Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 05:44 AM JST

PDB ID	:	7FJO
EMDB ID	:	EMD-31625
Title	:	Cryo-EM structure of South African (B.1.351) SARS-CoV-2 spike glycoprotein in complex with three T6 Fab
Authors	:	Wang, X.; Zhang, L.; Zhang, S.; Liang, Q.
Deposited on	:	2021-08-04
Resolution	:	3.34 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:

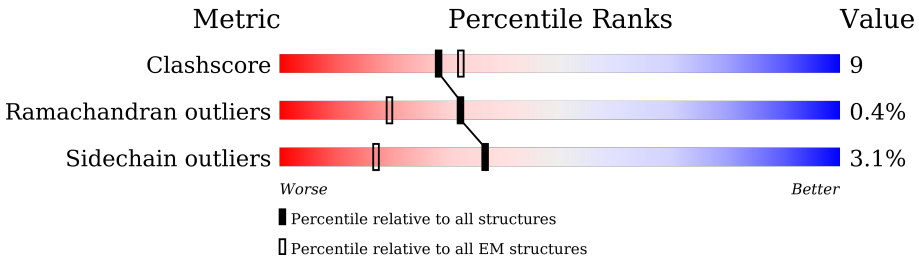
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.34 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 >=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 <=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	F	216	47% 31% 17% • 50%
1	H	216	41% 32% 16% • 50%
1	J	216	21% 32% 16% • 50%
2	G	220	37% 33% 16% • 49%
2	K	220	17% 34% 15% • 49%
2	L	220	38% 34% 15% • 49%
3	A	1280	15% 72% 6% 22%
3	B	1280	8% 72% 5% 22%

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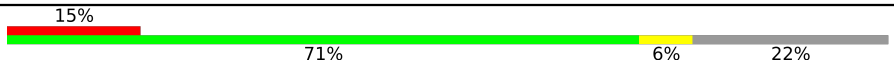
Mol	Chain	Length	Quality of chain
3	C	1280	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28547 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 T6 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			823	517	132	170	4		
1	H	107	Total	C	N	O	S	0	0
			823	517	132	170	4		
1	J	107	Total	C	N	O	S	0	0
			823	517	132	170	4		

- Molecule 2 is a protein called T6 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	113	Total	C	N	O	S	0	0
			886	564	146	174	2		
2	K	113	Total	C	N	O	S	0	0
			886	564	146	174	2		
2	L	113	Total	C	N	O	S	0	0
			886	564	146	174	2		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	994	Total	C	N	O	S	0	0
			7696	4924	1278	1459	35		
3	B	994	Total	C	N	O	S	0	0
			7696	4924	1278	1459	35		
3	C	992	Total	C	N	O	S	0	0
			7678	4916	1279	1448	35		

There are 321 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	305	THR	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	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	701	VAL	ALA	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
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	SER	-	expression tag	UNP P0DTC2
A	1291	ASP	-	expression tag	UNP P0DTC2
A	1292	TYR	-	expression tag	UNP P0DTC2
A	1293	LYS	-	expression tag	UNP P0DTC2
A	1294	ASP	-	expression tag	UNP P0DTC2
A	1295	ASP	-	expression tag	UNP P0DTC2
A	1296	ASP	-	expression tag	UNP P0DTC2
A	1297	ASP	-	expression tag	UNP P0DTC2
A	1298	LYS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	305	THR	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	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	701	VAL	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	SER	-	expression tag	UNP P0DTC2
B	1291	ASP	-	expression tag	UNP P0DTC2
B	1292	TYR	-	expression tag	UNP P0DTC2
B	1293	LYS	-	expression tag	UNP P0DTC2
B	1294	ASP	-	expression tag	UNP P0DTC2
B	1295	ASP	-	expression tag	UNP P0DTC2
B	1296	ASP	-	expression tag	UNP P0DTC2
B	1297	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1298	LYS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	305	THR	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	614	GLY	ASP	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	701	VAL	ALA	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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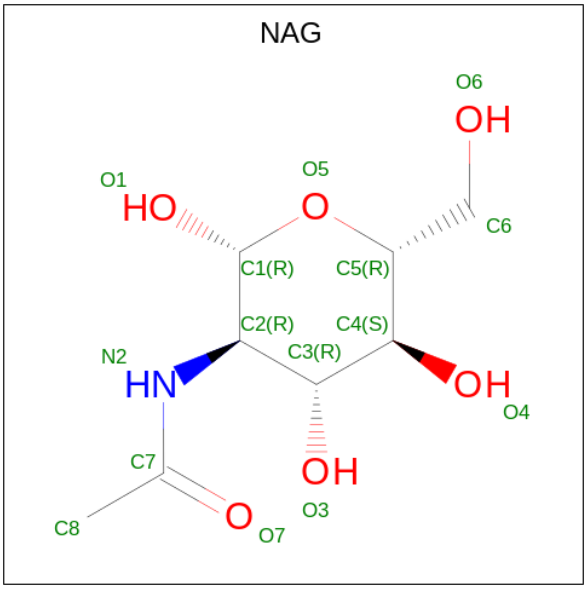
Chain	Residue	Modelled	Actual	Comment	Reference
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	SER	-	expression tag	UNP P0DTC2
C	1291	ASP	-	expression tag	UNP P0DTC2
C	1292	TYR	-	expression tag	UNP P0DTC2
C	1293	LYS	-	expression tag	UNP P0DTC2
C	1294	ASP	-	expression tag	UNP P0DTC2
C	1295	ASP	-	expression tag	UNP P0DTC2
C	1296	ASP	-	expression tag	UNP P0DTC2
C	1297	ASP	-	expression tag	UNP P0DTC2
C	1298	LYS	-	expression tag	UNP P0DTC2

- Molecule 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	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	
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	

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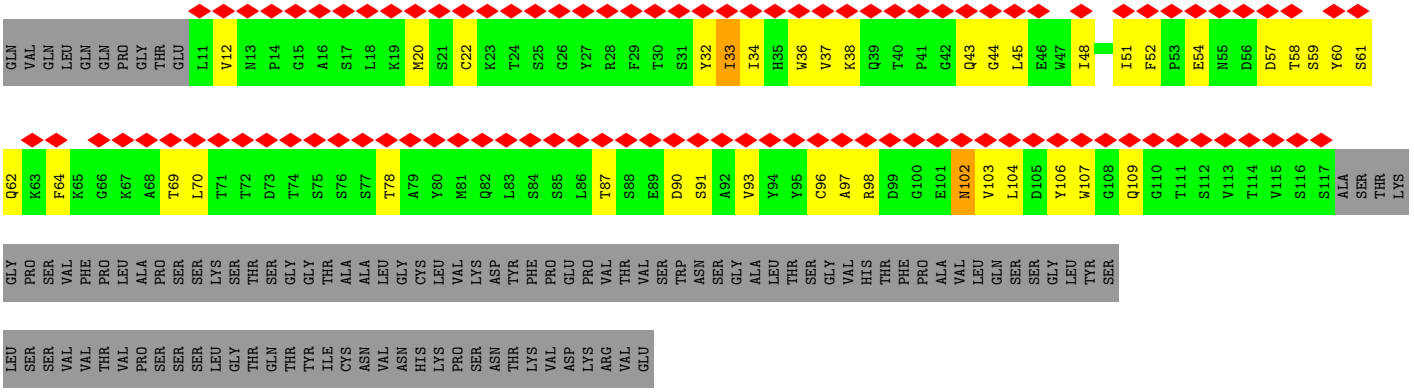
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

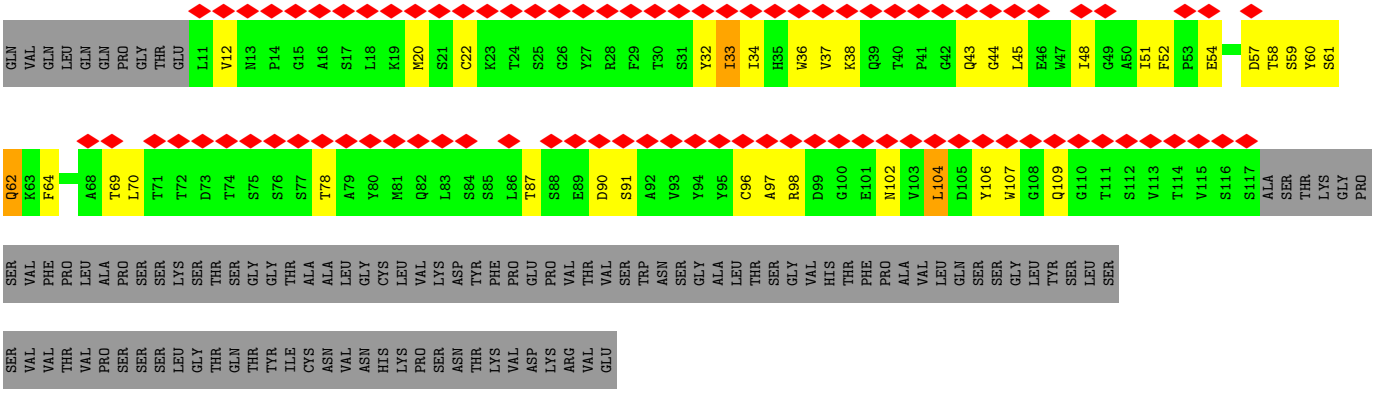
• Molecule 1: T6 heavy chain

Chain F:



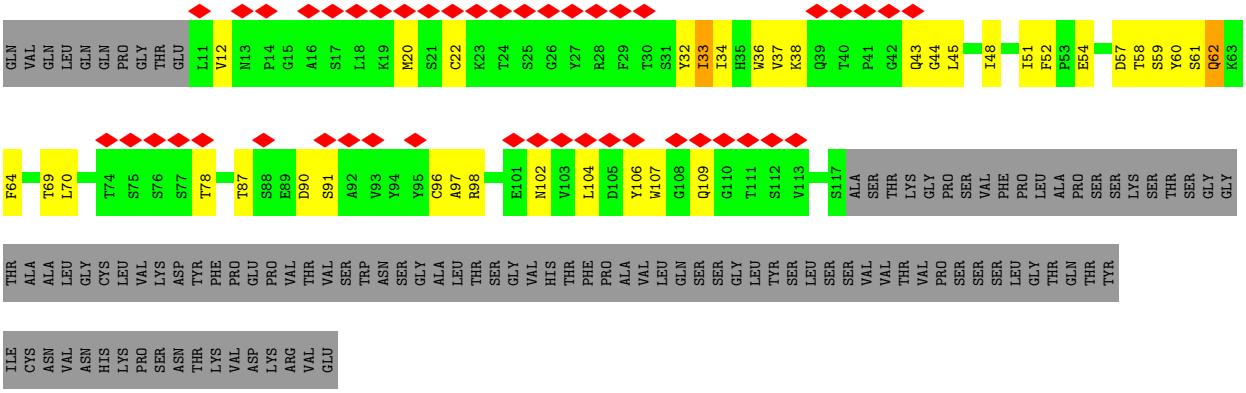
• Molecule 1: T6 heavy chain

Chain H:



