:TRP:CD2	2.49	0.48
1:C:981:ARG:HH12	1:C:982:LEU:HD13	1.78	0.48
1:C:499:TYR:HB3	1:C:504:GLN:HE22	1.78	0.48
1:B:288:ASP:OD1	1:B:289:CYS:N	2.47	0.48
1:A:34:ARG:HG3	1:A:214:LEU:HD11	1.95	0.48
1:C:213:ASP:OD2	1:C:264:TYR:OH	2.31	0.48
1:B:819:LEU:HD11	1:B:823:LYS:HE2	1.96	0.47
3:K:36:TRP:HB2	3:K:49:VAL:HG12	1.95	0.47
3:L:30:SER:OG	3:L:31:SER:N	2.47	0.47
1:A:287:VAL:HG21	1:A:298:LYS:HD2	1.97	0.47
1:A:327:PHE:HB3	1:A:328:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HB2	1:A:577:PRO:O	2.14	0.47
1:A:175:MET:SD	1:A:175:MET:N	2.87	0.47
1:B:95:LYS:H	1:B:98:ILE:HD13	1.80	0.47
1:C:1084:LYS:HA	1:C:1123:ASN:HA	1.94	0.47
1:C:437:ASN:HB3	1:C:504:GLN:HB3	1.95	0.47
2:H:34:MET:HB2	2:H:51:ILE:HG23	1.96	0.47
3:L:52:ALA:HB1	3:L:66:SER:HA	1.97	0.47
1:A:348:VAL:CG2	1:A:451:TYR:HB3	2.44	0.47
1:A:904:PHE:HB3	1:A:909:VAL:HG13	1.97	0.47
1:B:455:ARG:NH1	1:B:457:SER:O	2.45	0.47
3:K:6:GLN:HG2	3:K:23:CYS:HB2	1.97	0.47
1:B:470:ILE:HD13	1:B:488:PHE:HD1	1.80	0.47
1:B:328:PRO:HB3	1:B:577:PRO:C	2.39	0.47
1:A:334:CYS:HB2	1:A:360:VAL:O	2.14	0.46
1:A:360:VAL:HA	1:A:522:VAL:HA	1.97	0.46
2:I:4:LEU:HA	2:I:24:ALA:HA	1.97	0.46
1:A:98:ILE:HG22	1:A:240:LEU:HD11	1.98	0.46
1:A:344:ARG:HH22	1:A:439:LEU:CG	2.27	0.46
1:C:967:LYS:HE3	1:C:972:SER:HA	1.97	0.46
3:L:55:ARG:NE	3:L:63:ILE:O	2.45	0.46
2:G:3:GLN:NE2	2:G:4:LEU:O	2.48	0.46
1:A:295:SER:HA	1:A:298:LYS:HG2	1.98	0.46
1:A:349:TYR:HB3	1:A:452:ARG:H	1.80	0.46
1:A:355:ARG:HG2	1:A:393:VAL:O	2.16	0.46
1:B:603:SER:OG	1:B:604:ASN:N	2.48	0.46
1:B:1045:TYR:HB2	1:B:1065:TYR:HB3	1.97	0.46
1:C:125:VAL:HA	1:C:169:VAL:HG12	1.97	0.46
1:A:331:THR:HA	1:A:526:LYS:CE	2.45	0.46
1:A:334:CYS:SG	1:A:360:VAL:C	2.99	0.46
1:A:414:GLY:H	1:A:417:ALA:HB3	1.81	0.46
1:A:768:ILE:HD11	1:A:1010:LEU:HD23	1.97	0.46
1:A:1127:VAL:HG23	1:B:915:TYR:HB3	1.97	0.46
1:C:349:TYR:HD2	1:C:452:ARG:HH21	1.64	0.46
1:C:730:THR:OG1	1:C:953:ASN:OD1	2.34	0.46
1:B:116:LEU:HD13	1:B:131:PHE:HE2	1.81	0.46
2:I:23:ALA:HB2	2:I:77:THR:HG23	1.97	0.46
1:A:101:GLY:HA3	1:A:117:ILE:O	2.16	0.46
1:B:437:ASN:ND2	1:B:504:GLN:OE1	2.43	0.46
1:C:202:TYR:HD1	1:C:223:PRO:HA	1.80	0.46
1:C:1095:SER:HB2	1:C:1100:TRP:CD2	2.51	0.46
1:A:898:MET:HE2	1:A:898:MET:HB3	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:NH1	1:B:214:LEU:O	2.49	0.46
1:B:969:GLY:H	1:C:753:GLN:HE22	1.62	0.46
1:C:561:GLN:O	1:C:575:ARG:NH1	2.48	0.46
1:A:143:TYR:HB3	1:A:146:ASN:HB3	1.97	0.45
1:B:415:ASN:OD1	1:B:416:ILE:N	2.50	0.45
3:K:49:VAL:HG23	3:K:55:ARG:HA	1.98	0.45
3:L:65:GLY:HA2	3:L:74:LEU:HA	1.98	0.45
2:I:2:VAL:N	2:I:25:SER:O	2.49	0.45
1:A:362:ASP:OD1	1:A:362:ASP:N	2.44	0.45
1:B:37:TYR:OH	1:B:54:LEU:O	2.34	0.45
2:G:29:VAL:HG12	2:G:97:ARG:HD3	1.98	0.45
2:I:4:LEU:HD22	2:I:107:VAL:HG11	1.98	0.45
1:A:399:VAL:HA	1:A:507:ARG:HA	1.98	0.45
1:A:1082:ASP:O	1:A:1084:LYS:NZ	2.49	0.45
1:B:51:THR:O	1:B:272:THR:HA	2.16	0.45
3:J:6:GLN:HG2	3:J:103:THR:HG23	1.99	0.45
1:B:465:ASP:OD1	1:B:465:ASP:N	2.48	0.45
1:C:119:ASN:HA	1:C:124:VAL:HG12	1.99	0.45
3:J:4:LEU:HD23	3:J:100:GLY:HA3	1.98	0.45
1:A:99:ILE:HG13	1:A:240:LEU:HD13	1.99	0.45
1:A:348:VAL:HG13	1:A:400:ILE:HD12	1.99	0.45
1:C:240:LEU:HD21	1:C:242:LEU:HD22	1.99	0.45
2:G:4:LEU:HD12	2:G:24:ALA:HB2	1.98	0.45
2:I:104:GLY:HA2	3:K:47:LEU:HG	1.97	0.45
2:H:98:ASP:HA	2:H:103:GLY:HA2	1.98	0.45
2:I:29:VAL:HG22	2:I:76:ASN:HB3	1.99	0.45
1:A:609:LEU:HD12	1:A:648:LEU:HD13	1.99	0.44
1:B:212:ARG:NH1	1:B:213:ASP:O	2.50	0.44
1:B:1070:GLU:OE1	1:B:1070:GLU:N	2.45	0.44
1:C:51:THR:O	1:C:272:THR:HA	2.18	0.44
1:C:617:GLU:HG2	1:C:618:VAL:HG23	1.99	0.44
1:C:1113:ILE:HG22	1:C:1135:VAL:HG13	1.98	0.44
3:J:26:SER:OG	3:J:27:LEU:N	2.50	0.44
1:A:54:LEU:HD12	1:A:193:LYS:HD2	1.99	0.44
1:B:350:ALA:HB1	1:B:464:ARG:HH21	1.83	0.44
1:C:409:ALA:HB3	1:C:412:GLN:HG3	2.00	0.44
2:H:64:LYS:HA	2:H:64:LYS:HD2	1.85	0.44
1:A:488:PHE:HD2	1:A:490:LEU:HD23	1.82	0.44
1:C:391:THR:HA	1:C:520:ALA:HA	2.00	0.44
1:A:360:VAL:HG22	1:A:522:VAL:HA	1.99	0.44
1:B:615:CYS:HB3	1:B:647:CYS:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:HG13	1:C:172:PRO:HA	1.99	0.44
1:C:129:CYS:SG	1:C:130:GLU:N	2.91	0.44
1:C:317:ARG:HE	1:C:317:ARG:HB3	1.53	0.44
1:C:720:VAL:HG22	1:C:1063:VAL:HG22	1.98	0.44
1:C:326:ARG:HD3	1:C:530:ASN:N	2.32	0.44
1:C:452:ARG:NH2	1:C:465:ASP:O	2.46	0.44
3:J:11:LEU:HB2	3:J:105:LEU:HA	2.00	0.44
1:A:324:ILE:HD12	1:A:531:LEU:H	1.83	0.44
1:C:356:ILE:HB	1:C:393:VAL:HB	1.98	0.44
2:I:38:ARG:HH21	2:I:91:ALA:HB3	1.82	0.44
1:A:1095:SER:HB3	1:A:1100:TRP:CD2	2.53	0.44
2:H:36:TRP:CH2	2:H:93:TYR:HB3	2.53	0.44
2:I:108:TRP:CD1	2:I:108:TRP:H	2.36	0.44
1:A:202:TYR:HB3	1:A:221:LEU:HB3	1.99	0.44
1:A:329:ASN:OD1	1:A:578:GLN:HB3	2.18	0.44
1:A:453:LEU:HB2	1:A:491:GLN:HG2	2.00	0.44
1:A:720:VAL:HG22	1:A:1063:VAL:HG22	2.00	0.44
1:C:94:GLU:OE2	1:C:188:ARG:NH1	2.41	0.44
2:H:2:VAL:N	2:H:25:SER:O	2.51	0.44
3:J:38:GLN:HE21	3:J:85:ALA:HB3	1.83	0.44
1:A:94:GLU:OE2	1:A:188:ARG:NH1	2.43	0.43
1:A:702:SER:HB2	1:B:788:LYS:HZ3	1.83	0.43
1:C:471:TYR:HB2	1:C:489:PRO:HG3	2.00	0.43
1:A:823:LYS:HE2	1:A:823:LYS:HB3	1.86	0.43
1:A:863:LEU:HD22	1:A:867:MET:HE2	2.00	0.43
1:C:102:TRP:HB2	1:C:117:ILE:HB	2.00	0.43
1:A:98:ILE:HG23	1:A:242:LEU:HD21	2.00	0.43
1:A:125:VAL:HA	1:A:169:VAL:HG12	2.00	0.43
1:A:349:TYR:CD1	1:A:451:TYR:HA	2.53	0.43
1:A:351:TRP:CD2	1:A:421:TYR:CD1	3.06	0.43
1:A:41:LYS:HE2	1:C:560:PHE:HD2	1.84	0.43
1:A:355:ARG:HA	1:A:393:VAL:O	2.18	0.43
1:B:326:ARG:HD2	1:B:326:ARG:HA	1.75	0.43
1:B:377:CYS:HB3	1:B:382:PRO:HG3	1.99	0.43
1:B:488:PHE:HD2	1:B:490:LEU:HD23	1.83	0.43
1:C:337:ASP:OD1	1:C:338:GLU:N	2.51	0.43
2:G:64:LYS:HD2	2:G:64:LYS:HA	1.81	0.43
1:B:401:ARG:HD2	1:B:503:HIS:CD2	2.53	0.43
1:C:983:ASP:OD1	1:C:983:ASP:N	2.51	0.43
3:J:30:SER:OG	3:J:31:SER:N	2.51	0.43
1:A:342:ALA:O	1:A:343:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ARG:NH2	1:A:404:GLU:OE2	2.47	0.43
1:A:992:ASP:HA	1:A:995:ILE:HG22	2.00	0.43
1:A:1090:GLU:O	1:A:1105:ARG:NH1	2.51	0.43
