



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 08:20 PM JST

PDB ID : 7WLZ  
EMDB ID : EMD-32595  
Title : Cryo-EM structure of the Omicron S in complex with 35B5 Fab(1 down-, 1 up- and 1 invisible RBDs)  
Authors : Wang, X.; Zhu, Y.  
Deposited on : 2022-01-14  
Resolution : 2.98 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

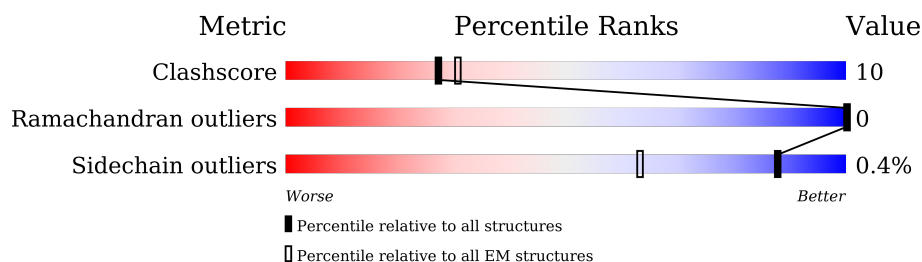
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.98 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1285	
1	B	1285	
1	C	1285	
2	P	237	
3	O	219	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25061 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	1028	Total	C	N	O	S	0	0
			8046	5159	1335	1517	35		
1	B	1042	Total	C	N	O	S	0	0
			8144	5216	1351	1540	37		
1	C	863	Total	C	N	O	S	0	0
			6692	4280	1110	1272	30		

There are 384 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213B	GLU	-	insertion	UNP P0DTC2
A	213C	PRO	-	insertion	UNP P0DTC2
A	214C	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213B	GLU	-	insertion	UNP P0DTC2
B	213C	PRO	-	insertion	UNP P0DTC2
B	214C	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213B	GLU	-	insertion	UNP P0DTC2
C	213C	PRO	-	insertion	UNP P0DTC2
C	214C	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called Heavy chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	127	Total	C	N	O	S	0	0
			967	605	171	185	6		

- Molecule 3 is a protein called Light chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	111	Total	C	N	O	S	0	0
			834	527	138	166	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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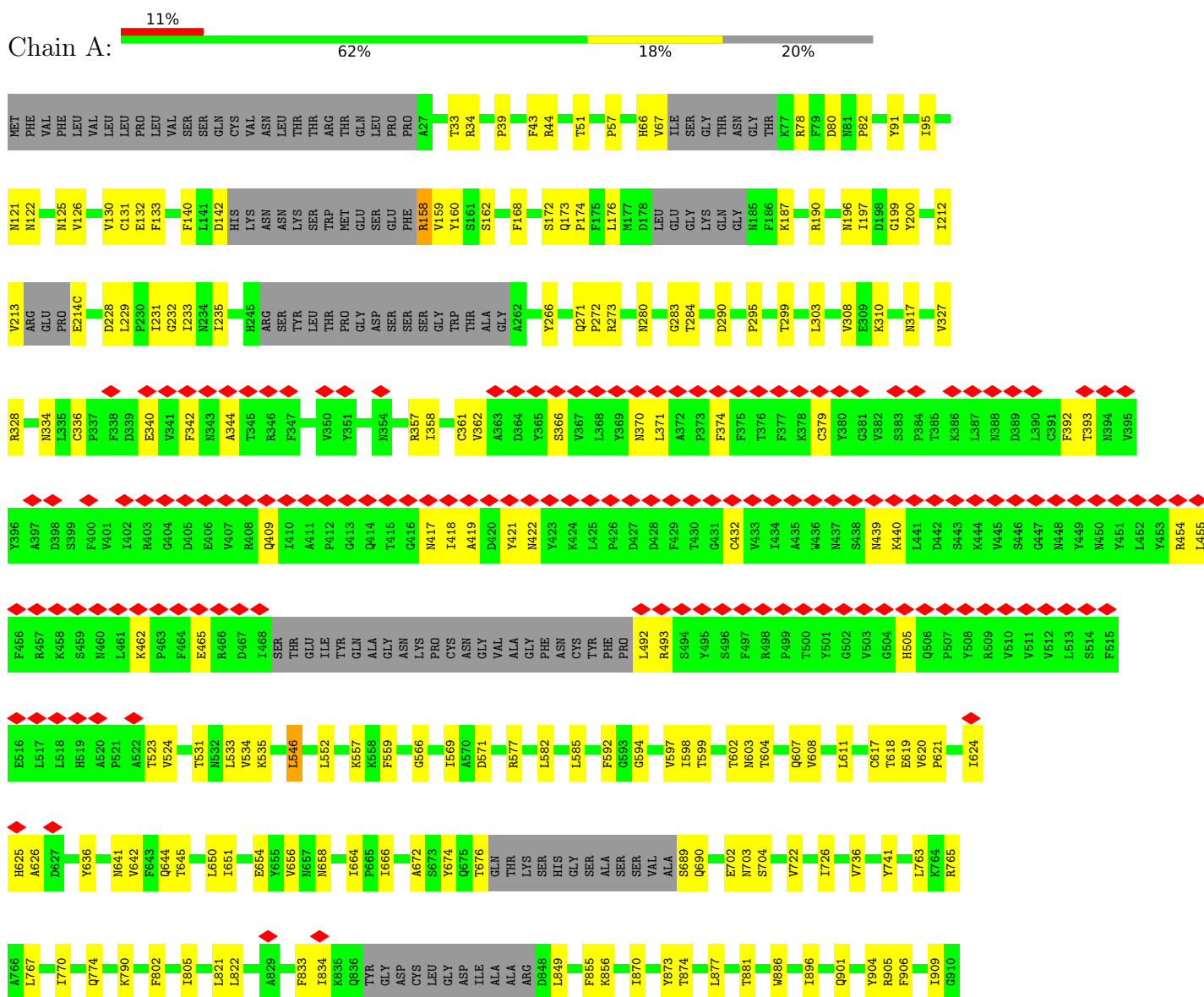
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

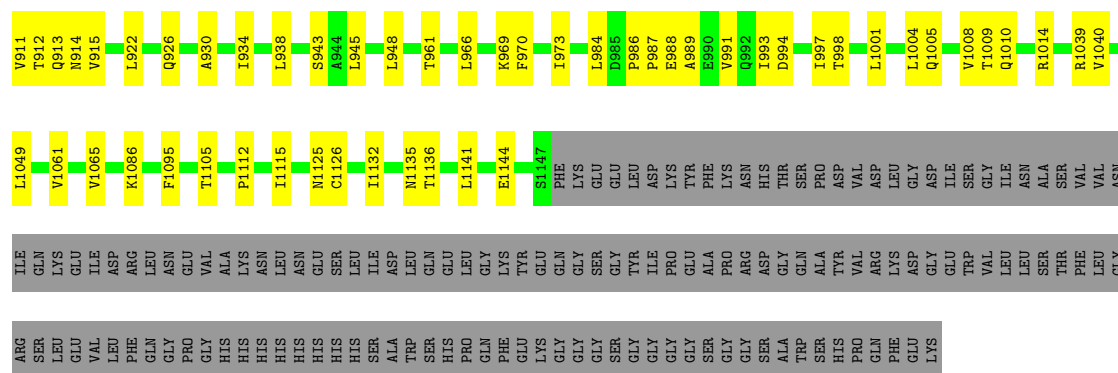
### 3 Residue-property plots

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.