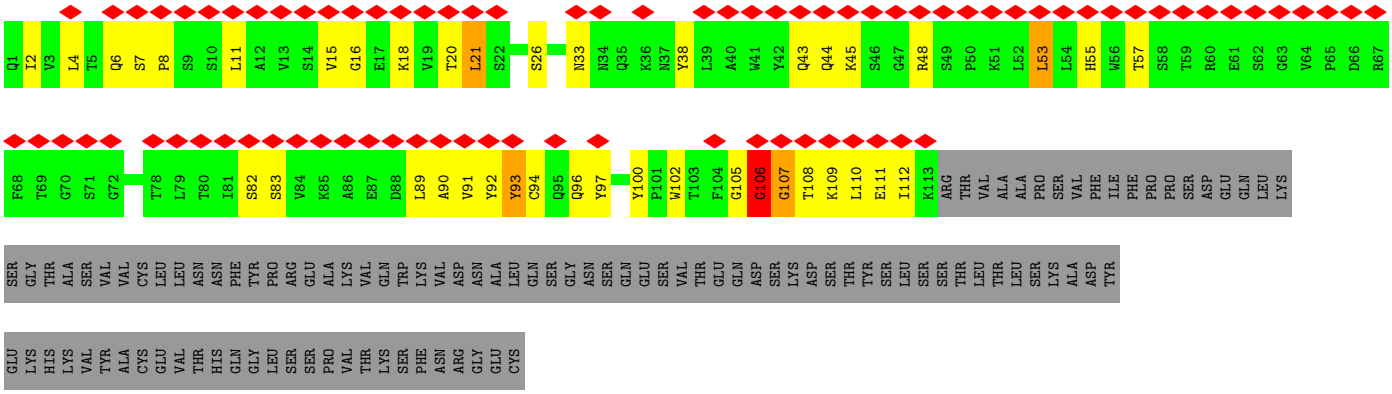
• Molecule 1: T6 heavy chain

Chain J:



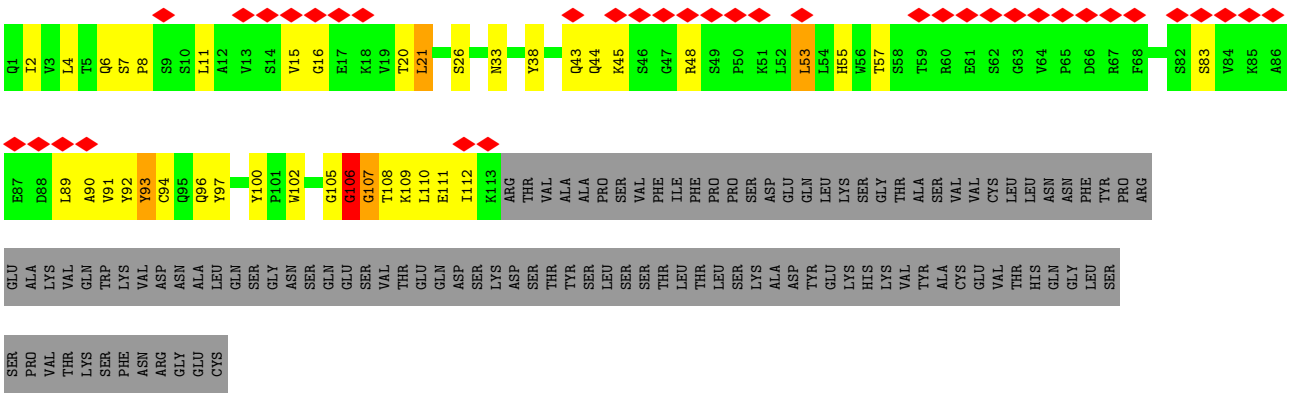
• Molecule 2: T6 light chain

Chain G:



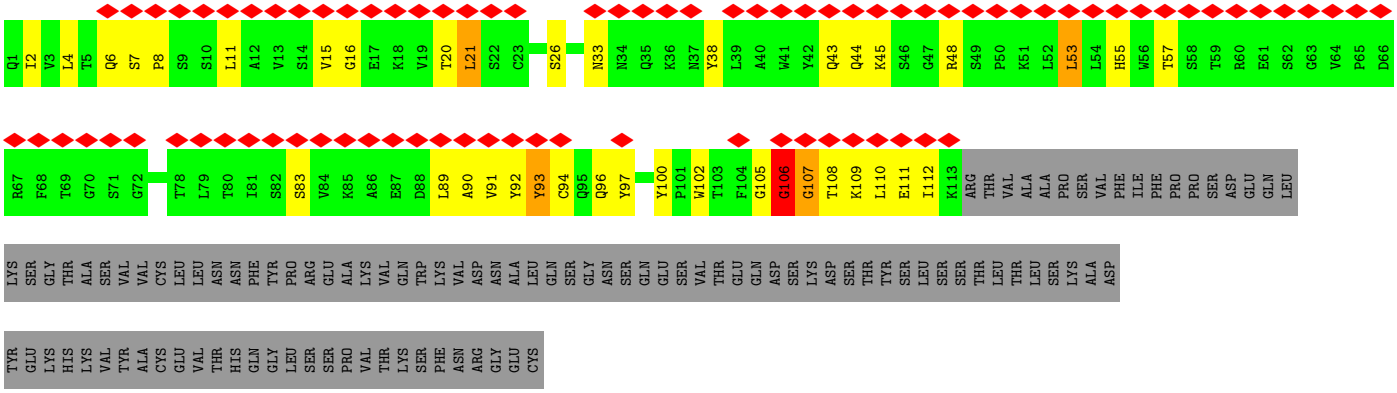
• Molecule 2: T6 light chain

Chain K:



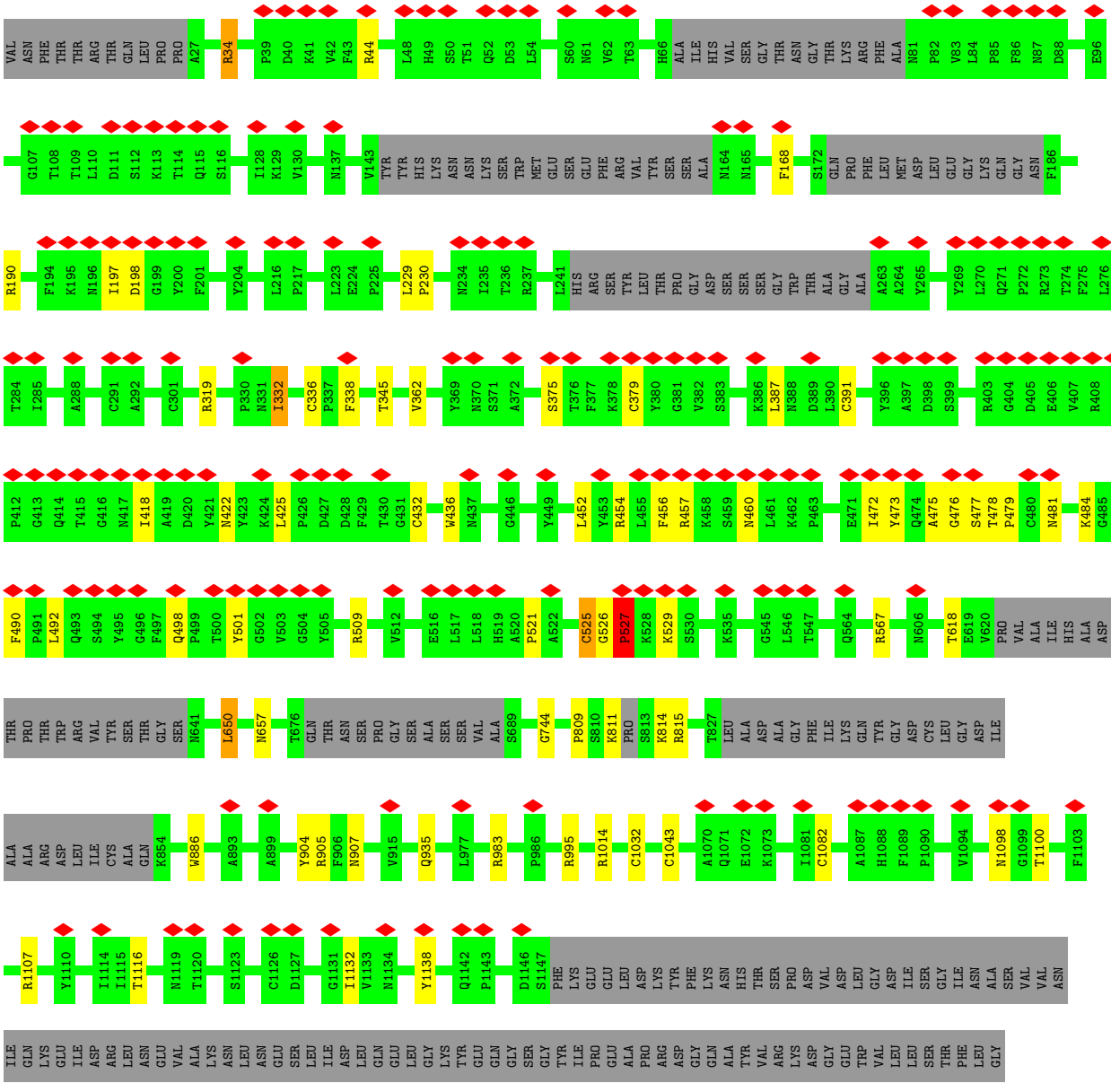
• Molecule 2: T6 light chain

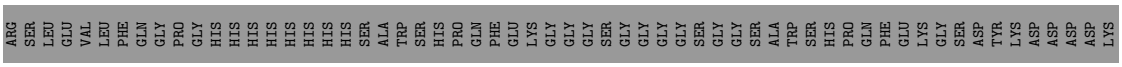
Chain L:



• Molecule 3: Spike glycoprotein

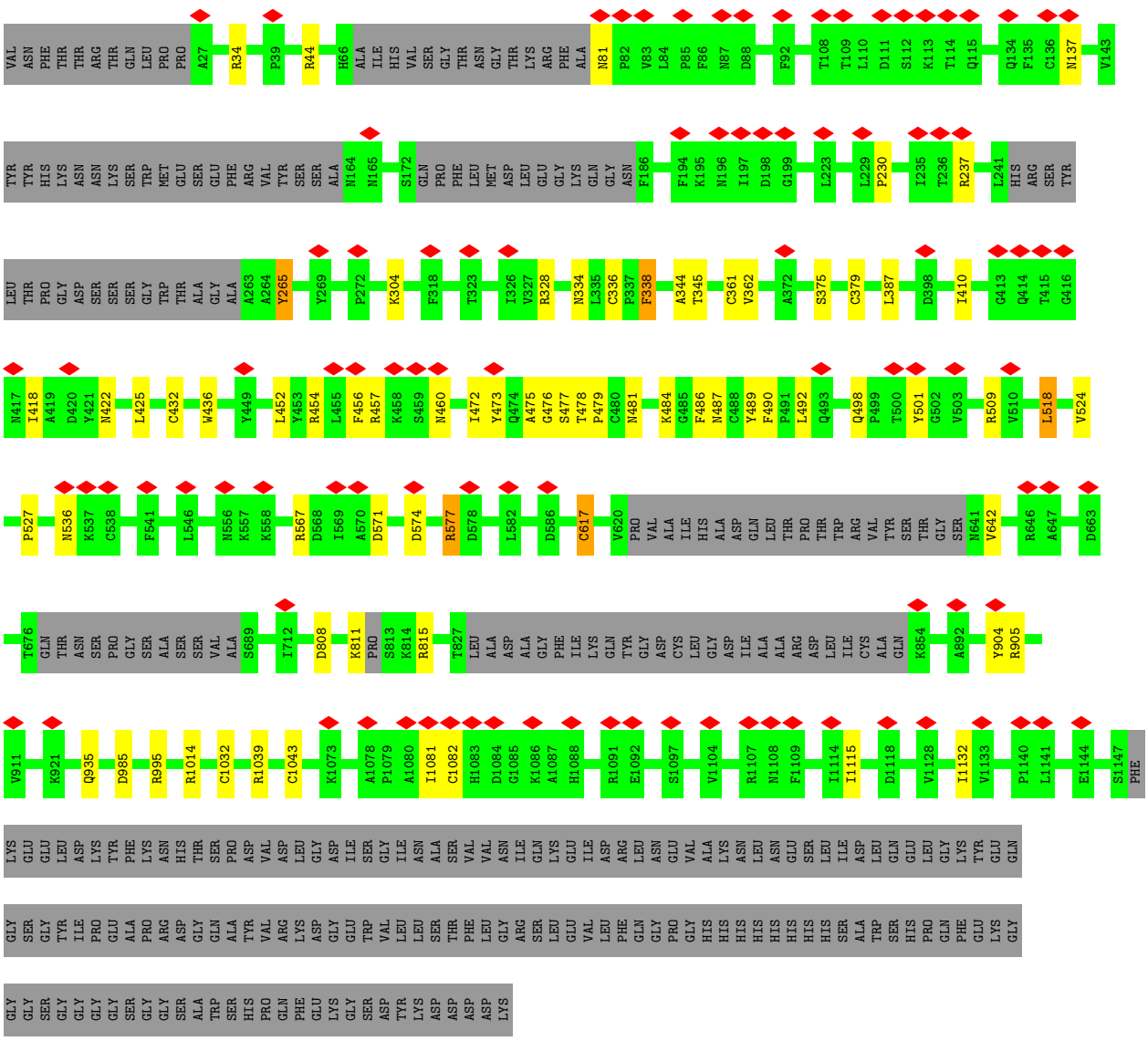
Chain A:





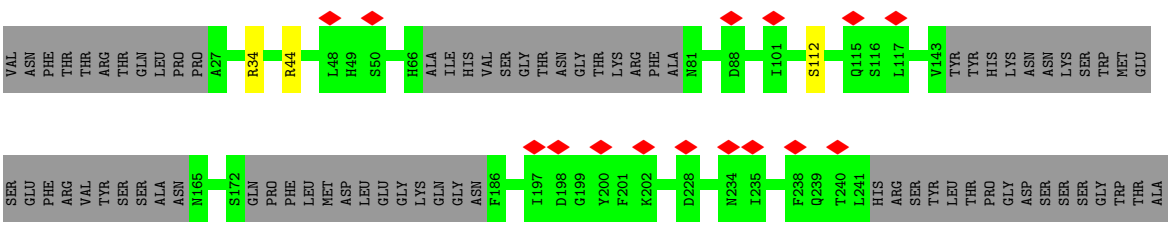
• Molecule 3: Spike glycoprotein

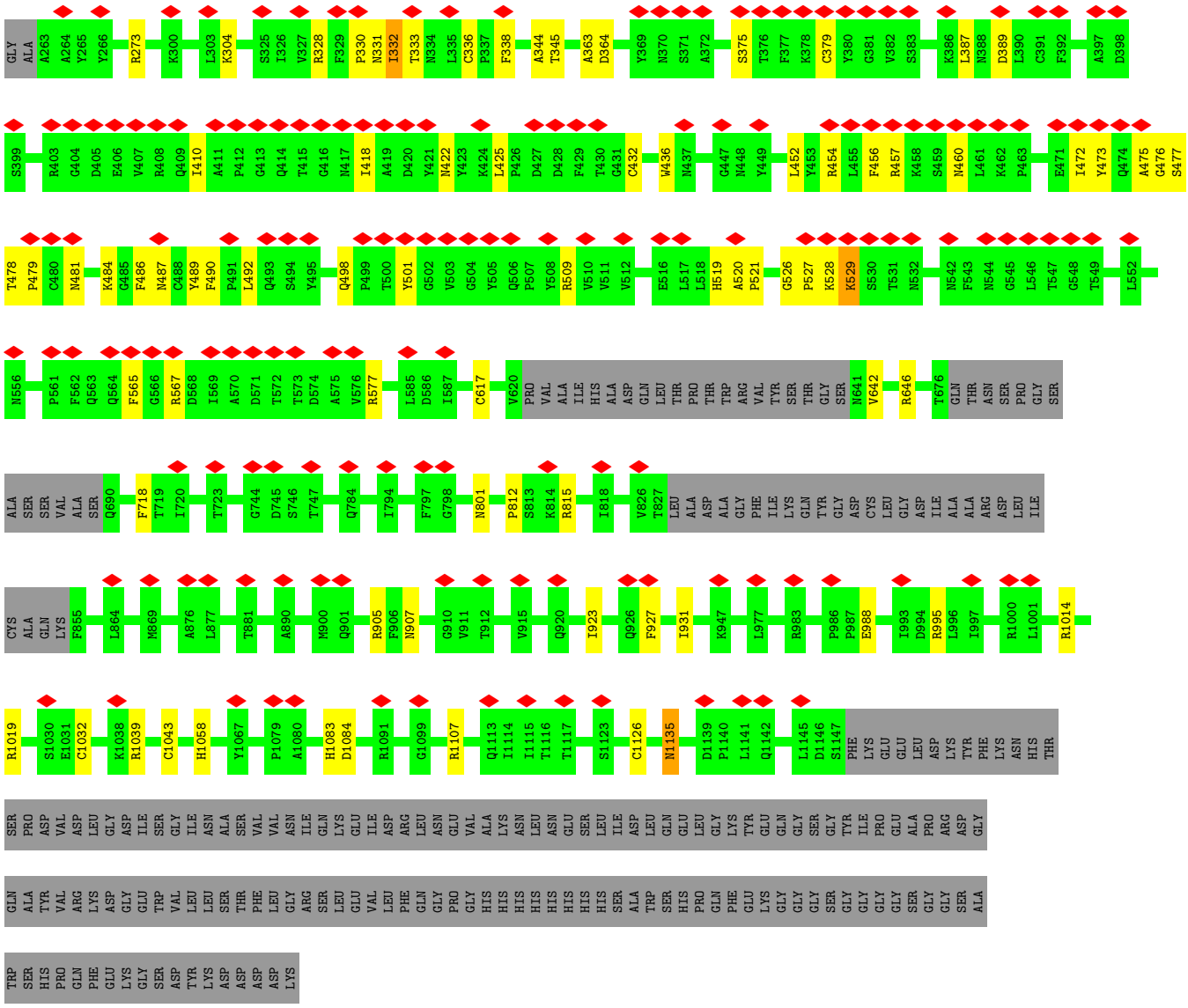
Chain B:



• Molecule 3: Spike glycoprotein

Chain C:




GLY ALA A263 A264 Y265 Y266 R273 K300 L303 K304 S325 I326 V327 R328 F329 P330 N331 I332 T333 N334 L335 C336 P337 F338 A344 T345 A363 D364 Y369 N370 S371 A372 S375 T376 F377 K378 C379 Y380 G381 V382 S383 K386 L387 N388 D389 L390 C391 F392 A397 D398
S399 R403 G404 D405 E406 V407 R408 Q409 I410 A411 P412 G413 Q414 T415 G416 N417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 W436 N437 G447 N448 Y449 L452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 P463 E471 I472 Y473 Q474 A475 G476 S477
T478 P479 C480 N481 K484 G485 F486 N487 C488 Y489 F490 P491 L492 Q493 S494 Y495 Q498 P499 T500 Y501 G502 V503 G504 Y505 Q506 P507 Y508 R509 V510 V511 V512 E516 L517 L518 H519 A520 P521 G526 P527 K528 K529 S530 T531 N532 N542 F543 N544 G545 L546 T547 G548 T549 L552
N556 P561 F562 Q563 Q564 F565 G566 R567 D568 I569 A570 D571 T572 T573 D574 A575 V576 R577 L585 D586 I587 C617 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER N641 V642 R646 T676 GLN THR ASN SER PRO GLY SER
ALA SER SER VAL ALA SER Q690 F718 T719 I720 T723 G744 D745 S746 T747 Q784 I794 F797 G798 N801 P812 S813 K814 R815 I818 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ARG ASP LEU ILE
CYS ALA GLN LYS F855 L864 M869 A876 L877 T881 A890 M900 Q901 R905 F906 N907 G910 V911 T912 V915 Q920 I923 Q926 F927 I931 K947 L977 R983 P986 P987 E988 I993 D994 R995 L996 I997 R1000 L1001 R1014
R1019 S1030 E1031 C1032 K1038 R1039 C1043 H1058 Y1067 P1079 A1080 H1083 D1084 R1091 G1099 R1107 Q1113 I1114 I1115 T1116 T1117 S1123 C1126 N1135 D1139 P1140 L1141 Q1142 L1145 D1146 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR
SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY
GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS SER LEU ILE SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA
TRP SER HIS PRO GLN PHE GLU LYS GLY SER ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	258463	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0083	Depositor
Map size (Å)	351.328, 351.328, 351.328	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

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	F	0.66	0/842	0.65	0/1144
1	H	0.66	0/842	0.65	0/1144
1	J	0.66	0/842	0.65	0/1144
2	G	0.70	1/907 (0.1%)	0.65	0/1231
2	K	0.70	1/907 (0.1%)	0.65	0/1231
2	L	0.70	1/907 (0.1%)	0.65	0/1231
3	A	0.58	0/7869	0.82	14/10713 (0.1%)
3	B	0.59	0/7869	0.84	13/10713 (0.1%)
3	C	0.57	0/7853	0.83	14/10696 (0.1%)
All	All	0.60	3/28838 (0.0%)	0.80	41/39247 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
2	K	0	1
2	L	0	1
3	A	0	1
3	B	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	106	GLY	CA-C	7.08	1.63	1.51
2	L	106	GLY	CA-C	7.04	1.63	1.51
2	G	106	GLY	CA-C	7.03	1.63	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	273	ARG	NE-CZ-NH1	8.42	124.51	120.30
3	B	904	TYR	CB-CG-CD2	-8.19	116.09	121.00
3	C	1014	ARG	NE-CZ-NH1	7.79	124.19	120.30
3	B	1014	ARG	NE-CZ-NH1	7.69	124.14	120.30
3	B	34	ARG	NE-CZ-NH1	7.66	124.13	120.30
3	C	577	ARG	NE-CZ-NH1	7.58	124.09	120.30
3	A	904	TYR	CB-CG-CD2	-7.20	116.68	121.00
3	C	328	ARG	NE-CZ-NH1	7.03	123.81	120.30
3	A	1014	ARG	NE-CZ-NH1	7.00	123.80	120.30
3	C	1107	ARG	NE-CZ-NH1	6.87	123.73	120.30
3	B	905	ARG	NE-CZ-NH1	6.78	123.69	120.30
3	C	905	ARG	NE-CZ-NH1	6.77	123.68	120.30
3	C	815	ARG	NE-CZ-NH1	6.67	123.64	120.30
3	B	577	ARG	NE-CZ-NH1	6.44	123.52	120.30
3	C	995	ARG	NE-CZ-NH1	6.38	123.49	120.30
3	B	995	ARG	NE-CZ-NH1	6.13	123.36	120.30
3	A	319	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	B	815	ARG	NE-CZ-NH1	6.11	123.35	120.30
3	C	567	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	C	34	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	A	525	CYS	C-N-CA	-6.06	109.58	122.30
3	B	567	ARG	NE-CZ-NH1	6.06	123.33	120.30
3	A	905	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	A	567	ARG	NE-CZ-NH1	5.77	123.18	120.30
3	B	237	ARG	NE-CZ-NH1	5.75	123.17	120.30
3	B	1039	ARG	NE-CZ-NH1	5.72	123.16	120.30
3	C	44	ARG	NE-CZ-NH1	5.67	123.13	120.30
3	C	646	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	A	527	PRO	CA-N-CD	-5.66	103.58	111.50
3	A	815	ARG	NE-CZ-NH1	5.64	123.12	120.30
3	B	1039	ARG	NE-CZ-NH2	-5.49	117.55	120.30
3	C	1039	ARG	NE-CZ-NH2	-5.39	117.61	120.30
3	A	995	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	B	44	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	A	34	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	C	1019	ARG	NE-CZ-NH2	5.28	122.94	120.30
3	A	1107	ARG	NE-CZ-NH1	5.23	122.91	120.30
3	A	190	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	A	44	ARG	NE-CZ-NH1	5.09	122.85	120.30
3	A	983	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	B	328	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	34	ARG	Sidechain
3	B	577	ARG	Sidechain
2	G	106	GLY	Mainchain
2	K	106	GLY	Mainchain
2	L	106	GLY	Mainchain