1:B:63:THR:HB	1:B:65:PHE:CE2	2.54	0.43
2:G:40:ALA:HB3	2:G:43:LYS:HB3	2.01	0.43
1:B:113:GLN:HA	1:B:130:GLU:HG3	2.00	0.43
1:A:331:THR:HA	1:A:526:LYS:HE2	2.01	0.43
1:A:361:ALA:H	1:A:522:VAL:HB	1.83	0.43
1:A:1035:SER:OG	1:A:1041:CYS:SG	2.67	0.43
2:G:36:TRP:CH2	2:G:93:TYR:HB3	2.54	0.43
1:B:71:THR:O	1:B:144:HIS:NE2	2.52	0.43
1:C:30:ASN:HA	1:C:61:ASN:HA	2.00	0.43
1:A:355:ARG:HE	1:A:355:ARG:HB3	1.45	0.42
1:A:403:ASN:N	1:A:502:GLY:O	2.52	0.42
1:B:170:SER:OG	1:B:171:GLN:N	2.52	0.42
2:H:69:ILE:HD11	2:H:78:LEU:HD12	2.00	0.42
3:K:38:GLN:OE1	3:K:46:ARG:NH2	2.48	0.42
1:B:328:PRO:HG2	1:B:330:ILE:HG12	2.01	0.42
1:B:331:THR:HG21	1:B:525:PRO:CG	2.39	0.42
1:B:564:GLY:HA2	1:C:43:PHE:HB3	2.01	0.42
1:C:110:SER:HA	1:C:130:GLU:HB3	2.00	0.42
3:J:34:LEU:HA	3:J:90:GLN:O	2.18	0.42
3:J:36:TRP:HA	3:J:88:TYR:O	2.19	0.42
1:C:554:ASN:OD1	1:C:554:ASN:N	2.52	0.42
1:A:848:ILE:O	1:A:852:LYS:NZ	2.47	0.42
1:B:349:TYR:HD2	1:B:452:ARG:HH21	1.66	0.42
2:H:48:VAL:HA	2:H:60:ALA:HB2	2.01	0.42
2:G:50:LEU:HD11	3:J:97:TRP:HE1	1.85	0.42
1:A:329:ASN:CG	1:A:330:ILE:N	2.78	0.42
1:B:334:CYS:C	1:B:336:PHE:H	2.27	0.42
1:B:579:THR:O	1:B:580:LEU:C	2.62	0.42
1:C:326:ARG:HD3	1:C:530:ASN:HB2	2.01	0.42
2:I:22:CYS:HB3	2:I:78:LEU:HB3	2.01	0.42
1:A:192:PHE:HD1	1:A:201:ILE:HG12	1.85	0.42
1:C:372:PHE:HB2	1:C:375:PHE:HE1	1.85	0.42
1:A:735:ASP:OD2	1:C:315:ASN:ND2	2.44	0.42
1:A:347:SER:HB2	1:A:350:ALA:HB3	2.00	0.42
1:B:115:LEU:HD13	1:B:128:VAL:HG22	2.02	0.42
1:C:1051:PRO:O	1:C:1052:GLN:NE2	2.48	0.42
3:L:24:ARG:NH1	3:L:71:ASP:OD1	2.53	0.42
2:G:22:CYS:HB3	2:G:78:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HB	1:A:165:THR:HB	2.02	0.42
1:A:334:CYS:CA	1:A:359:CYS:HB2	2.49	0.42
1:A:856:LEU:HD13	1:A:957:LEU:HD22	2.01	0.42
1:A:867:MET:HB2	1:C:697:LEU:HD21	2.01	0.42
1:B:37:TYR:HB3	1:B:221:LEU:HB2	2.01	0.42
1:B:1079:ILE:O	1:B:1086:HIS:N	2.53	0.42
1:A:697:LEU:HB3	1:B:871:TYR:HE1	1.85	0.41
2:H:20:LEU:HD23	2:H:80:LEU:HD11	2.00	0.41
1:B:566:ASP:OD1	1:B:570:THR:OG1	2.35	0.41
1:B:758:CYS:HA	1:B:761:LEU:HB2	2.01	0.41
1:A:330:ILE:O	1:A:331:THR:HB	2.19	0.41
1:A:558:LEU:HB2	1:A:561:GLN:HE21	1.85	0.41
1:A:753:GLN:HE21	1:C:967:LYS:HB2	1.85	0.41
2:G:14:PRO:HA	2:G:85:LEU:HB2	2.02	0.41
1:A:382:PRO:HA	1:A:385:LEU:HG	2.02	0.41
1:A:525:PRO:O	1:A:526:LYS:C	2.63	0.41
2:G:17:SER:HB3	2:G:81:GLN:HE21	1.86	0.41
1:A:917:ASN:O	1:A:921:ILE:HG12	2.20	0.41
1:C:189:GLU:OE2	1:C:206:THR:OG1	2.37	0.41
1:C:302:LYS:HB3	1:C:302:LYS:HE2	1.82	0.41
1:B:334:CYS:N	1:B:360:VAL:O	2.54	0.41
1:C:275:LEU:HD23	1:C:283:ILE:HD12	2.02	0.41
1:C:330:ILE:HG22	1:C:331:THR:N	2.36	0.41
1:C:757:PHE:HD2	1:C:999:LEU:HD21	1.86	0.41
2:H:4:LEU:HD21	2:H:97:ARG:NE	2.35	0.41
3:K:65:GLY:HA2	3:K:74:LEU:HA	2.03	0.41
1:A:603:SER:OG	1:A:604:ASN:N	2.54	0.41
1:A:823:LYS:NZ	1:A:936:LEU:O	2.46	0.41
1:B:192:PHE:HD1	1:B:201:ILE:HG12	1.86	0.41
1:B:333:LEU:HA	1:B:360:VAL:O	2.20	0.41
1:B:903:ARG:NH1	1:B:1047:LEU:O	2.48	0.41
1:C:329:ASN:O	1:C:331:THR:HG23	2.20	0.41
1:C:129:CYS:HB2	1:C:164:CYS:HB3	1.81	0.41
2:G:110:GLN:NE2	2:G:111:GLY:O	2.53	0.41
1:A:1127:VAL:HG13	1:A:1130:ILE:HB	2.02	0.41
1:B:188:ARG:HB3	1:B:190:PHE:CE2	2.56	0.41
1:B:356:ILE:HD13	1:B:393:VAL:HG12	2.03	0.41
1:C:354:LYS:HE3	1:C:354:LYS:HB2	1.89	0.41
1:C:465:ASP:OD1	1:C:465:ASP:N	2.53	0.41
1:C:603:SER:OG	1:C:604:ASN:N	2.54	0.41
2:H:51:ILE:HG21	2:H:69:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1137:ASP:OD1	1:B:1137:ASP:N	2.52	0.41
1:A:288:ASP:OD1	1:A:289:CYS:N	2.54	0.40
1:A:397:SER:HA	1:A:509:VAL:HA	2.02	0.40
1:C:765:LEU:HD23	1:C:765:LEU:HA	1.93	0.40
2:G:50:LEU:HB2	2:G:58:PHE:HB2	2.03	0.40
1:A:778:GLU:O	1:A:782:GLN:NE2	2.54	0.40
1:A:880:ILE:HG13	1:A:881:THR:HG23	2.03	0.40
1:C:372:PHE:HB2	1:C:375:PHE:CE1	2.57	0.40
1:A:753:GLN:NE2	1:C:967:LYS:HB2	2.35	0.40
3:K:55:ARG:HH21	3:K:64:SER:HA	1.87	0.40
1:A:553:SER:HB3	1:A:584:ASP:HB2	2.03	0.40
1:B:116:LEU:HD13	1:B:131:PHE:CE2	2.56	0.40
1:B:355:ARG:HH11	1:B:394:TYR:HE1	1.69	0.40
1:B:440:ASP:OD1	1:B:440:ASP:N	2.52	0.40
1:B:561:GLN:HA	1:C:41:LYS:HD2	2.02	0.40
1:B:817:GLU:HA	1:B:820:LEU:HD12	2.02	0.40
2:I:98:ASP:HA	2:I:103:GLY:HA2	2.04	0.40
1:A:710:ILE:O	1:A:1073:PHE:N	2.49	0.40
3:K:34:LEU:HA	3:K:90:GLN:O	2.21	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	1036/1289 (80%)	956 (92%)	74 (7%)	6 (1%)	21	54
1	B	1045/1289 (81%)	978 (94%)	65 (6%)	2 (0%)	43	73
1	C	1040/1289 (81%)	963 (93%)	76 (7%)	1 (0%)	48	79
2	G	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	H	113/115 (98%)	109 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
3	J	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	K	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	L	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
All	All	3775/4533 (83%)	3520 (93%)	246 (6%)	9 (0%)	44	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	ALA
1	A	343	THR
1	B	579	THR
1	A	331	THR
1	C	330	ILE
1	A	359	CYS
1	B	335	PRO
1	A	328	PRO
1	A	524	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	916/1115 (82%)	908 (99%)	8 (1%)	70	76
1	B	922/1115 (83%)	921 (100%)	1 (0%)	88	87
1	C	916/1115 (82%)	916 (100%)	0	100	100
2	G	90/90 (100%)	90 (100%)	0	100	100
2	H	90/90 (100%)	90 (100%)	0	100	100
2	I	90/90 (100%)	90 (100%)	0	100	100
3	J	90/90 (100%)	90 (100%)	0	100	100
3	K	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	90/90 (100%)	90 (100%)	0	100	100
All	All	3294/3885 (85%)	3285 (100%)	9 (0%)	84	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	LEU
1	A	336	PHE
1	A	337	ASP
1	A	348	VAL
1	A	352	ASN
1	A	353	ARG
1	A	356	ILE
1	A	360	VAL
1	B	578	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	144	HIS
1	A	332	ASN
1	A	403	ASN
1	A	435	ASN
1	A	753	GLN
1	A	953	ASN
1	A	1052	GLN
1	A	1104	GLN
1	A	1117	ASN
1	B	578	GLN
1	B	601	ASN
1	B	688	GLN
1	B	749	ASN
1	B	785	GLN
1	B	1104	GLN
1	C	79	ASN
1	C	97	ASN
1	C	194	ASN
1	C	269	GLN
1	C	435	ASN
1	C	538	ASN