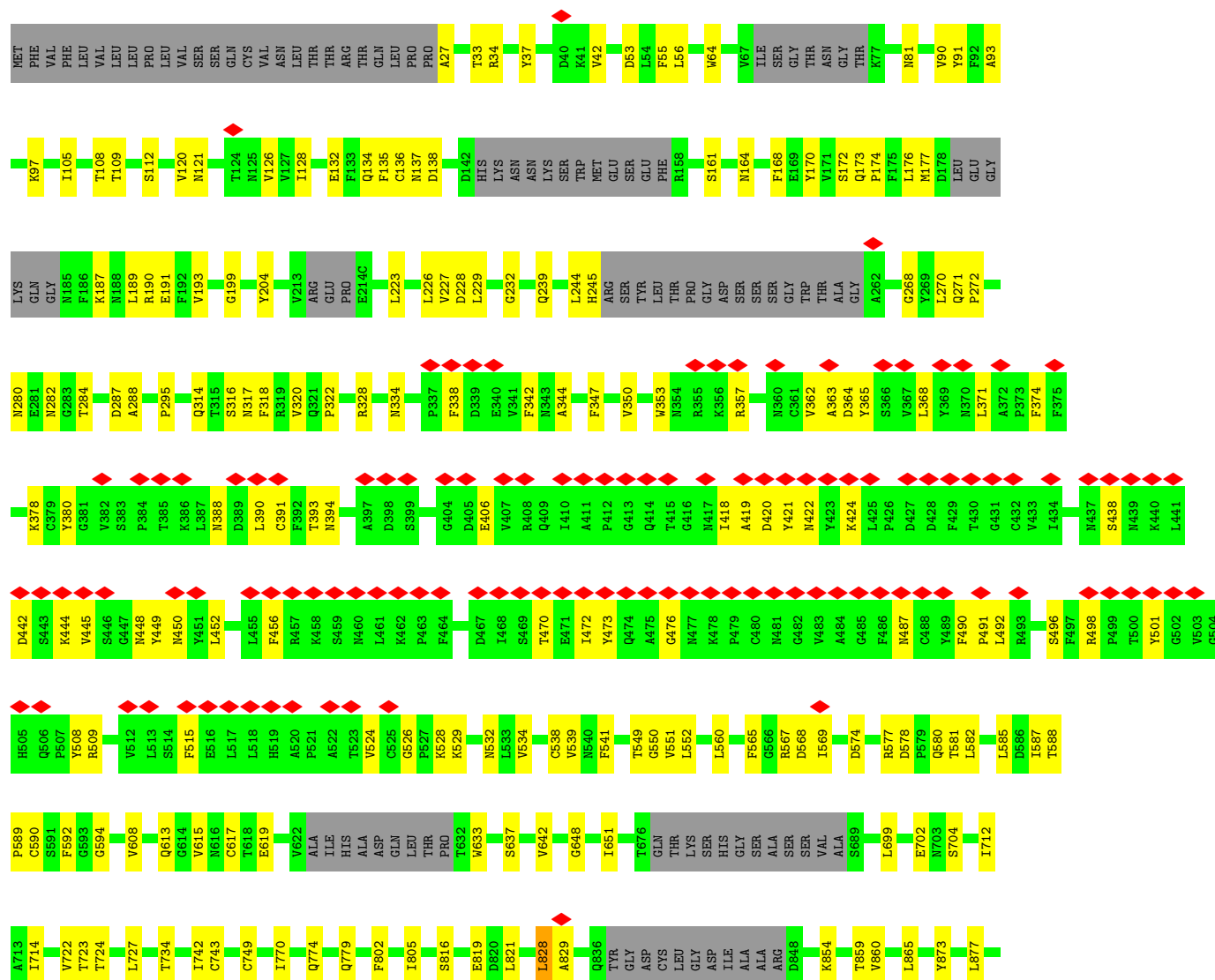
#### • Molecule 1: Spike glycoprotein

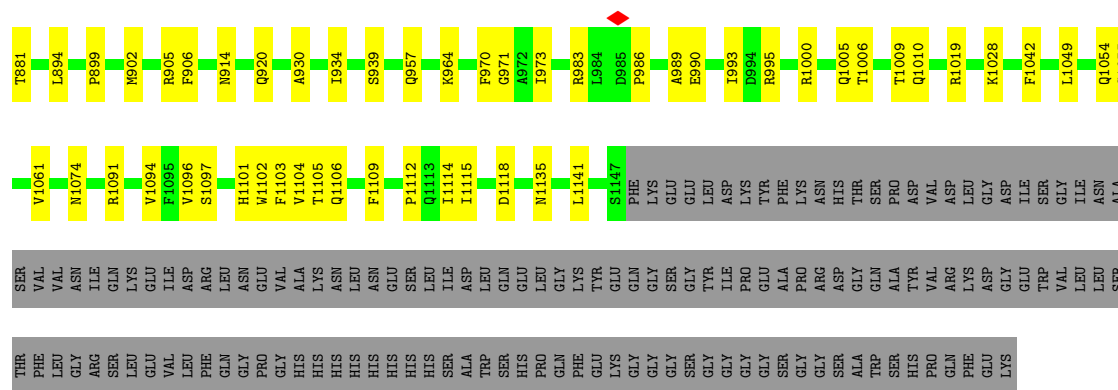




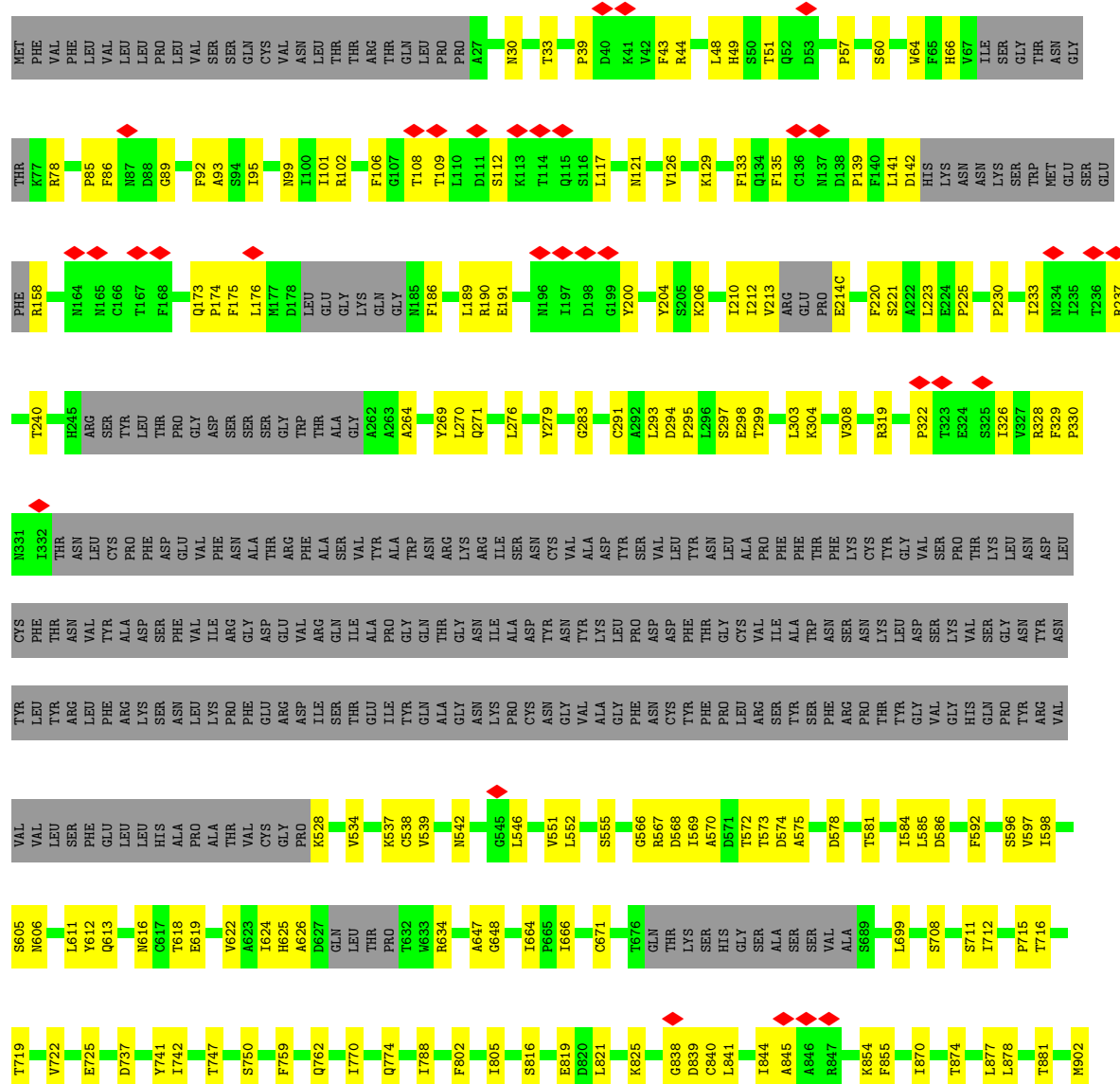


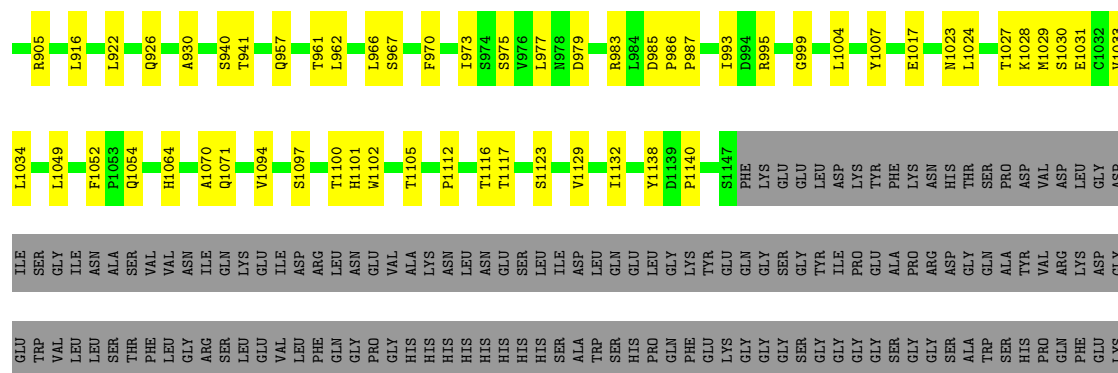
### • Molecule 1: Spike glycoprotein



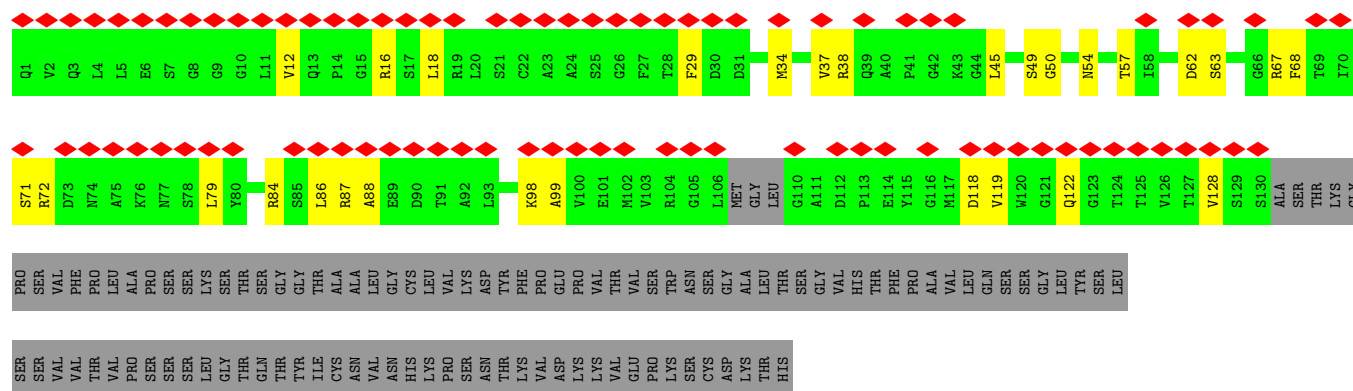


# Molecule 1: Spike glycoprotein

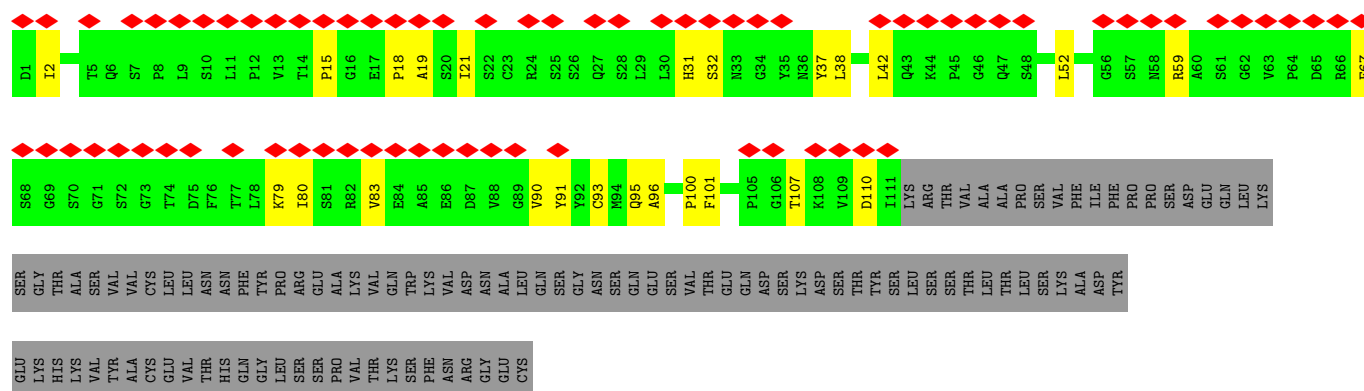
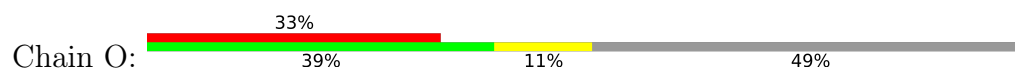