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	F	823	0	779	53	0
1	H	823	0	779	54	0
1	J	823	0	779	52	0
2	G	886	0	872	55	0
2	K	886	0	872	56	0
2	L	886	0	872	54	0
3	A	7696	0	7484	133	0
3	B	7696	0	7484	115	0
3	C	7678	0	7476	133	0
4	A	112	0	104	0	0
4	B	112	0	104	0	0
4	C	126	0	117	2	0
All	All	28547	0	27722	523	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:GLU:HG2	3:A:456:PHE:CZ	1.22	1.71
1:J:54:GLU:HG2	3:B:456:PHE:CZ	1.22	1.68
1:F:54:GLU:HG2	3:C:456:PHE:CZ	1.22	1.60
3:C:498:GLN:HB2	3:C:501:TYR:CE2	1.50	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:498:GLN:HB2	3:A:501:TYR:CE2	1.50	1.45
3:B:498:GLN:HB2	3:B:501:TYR:CE2	1.50	1.43
3:A:498:GLN:HB2	3:A:501:TYR:CD2	1.55	1.41
3:B:484:LYS:NZ	3:B:490:PHE:CD1	1.89	1.40
3:C:484:LYS:NZ	3:C:490:PHE:CD1	1.89	1.40
3:C:498:GLN:HB2	3:C:501:TYR:CD2	1.55	1.40
3:A:484:LYS:NZ	3:A:490:PHE:CD1	1.89	1.40
3:B:498:GLN:HB2	3:B:501:TYR:CD2	1.55	1.40
3:A:521:PRO:HG3	3:B:230:PRO:CB	1.52	1.36
1:H:33:ILE:CD1	3:A:476:GLY:HA3	1.56	1.35
1:H:54:GLU:CG	3:A:456:PHE:HZ	1.40	1.34
1:J:33:ILE:CD1	3:B:476:GLY:HA3	1.56	1.33
1:J:54:GLU:CG	3:B:456:PHE:CZ	2.10	1.33
3:B:498:GLN:CG	3:B:501:TYR:HE2	1.41	1.33
1:H:54:GLU:CG	3:A:456:PHE:CZ	2.10	1.33
1:F:54:GLU:CG	3:C:456:PHE:HZ	1.40	1.33
1:F:33:ILE:CD1	3:C:476:GLY:HA3	1.56	1.32
1:F:54:GLU:CG	3:C:456:PHE:CZ	2.10	1.32
3:C:498:GLN:CG	3:C:501:TYR:HE2	1.41	1.31
3:A:230:PRO:HB2	3:C:519:HIS:O	1.26	1.31
3:A:498:GLN:CG	3:A:501:TYR:HE2	1.41	1.31
1:J:54:GLU:CG	3:B:456:PHE:HZ	1.40	1.31
3:A:230:PRO:HG2	3:C:520:ALA:CA	1.62	1.29
1:H:32:TYR:CE1	3:A:473:TYR:OH	1.83	1.29
2:K:94:CYS:H	2:K:106:GLY:CA	1.47	1.26
2:G:94:CYS:H	2:G:106:GLY:CA	1.47	1.26
1:J:59:SER:CB	3:B:486:PHE:HE1	1.49	1.25
2:L:94:CYS:H	2:L:106:GLY:CA	1.47	1.25
3:A:521:PRO:CG	3:B:230:PRO:HB2	1.67	1.25
1:H:59:SER:CB	3:A:486:PHE:HE1	1.49	1.25
1:F:59:SER:CB	3:C:486:PHE:HE1	1.49	1.23
3:B:498:GLN:CB	3:B:501:TYR:CE2	2.20	1.23
3:C:498:GLN:CB	3:C:501:TYR:CE2	2.20	1.23
3:A:498:GLN:CB	3:A:501:TYR:CE2	2.20	1.23
1:F:32:TYR:CE1	3:C:473:TYR:OH	1.83	1.22
1:J:32:TYR:CE1	3:B:473:TYR:OH	1.83	1.22
1:J:59:SER:OG	3:B:486:PHE:CE1	1.93	1.21
1:H:59:SER:OG	3:A:486:PHE:CE1	1.93	1.21
1:F:59:SER:CB	3:C:486:PHE:CE1	2.24	1.21
1:J:59:SER:CB	3:B:486:PHE:CE1	2.24	1.20
2:G:100:TYR:CZ	3:C:486:PHE:CE2	2.27	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:SER:OG	3:C:486:PHE:CE1	1.93	1.19
1:H:33:ILE:HD11	3:A:476:GLY:CA	1.73	1.18
1:H:59:SER:CB	3:A:486:PHE:CE1	2.24	1.18
1:F:59:SER:HB2	3:C:486:PHE:CE1	1.79	1.17
2:L:100:TYR:CZ	3:A:486:PHE:CE2	2.27	1.17
3:B:498:GLN:CB	3:B:501:TYR:HE2	1.57	1.17
1:H:59:SER:HB2	3:A:486:PHE:CE1	1.79	1.17
1:J:33:ILE:HD11	3:B:476:GLY:CA	1.72	1.17
1:J:59:SER:HB2	3:B:486:PHE:CE1	1.79	1.17
2:K:100:TYR:CZ	3:B:486:PHE:CE2	2.27	1.17
1:F:33:ILE:HD11	3:C:476:GLY:CA	1.73	1.16
1:F:59:SER:HB2	3:C:486:PHE:HE1	1.08	1.15
2:K:100:TYR:CE1	3:B:486:PHE:HE2	1.65	1.15
3:C:498:GLN:CB	3:C:501:TYR:HE2	1.57	1.15
2:L:100:TYR:CE1	3:A:486:PHE:HE2	1.65	1.14
2:G:100:TYR:CE1	3:C:486:PHE:HE2	1.65	1.13
1:H:57:ASP:OD1	3:A:489:TYR:OH	1.66	1.12
3:A:498:GLN:CB	3:A:501:TYR:HE2	1.57	1.12
3:A:230:PRO:CG	3:C:520:ALA:HA	1.79	1.12
3:A:168:PHE:CE1	3:C:520:ALA:HB1	1.84	1.11
3:A:168:PHE:CD1	3:C:520:ALA:HB1	1.84	1.11
1:F:57:ASP:OD1	3:C:489:TYR:OH	1.66	1.11
1:F:59:SER:OG	3:C:486:PHE:CZ	2.03	1.11
1:J:57:ASP:OD1	3:B:489:TYR:OH	1.66	1.11
2:K:94:CYS:H	2:K:106:GLY:HA2	0.94	1.10
1:J:59:SER:OG	3:B:486:PHE:CZ	2.03	1.10
3:C:498:GLN:CG	3:C:501:TYR:CE2	2.34	1.10
3:A:498:GLN:CG	3:A:501:TYR:CE2	2.34	1.10
1:H:59:SER:OG	3:A:486:PHE:CZ	2.03	1.09
3:B:498:GLN:CG	3:B:501:TYR:CE2	2.34	1.09
2:G:94:CYS:H	2:G:106:GLY:HA2	0.94	1.08
2:K:4:LEU:HB2	2:K:105:GLY:HA3	1.34	1.08
3:C:484:LYS:NZ	3:C:490:PHE:CE1	2.22	1.07
2:L:94:CYS:H	2:L:106:GLY:HA2	0.94	1.07
3:A:168:PHE:HD1	3:C:520:ALA:CB	1.67	1.07
1:H:59:SER:HB2	3:A:486:PHE:HE1	1.08	1.07
1:J:59:SER:HB2	3:B:486:PHE:HE1	1.07	1.06
1:J:52:PHE:CE1	3:B:475:ALA:CB	2.39	1.06
1:F:52:PHE:CE1	3:C:475:ALA:CB	2.39	1.06
2:L:100:TYR:CZ	3:A:486:PHE:HE2	1.46	1.06
3:A:168:PHE:CD1	3:C:520:ALA:CB	2.39	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:498:GLN:CD	3:C:501:TYR:CE2	2.30	1.05
2:G:4:LEU:HB2	2:G:105:GLY:HA3	1.34	1.05
2:G:94:CYS:N	2:G:106:GLY:HA2	1.70	1.05
2:G:93:TYR:CD2	2:G:106:GLY:CA	2.40	1.05
2:K:94:CYS:N	2:K:106:GLY:CA	2.20	1.05
2:L:94:CYS:N	2:L:106:GLY:CA	2.20	1.05
1:H:33:ILE:CG1	3:A:476:GLY:HA3	1.87	1.04
1:H:52:PHE:CE1	3:A:475:ALA:CB	2.39	1.04
2:L:93:TYR:CD2	2:L:106:GLY:CA	2.40	1.04
3:B:498:GLN:CD	3:B:501:TYR:CE2	2.30	1.04
1:J:33:ILE:CG1	3:B:476:GLY:HA3	1.87	1.04
2:K:93:TYR:CD2	2:K:106:GLY:CA	2.40	1.04
2:L:94:CYS:N	2:L:106:GLY:HA2	1.70	1.04
3:A:498:GLN:CD	3:A:501:TYR:CE2	2.30	1.04
2:K:94:CYS:N	2:K:106:GLY:HA2	1.70	1.04
1:F:33:ILE:CG1	3:C:476:GLY:HA3	1.87	1.03
3:B:484:LYS:NZ	3:B:490:PHE:CE1	2.21	1.03
2:L:4:LEU:HB2	2:L:105:GLY:HA3	1.34	1.02
2:G:94:CYS:N	2:G:106:GLY:CA	2.20	1.02
1:J:52:PHE:HE1	3:B:475:ALA:CB	1.74	1.01
2:G:100:TYR:CZ	3:C:486:PHE:HE2	1.46	1.01
3:A:230:PRO:CB	3:C:519:HIS:O	2.06	1.01
1:H:52:PHE:HE1	3:A:475:ALA:CB	1.74	1.01
1:F:52:PHE:HE1	3:C:475:ALA:CB	1.74	1.00
3:A:168:PHE:HD1	3:C:520:ALA:HB2	1.25	0.99
1:H:33:ILE:HD11	3:A:476:GLY:HA3	1.00	0.99
2:G:102:TRP:HZ2	3:C:477:SER:HG	1.07	0.99
1:F:52:PHE:CE1	3:C:475:ALA:HB2	1.97	0.99
2:G:93:TYR:CG	2:G:106:GLY:HA3	1.97	0.99
1:J:33:ILE:HD11	3:B:476:GLY:HA3	1.00	0.98
1:F:33:ILE:HD11	3:C:476:GLY:HA3	1.00	0.98
1:H:52:PHE:CE1	3:A:475:ALA:HB2	1.97	0.98
2:K:93:TYR:CD2	2:K:106:GLY:HA3	1.98	0.98
2:L:93:TYR:CG	2:L:106:GLY:HA3	1.97	0.98
2:G:93:TYR:CD2	2:G:106:GLY:HA3	1.98	0.98
3:C:498:GLN:OE1	3:C:501:TYR:CE2	2.17	0.98
3:A:498:GLN:OE1	3:A:501:TYR:CE2	2.17	0.97
2:K:93:TYR:CG	2:K:106:GLY:HA3	1.97	0.97
1:J:52:PHE:CE1	3:B:475:ALA:HB2	1.97	0.97
3:B:498:GLN:OE1	3:B:501:TYR:CE2	2.17	0.96
3:A:230:PRO:CG	3:C:520:ALA:CA	2.41	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:GLN:OE1	2:L:106:GLY:HA2	1.65	0.96