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Mol	Chain	Res	Type
1	C	542	ASN
1	C	604	ASN
1	C	753	GLN
1	C	777	GLN
1	C	893	GLN
1	C	1003	GLN
1	C	1009	GLN
2	H	6	GLN
3	L	38	GLN
3	K	39	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

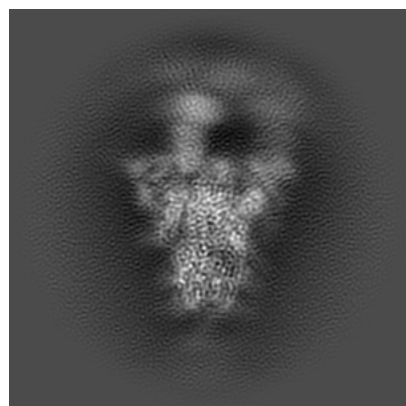
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38616. These allow visual inspection of the internal detail of the map and identification of artifacts.

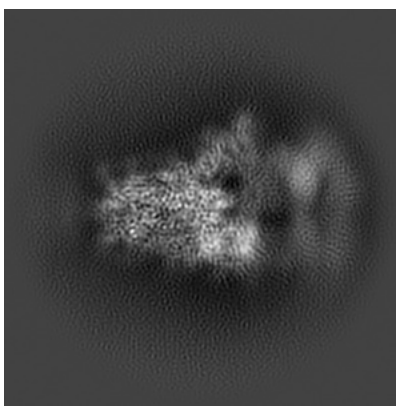
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