### • Molecule 2: Heavy chain of 35B5 Fab



### • Molecule 3: Light chain of 35B5 Fab



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	243427	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.390	Depositor
Minimum map value	-0.612	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	391.40402, 391.40402, 391.40402	wwPDB
Map dimensions	386, 386, 386	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.31	0/8233	0.49	1/11205 (0.0%)
1	B	0.36	0/8336	0.53	0/11345
1	C	0.35	0/6838	0.51	0/9301
2	P	0.43	0/987	0.57	0/1334
3	O	0.41	0/855	0.53	0/1166
All	All	0.34	0/25249	0.51	1/34351 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	546	LEU	CA-CB-CG	5.86	128.78	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8046	0	7871	168	0
1	B	8144	0	7919	162	0
1	C	6692	0	6547	140	0
2	P	967	0	932	21	0
3	O	834	0	799	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	126	0	117	0	0
4	B	126	0	117	2	0
4	C	126	0	117	1	0
All	All	25061	0	24419	476	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 (476) 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:B:1097:SER:HB3	1:B:1102:TRP:HA	1.73	0.71
1:C:294:ASP:HB2	1:C:295:PRO:HD2	1.79	0.64
1:C:293:LEU:HB3	1:C:297:SER:OG	1.96	0.64
1:A:656:VAL:HG12	1:A:658:ASN:H	1.64	0.62
1:A:566:GLY:HA2	1:C:43:PHE:HB3	1.82	0.62
1:A:855:PHE:O	1:A:856:LYS:HB2	2.00	0.61
1:C:49:HIS:HD2	1:C:279:TYR:CE1	2.19	0.60
1:C:566:GLY:O	1:C:574:ASP:N	2.32	0.60
1:A:644:GLN:NE2	1:A:645:THR:O	2.34	0.60
1:A:130:VAL:CG1	1:A:168:PHE:HB3	2.32	0.60
1:A:214(C):GLU:N	1:A:266:TYR:HH	1.99	0.60
1:C:666:ILE:HG12	1:C:671:CYS:HA	1.83	0.60
1:B:1005:GLN:O	1:B:1009:THR:HG23	2.01	0.60
1:A:873:TYR:HE1	1:B:699:LEU:HB3	1.68	0.59
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.85	0.59
1:C:328:ARG:NH1	1:C:578:ASP:OD1	2.36	0.59
1:B:642:VAL:HG12	1:B:651:ILE:HG12	1.85	0.59
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.85	0.58
1:B:108:THR:HG23	1:B:109:THR:HG23	1.83	0.58
1:B:450:ASN:HB3	2:P:57:THR:HG23	1.86	0.58
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	1.85	0.58
1:C:986:PRO:N	1:C:987:PRO:HD2	2.19	0.58
1:A:357:ARG:NH1	1:A:358:ILE:O	2.37	0.57
1:A:624:ILE:HG12	1:A:625:HIS:H	1.70	0.57
1:B:550:GLY:HA2	1:B:589:PRO:HA	1.86	0.57
1:C:93:ALA:HB1	1:C:189:LEU:HD11	1.85	0.57
1:C:319:ARG:HG2	1:C:592:PHE:HB3	1.86	0.57
1:B:723:THR:HG22	1:B:724:THR:H	1.69	0.57
1:A:603:ASN:OD1	1:A:604:THR:N	2.37	0.57
1:B:714:ILE:HD11	1:B:1094:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TYR:O	1:B:450:ASN:ND2	2.34	0.57
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.20	0.57
1:A:505:HIS:O	1:A:505:HIS:ND1	2.35	0.57
1:A:642:VAL:HG22	1:A:651:ILE:HG12	1.86	0.56
1:A:912:THR:HG22	1:A:913:GLN:H	1.70	0.56
1:C:206:LYS:HZ3	1:C:221:SER:HG	1.51	0.56
1:C:962:LEU:HD11	1:C:1007:TYR:CG	2.41	0.56
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.37	0.56
1:A:911:VAL:HG12	1:A:915:VAL:HG11	1.86	0.56
1:B:1105:THR:HG22	1:B:1112:PRO:HA	1.87	0.56
1:B:894:LEU:HD21	1:C:715:PRO:HD3	1.87	0.56
1:A:231:ILE:HG22	1:A:233:ILE:HG23	1.88	0.56
1:A:571:ASP:N	1:C:967:SER:OG	2.38	0.56
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.88	0.56
1:B:1101:HIS:CE1	4:B:1308:NAG:H3	2.40	0.55
1:B:819:GLU:OE2	1:B:1055:SER:OG	2.24	0.55
1:C:142:ASP:HB2	1:C:158:ARG:HG2	1.89	0.55
1:A:534:VAL:HG12	1:A:535:LYS:N	2.21	0.55
1:A:703:ASN:OD1	1:A:704:SER:N	2.39	0.55
1:B:176:LEU:HB3	1:B:190:ARG:NH1	2.20	0.55
1:B:854:LYS:HE2	1:B:859:THR:HG23	1.88	0.55
1:C:204:TYR:HA	1:C:225:PRO:HA	1.87	0.55
1:C:322:PRO:HA	1:C:538:CYS:O	2.06	0.55
1:A:439:ASN:OD1	1:A:440:LYS:N	2.40	0.55
1:C:552:LEU:HD12	1:C:585:LEU:HD21	1.89	0.55
1:A:455:LEU:HG	1:A:493:ARG:HH21	1.69	0.55
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.54	0.55
1:B:821:LEU:HD21	1:B:939:SER:HB3	1.89	0.55
1:C:108:THR:HG23	1:C:109:THR:HG23	1.87	0.55
1:A:126:VAL:HB	1:A:174:PRO:HA	1.89	0.55
1:C:957:GLN:O	1:C:961:THR:HG23	2.08	0.54
1:B:316:SER:OG	1:B:317:ASN:N	2.40	0.54
1:A:790:LYS:NZ	1:B:702:GLU:HG2	2.23	0.54
1:A:1141:LEU:HD13	1:B:1141:LEU:HD11	1.88	0.54
1:B:615:VAL:HG12	1:B:617:CYS:H	1.72	0.54
1:B:828:LEU:HD23	1:B:829:ALA:H	1.73	0.54
1:A:197:ILE:O	1:A:200:TYR:N	2.41	0.54
1:B:81:ASN:OD1	1:B:239:GLN:NE2	2.36	0.54
1:B:176:LEU:HB3	1:B:190:ARG:HH11	1.72	0.54
2:P:62:ASP:OD1	2:P:63:SER:N	2.41	0.54
1:A:140:PHE:H	1:A:159:VAL:HG21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:31:HIS:CD2	3:O:32:SER:H	2.25	0.54
1:A:299:THR:HG21	1:A:597:VAL:HG11	1.89	0.53
2:P:12:VAL:HG11	2:P:18:LEU:HD11	1.89	0.53
3:O:15:PRO:HA	3:O:83:VAL:HG13	1.90	0.53
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.42	0.53
1:B:228:ASP:OD1	1:B:229:LEU:N	2.40	0.53
1:A:439:ASN:OD1	1:A:440:LYS:HG2	2.09	0.53
1:C:102:ARG:NH2	1:C:141:LEU:O	2.41	0.53
1:C:206:LYS:NZ	1:C:221:SER:OG	2.40	0.53
1:B:406:GLU:HG2	1:B:418:ILE:HG13	1.89	0.53
1:B:970:PHE:O	1:B:995:ARG:NH1	2.42	0.53
1:B:779:GLN:OE1	1:B:865:LEU:HD21	2.09	0.53
1:A:619:GLU:OE2	1:A:619:GLU:N	2.38	0.53
1:B:56:LEU:HB2	1:B:270:LEU:HD23	1.91	0.53
1:B:496:SER:HB2	1:B:498:ARG:NH2	2.24	0.53
1:A:196:ASN:HD22	1:A:235:ILE:HD12	1.74	0.53
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.91	0.53
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.90	0.53
2:P:118:ASP:OD1	2:P:119:VAL:N	2.42	0.53
1:A:1040:VAL:HG22	1:C:1031:GLU:HA	1.91	0.52
1:B:105:ILE:HG21	1:B:135:PHE:HE2	1.73	0.52
1:B:420:ASP:C	1:B:421:TYR:HD2	2.13	0.52
1:C:191:GLU:HB2	1:C:206:LYS:HB3	1.90	0.52
1:C:719:THR:HG23	1:C:1070:ALA:HB2	1.91	0.52
1:A:160:TYR:HD2	1:A:162:SER:H	1.56	0.52
1:A:855:PHE:HZ	1:B:588:THR:HG23	1.75	0.52
1:C:546:LEU:HD21	1:C:573:THR:HG21	1.92	0.52
1:A:599:THR:HB	1:A:608:VAL:HG23	1.91	0.52
1:A:855:PHE:CE1	1:B:589:PRO:HD2	2.45	0.52
1:B:328:ARG:HD3	1:B:532:ASN:O	2.10	0.52
2:P:37:VAL:CG1	2:P:45:LEU:HD22	2.40	0.52
3:O:18:PRO:HA	3:O:80:ILE:O	2.10	0.52
1:A:131:CYS:HB2	1:A:133:PHE:CZ	2.44	0.51
1:A:142:ASP:HB2	1:A:158:ARG:HH22	1.75	0.51
1:A:327:VAL:H	1:A:531:THR:HG22	1.75	0.51
1:A:557:LYS:HZ2	1:A:559:PHE:HE1	1.56	0.51
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.92	0.51
1:C:1030:SER:O	1:C:1034:LEU:HB2	2.10	0.51
2:P:122:GLN:O	2:P:122:GLN:HG2	2.10	0.51
1:A:172:SER:OG	1:A:173:GLN:OE1	2.28	0.51
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG23	1:B:223:LEU:HD22	1.92	0.51
1:A:736:VAL:HG12	1:A:767:LEU:HD12	1.92	0.51
1:C:33:THR:HG22	1:C:220:PHE:HD1	1.76	0.51
1:B:132:GLU:HB2	1:B:164:ASN:HB3	1.91	0.51
1:B:33:THR:O	1:B:34:ARG:HD2	2.11	0.51
1:C:970:PHE:O	1:C:995:ARG:HG2	2.11	0.51
1:A:922:LEU:O	1:A:926:GLN:HG3	2.10	0.51
1:B:37:TYR:HB2	1:B:204:TYR:CD2	2.46	0.51
1:C:64:TRP:CZ2	1:C:214(C):GLU:HB2	2.46	0.51
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.93	0.51
1:C:85:PRO:HA	1:C:237:ARG:HA	1.93	0.51
1:C:870:ILE:O	1:C:874:THR:HG23	2.11	0.51
3:O:42:LEU:HD12	3:O:90:VAL:O	2.11	0.51
1:A:571:ASP:OD2	1:C:975:SER:OG	2.29	0.50
1:C:212:ILE:HG22	1:C:213:VAL:HG23	1.92	0.50
1:C:612:TYR:O	1:C:648:GLY:HA3	2.11	0.50
2:P:88:ALA:HA	2:P:128:VAL:HG23	1.93	0.50
1:A:676:THR:HA	1:A:690:GLN:HA	1.91	0.50
1:A:822:LEU:HD21	1:A:938:LEU:HD21	1.92	0.50
1:C:121:ASN:HD22	1:C:176:LEU:HD12	1.75	0.50
1:B:973:ILE:HG22	1:B:983:ARG:HH22	1.76	0.50
1:C:816:SER:OG	1:C:819:GLU:HG3	2.11	0.50
1:A:969:LYS:NZ	1:A:973:ILE:O	2.34	0.50
1:B:320:VAL:HB	1:B:590:CYS:HB3	1.92	0.50
1:B:444:LYS:HG2	1:B:445:VAL:N	2.27	0.50
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.76	0.50
1:A:462:LYS:HB3	1:A:465:GLU:HB2	1.93	0.50
1:A:546:LEU:HD12	1:A:546:LEU:O	2.11	0.50
1:C:922:LEU:O	1:C:926:GLN:HG3	2.10	0.50
1:A:57:PRO:HG3	1:A:273:ARG:HE	1.76	0.50
1:A:67:VAL:O	1:A:78:ARG:N	2.37	0.50
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.93	0.50
3:O:38:LEU:HD21	3:O:93:CYS:HB2	1.92	0.50
1:A:44:ARG:HG2	1:B:567:ARG:HB2	1.93	0.50
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.94	0.50
1:B:338:PHE:CE2	1:B:363:ALA:HB1	2.47	0.50
1:B:1094:VAL:HG23	1:B:1096:VAL:HG13	1.94	0.50
1:C:747:THR:O	1:C:750:SER:OG	2.22	0.50
1:C:970:PHE:CD2	1:C:999:GLY:HA3	2.46	0.50