3:A:484:LYS:NZ	3:A:490:PHE:CE1	2.21	0.96
2:G:6:GLN:OE1	2:G:106:GLY:HA2	1.65	0.96
2:K:6:GLN:OE1	2:K:106:GLY:HA2	1.65	0.96
2:G:93:TYR:CA	2:G:106:GLY:HA3	1.97	0.94
2:L:93:TYR:CD2	2:L:106:GLY:HA3	1.98	0.94
2:L:93:TYR:CA	2:L:106:GLY:HA3	1.97	0.94
2:K:93:TYR:CA	2:K:106:GLY:HA3	1.97	0.94
2:K:100:TYR:CE1	3:B:486:PHE:CE2	2.53	0.94
2:L:100:TYR:CE1	3:A:486:PHE:CE2	2.53	0.94
1:F:32:TYR:CZ	3:C:473:TYR:OH	2.21	0.94
3:A:168:PHE:CE1	3:C:521:PRO:HD2	2.01	0.94
1:H:32:TYR:CZ	3:A:473:TYR:OH	2.21	0.93
1:J:32:TYR:CZ	3:B:473:TYR:OH	2.21	0.93
3:A:484:LYS:NZ	3:A:490:PHE:HD1	1.48	0.93
3:A:498:GLN:OE1	3:A:501:TYR:CZ	2.23	0.92
1:J:52:PHE:CE1	3:B:475:ALA:HB1	2.04	0.92
1:H:52:PHE:CE1	3:A:475:ALA:HB1	2.04	0.91
3:B:1082:CYS:SG	3:B:1132:ILE:CD1	2.58	0.91
3:B:498:GLN:OE1	3:B:501:TYR:CZ	2.23	0.91
2:K:102:TRP:HZ2	3:B:477:SER:HG	1.07	0.91
2:K:100:TYR:CZ	3:B:486:PHE:HE2	1.46	0.91
3:C:498:GLN:OE1	3:C:501:TYR:CZ	2.23	0.91
2:L:102:TRP:HZ2	3:A:477:SER:HG	1.08	0.91
1:F:52:PHE:CE1	3:C:475:ALA:HB1	2.04	0.90
2:G:100:TYR:CE1	3:C:486:PHE:CE2	2.53	0.90
2:K:93:TYR:CB	2:K:106:GLY:HA3	2.02	0.90
2:L:93:TYR:CB	2:L:106:GLY:HA3	2.02	0.89
3:A:230:PRO:CG	3:C:520:ALA:C	2.36	0.89
3:C:498:GLN:HB2	3:C:501:TYR:HD2	1.37	0.89
2:G:93:TYR:CB	2:G:106:GLY:HA3	2.02	0.89
3:B:498:GLN:CD	3:B:501:TYR:HE2	1.72	0.89
3:C:484:LYS:HZ3	3:C:490:PHE:HD1	0.90	0.89
3:B:498:GLN:HB2	3:B:501:TYR:HD2	1.37	0.88
3:C:498:GLN:CD	3:C:501:TYR:HE2	1.72	0.87
3:A:498:GLN:CD	3:A:501:TYR:HE2	1.72	0.87
3:A:498:GLN:CB	3:A:501:TYR:CD2	2.52	0.87
3:B:484:LYS:NZ	3:B:490:PHE:HD1	1.48	0.87
3:B:1082:CYS:SG	3:B:1132:ILE:HD13	2.16	0.86
2:K:6:GLN:OE1	2:K:106:GLY:CA	2.24	0.85
2:L:6:GLN:OE1	2:L:106:GLY:CA	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:GLN:OE1	2:G:106:GLY:CA	2.24	0.84
3:B:484:LYS:HZ3	3:B:490:PHE:HD1	1.00	0.84
3:A:230:PRO:HG2	3:C:520:ALA:HA	0.84	0.84
1:F:33:ILE:HD11	3:C:477:SER:N	1.93	0.83
3:A:498:GLN:CD	3:A:501:TYR:OH	2.17	0.83
3:C:498:GLN:CD	3:C:501:TYR:OH	2.17	0.83
1:H:33:ILE:HD11	3:A:477:SER:N	1.93	0.83
3:B:1082:CYS:SG	3:B:1132:ILE:HD11	2.18	0.83
2:K:93:TYR:HA	2:K:106:GLY:CA	2.09	0.82
3:B:498:GLN:CD	3:B:501:TYR:OH	2.17	0.82
2:L:93:TYR:HA	2:L:106:GLY:CA	2.09	0.82
3:B:484:LYS:CE	3:B:490:PHE:HD1	1.93	0.82
3:C:498:GLN:CB	3:C:501:TYR:CD2	2.51	0.82
3:A:484:LYS:CE	3:A:490:PHE:HD1	1.92	0.82
3:B:617:CYS:SG	3:B:642:VAL:HG11	2.18	0.82
2:K:16:GLY:HA2	2:K:83:SER:HA	1.62	0.82
2:G:93:TYR:HA	2:G:106:GLY:CA	2.09	0.82
3:A:498:GLN:CD	3:A:501:TYR:CZ	2.53	0.81
1:J:33:ILE:HD11	3:B:477:SER:N	1.93	0.81
3:B:498:GLN:CB	3:B:501:TYR:CD2	2.52	0.81
3:A:484:LYS:HZ1	3:A:490:PHE:HE1	1.24	0.80
3:C:498:GLN:CD	3:C:501:TYR:CZ	2.53	0.80
3:B:498:GLN:CD	3:B:501:TYR:CZ	2.54	0.80
3:C:484:LYS:CE	3:C:490:PHE:HD1	1.93	0.80
2:G:16:GLY:HA2	2:G:83:SER:HA	1.62	0.80
3:C:472:ILE:CD1	3:C:484:LYS:HE2	2.12	0.80
2:L:16:GLY:HA2	2:L:83:SER:HA	1.62	0.80
3:B:472:ILE:HD12	3:B:484:LYS:HE2	1.64	0.79
3:A:472:ILE:HD12	3:A:484:LYS:HE2	1.65	0.79
3:B:472:ILE:CD1	3:B:484:LYS:HE2	2.12	0.79
3:A:472:ILE:CD1	3:A:484:LYS:HE2	2.12	0.79
1:F:98:ARG:HB2	1:F:106:TYR:HB3	1.65	0.79
3:C:484:LYS:NZ	3:C:490:PHE:HD1	1.49	0.79
1:H:54:GLU:HG2	3:A:456:PHE:CE1	2.13	0.79
2:G:93:TYR:CG	2:G:106:GLY:CA	2.64	0.78
1:J:98:ARG:HB2	1:J:106:TYR:HB3	1.65	0.78
2:K:93:TYR:CG	2:K:106:GLY:CA	2.64	0.78
1:F:33:ILE:HD11	3:C:477:SER:H	1.48	0.78
1:H:59:SER:CB	3:A:486:PHE:CZ	2.66	0.78
2:L:100:TYR:CD1	3:A:486:PHE:CE2	2.63	0.78
3:A:498:GLN:HB2	3:A:501:TYR:HD2	1.37	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:330:PRO:HB2	3:C:527:PRO:HD2	1.64	0.78
3:C:472:ILE:HD12	3:C:484:LYS:HE2	1.65	0.77
1:J:52:PHE:HE1	3:B:475:ALA:HB2	1.38	0.77
1:H:33:ILE:HD11	3:A:477:SER:H	1.48	0.77
1:H:98:ARG:HB2	1:H:106:TYR:HB3	1.65	0.77
1:J:33:ILE:HD11	3:B:477:SER:H	1.48	0.77
2:G:93:TYR:CA	2:G:106:GLY:CA	2.63	0.77
2:L:93:TYR:CG	2:L:106:GLY:CA	2.64	0.76
1:F:54:GLU:HG2	3:C:456:PHE:CE1	2.13	0.76
2:L:93:TYR:CA	2:L:106:GLY:CA	2.63	0.75
2:K:93:TYR:CA	2:K:106:GLY:CA	2.63	0.75
1:F:59:SER:CB	3:C:486:PHE:CZ	2.66	0.75
3:A:521:PRO:HG3	3:B:230:PRO:CG	2.16	0.75
3:A:168:PHE:HE1	3:C:520:ALA:HB1	1.48	0.75
1:F:52:PHE:HE1	3:C:475:ALA:HB1	1.47	0.74
1:F:52:PHE:HE1	3:C:475:ALA:HB2	1.38	0.74
1:H:52:PHE:HE1	3:A:475:ALA:HB1	1.47	0.73
3:A:1082:CYS:SG	3:A:1132:ILE:CD1	2.76	0.73
2:K:38:TYR:HB3	2:K:97:TYR:HB3	1.71	0.73
1:J:54:GLU:HG2	3:B:456:PHE:CE1	2.13	0.73
2:L:38:TYR:HB3	2:L:97:TYR:HB3	1.71	0.72
3:A:498:GLN:NE2	3:A:501:TYR:OH	2.23	0.72
1:F:32:TYR:CD1	3:C:473:TYR:OH	2.36	0.72
2:L:6:GLN:OE1	2:L:106:GLY:C	2.28	0.72
2:G:6:GLN:OE1	2:G:106:GLY:C	2.28	0.72
3:C:498:GLN:NE2	3:C:501:TYR:OH	2.23	0.72
1:J:33:ILE:HD11	3:B:476:GLY:C	2.10	0.71
1:H:33:ILE:HD11	3:A:476:GLY:C	2.10	0.71
2:L:93:TYR:CD2	2:L:106:GLY:C	2.63	0.71
3:C:389:ASP:HB2	3:C:527:PRO:HA	1.72	0.71
2:G:38:TYR:HB3	2:G:97:TYR:HB3	1.71	0.71
2:K:93:TYR:CD2	2:K:106:GLY:C	2.63	0.71
2:K:6:GLN:OE1	2:K:106:GLY:C	2.28	0.71
2:G:93:TYR:CD2	2:G:106:GLY:C	2.63	0.71
2:K:93:TYR:CD2	2:K:106:GLY:N	2.59	0.71
3:B:484:LYS:HZ1	3:B:490:PHE:HE1	1.29	0.71
1:J:52:PHE:CD1	3:B:475:ALA:HB1	2.26	0.71
3:B:498:GLN:NE2	3:B:501:TYR:OH	2.23	0.71
1:F:33:ILE:HD11	3:C:476:GLY:C	2.10	0.70
2:G:93:TYR:CD2	2:G:106:GLY:N	2.59	0.70
2:G:100:TYR:CD1	3:C:486:PHE:CE2	2.63	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:100:TYR:CD1	3:B:486:PHE:CE2	2.63	0.70
1:F:52:PHE:CD1	3:C:475:ALA:HB1	2.26	0.70
2:K:33:ASN:ND2	3:B:481:ASN:HD22	1.90	0.69
2:L:33:ASN:ND2	3:A:481:ASN:HD22	1.90	0.69
2:L:93:TYR:CD2	2:L:106:GLY:N	2.59	0.69
1:H:52:PHE:CD1	3:A:475:ALA:HB1	2.26	0.69
1:J:59:SER:CB	3:B:486:PHE:CZ	2.66	0.69
2:G:94:CYS:N	2:G:106:GLY:HA3	2.06	0.69
1:H:52:PHE:HE1	3:A:475:ALA:HB2	1.38	0.69
2:K:94:CYS:N	2:K:106:GLY:HA3	2.06	0.69
3:C:389:ASP:CB	3:C:527:PRO:HA	2.24	0.68
2:L:94:CYS:N	2:L:106:GLY:HA3	2.06	0.68
3:A:230:PRO:HG3	3:C:520:ALA:C	1.79	0.68
1:H:33:ILE:HG13	3:A:476:GLY:HA3	1.76	0.68
2:G:33:ASN:ND2	3:C:481:ASN:HD22	1.90	0.68