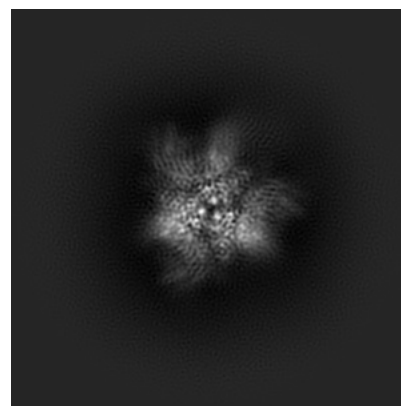
6.1.1 Primary map



X

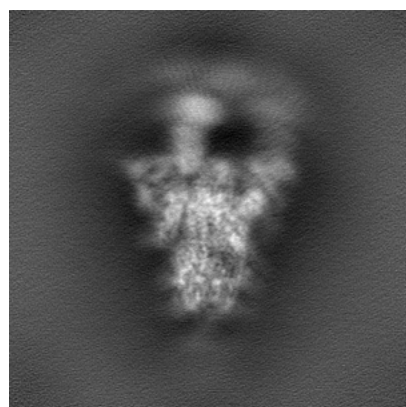


Y

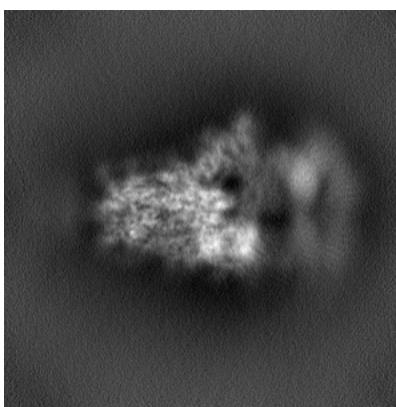


Z

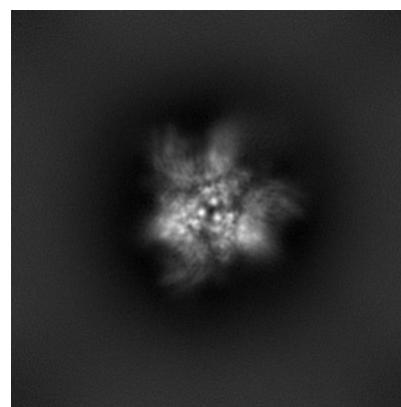
6.1.2 Raw map



X



Y

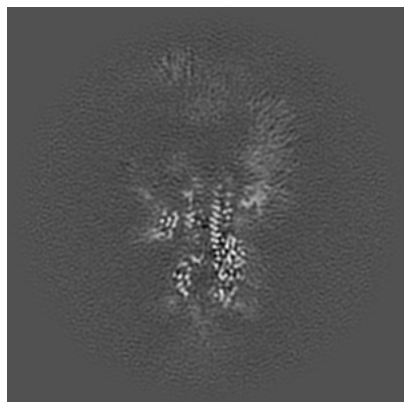


Z

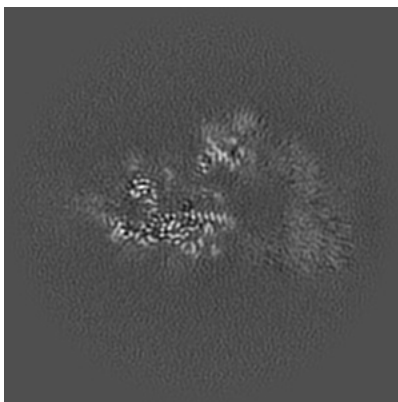
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

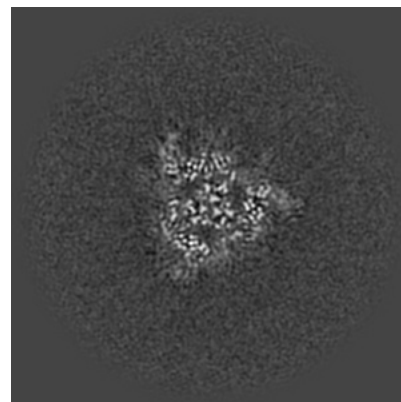
6.2.1 Primary map



X Index: 160

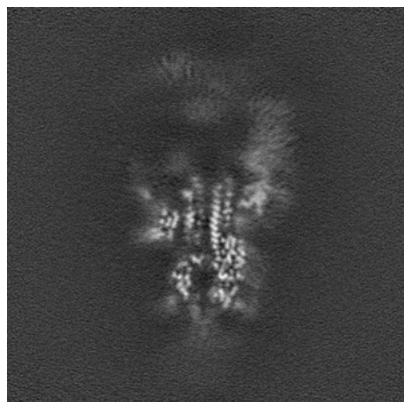


Y Index: 160

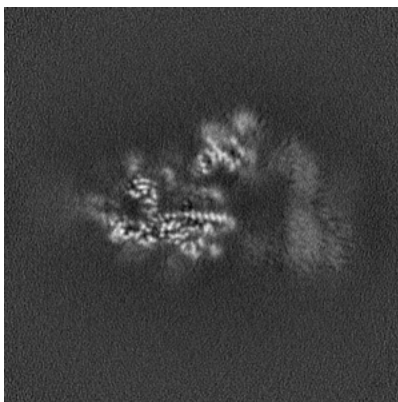


Z Index: 160

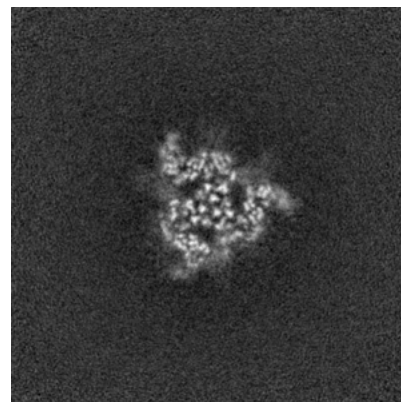
6.2.2 Raw map



X Index: 160



Y Index: 160

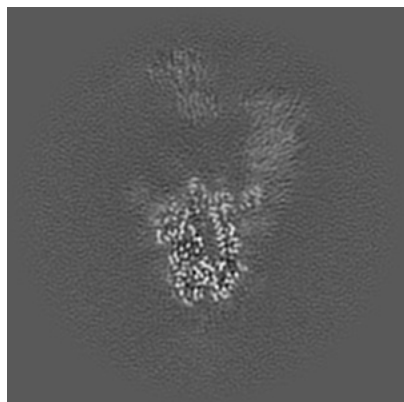


Z Index: 160

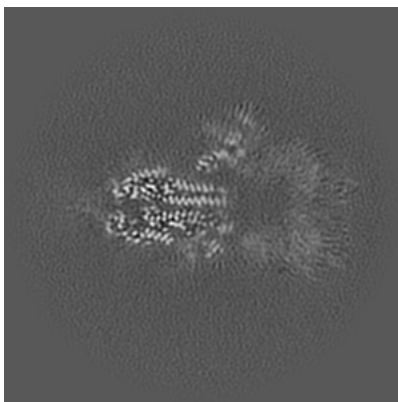
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