1:B:365:TYR:HH	1:B:515:PHE:HE1	1.60	0.49
1:B:930:ALA:O	1:B:934:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:ILE:HD11	1:B:1135:ASN:OD1	2.12	0.49
1:A:930:ALA:O	1:A:934:ILE:HG12	2.13	0.49
1:A:130:VAL:HG12	1:A:168:PHE:HD2	1.78	0.49
1:B:280:ASN:HD21	1:B:282:ASN:HB2	1.77	0.49
1:B:287:ASP:OD1	1:B:288:ALA:N	2.43	0.49
1:B:873:TYR:CE1	1:C:699:LEU:HD22	2.47	0.49
1:C:878:LEU:HD11	1:C:1054:GLN:HE22	1.77	0.49
3:O:95:GLN:NE2	3:O:100:PRO:O	2.46	0.49
1:A:1005:GLN:O	1:A:1009:THR:HG23	2.13	0.49
1:B:342:PHE:CD2	1:B:374:PHE:HE1	2.30	0.49
1:B:906:PHE:CD1	1:B:1049:LEU:HD11	2.48	0.49
1:A:870:ILE:O	1:A:874:THR:HG23	2.13	0.49
1:B:334:ASN:O	1:B:362:VAL:HG22	2.12	0.49
1:B:526:GLY:O	1:B:528:LYS:NZ	2.40	0.49
1:C:299:THR:OG1	1:C:597:VAL:HG11	2.12	0.49
1:C:303:LEU:HD22	1:C:308:VAL:HG12	1.95	0.49
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.12	0.49
1:A:295:PRO:O	1:A:299:THR:HG23	2.13	0.49
1:C:64:TRP:NE1	1:C:66:HIS:HB3	2.28	0.49
1:B:734:THR:HG22	1:B:860:VAL:HG12	1.95	0.48
1:A:912:THR:HG22	1:A:913:GLN:N	2.28	0.48
1:B:723:THR:HG22	1:B:724:THR:N	2.28	0.48
1:C:270:LEU:O	1:C:271:GLN:HG3	2.13	0.48
1:A:393:THR:HB	1:A:523:THR:H	1.78	0.48
1:A:970:PHE:HE1	1:C:759:PHE:HE2	1.58	0.48
1:B:120:VAL:O	1:B:126:VAL:HG23	2.13	0.48
1:C:85:PRO:O	1:C:269:TYR:OH	2.27	0.48
1:A:896:ILE:HD13	1:B:712:ILE:HD13	1.95	0.48
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.94	0.48
1:B:344:ALA:HB1	2:P:54:ASN:ND2	2.28	0.48
1:C:605:SER:OG	1:C:606:ASN:N	2.47	0.48
1:A:624:ILE:HG23	1:A:626:ALA:H	1.78	0.48
1:A:310:LYS:HG3	1:A:664:ILE:HD11	1.96	0.48
1:A:552:LEU:HB3	1:A:585:LEU:HD13	1.95	0.48
1:A:569:ILE:HD12	1:A:569:ILE:H	1.77	0.48
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.95	0.48
1:C:39:PRO:HG2	1:C:51:THR:HG21	1.95	0.48
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.96	0.48
1:A:984:LEU:HD21	1:A:988:GLU:HG2	1.95	0.48
1:C:57:PRO:HB2	1:C:60:SER:HB2	1.95	0.48
1:C:295:PRO:HA	1:C:298:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:CG1	1:A:621:PRO:HD3	2.43	0.47
1:C:1029:MET:O	1:C:1033:VAL:HB	2.14	0.47
1:A:988:GLU:O	1:A:991:VAL:HG12	2.15	0.47
1:A:1126:CYS:HB2	1:A:1132:ILE:HG12	1.95	0.47
1:C:613:GLN:HA	1:C:647:ALA:O	2.14	0.47
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.96	0.47
1:B:1019:ARG:HH22	1:C:1017:GLU:HG2	1.79	0.47
1:C:44:ARG:HD3	1:C:49:HIS:CD2	2.50	0.47
1:C:48:LEU:HB3	1:C:276:LEU:HD11	1.96	0.47
1:C:625:HIS:CD2	1:C:634:ARG:HH12	2.32	0.47
1:C:821:LEU:O	1:C:825:LYS:HG3	2.14	0.47
3:O:2:ILE:HB	3:O:95:GLN:OE1	2.15	0.47
1:A:66:HIS:N	1:A:80:ASP:OD2	2.47	0.47
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.96	0.47
1:B:328:ARG:NH1	1:B:580:GLN:OE1	2.48	0.47
1:B:552:LEU:HD12	1:B:585:LEU:HD13	1.96	0.47
1:B:816:SER:HB3	1:B:819:GLU:HG3	1.96	0.47
1:C:596:SER:HB2	1:C:613:GLN:HE22	1.79	0.47
1:A:43:PHE:HB3	1:B:565:PHE:O	2.14	0.47
1:A:303:LEU:HD22	1:A:308:VAL:HG12	1.95	0.47
1:A:422:ASN:ND2	1:A:454:ARG:HB3	2.29	0.47
1:B:476:GLY:H	1:B:487:ASN:HB3	1.79	0.47
1:C:176:LEU:HD22	1:C:190:ARG:CZ	2.43	0.47
1:C:844:ILE:HG22	1:C:845:ALA:N	2.29	0.47
1:A:417:ASN:OD1	1:A:418:ILE:N	2.46	0.47
1:A:765:ARG:HD3	1:B:957:GLN:HE22	1.80	0.47
1:A:790:LYS:HG2	1:B:704:SER:HB2	1.96	0.47
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.97	0.47
1:C:44:ARG:HD3	1:C:49:HIS:NE2	2.30	0.47
1:C:902:MET:HB3	1:C:916:LEU:HD11	1.95	0.47
2:P:67:ARG:HD3	2:P:84:ARG:O	2.14	0.47
1:A:421:TYR:C	1:A:422:ASN:HD22	2.19	0.47
1:A:997:ILE:O	1:A:1001:LEU:HD23	2.15	0.47
1:B:193:VAL:HB	1:B:204:TYR:HB2	1.97	0.47
1:C:555:SER:CB	1:C:584:ILE:HG22	2.45	0.47
1:A:172:SER:HG	1:A:173:GLN:H	1.63	0.47
1:A:392:PHE:O	1:A:524:VAL:N	2.46	0.47
1:B:456:PHE:HB3	1:B:473:TYR:CG	2.50	0.47
1:C:1129:VAL:HG13	1:C:1132:ILE:HB	1.95	0.47
3:O:19:ALA:O	3:O:79:LYS:HA	2.15	0.47
1:B:613:GLN:HA	1:B:648:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ILE:O	1:B:774:GLN:HG2	2.15	0.46
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.50	0.46
1:C:95:ILE:HD13	1:C:189:LEU:HB2	1.97	0.46
1:C:142:ASP:OD1	1:C:158:ARG:NH1	2.48	0.46
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.97	0.46
1:B:244:LEU:HD12	1:B:245:HIS:N	2.31	0.46
2:P:71:SER:O	2:P:79:LEU:HD12	2.14	0.46
1:A:176:LEU:HB3	1:A:190:ARG:HH11	1.79	0.46
1:C:48:LEU:HD22	1:C:304:LYS:O	2.16	0.46
1:C:92:PHE:CE2	1:C:240:THR:HB	2.50	0.46
2:P:98:LYS:HE2	2:P:119:VAL:HG12	1.96	0.46
1:A:121:ASN:ND2	1:A:176:LEU:HB2	2.31	0.46
1:B:529:LYS:O	1:B:529:LYS:HD3	2.15	0.46
1:C:838:GLY:O	1:C:841:LEU:HG	2.16	0.46
1:A:422:ASN:HD21	1:A:454:ARG:HB3	1.80	0.46
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.49	0.46
1:C:326:ILE:O	1:C:542:ASN:N	2.49	0.46
1:A:722:VAL:O	1:A:934:ILE:HD11	2.16	0.46
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.80	0.46
1:B:393:THR:C	1:B:394:ASN:HD22	2.18	0.46
1:B:986:PRO:O	1:B:990:GLU:HG2	2.16	0.46
1:C:186:PHE:HB3	1:C:210:ILE:O	2.16	0.46
1:C:940:SER:OG	1:C:941:THR:N	2.47	0.46
1:A:409:GLN:NE2	1:A:419:ALA:H	2.14	0.46
1:A:620:VAL:HG13	1:A:621:PRO:HD3	1.97	0.46
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.51	0.46
1:B:722:VAL:O	1:B:934:ILE:HD11	2.16	0.46
1:B:577:ARG:HD3	1:B:582:LEU:HD22	1.97	0.46
1:C:741:TYR:HE1	1:C:966:LEU:HD11	1.81	0.46
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.51	0.45
1:A:1144:GLU:N	1:A:1144:GLU:OE2	2.49	0.45
1:C:611:LEU:HD22	1:C:666:ILE:HG23	1.98	0.45
1:A:534:VAL:CG1	1:A:535:LYS:N	2.79	0.45
1:B:97:LYS:HD3	1:B:187:LYS:HG2	1.99	0.45
2:P:87:ARG:HB3	2:P:87:ARG:CZ	2.44	0.45
1:B:350:VAL:HG21	1:B:418:ILE:HG23	1.98	0.45
1:C:1117:THR:HG22	1:C:1140:PRO:HD3	1.98	0.45
3:O:59:ARG:NH1	3:O:67:PHE:O	2.45	0.45
1:B:470:THR:HA	1:B:491:PRO:HG2	1.99	0.45
1:C:725:GLU:OE2	1:C:1064:HIS:NE2	2.39	0.45
3:O:91:TYR:HB2	3:O:107:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HH12	1:A:533:LEU:HD23	1.80	0.45
1:B:112:SER:HA	1:B:132:GLU:HB3	1.97	0.45
1:B:134:GLN:H	1:B:161:SER:HB2	1.81	0.45
1:B:388:ASN:OD1	1:B:388:ASN:O	2.35	0.45
2:P:49:SER:OG	2:P:50:GLY:N	2.47	0.45
3:O:110:ASP:OD1	3:O:110:ASP:C	2.54	0.45
1:A:80:ASP:C	1:A:82:PRO:HD3	2.37	0.45
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.82	0.45
1:B:1103:PHE:HE1	1:B:1114:ILE:HD13	1.82	0.45
1:A:1010:GLN:O	1:A:1014:ARG:HG3	2.17	0.45
1:B:378:LYS:HD2	1:B:380:TYR:OH	2.17	0.45
1:B:712:ILE:HG21	1:B:1096:VAL:HG12	1.99	0.45
1:C:708:SER:HB3	1:C:711:SER:HB3	1.98	0.45
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.86	0.45
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.51	0.45
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.99	0.45
1:A:176:LEU:HB3	1:A:190:ARG:NH1	2.31	0.44
1:A:280:ASN:OD1	1:A:284:THR:N	2.50	0.44
1:A:901:GLN:O	1:A:905:ARG:HG2	2.17	0.44
1:B:877:LEU:O	1:B:881:THR:HG22	2.17	0.44
2:P:98:LYS:HG2	2:P:99:ALA:N	2.31	0.44
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.49	0.44
1:A:592:PHE:HZ	1:C:854:LYS:O	1.99	0.44
1:C:1023:ASN:O	1:C:1027:THR:HG23	2.17	0.44
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.98	0.44
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.98	0.44
1:C:129:LYS:HE2	1:C:133:PHE:HZ	1.82	0.44
1:C:200:TYR:HA	1:C:230:PRO:HA	1.98	0.44
1:C:598:ILE:HG23	1:C:664:ILE:HG21	2.00	0.44
1:A:833:PHE:HD1	1:A:834:ILE:HG13	1.83	0.44
1:B:121:ASN:ND2	1:B:176:LEU:HB2	2.33	0.44
1:B:989:ALA:O	1:B:993:ILE:HG12	2.18	0.44
1:B:1006:THR:O	1:B:1010:GLN:OE1	2.36	0.44
1:C:568:ASP:OD1	1:C:569:ILE:N	2.47	0.44
1:A:336:CYS:HA	1:A:361:CYS:HB2	1.99	0.44
1:C:294:ASP:H	1:C:297:SER:HB2	1.82	0.44
1:C:1100:THR:HG1	1:C:1101:HIS:HD1	1.62	0.44
1:A:328:ARG:NH1	1:A:533:LEU:HB3	2.33	0.44
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.53	0.44
1:C:537:LYS:N	1:C:551:VAL:HG23	2.33	0.44
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:21:ILE:HG21	3:O:107:THR:HG21	1.99	0.44
1:A:914:ASN:OD1	1:A:915:VAL:N	2.51	0.44
1:B:914:ASN:HD22	1:C:1123:SER:HB3	1.82	0.44
1:C:135:PHE:HB3	1:C:139:PRO:HG3	2.00	0.44
2:P:38:ARG:O	2:P:45:LEU:HD23	2.18	0.44
1:A:577:ARG:HD2	1:A:582:LEU:HD12	2.00	0.43
1:A:989:ALA:O	1:A:993:ILE:HG12	2.18	0.43