2:G:6:GLN:OE1	2:G:107:GLY:N	2.27	0.68
1:H:33:ILE:CD1	3:A:477:SER:H	2.07	0.67
1:J:52:PHE:HE1	3:B:475:ALA:HB1	1.47	0.67
2:L:6:GLN:OE1	2:L:107:GLY:N	2.27	0.67
1:J:33:ILE:CD1	3:B:477:SER:H	2.07	0.67
2:K:6:GLN:OE1	2:K:107:GLY:N	2.27	0.67
3:C:484:LYS:HZ1	3:C:490:PHE:HE1	1.39	0.67
1:J:32:TYR:CD1	3:B:473:TYR:OH	2.36	0.67
1:F:33:ILE:CD1	3:C:477:SER:H	2.07	0.67
3:A:521:PRO:HG3	3:B:230:PRO:HB2	0.72	0.67
3:C:498:GLN:HG3	3:C:501:TYR:HE2	1.54	0.67
1:F:33:ILE:HG13	3:C:476:GLY:HA3	1.76	0.66
1:J:36:TRP:HE1	1:J:51:ILE:HD11	1.61	0.66
1:H:36:TRP:HE1	1:H:51:ILE:HD11	1.60	0.66
3:B:617:CYS:SG	3:B:642:VAL:CG1	2.83	0.66
1:H:32:TYR:CD1	3:A:473:TYR:OH	2.36	0.66
1:F:36:TRP:HE1	1:F:51:ILE:HD11	1.61	0.65
1:J:33:ILE:HG13	3:B:476:GLY:HA3	1.76	0.65
3:B:336:CYS:HA	3:B:361:CYS:HB2	1.80	0.64
3:A:498:GLN:HG3	3:A:501:TYR:HE2	1.54	0.64
3:A:168:PHE:HE1	3:C:521:PRO:HD2	1.62	0.64
3:A:521:PRO:CG	3:B:230:PRO:CB	2.47	0.64
3:C:332:ILE:HD13	3:C:363:ALA:O	1.99	0.63
1:F:54:GLU:CB	3:C:456:PHE:CZ	2.82	0.63
1:J:54:GLU:CB	3:B:456:PHE:CZ	2.82	0.63
2:G:89:LEU:HA	2:G:110:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:SER:OG	3:B:486:PHE:HZ	1.79	0.62
2:K:89:LEU:HA	2:K:110:LEU:HD23	1.81	0.62
2:L:89:LEU:HA	2:L:110:LEU:HD23	1.81	0.62
1:F:51:ILE:HG12	1:F:70:LEU:HD13	1.81	0.62
2:K:93:TYR:CG	2:K:106:GLY:C	2.73	0.62
2:L:43:GLN:HB2	2:L:53:LEU:HD23	1.82	0.62
3:B:808:ASP:HB3	3:B:811:LYS:HE2	1.82	0.62
1:F:59:SER:OG	3:C:486:PHE:HZ	1.79	0.62
1:H:51:ILE:HG12	1:H:70:LEU:HD13	1.81	0.61
3:A:472:ILE:HD11	3:A:484:LYS:CE	2.30	0.61
3:B:472:ILE:HD11	3:B:484:LYS:CE	2.30	0.61
2:G:93:TYR:CG	2:G:106:GLY:C	2.73	0.61
1:H:54:GLU:CB	3:A:456:PHE:CZ	2.82	0.61
1:H:59:SER:OG	3:A:486:PHE:HZ	1.79	0.61
3:C:333:THR:H	4:C:1302:NAG:H81	1.65	0.61
2:K:43:GLN:HB2	2:K:53:LEU:HD23	1.82	0.61
1:J:51:ILE:HG12	1:J:70:LEU:HD13	1.81	0.61
2:L:93:TYR:CG	2:L:106:GLY:C	2.73	0.61
2:G:43:GLN:HB2	2:G:53:LEU:HD23	1.82	0.61
3:A:498:GLN:OE1	3:A:501:TYR:OH	2.19	0.61
3:C:472:ILE:HD11	3:C:484:LYS:CE	2.30	0.61
2:G:4:LEU:HD11	2:G:96:GLN:HB3	1.84	0.60
3:C:484:LYS:HE2	3:C:490:PHE:HD1	1.67	0.60
3:A:484:LYS:HE2	3:A:490:PHE:HD1	1.67	0.60
2:G:33:ASN:ND2	3:C:481:ASN:ND2	2.50	0.60
2:K:4:LEU:HD11	2:K:96:GLN:HB3	1.84	0.59
3:B:484:LYS:HE2	3:B:490:PHE:HD1	1.67	0.59
2:L:33:ASN:ND2	3:A:481:ASN:ND2	2.50	0.59
2:L:4:LEU:HD11	2:L:96:GLN:HB3	1.84	0.59
1:F:34:ILE:HA	1:F:98:ARG:HA	1.85	0.59
2:K:33:ASN:ND2	3:B:481:ASN:ND2	2.50	0.59
1:J:34:ILE:HA	1:J:98:ARG:HA	1.85	0.59
3:C:498:GLN:OE1	3:C:501:TYR:OH	2.19	0.58
1:F:33:ILE:CD1	3:C:476:GLY:CA	2.49	0.58
1:H:87:THR:H	1:H:90:ASP:HB2	1.68	0.58
1:H:34:ILE:HA	1:H:98:ARG:HA	1.85	0.58
1:J:87:THR:H	1:J:90:ASP:HB2	1.68	0.58
3:B:498:GLN:OE1	3:B:501:TYR:OH	2.19	0.58
3:B:498:GLN:HG3	3:B:501:TYR:HE2	1.54	0.58
1:F:87:THR:H	1:F:90:ASP:HB2	1.68	0.57
3:A:1082:CYS:SG	3:A:1132:ILE:HD13	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:472:ILE:HD11	3:B:484:LYS:HE2	1.86	0.57
2:G:38:TYR:OH	3:C:479:PRO:HG2	2.05	0.57
2:K:38:TYR:OH	3:B:479:PRO:HG2	2.05	0.57
2:L:38:TYR:OH	3:A:479:PRO:HG2	2.05	0.57
3:A:362:VAL:HG13	3:A:526:GLY:HA2	1.87	0.56
3:B:379:CYS:HA	3:B:432:CYS:HA	1.87	0.56
2:K:93:TYR:HA	2:K:106:GLY:HA3	1.74	0.56
3:B:472:ILE:CD1	3:B:484:LYS:CE	2.83	0.56
3:C:333:THR:N	4:C:1302:NAG:H81	2.20	0.56
3:C:379:CYS:HA	3:C:432:CYS:HA	1.87	0.56
3:C:927:PHE:CZ	3:C:931:ILE:HD11	2.40	0.56
1:F:54:GLU:CD	3:C:456:PHE:CZ	2.78	0.56
3:A:391:CYS:HA	3:A:525:CYS:HA	1.87	0.56
3:A:1082:CYS:SG	3:A:1132:ILE:HD11	2.45	0.56
3:C:472:ILE:CD1	3:C:484:LYS:CE	2.84	0.56
1:J:54:GLU:CD	3:B:456:PHE:CZ	2.78	0.55
3:A:1032:CYS:HG	3:A:1043:CYS:HG	1.55	0.55
1:H:54:GLU:CD	3:A:456:PHE:CZ	2.78	0.55
3:A:379:CYS:HA	3:A:432:CYS:HA	1.87	0.55
3:A:521:PRO:CG	3:B:230:PRO:CG	2.82	0.55
3:A:811:LYS:HG2	3:A:814:LYS:H	1.72	0.55
2:L:2:ILE:HG23	2:L:26:SER:HB3	1.90	0.54
3:A:230:PRO:CG	3:C:519:HIS:O	2.55	0.54
3:A:1116:THR:HG22	3:A:1138:TYR:HD2	1.72	0.54
3:B:334:ASN:HB3	3:B:362:VAL:HG21	1.89	0.54
2:G:2:ILE:HG23	2:G:26:SER:HB3	1.90	0.54
2:K:93:TYR:CE2	2:K:106:GLY:C	2.82	0.54
1:F:52:PHE:CD1	3:C:475:ALA:CB	2.86	0.54
2:L:93:TYR:C	2:L:106:GLY:HA3	2.28	0.54
2:L:93:TYR:CE2	2:L:106:GLY:C	2.82	0.54
2:K:2:ILE:HG23	2:K:26:SER:HB3	1.90	0.54
3:A:168:PHE:CD1	3:C:520:ALA:HB2	2.16	0.54
2:G:93:TYR:CE2	2:G:106:GLY:C	2.82	0.53
3:C:330:PRO:CB	3:C:527:PRO:HD2	2.34	0.53
2:K:93:TYR:C	2:K:106:GLY:HA3	2.28	0.53
3:A:457:ARG:NH2	3:A:460:ASN:O	2.42	0.53
1:H:54:GLU:CG	3:A:456:PHE:CE1	2.86	0.53
2:K:94:CYS:SG	2:K:105:GLY:C	2.88	0.53
2:G:93:TYR:C	2:G:106:GLY:HA3	2.28	0.53
3:C:457:ARG:NH2	3:C:460:ASN:O	2.42	0.53
3:A:1098:ASN:ND2	3:A:1100:THR:OG1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:457:ARG:NH2	3:B:460:ASN:O	2.42	0.52
3:A:498:GLN:HG3	3:A:501:TYR:CE2	2.36	0.52
1:F:38:LYS:HB2	1:F:48:ILE:HD11	1.92	0.52
2:L:94:CYS:SG	2:L:105:GLY:C	2.88	0.52
3:A:809:PRO:HA	3:A:814:LYS:HE3	1.92	0.52
3:B:484:LYS:CE	3:B:490:PHE:CD1	2.76	0.52
2:G:94:CYS:SG	2:G:105:GLY:C	2.88	0.52
2:L:93:TYR:CE2	2:L:106:GLY:O	2.64	0.51
3:B:498:GLN:HG3	3:B:501:TYR:CE2	2.37	0.51
1:H:33:ILE:CG1	3:A:476:GLY:CA	2.76	0.51
1:J:38:LYS:HB2	1:J:48:ILE:HD11	1.92	0.51
2:K:93:TYR:CE2	2:K:106:GLY:O	2.64	0.51
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.92	0.51
1:H:52:PHE:CD1	3:A:475:ALA:CB	2.87	0.51
1:F:54:GLU:CD	3:C:456:PHE:CE1	2.85	0.51
2:G:93:TYR:CE2	2:G:106:GLY:O	2.64	0.50
1:J:52:PHE:CD1	3:B:475:ALA:CB	2.87	0.50
1:H:54:GLU:CD	3:A:456:PHE:CE1	2.85	0.50
1:F:54:GLU:CG	3:C:456:PHE:CE1	2.86	0.50
1:F:33:ILE:CG1	3:C:476:GLY:CA	2.76	0.50
1:J:54:GLU:CD	3:B:456:PHE:CE1	2.85	0.50
2:L:93:TYR:C	2:L:106:GLY:CA	2.81	0.49
3:C:484:LYS:CE	3:C:490:PHE:CD1	2.76	0.49
3:A:472:ILE:CD1	3:A:484:LYS:CE	2.83	0.49
1:H:44:GLY:HA3	2:L:93:TYR:OH	2.12	0.49
1:J:44:GLY:HA3	2:K:93:TYR:OH	2.12	0.49
3:A:229:LEU:HA	3:C:521:PRO:HG3	1.94	0.49
3:C:472:ILE:HD11	3:C:484:LYS:HE3	1.95	0.49
2:K:93:TYR:C	2:K:106:GLY:CA	2.81	0.49
2:L:44:GLN:HB2	2:L:91:VAL:HB	1.95	0.49
2:G:44:GLN:HB2	2:G:91:VAL:HB	1.95	0.49