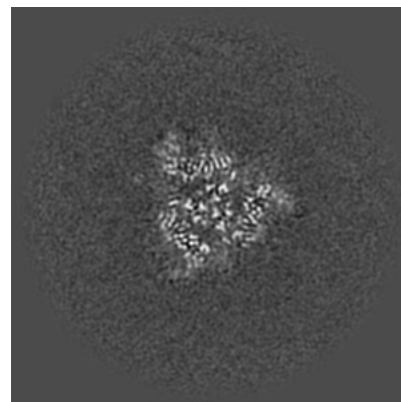
6.3.1 Primary map



X Index: 171

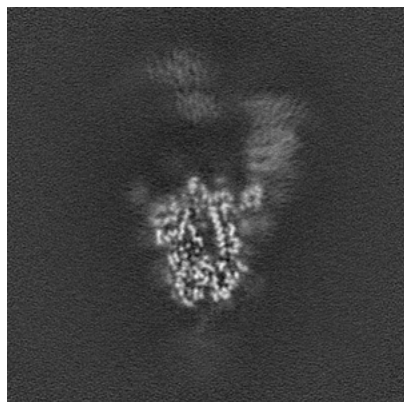


Y Index: 155

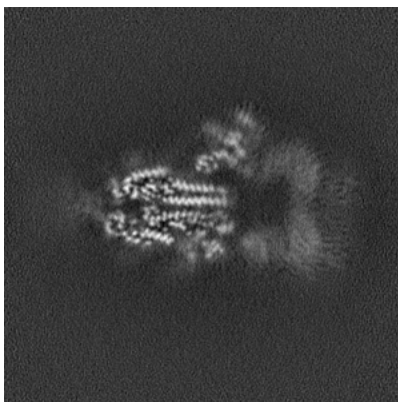


Z Index: 161

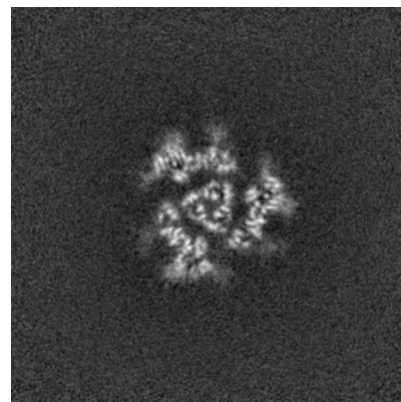
6.3.2 Raw map



X Index: 171



Y Index: 155

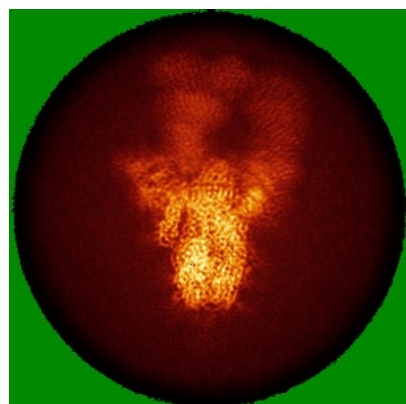


Z Index: 169

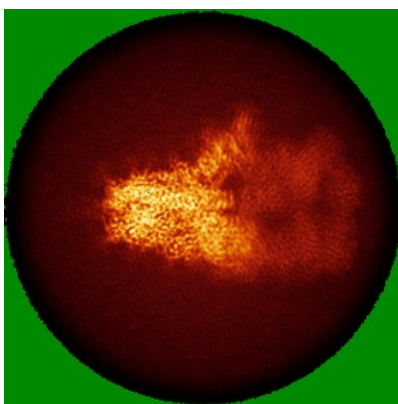
The images above show the largest variance slices of the map in three orthogonal directions.

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

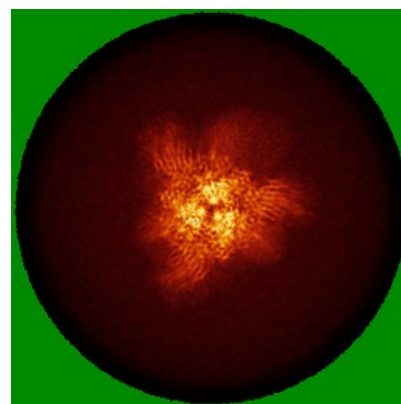
6.4.1 Primary map



X

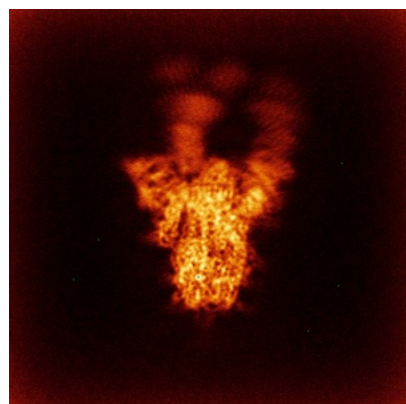


Y

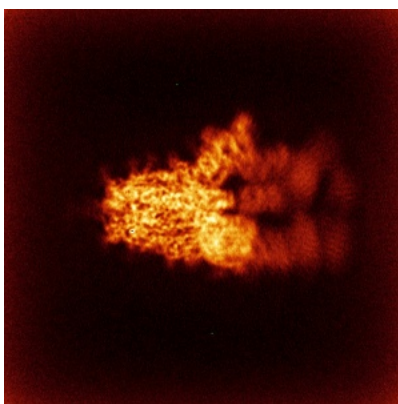


Z

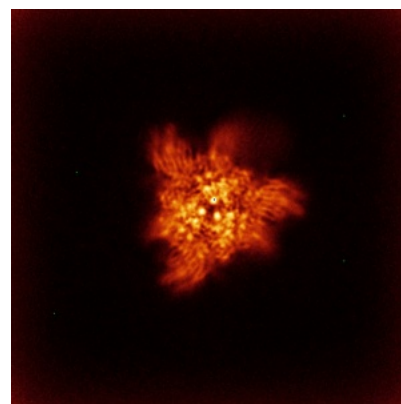
6.4.2 Raw map



X



Y

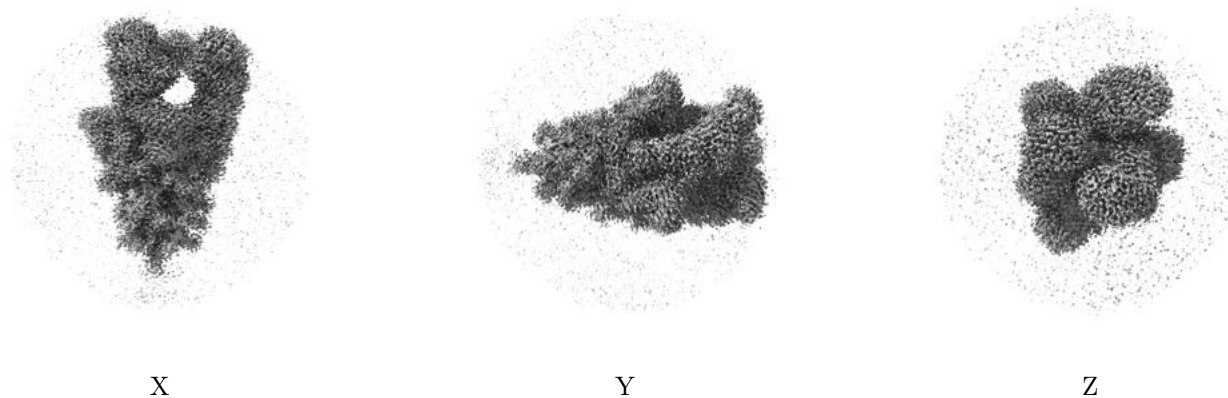


Z

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.

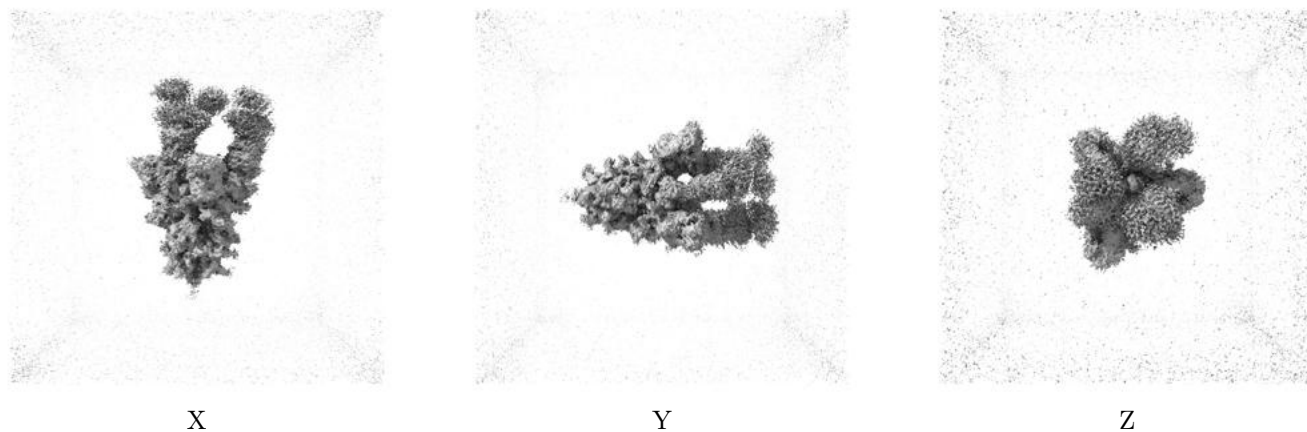
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