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.99	0.43
1:B:633:TRP:O	1:B:637:SER:OG	2.21	0.43
1:A:212:ILE:N	1:A:212:ILE:HD12	2.33	0.43
1:A:284:THR:HG22	1:B:560:LEU:HD11	2.01	0.43
1:A:636:TYR:O	1:A:651:ILE:HG21	2.19	0.43
1:A:943:SER:O	1:A:943:SER:OG	2.36	0.43
1:B:472:ILE:HD13	1:B:490:PHE:HA	2.00	0.43
1:C:176:LEU:HD22	1:C:190:ARG:NE	2.34	0.43
1:A:122:ASN:HB3	1:A:125:ASN:HB2	2.00	0.43
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.54	0.43
1:B:271:GLN:HB2	1:B:272:PRO:HD2	2.01	0.43
1:C:712:ILE:HD13	1:C:1094:VAL:HG21	2.00	0.43
1:A:271:GLN:HB2	1:A:272:PRO:HD2	2.01	0.43
1:A:618:THR:C	1:A:621:PRO:HD2	2.39	0.43
1:A:736:VAL:HG21	1:A:1004:LEU:HD21	2.01	0.43
1:B:322:PRO:HB3	1:B:549:THR:HG21	2.00	0.43
1:A:121:ASN:HD22	1:A:176:LEU:HB2	1.83	0.43
1:A:379:CYS:HA	1:A:432:CYS:HA	2.00	0.43
1:A:904:TYR:OH	1:B:1094:VAL:HG12	2.18	0.43
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.18	0.43
1:C:979:ASP:CG	1:C:983:ARG:HE	2.22	0.43
1:A:366:SER:OG	1:A:370:ASN:ND2	2.52	0.43
1:A:650:LEU:HD22	1:A:666:ILE:HD13	2.00	0.43
1:B:578:ASP:OD2	1:B:581:THR:OG1	2.36	0.43
1:C:30:ASN:HA	1:C:60:SER:O	2.18	0.43
1:C:99:ASN:ND2	1:C:101:ILE:O	2.52	0.43
1:C:624:ILE:HD12	1:C:626:ALA:HB3	2.00	0.43
1:B:568:ASP:HB2	1:B:574:ASP:OD2	2.19	0.43
1:C:534:VAL:HG21	1:C:539:VAL:HG21	2.00	0.43
1:A:454:ARG:HB2	1:A:492:LEU:HD23	2.01	0.43
1:C:330:PRO:HB3	4:C:1302:NAG:H82	2.01	0.43
1:C:770:ILE:O	1:C:774:GLN:HG2	2.19	0.43
1:A:228:ASP:OD2	1:A:229:LEU:N	2.52	0.43
1:A:994:ASP:O	1:A:998:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ALA:HB1	1:B:189:LEU:HD11	2.01	0.43
1:A:765:ARG:HD3	1:B:957:GLN:NE2	2.34	0.43
1:C:877:LEU:O	1:C:881:THR:HG22	2.19	0.43
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.19	0.42
1:B:873:TYR:HE1	1:C:699:LEU:HB3	1.84	0.42
1:B:199:GLY:HA2	1:B:232:GLY:HA2	2.01	0.42
1:B:444:LYS:HE3	1:B:448:ASN:HA	2.02	0.42
1:C:570:ALA:O	1:C:572:THR:HG23	2.19	0.42
1:A:273:ARG:HD3	1:A:290:ASP:OD1	2.20	0.42
1:A:607:GLN:NE2	1:A:674:TYR:OH	2.53	0.42
1:A:1095:PHE:HE1	1:A:1115:ILE:HD12	1.85	0.42
1:B:350:VAL:O	1:B:353:TRP:HD1	2.03	0.42
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.55	0.42
1:B:828:LEU:HD23	1:B:829:ALA:N	2.33	0.42
1:B:902:MET:SD	1:B:1049:LEU:HD12	2.59	0.42
2:P:34:MET:CB	2:P:79:LEU:HD22	2.50	0.42
1:A:1039:ARG:H	1:A:1039:ARG:HG2	1.64	0.42
1:B:42:VAL:HG11	1:C:567:ARG:HG3	2.02	0.42
1:B:280:ASN:OD1	1:B:284:THR:N	2.43	0.42
1:B:391:CYS:HB3	1:B:524:VAL:O	2.20	0.42
1:C:840:CYS:HB3	1:C:855:PHE:CZ	2.54	0.42
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	2.01	0.42
2:P:37:VAL:HG12	2:P:45:LEU:HD22	2.02	0.42
1:A:770:ILE:O	1:A:774:GLN:HG2	2.19	0.42
1:A:1095:PHE:CE1	1:A:1115:ILE:HD12	2.54	0.42
1:B:314:GLN:HE21	1:B:594:GLY:HA3	1.83	0.42
1:B:538:CYS:HB3	1:B:549:THR:HG22	2.00	0.42
1:A:280:ASN:OD1	1:A:283:GLY:N	2.52	0.42
1:A:317:ASN:ND2	1:C:737:ASP:OD2	2.51	0.42
1:A:961:THR:HG21	1:C:762:GLN:NE2	2.34	0.42
1:B:91:TYR:OH	1:B:191:GLU:OE2	2.26	0.42
1:B:328:ARG:HH21	1:B:578:ASP:CG	2.23	0.42
1:B:364:ASP:OD1	1:B:364:ASP:N	2.52	0.42
1:B:371:LEU:HB2	1:B:374:PHE:CD2	2.54	0.42
1:B:551:VAL:HG23	1:B:551:VAL:O	2.19	0.42
1:A:91:TYR:CG	1:A:91:TYR:O	2.72	0.42
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.84	0.42
1:A:906:PHE:O	1:A:909:ILE:HG12	2.20	0.42
1:B:419:ALA:O	1:B:424:LYS:HD3	2.19	0.42
1:C:112:SER:OG	1:C:133:PHE:O	2.34	0.42
1:A:33:THR:HG23	1:A:33:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:OD1	1:B:138:ASP:N	2.53	0.42
1:B:971:GLY:C	1:B:995:ARG:HH12	2.23	0.42
1:B:1074:ASN:CG	4:B:1306:NAG:HN2	2.23	0.42
1:B:1094:VAL:O	1:B:1104:VAL:HA	2.19	0.42
1:C:191:GLU:HB3	1:C:223:LEU:HD21	2.02	0.42
1:C:578:ASP:OD2	1:C:581:THR:N	2.53	0.42
3:O:37:TYR:HB3	3:O:96:ALA:HB3	2.02	0.42
1:A:132:GLU:N	1:A:132:GLU:OE1	2.53	0.41
1:A:1086:LYS:HA	1:A:1125:ASN:HA	2.01	0.41
1:B:552:LEU:HD23	1:B:552:LEU:H	1.85	0.41
1:A:212:ILE:O	1:A:213:VAL:C	2.58	0.41
1:A:641:ASN:ND2	1:A:654:GLU:OE2	2.34	0.41
2:P:16:ARG:O	2:P:86:LEU:HG	2.19	0.41
1:A:986:PRO:N	1:A:987:PRO:HD2	2.35	0.41
1:C:619:GLU:O	1:C:622:VAL:HB	2.20	0.41
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.55	0.41
1:A:617:CYS:SG	1:A:644:GLN:HB2	2.60	0.41
1:A:618:THR:O	1:A:621:PRO:HD2	2.20	0.41
1:B:121:ASN:HD22	1:B:176:LEU:HB2	1.85	0.41
1:B:899:PRO:HB3	1:B:920:GLN:NE2	2.36	0.41
1:C:117:LEU:HD23	1:C:233:ILE:HD11	2.02	0.41
1:C:716:THR:HG22	1:C:1071:GLN:O	2.19	0.41
1:C:973:ILE:HD12	1:C:973:ILE:H	1.86	0.41
1:A:122:ASN:N	1:A:125:ASN:O	2.54	0.41
1:A:611:LEU:HD22	1:A:666:ILE:HG23	2.01	0.41
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.76	0.41
1:A:689:SER:O	1:A:689:SER:OG	2.31	0.41
1:A:986:PRO:HA	1:A:989:ALA:HB3	2.01	0.41
1:B:541:PHE:CZ	1:B:587:ILE:HD12	2.55	0.41
1:B:983:ARG:O	1:B:983:ARG:HG2	2.21	0.41
1:C:962:LEU:HD11	1:C:1007:TYR:CD2	2.55	0.41
3:O:42:LEU:HD13	3:O:91:TYR:CE1	2.55	0.41
1:A:702:GLU:HA	1:C:788:ILE:HB	2.02	0.41
1:A:1004:LEU:O	1:A:1008:VAL:HG23	2.21	0.41
1:B:90:VAL:HA	1:B:268:GLY:O	2.21	0.41
1:B:452:LEU:HB3	1:B:492:LEU:HB3	2.02	0.41
1:C:575:ALA:HA	1:C:586:ASP:HA	2.02	0.41
1:C:742:ILE:HD11	1:C:1004:LEU:HD12	2.03	0.41
1:A:877:LEU:O	1:A:881:THR:HG22	2.21	0.41
1:B:121:ASN:HD22	1:B:176:LEU:HD12	1.85	0.41
1:B:136:CYS:SG	1:B:137:ASN:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PHE:O	1:B:592:PHE:HA	2.21	0.41
1:B:390:LEU:HD12	1:B:391:CYS:H	1.84	0.41
1:C:86:PHE:CZ	1:C:89:GLY:HA2	2.55	0.41
1:C:106:PHE:CD1	1:C:117:LEU:HD11	2.55	0.41
1:C:173:GLN:HG2	1:C:174:PRO:HD2	2.02	0.41
1:C:319:ARG:HG2	1:C:592:PHE:CB	2.51	0.41
1:C:839:ASP:OD1	1:C:840:CYS:N	2.54	0.41
1:C:977:LEU:HD13	1:C:993:ILE:HD12	2.02	0.41
1:A:39:PRO:HG2	1:A:51:THR:HG21	2.02	0.41
1:A:821:LEU:HA	1:A:821:LEU:HD23	1.90	0.41
1:C:291:CYS:O	1:C:298:GLU:HG3	2.21	0.41
1:C:1024:LEU:O	1:C:1028:LYS:HG3	2.21	0.41
1:A:340:GLU:O	1:A:344:ALA:HB2	2.21	0.40
1:A:849:LEU:H	1:A:849:LEU:HD23	1.86	0.40
1:B:172:SER:OG	1:B:173:GLN:N	2.54	0.40
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.86	0.40
1:C:95:ILE:HG23	1:C:95:ILE:O	2.20	0.40
1:A:342:PHE:HB3	1:A:374:PHE:CZ	2.56	0.40
1:B:1106:GLN:NE2	1:B:1109:PHE:HB3	2.36	0.40
1:C:616:ASN:C	1:C:618:THR:H	2.24	0.40
1:A:95:ILE:HD11	1:A:187:LYS:HB3	2.04	0.40
1:B:568:ASP:CG	1:B:569:ILE:H	2.24	0.40
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	2.03	0.40
3:O:95:GLN:HE21	3:O:101:PHE:HA	1.87	0.40
1:B:1054:GLN:HB2	1:B:1061:VAL:HG13	2.02	0.40
1:C:598:ILE:HG12	1:C:666:ILE:HD11	2.03	0.40
2:P:88:ALA:HA	2:P:128:VAL:CG2	2.51	0.40
1:A:334:ASN:O	1:A:362:VAL:HG12	2.21	0.40
1:A:909:ILE:HG13	1:A:911:VAL:HG23	2.04	0.40
1:B:174:PRO:HG2	1:B:177:MET:SD	2.62	0.40
1:B:496:SER:HB2	1:B:498:ARG:HH21	1.87	0.40
1:B:619:GLU:N	1:B:619:GLU:OE1	2.54	0.40
1:C:126:VAL:HG21	1:C:175:PHE:CE2	2.56	0.40
1:C:303:LEU:CD2	1:C:308:VAL:HG12	2.51	0.40
2:P:29:PHE:O	2:P:72:ARG:NH2	2.54	0.40
2:P:67:ARG:HG3	2:P:68:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1010/1285 (79%)	969 (96%)	41 (4%)	0	100	100
1	B	1024/1285 (80%)	968 (94%)	56 (6%)	0	100	100
1	C	845/1285 (66%)	804 (95%)	41 (5%)	0	100	100
2	P	123/237 (52%)	116 (94%)	7 (6%)	0	100	100
3	O	109/219 (50%)	102 (94%)	7 (6%)	0	100	100
All	All	3111/4311 (72%)	2959 (95%)	152 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	897/1116 (80%)	895 (100%)	2 (0%)	92	97
1	B	905/1116 (81%)	898 (99%)	7 (1%)	79	90
1	C	744/1116 (67%)	742 (100%)	2 (0%)	91	96
2	P	100/195 (51%)	100 (100%)	0	100	100
3	O	93/193 (48%)	92 (99%)	1 (1%)	70	86
All	All	2739/3736 (73%)	2727 (100%)	12 (0%)	88	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	158	ARG
1	B	357	ARG
1	B	368	LEU
1	B	442	ASP
1	B	501	TYR
1	B	508	TYR
1	B	828	LEU
1	B	964	LYS
1	C	78	ARG
1	C	985	ASP
3	O	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	134	GLN
1	A	164	ASN
1	A	196	ASN
1	A	314	GLN
1	A	370	ASN
1	A	409	GLN
1	A	422	ASN
1	A	506	GLN
1	A	542	ASN
1	A	755	GLN
1	A	784	GLN
1	A	901	GLN
1	A	919	ASN
1	A	957	GLN
1	B	87	ASN
1	B	121	ASN
1	B	218	GLN
1	B	317	ASN
1	B	448	ASN
1	B	606	ASN
1	B	755	GLN
1	B	957	GLN
1	B	960	ASN
1	C	49	HIS
1	C	121	ASN
1	C	271	GLN