2:K:44:GLN:HB2	2:K:91:VAL:HB	1.95	0.48
3:A:472:ILE:HD11	3:A:484:LYS:HE2	1.86	0.48
2:L:55:HIS:C	2:L:57:THR:H	2.17	0.48
1:F:44:GLY:HA3	2:G:93:TYR:OH	2.12	0.48
2:K:92:TYR:HE2	2:K:110:LEU:HD22	1.79	0.48
2:L:92:TYR:HE2	2:L:110:LEU:HD22	1.79	0.48
2:G:55:HIS:C	2:G:57:THR:H	2.17	0.47
1:J:33:ILE:CD1	3:B:476:GLY:CA	2.48	0.47
3:C:617:CYS:SG	3:C:642:VAL:CG1	3.02	0.47
3:C:454:ARG:HH21	3:C:457:ARG:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:TYR:HE2	2:G:110:LEU:HD22	1.79	0.47
2:K:33:ASN:HD22	3:B:481:ASN:ND2	2.13	0.47
3:C:498:GLN:HG3	3:C:501:TYR:CE2	2.37	0.47
3:A:452:LEU:HD23	3:A:492:LEU:HB3	1.97	0.47
3:A:472:ILE:HD11	3:A:484:LYS:HE3	1.94	0.47
3:C:452:LEU:HD23	3:C:492:LEU:HB3	1.97	0.47
3:B:472:ILE:HD11	3:B:484:LYS:HE3	1.94	0.47
1:H:33:ILE:CD1	3:A:476:GLY:CA	2.49	0.47
3:B:1032:CYS:HG	3:B:1043:CYS:HG	1.58	0.47
2:K:55:HIS:C	2:K:57:THR:H	2.17	0.46
2:L:33:ASN:HD22	3:A:481:ASN:ND2	2.13	0.46
3:C:389:ASP:HA	3:C:526:GLY:O	2.15	0.46
2:G:93:TYR:C	2:G:106:GLY:CA	2.81	0.46
1:H:62:GLN:H	1:H:62:GLN:HG3	1.56	0.46
3:B:452:LEU:HD23	3:B:492:LEU:HB3	1.97	0.46
3:C:472:ILE:HD11	3:C:484:LYS:HE2	1.86	0.46
2:G:33:ASN:HD22	3:C:481:ASN:ND2	2.13	0.46
3:A:454:ARG:HH21	3:A:457:ARG:HG3	1.79	0.46
3:A:650:LEU:HD13	3:A:650:LEU:HA	1.77	0.46
3:B:81:ASN:N	3:B:265:TYR:HH	2.13	0.46
1:J:62:GLN:H	1:J:62:GLN:HG3	1.56	0.46
1:J:61:SER:HB3	1:J:64:PHE:HD2	1.81	0.46
3:C:332:ILE:HG23	3:C:364:ASP:HB2	1.97	0.46
3:C:389:ASP:HB3	3:C:528:LYS:N	2.31	0.46
3:B:454:ARG:HH21	3:B:457:ARG:HG3	1.79	0.45
1:J:33:ILE:HG13	3:B:476:GLY:CA	2.44	0.45
1:F:61:SER:HB3	1:F:64:PHE:HD2	1.81	0.45
3:C:336:CYS:O	3:C:338:PHE:N	2.49	0.45
3:A:168:PHE:CE1	3:C:520:ALA:CB	2.74	0.45
3:B:336:CYS:HB2	3:B:362:VAL:O	2.15	0.45
2:G:11:LEU:HD11	2:G:21:LEU:HB3	1.99	0.45
2:L:11:LEU:HD11	2:L:21:LEU:HB3	1.99	0.45
2:K:11:LEU:HD11	2:K:21:LEU:HB3	1.99	0.44
3:A:375:SER:H	3:A:436:TRP:HA	1.83	0.44
1:H:61:SER:HB3	1:H:64:PHE:HD2	1.81	0.44
3:A:336:CYS:O	3:A:338:PHE:N	2.49	0.44
3:A:478:THR:HB	3:A:487:ASN:HB2	2.00	0.44
1:F:60:TYR:HE1	1:F:70:LEU:HG	1.83	0.44
1:F:33:ILE:HG13	3:C:476:GLY:CA	2.44	0.44
1:J:60:TYR:HE1	1:J:70:LEU:HG	1.83	0.44
1:H:60:TYR:HE1	1:H:70:LEU:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:418:ILE:HG23	3:C:422:ASN:HD22	1.84	0.43
2:K:43:GLN:HG2	2:K:90:ALA:HB3	2.01	0.43
3:A:418:ILE:HG23	3:A:422:ASN:HD22	1.84	0.43
2:K:38:TYR:HD2	2:K:97:TYR:HD2	1.67	0.43
2:L:38:TYR:HD2	2:L:97:TYR:HD2	1.67	0.43
3:B:375:SER:H	3:B:436:TRP:HA	1.83	0.43
3:B:478:THR:HB	3:B:487:ASN:HB2	2.00	0.43
3:A:410:ILE:HG23	3:A:425:LEU:HD11	2.01	0.43
3:B:410:ILE:HG23	3:B:425:LEU:HD11	2.01	0.43
3:C:375:SER:H	3:C:436:TRP:HA	1.83	0.43
1:J:38:LYS:NZ	1:J:90:ASP:HA	2.34	0.43
2:K:45:LYS:HB2	2:K:48:ARG:HG3	2.01	0.43
3:C:478:THR:HB	3:C:487:ASN:HB2	2.00	0.43
1:H:33:ILE:HG13	3:A:476:GLY:CA	2.44	0.43
1:H:38:LYS:NZ	1:H:90:ASP:HA	2.34	0.43
1:J:97:ALA:HA	1:J:107:TRP:HA	2.01	0.43
3:C:1032:CYS:HG	3:C:1043:CYS:HG	1.65	0.43
1:F:38:LYS:NZ	1:F:90:ASP:HA	2.34	0.42
3:A:525:CYS:C	3:A:527:PRO:HD3	2.39	0.42
1:F:97:ALA:HA	1:F:107:TRP:HA	2.01	0.42
3:B:518:LEU:HD13	3:B:518:LEU:HA	1.88	0.42
2:G:43:GLN:HG2	2:G:90:ALA:HB3	2.01	0.42
2:G:45:LYS:HB2	2:G:48:ARG:HG3	2.01	0.42
3:A:490:PHE:CE2	3:A:492:LEU:HB2	2.55	0.42
3:A:526:GLY:N	3:A:527:PRO:HD3	2.34	0.42
3:B:418:ILE:HG23	3:B:422:ASN:HD22	1.84	0.42
3:B:490:PHE:CE2	3:B:492:LEU:HB2	2.54	0.42
1:J:33:ILE:CG1	3:B:476:GLY:CA	2.76	0.42
2:L:43:GLN:HG2	2:L:90:ALA:HB3	2.01	0.42
2:G:43:GLN:HG2	2:G:90:ALA:CB	2.50	0.42
2:K:43:GLN:HG2	2:K:90:ALA:CB	2.50	0.42
2:L:45:LYS:HB2	2:L:48:ARG:HG3	2.01	0.42
3:C:331:ASN:HB3	3:C:529:LYS:HA	2.01	0.42
3:C:410:ILE:HG23	3:C:425:LEU:HD11	2.01	0.42
2:K:38:TYR:CZ	3:B:479:PRO:HG2	2.55	0.42
2:L:38:TYR:CZ	3:A:479:PRO:HG2	2.55	0.42
1:H:104:LEU:HD13	1:H:104:LEU:HA	1.79	0.42
2:G:38:TYR:HD2	2:G:97:TYR:HD2	1.67	0.41
1:H:37:VAL:HG11	1:H:45:LEU:HB3	2.02	0.41
3:C:330:PRO:CG	3:C:527:PRO:HD2	2.50	0.41
3:C:1083:HIS:CG	3:C:1084:ASP:H	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:345:THR:HA	3:A:509:ARG:HH12	1.85	0.41
3:B:1081:ILE:HD11	3:B:1115:ILE:HG21	2.01	0.41
3:C:345:THR:HA	3:C:509:ARG:HH12	1.85	0.41
1:J:37:VAL:HG11	1:J:45:LEU:HB3	2.02	0.41
2:L:43:GLN:HG2	2:L:90:ALA:CB	2.50	0.41
2:L:94:CYS:O	2:L:106:GLY:N	2.53	0.41
3:A:521:PRO:CD	3:B:230:PRO:O	2.68	0.41
3:C:344:ALA:O	3:C:509:ARG:NH1	2.52	0.41
1:F:37:VAL:HG11	1:F:45:LEU:HB3	2.02	0.41
3:C:490:PHE:CE2	3:C:492:LEU:HB2	2.54	0.41
3:C:1135:ASN:HD22	3:C:1135:ASN:HA	1.71	0.41
1:H:97:ALA:HA	1:H:107:TRP:HA	2.01	0.41
2:G:94:CYS:O	2:G:106:GLY:N	2.53	0.41
2:K:94:CYS:O	2:K:106:GLY:N	2.53	0.41
3:C:718:PHE:HZ	3:C:923:ILE:HD11	1.86	0.41
2:G:38:TYR:CZ	3:C:479:PRO:HG2	2.55	0.41
2:G:7:SER:HB2	2:G:8:PRO:HA	2.03	0.41
2:K:7:SER:HB2	2:K:8:PRO:HA	2.03	0.41
2:G:18:LYS:HA	2:G:82:SER:HA	2.03	0.40
2:L:7:SER:HB2	2:L:8:PRO:HA	2.03	0.40
2:K:94:CYS:SG	2:K:105:GLY:O	2.79	0.40
3:A:811:LYS:HZ3	3:A:814:LYS:HG2	1.86	0.40
3:B:344:ALA:O	3:B:509:ARG:NH1	2.52	0.40
1:F:102:ASN:HB2	1:F:103:VAL:H	1.73	0.40
3:B:304:LYS:HD3	3:B:304:LYS:HA	1.94	0.40
3:B:345:THR:HA	3:B:509:ARG:HH12	1.86	0.40
3:B:361:CYS:H	3:B:524:VAL:HG22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/216 (49%)	97 (92%)	8 (8%)	0	100	100
1	H	105/216 (49%)	97 (92%)	8 (8%)	0	100	100
1	J	105/216 (49%)	97 (92%)	8 (8%)	0	100	100
2	G	111/220 (50%)	108 (97%)	2 (2%)	1 (1%)	14	44
2	K	111/220 (50%)	108 (97%)	2 (2%)	1 (1%)	14	44
2	L	111/220 (50%)	108 (97%)	2 (2%)	1 (1%)	14	44
3	A	976/1280 (76%)	893 (92%)	78 (8%)	5 (0%)	25	56
3	B	976/1280 (76%)	895 (92%)	76 (8%)	5 (0%)	25	56
3	C	976/1280 (76%)	901 (92%)	72 (7%)	3 (0%)	37	66
All	All	3576/5148 (70%)	3304 (92%)	256 (7%)	16 (0%)	32	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	527	PRO
3	A	197	ILE
3	C	112	SER
2	G	107	GLY
2	K	107	GLY
2	L	107	GLY
3	B	137	ASN
3	B	338	PHE
3	B	527	PRO
3	A	198	ASP
3	C	801	ASN
3	B	536	ASN
3	B	571	ASP
3	C	812	PRO
3	A	332	ILE
3	A	744	GLY