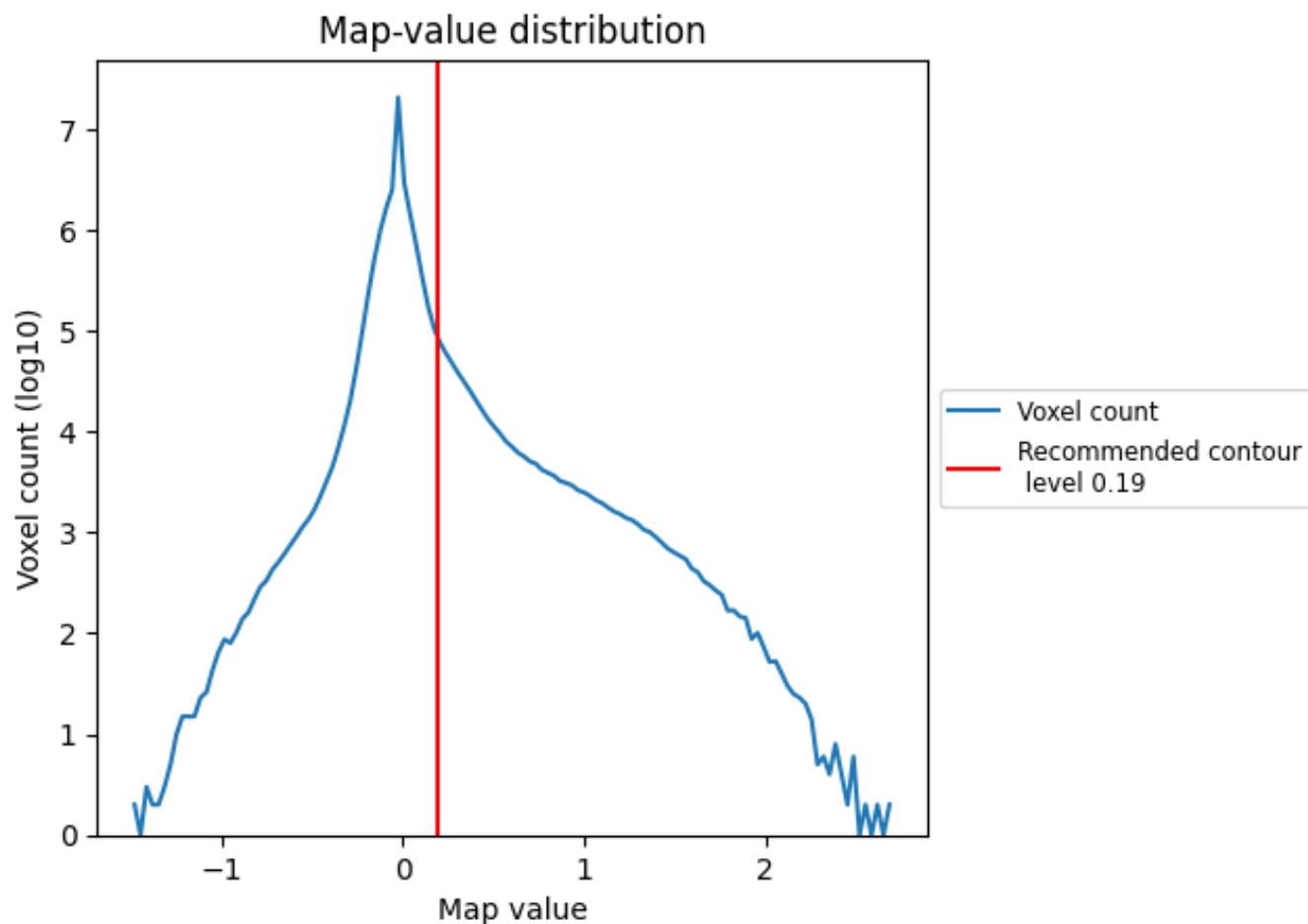
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

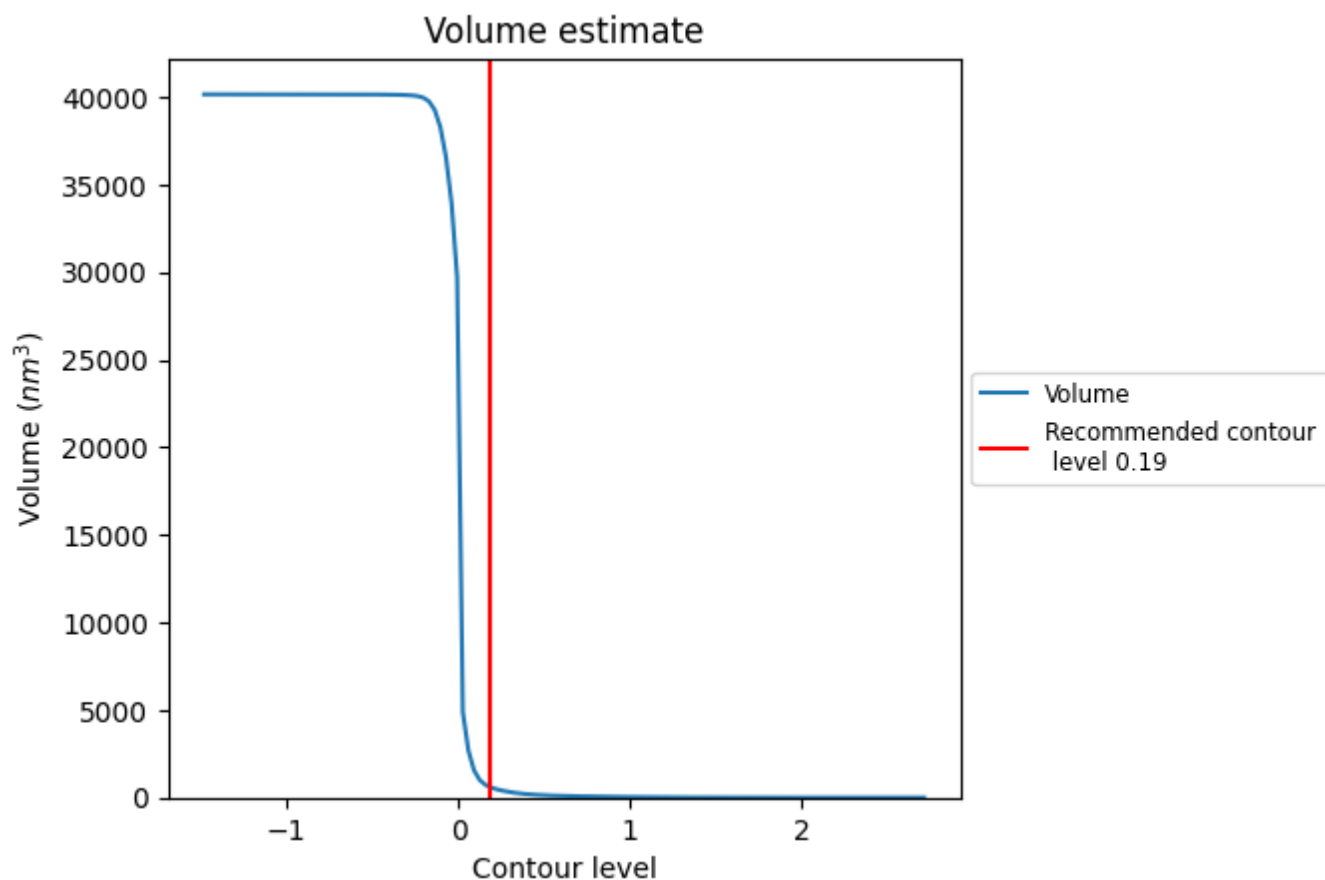
This section contains the results of statistical analysis of the map.

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.