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Mol	Chain	Res	Type
1	C	280	ASN
1	C	625	HIS
1	C	644	GLN
1	C	751	ASN
1	C	762	GLN
1	C	935	GLN
1	C	965	GLN
2	P	13	GLN
2	P	39	GLN
3	O	31	HIS

### 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](#)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	C	1307	1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	C	1308	1	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1302	1	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	A	1306	1	14,14,15	0.18	0	17,19,21	0.58	0
4	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	B	1306	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	B	1308	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	A	1303	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
4	NAG	C	1303	1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.49	0
4	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.67	0
4	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.60	0
4	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.69	0
4	NAG	B	1302	1	14,14,15	0.89	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	A	1305	1	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.52	0
4	NAG	C	1309	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	B	1304	1	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	A	1308	1	14,14,15	0.20	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1302	NAG	O5-C1	3.19	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1302	NAG	C1-O5-C5	4.91	118.85	112.19
4	A	1301	NAG	C1-O5-C5	-2.10	109.35	112.19

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C3-C2-N2-C7
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1304	NAG	C3-C2-N2-C7
4	A	1304	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1304	NAG	O7-C7-N2-C2
4	A	1305	NAG	C3-C2-N2-C7
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	B	1308	NAG	C3-C2-N2-C7
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	B	1309	NAG	C3-C2-N2-C7
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	C	1301	NAG	C3-C2-N2-C7
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	A	1309	NAG	C4-C5-C6-O6
4	C	1306	NAG	C8-C7-N2-C2
4	B	1307	NAG	O5-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	C	1304	NAG	C8-C7-N2-C2

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
4	C	1304	NAG	O7-C7-N2-C2
4	B	1302	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	B	1306	NAG	C1-C2-N2-C7
4	B	1303	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	B	1306	NAG	C3-C2-N2-C7
4	A	1306	NAG	C4-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	A	1304	NAG	C1-C2-N2-C7
4	A	1306	NAG	C3-C2-N2-C7
4	A	1309	NAG	C3-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	C	1303	NAG	C3-C2-N2-C7
4	C	1305	NAG	O5-C5-C6-O6
4	B	1308	NAG	C1-C2-N2-C7
4	C	1301	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1302	NAG	1	0
4	B	1306	NAG	1	0
4	B	1308	NAG	1	0

## 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.

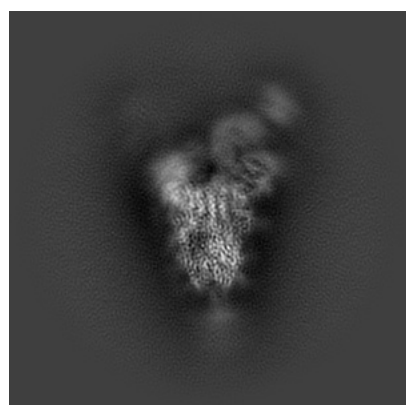
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32595. These allow visual inspection of the internal detail of the map and identification of artifacts.

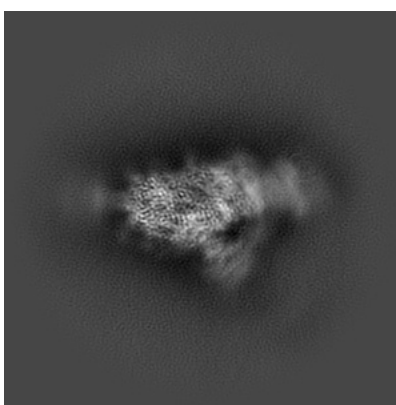
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

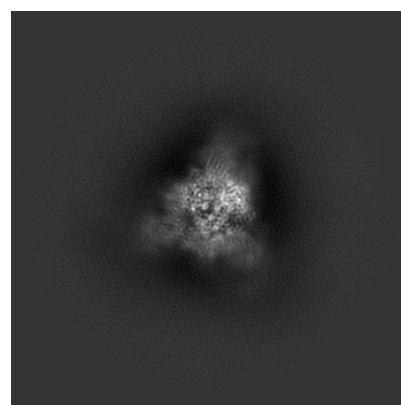
#### 6.1.1 Primary map



X



Y

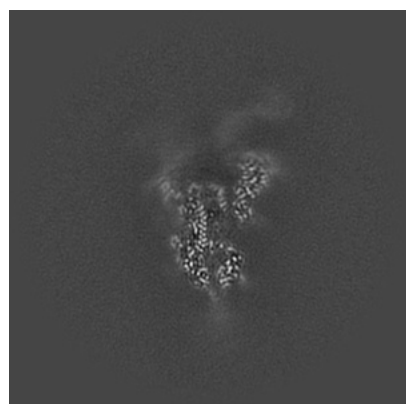


Z

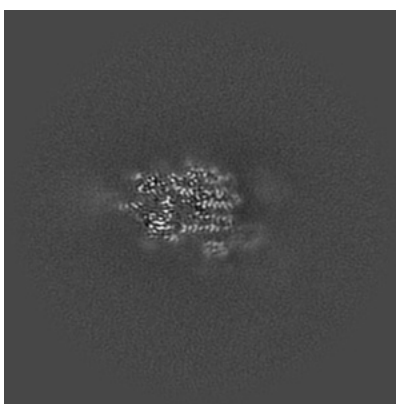
The images above show the map projected in three orthogonal directions.

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

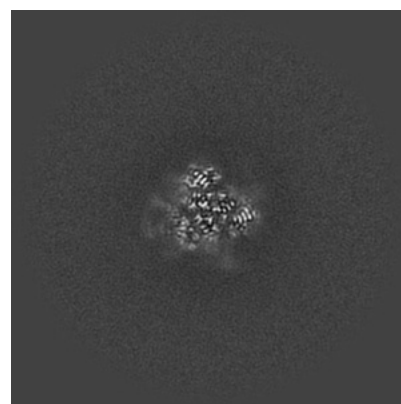
#### 6.2.1 Primary map



X Index: 193



Y Index: 193

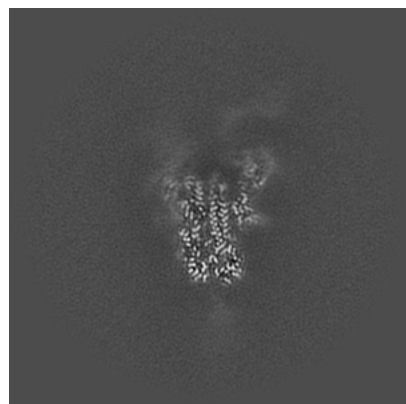


Z Index: 193

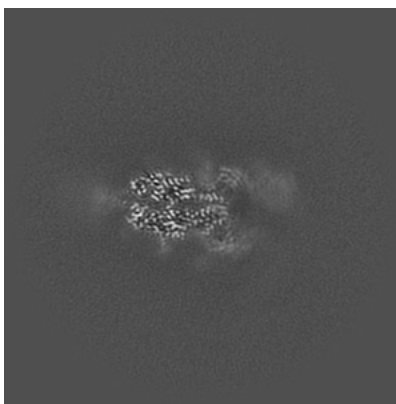
The images above show central slices of the map in three orthogonal directions.

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

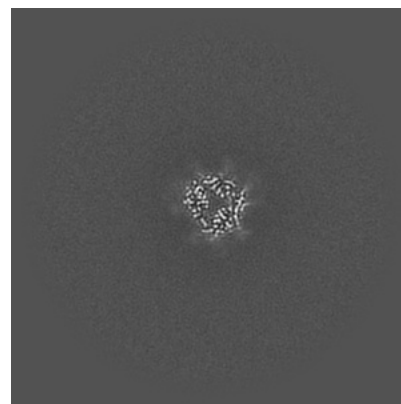
### 6.3.1 Primary map



X Index: 188



Y Index: 204

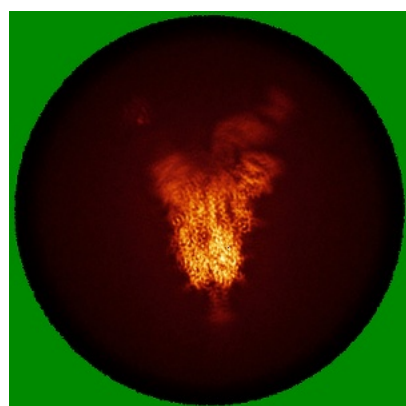


Z Index: 144

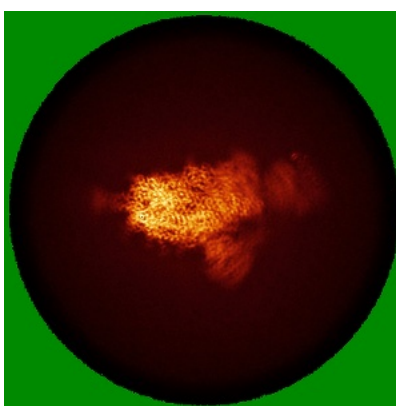
The images above show the largest variance slices of the map in three orthogonal directions.

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

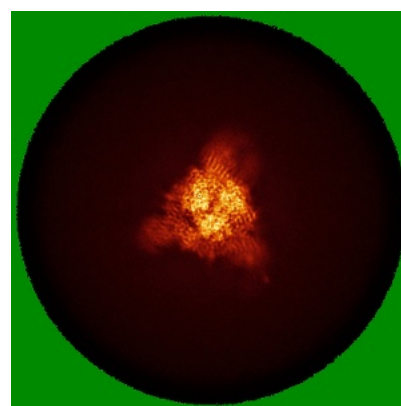
### 6.4.1 Primary map



X



Y

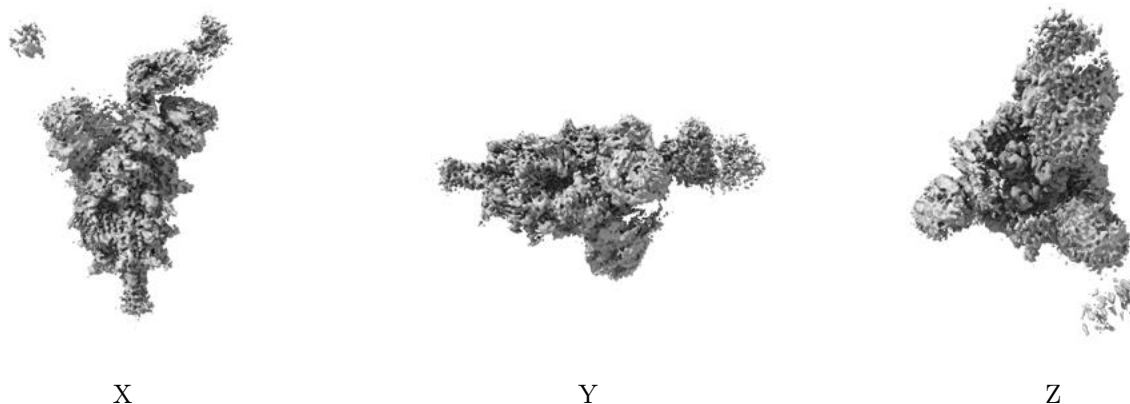


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

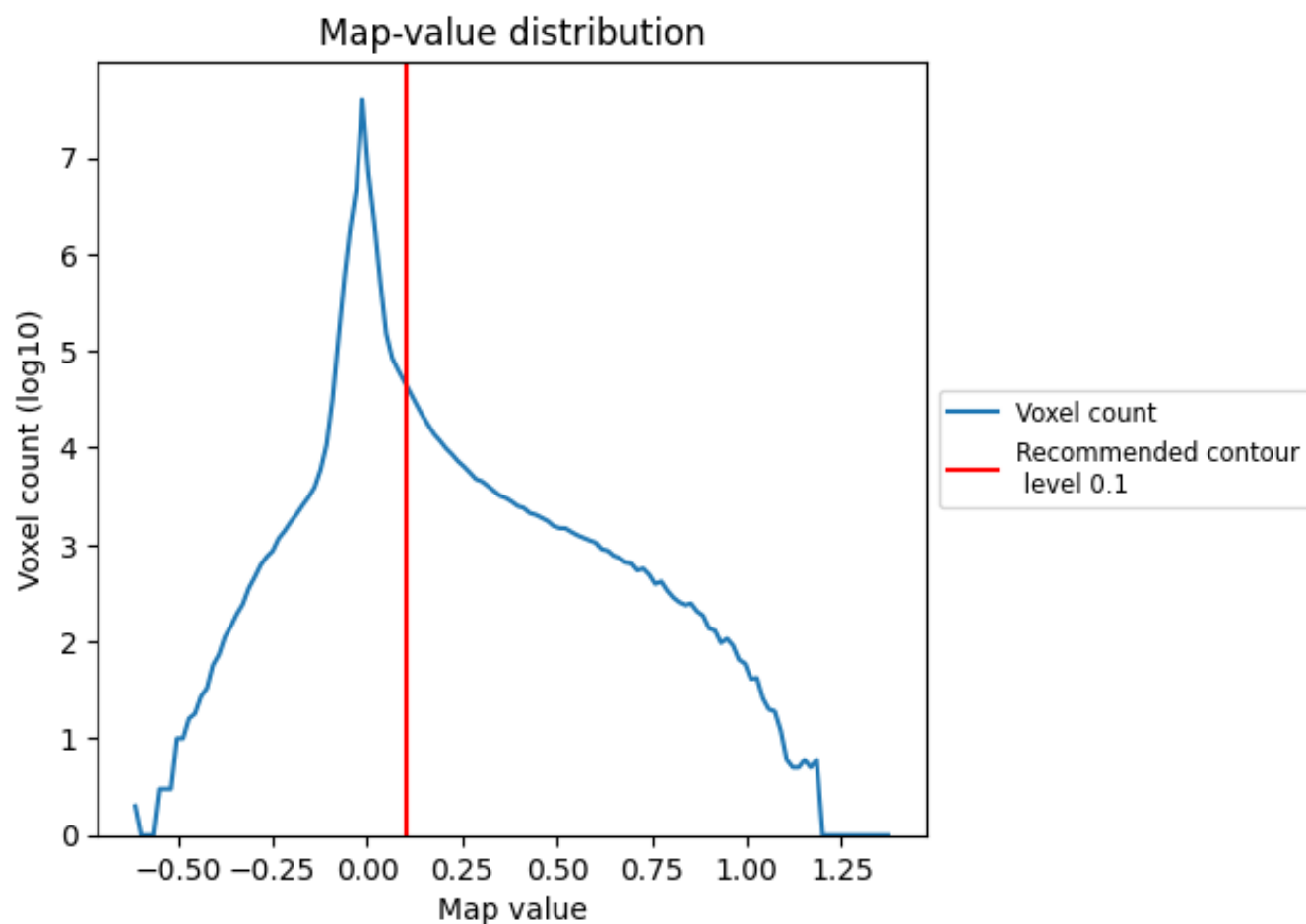
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

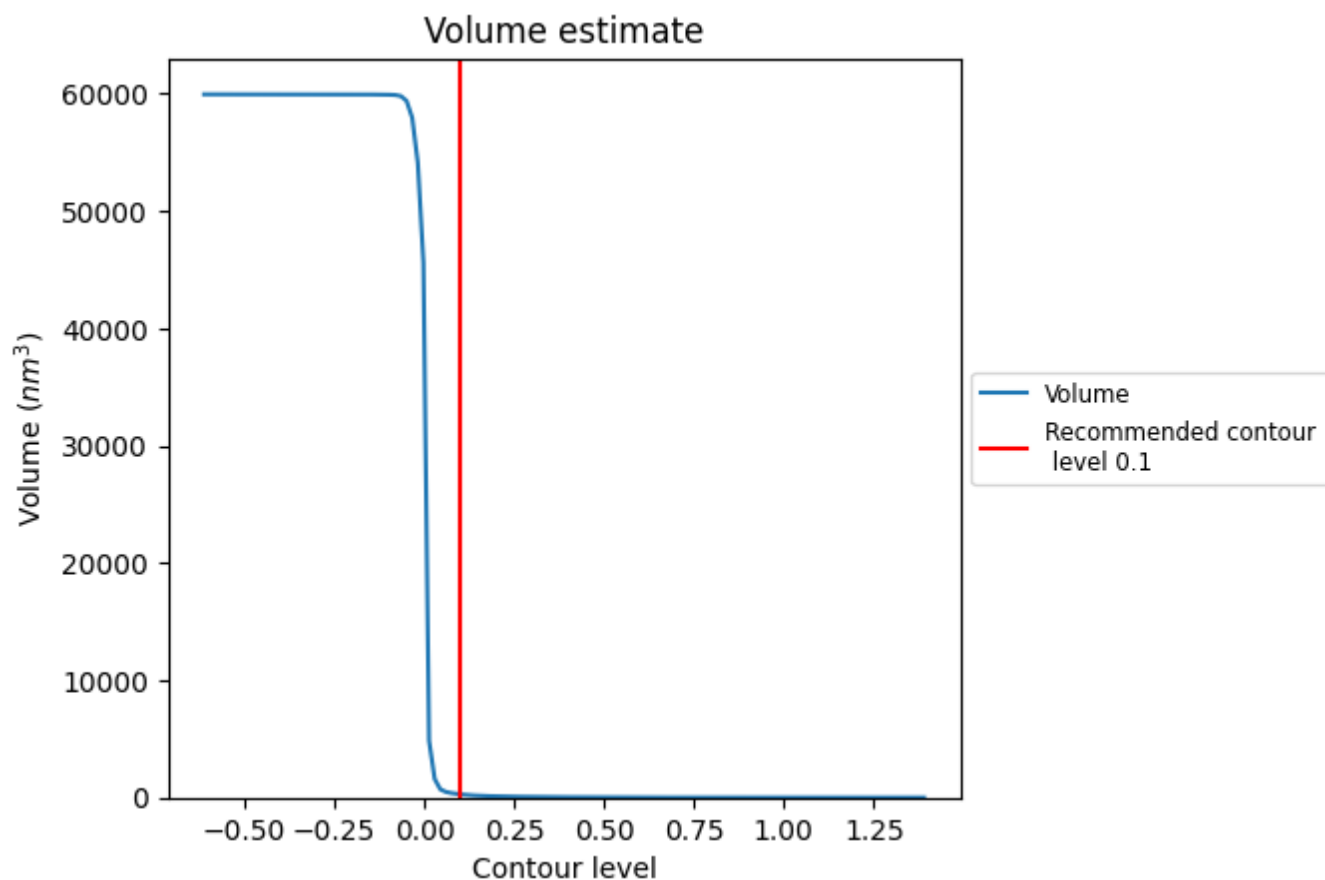
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