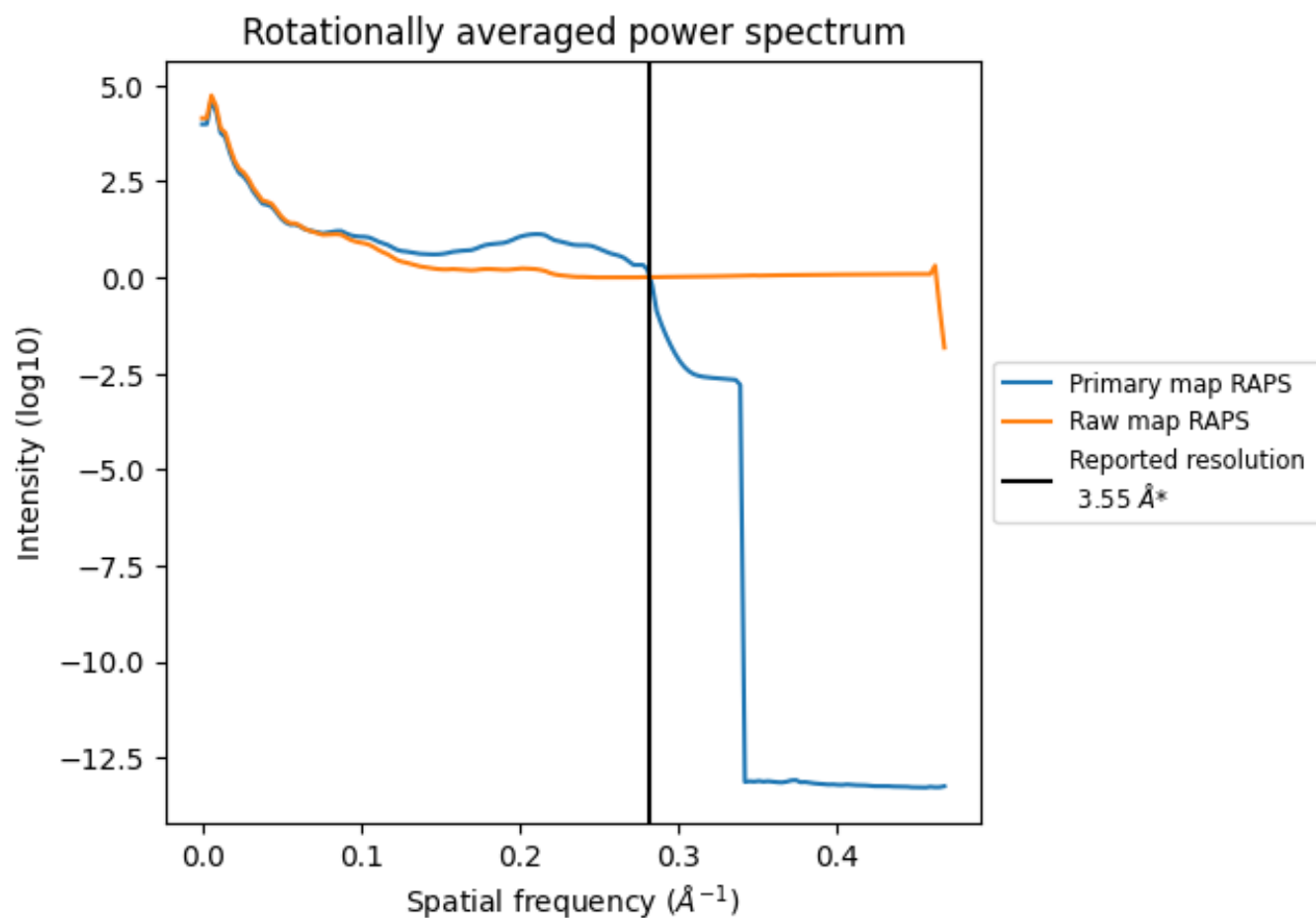
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 587 nm^3 ; this corresponds to an approximate mass of 530 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 ⓘ

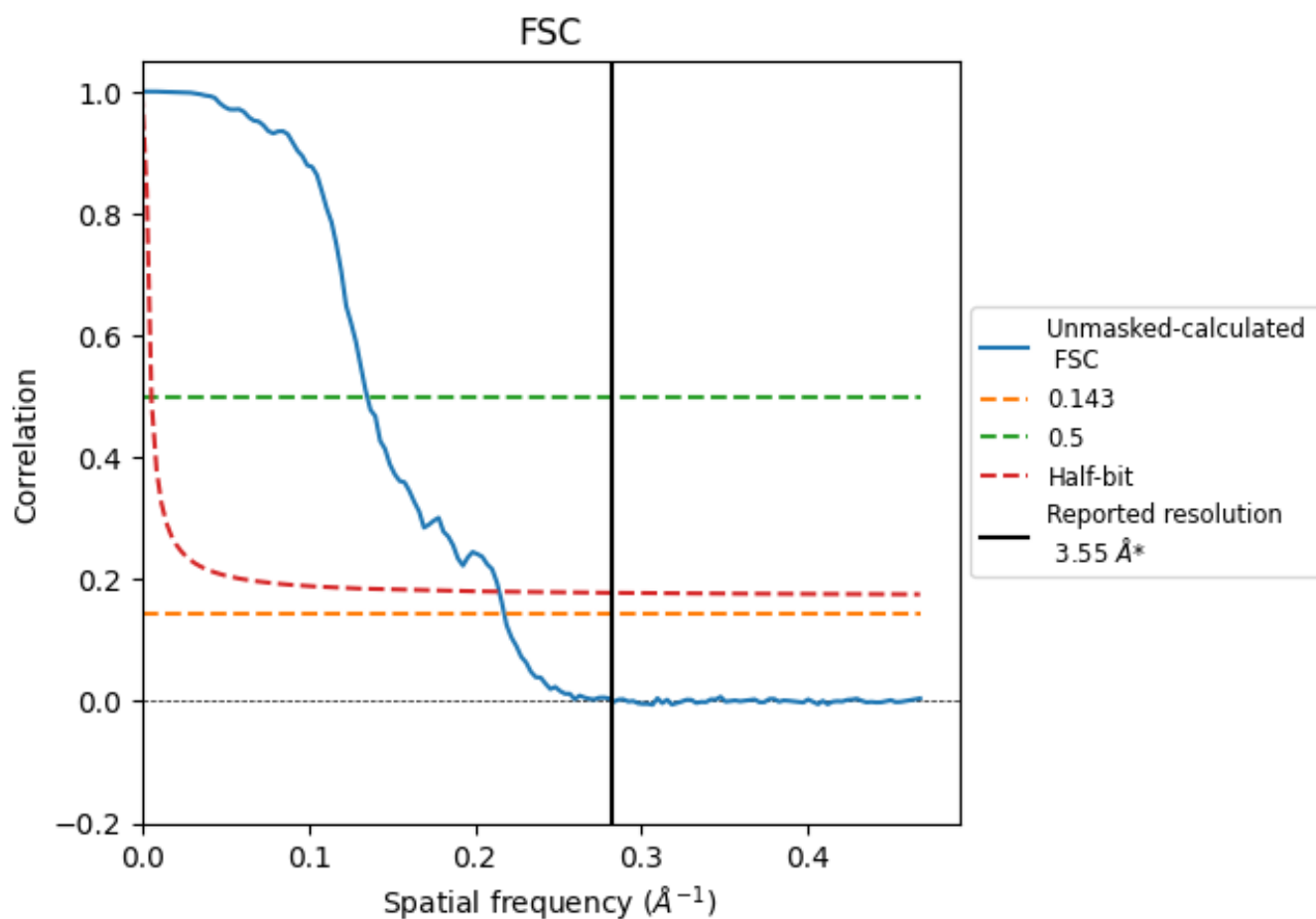


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 $0.282 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

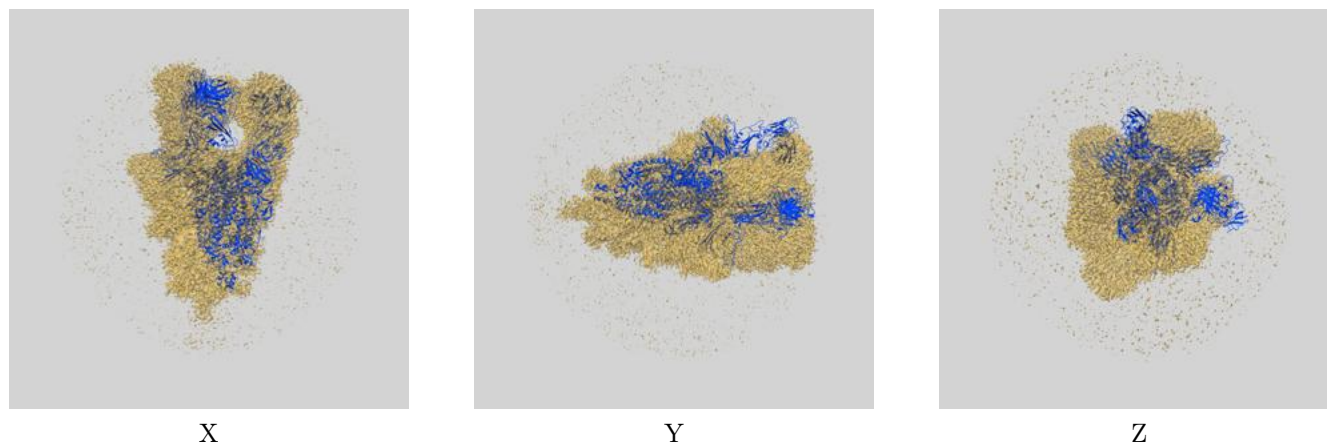
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.60	7.39	4.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

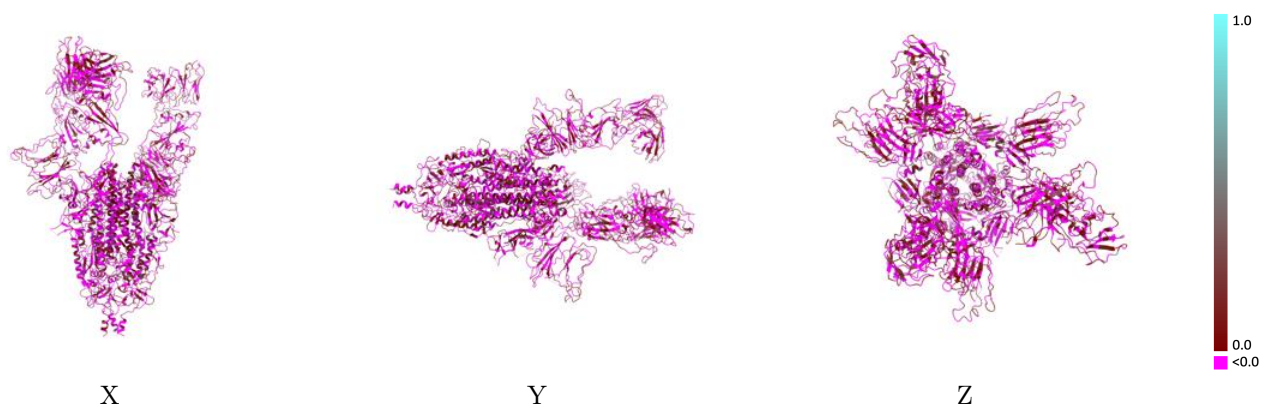
This section contains information regarding the fit between EMDB map EMD-38616 and PDB model 8XSD. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



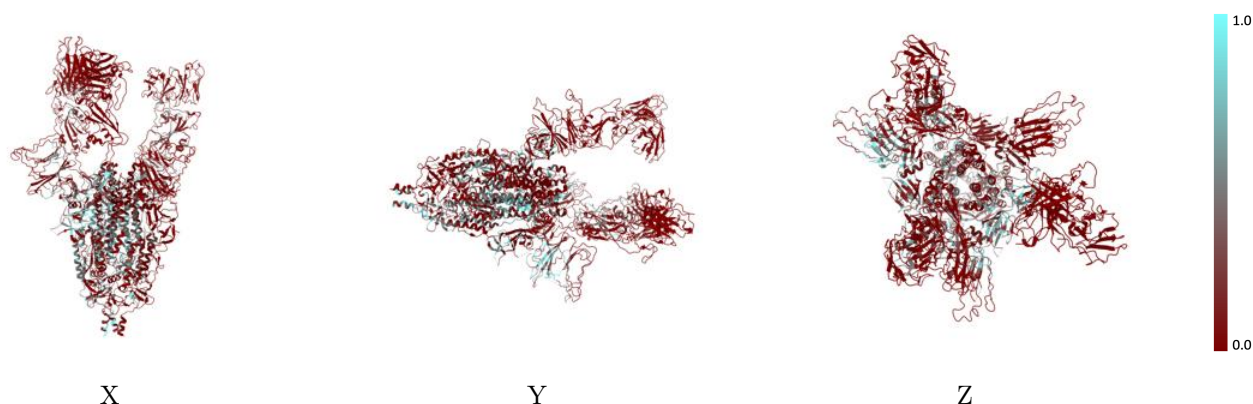
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



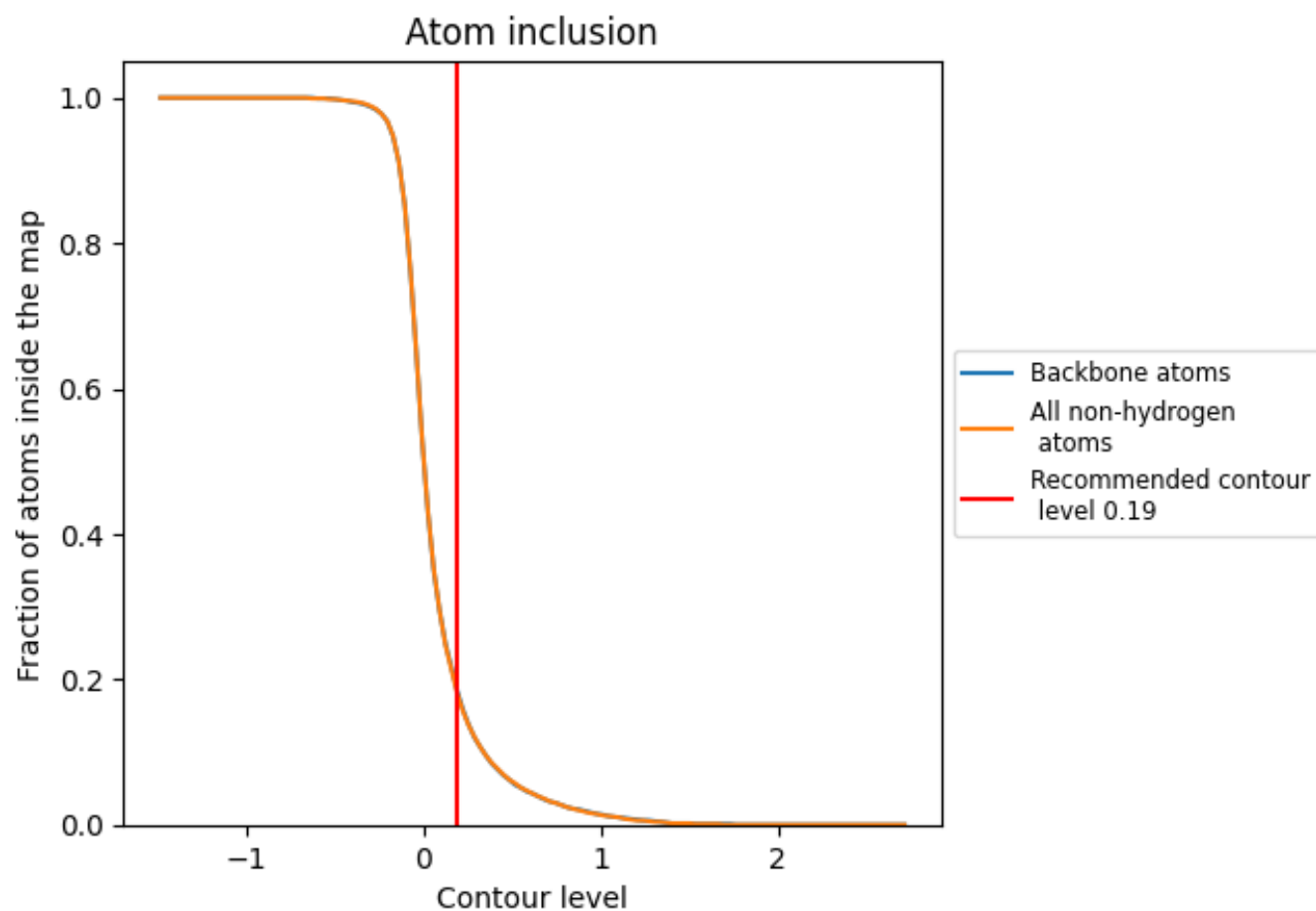
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 19% of all backbone atoms, 18% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1830	-0.0080
A	0.2390	-0.0080
B	0.1410	-0.0070
C	0.2580	-0.0140
G	0.0020	0.0170
H	0.1140	0.0000
I	0.0380	-0.0250
J	0.0000	-0.0120
K	0.0060	0.0260
L	0.0620	0.0110

1.0

0.0

<0.0