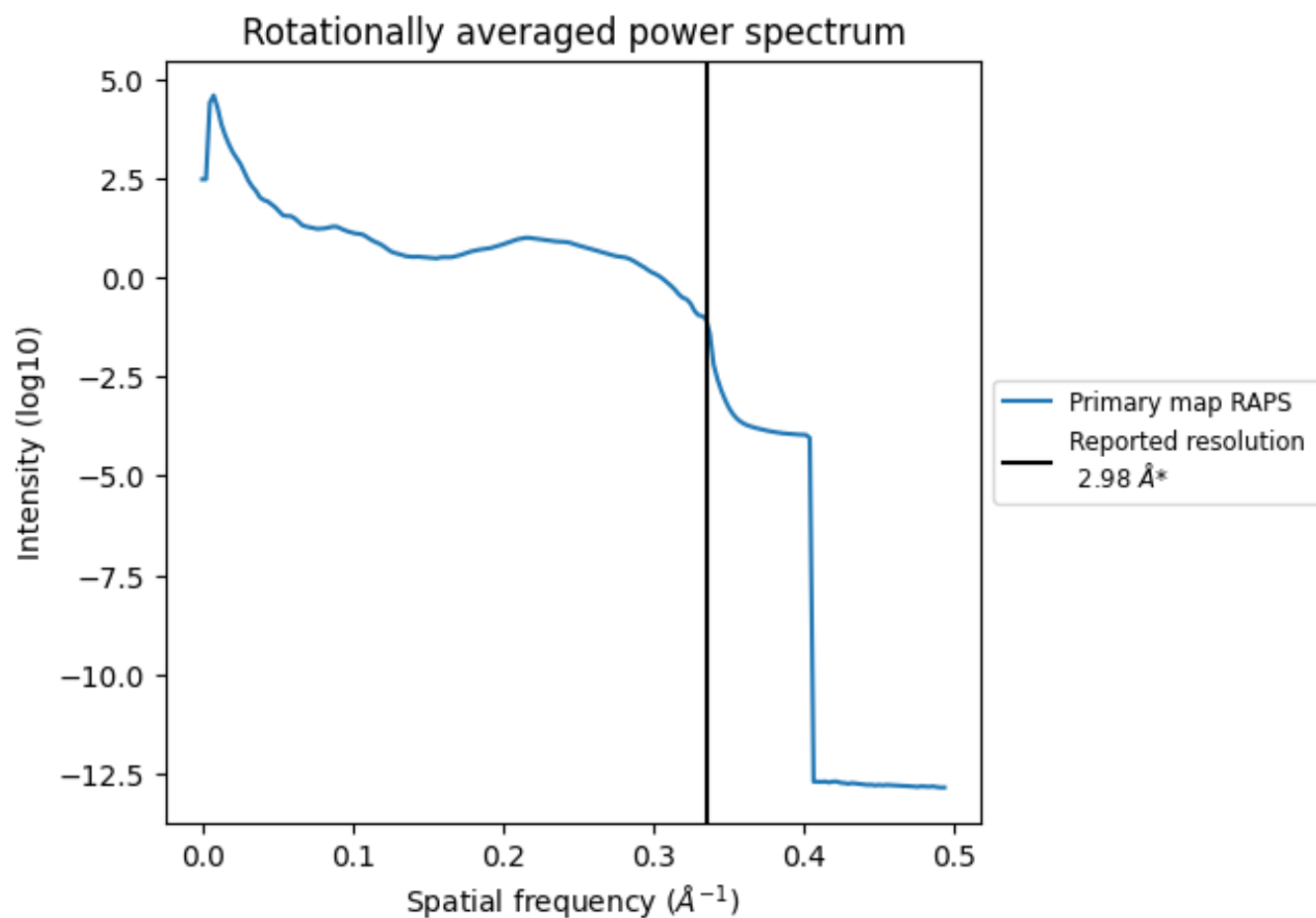


The volume at the recommended contour level is 279  $\text{nm}^3$ ; this corresponds to an approximate mass of 252 kDa.

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 0.336 Å<sup>-1</sup>

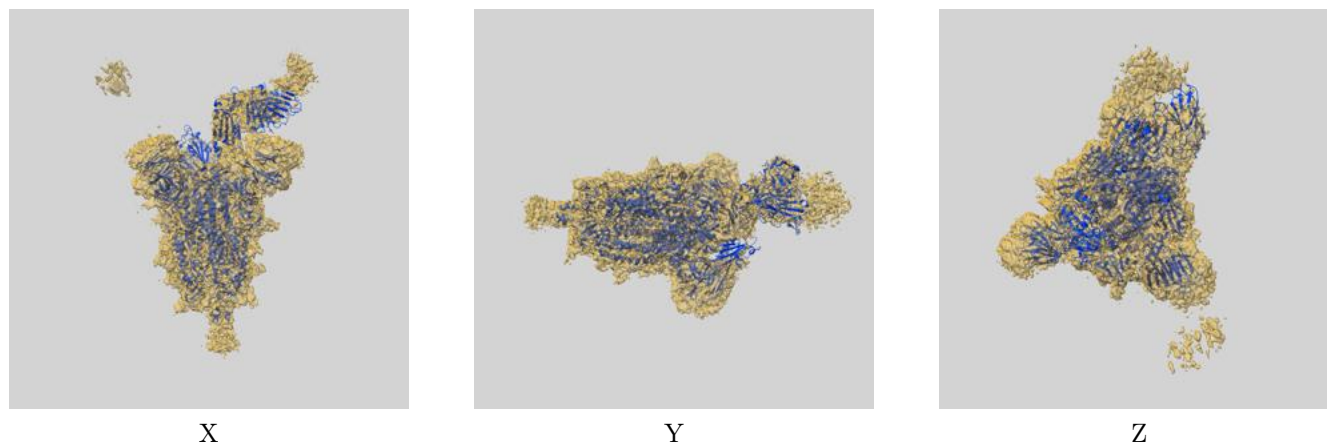
## 8 Fourier-Shell correlation ⓘ

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

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

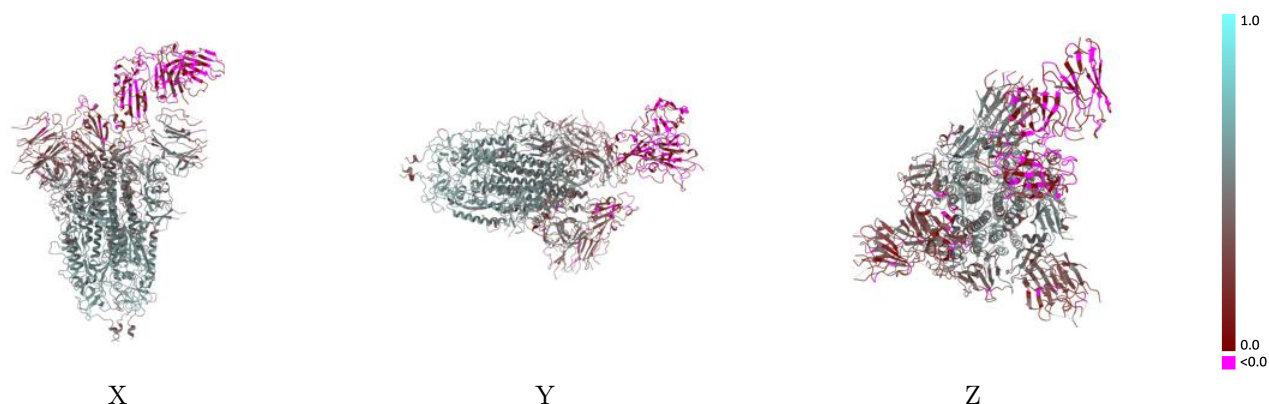
This section contains information regarding the fit between EMDB map EMD-32595 and PDB model 7WLZ. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



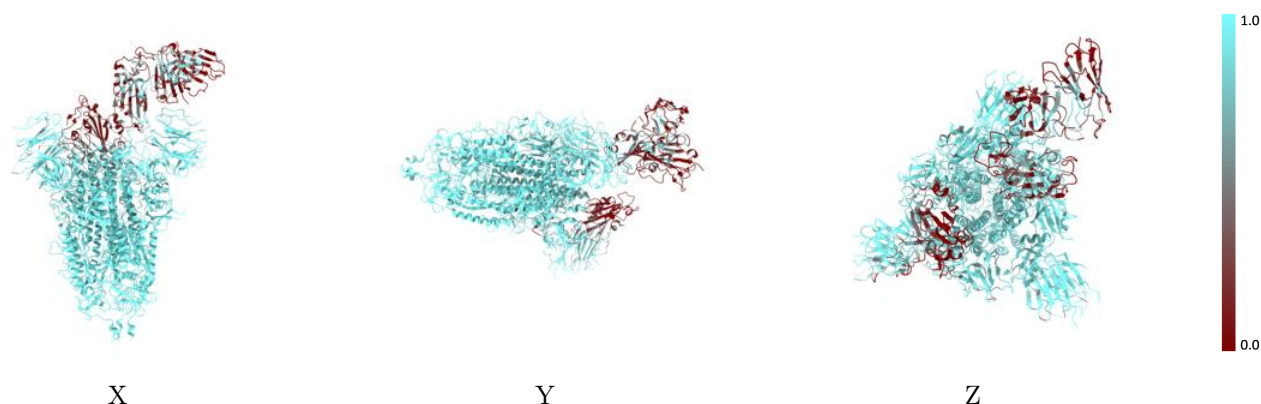
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



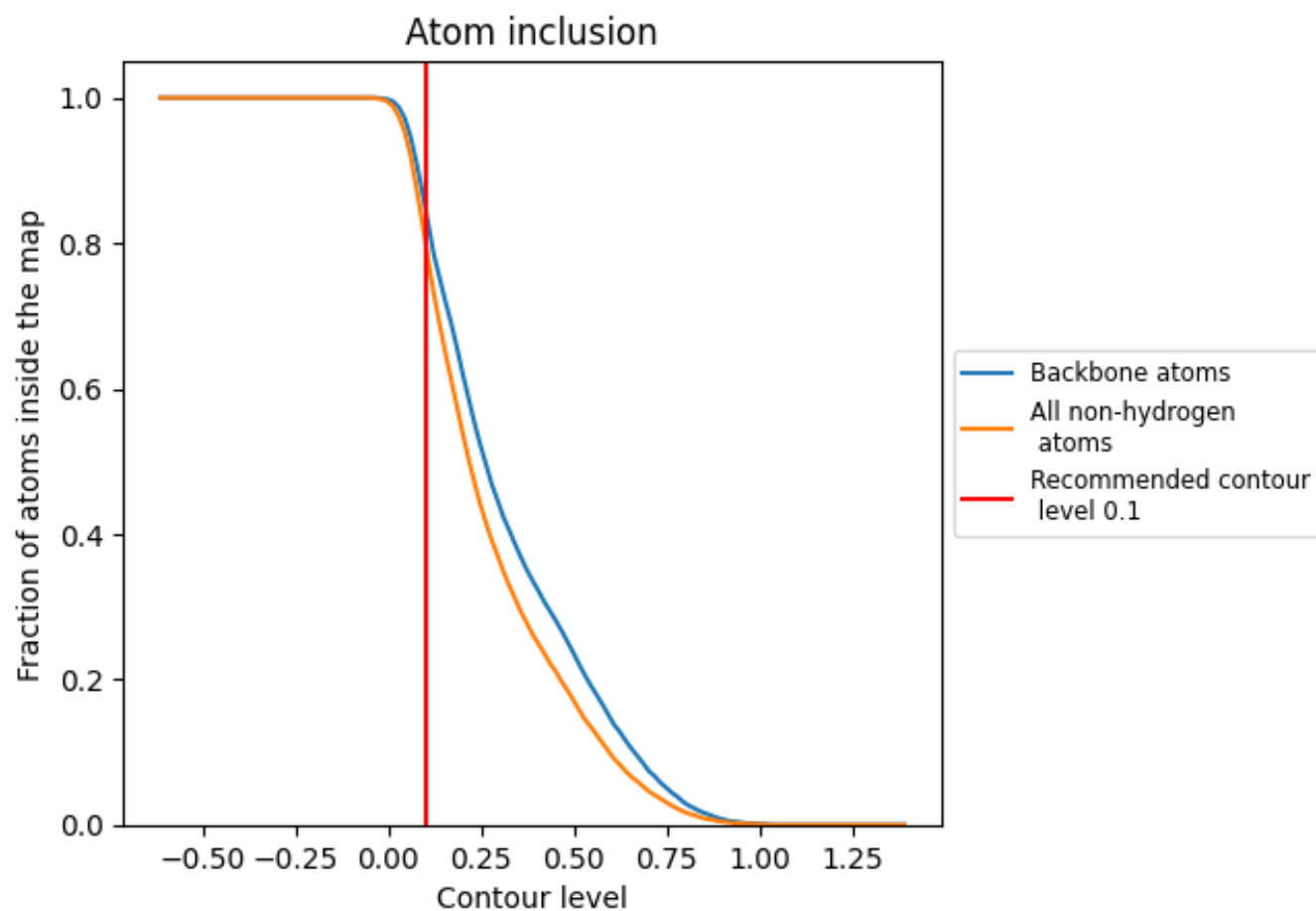
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8040	<div></div> 0.3950
A	<div></div> 0.8080	<div></div> 0.4400
B	<div></div> 0.8300	<div></div> 0.3850
C	<div></div> 0.8950	<div></div> 0.4410
O	<div></div> 0.3200	<div></div> 0.0500
P	<div></div> 0.3140	<div></div> 0.0570