5.3.2 Protein sidechains (i)

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	F	92/186 (50%)	77 (84%)	15 (16%)	2 8
1	H	92/186 (50%)	78 (85%)	14 (15%)	2 10
1	J	92/186 (50%)	78 (85%)	14 (15%)	2 10
2	G	100/196 (51%)	91 (91%)	9 (9%)	8 29
2	K	100/196 (51%)	91 (91%)	9 (9%)	8 29
2	L	100/196 (51%)	91 (91%)	9 (9%)	8 29
3	A	851/1103 (77%)	842 (99%)	9 (1%)	70 82
3	B	851/1103 (77%)	843 (99%)	8 (1%)	75 85
3	C	848/1103 (77%)	838 (99%)	10 (1%)	67 80
All	All	3126/4455 (70%)	3029 (97%)	97 (3%)	37 62

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	12	VAL
1	F	20	MET
1	F	22	CYS
1	F	33	ILE
1	F	43	GLN
1	F	58	THR
1	F	62	GLN
1	F	69	THR
1	F	78	THR
1	F	91	SER
1	F	93	VAL
1	F	96	CYS
1	F	102	ASN
1	F	104	LEU
1	F	109	GLN
2	G	15	VAL
2	G	20	THR
2	G	21	LEU
2	G	53	LEU
2	G	93	TYR
2	G	108	THR
2	G	109	LYS
2	G	111	GLU
2	G	112	ILE
1	H	12	VAL
1	H	20	MET

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Mol	Chain	Res	Type
1	H	22	CYS
1	H	33	ILE
1	H	43	GLN
1	H	58	THR
1	H	62	GLN
1	H	69	THR
1	H	78	THR
1	H	91	SER
1	H	96	CYS
1	H	102	ASN
1	H	104	LEU
1	H	109	GLN
1	J	12	VAL
1	J	20	MET
1	J	22	CYS
1	J	33	ILE
1	J	43	GLN
1	J	58	THR
1	J	62	GLN
1	J	69	THR
1	J	78	THR
1	J	91	SER
1	J	96	CYS
1	J	102	ASN
1	J	104	LEU
1	J	109	GLN
2	K	15	VAL
2	K	20	THR
2	K	21	LEU
2	K	53	LEU
2	K	93	TYR
2	K	108	THR
2	K	109	LYS
2	K	111	GLU
2	K	112	ILE
2	L	15	VAL
2	L	20	THR
2	L	21	LEU
2	L	53	LEU
2	L	93	TYR
2	L	108	THR
2	L	109	LYS

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Mol	Chain	Res	Type
2	L	111	GLU
2	L	112	ILE
3	A	332	ILE
3	A	387	LEU
3	A	529	LYS
3	A	618	THR
3	A	650	LEU
3	A	657	ASN
3	A	886	TRP
3	A	907	ASN
3	A	935	GLN
3	B	265	TYR
3	B	338	PHE
3	B	387	LEU
3	B	518	LEU
3	B	574	ASP
3	B	617	CYS
3	B	935	GLN
3	B	985	ASP
3	C	304	LYS
3	C	332	ILE
3	C	387	LEU
3	C	529	LYS
3	C	565	PHE
3	C	907	ASN
3	C	988	GLU
3	C	1058	HIS
3	C	1126	CYS
3	C	1135	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	33	ASN
2	K	33	ASN
2	L	33	ASN
3	A	409	GLN
3	A	448	ASN
3	A	450	ASN
3	A	493	GLN
3	A	498	GLN
3	B	409	GLN

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Mol	Chain	Res	Type
3	B	448	ASN
3	B	450	ASN
3	B	493	GLN
3	C	409	GLN
3	C	448	ASN
3	C	450	ASN
3	C	493	GLN
3	C	580	GLN
3	C	1135	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

25 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	C	1301	3	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	C	1303	3	14,14,15	0.27	0	17,19,21	1.10	2 (11%)
4	NAG	A	1301	3	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
4	NAG	C	1304	3	14,14,15	0.25	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1303	3	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	1306	3	14,14,15	0.28	0	17,19,21	0.69	0
4	NAG	C	1306	3	14,14,15	0.25	0	17,19,21	1.00	1 (5%)
4	NAG	A	1304	3	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	B	1301	3	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	B	1302	3	14,14,15	0.25	0	17,19,21	0.94	1 (5%)
4	NAG	B	1305	3	14,14,15	0.25	0	17,19,21	0.95	0
4	NAG	A	1308	3	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
4	NAG	B	1307	3	14,14,15	0.29	0	17,19,21	0.72	0
4	NAG	B	1304	3	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	C	1305	3	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	A	1305	3	14,14,15	0.28	0	17,19,21	0.69	0
4	NAG	A	1307	3	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	B	1306	3	14,14,15	0.25	0	17,19,21	0.98	1 (5%)
4	NAG	C	1302	3	14,14,15	0.30	0	17,19,21	0.76	0
4	NAG	C	1307	3	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	C	1309	3	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	A	1302	3	14,14,15	0.28	0	17,19,21	0.81	1 (5%)
4	NAG	B	1308	3	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	A	1303	3	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	C	1308	3	14,14,15	0.29	0	17,19,21	1.15	2 (11%)

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	C	1301	3	-	3/6/23/26	0/1/1/1
4	NAG	C	1303	3	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	3	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	3	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	3	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	3	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	3	-	3/6/23/26	0/1/1/1
4	NAG	A	1304	3	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	3	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	3	-	4/6/23/26	0/1/1/1
4	NAG	B	1305	3	-	4/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1301	NAG	C2-N2-C7	2.99	127.17	122.90
4	C	1308	NAG	C1-O5-C5	2.66	115.80	112.19
4	C	1303	NAG	C2-N2-C7	2.61	126.62	122.90
4	C	1308	NAG	C2-N2-C7	2.57	126.57	122.90
4	C	1303	NAG	C1-O5-C5	2.34	115.36	112.19
4	B	1302	NAG	C2-N2-C7	2.30	126.18	122.90
4	B	1306	NAG	C2-N2-C7	2.18	126.01	122.90
4	A	1308	NAG	C1-O5-C5	2.18	115.14	112.19
4	C	1306	NAG	C2-N2-C7	2.11	125.91	122.90
4	A	1302	NAG	O5-C5-C6	2.08	110.47	107.20

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1307	NAG	C8-C7-N2-C2
4	A	1307	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1301	NAG	C8-C7-N2-C2
4	B	1301	NAG	O7-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	B	1307	NAG	C8-C7-N2-C2
4	B	1307	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	C	1308	NAG	C8-C7-N2-C2
4	C	1308	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	A	1301	NAG	C1-C2-N2-C7
4	C	1307	NAG	C8-C7-N2-C2
4	B	1302	NAG	C1-C2-N2-C7
4	B	1306	NAG	C1-C2-N2-C7
4	C	1303	NAG	C1-C2-N2-C7
4	C	1307	NAG	O7-C7-N2-C2
4	B	1305	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	C	1301	NAG	C8-C7-N2-C2
4	C	1308	NAG	C1-C2-N2-C7
4	C	1301	NAG	O7-C7-N2-C2
4	B	1305	NAG	C3-C2-N2-C7
4	C	1306	NAG	C3-C2-N2-C7
4	A	1305	NAG	C8-C7-N2-C2
4	C	1308	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1302	NAG	2	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.

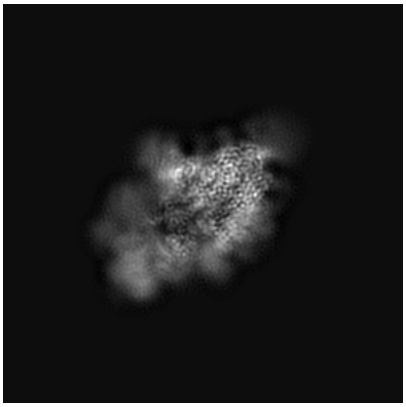
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31625. These allow visual inspection of the internal detail of the map and identification of artifacts.

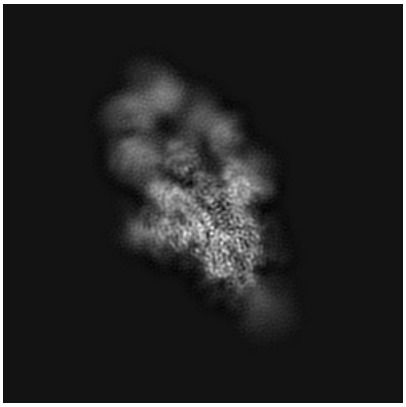
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

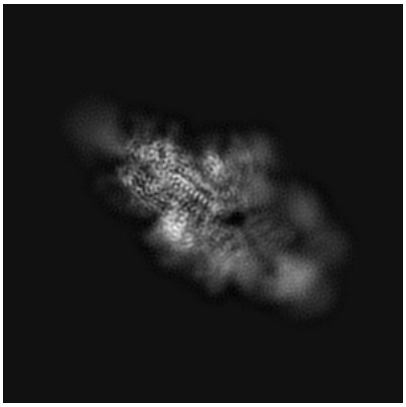
6.1.1 Primary map



X



Y

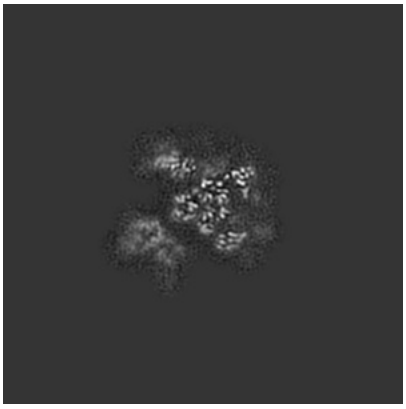


Z

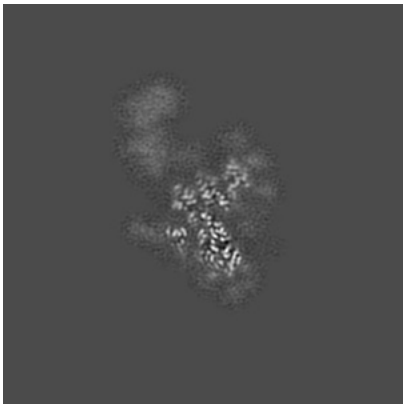
The images above show the map projected in three orthogonal directions.

6.2 Central slices

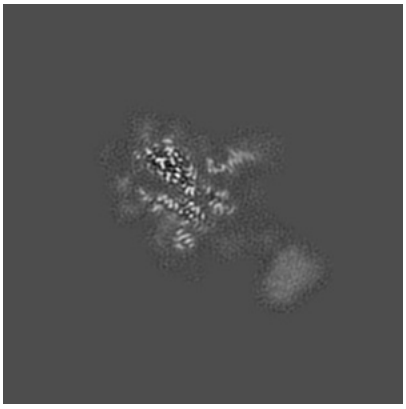
6.2.1 Primary map



X Index: 160



Y Index: 160

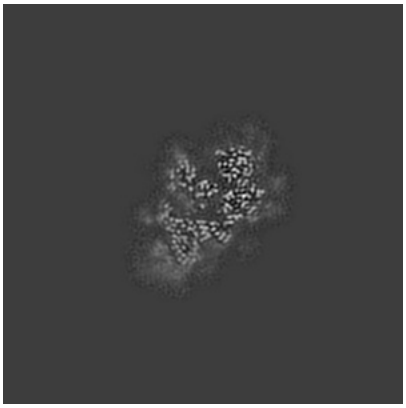


Z Index: 160

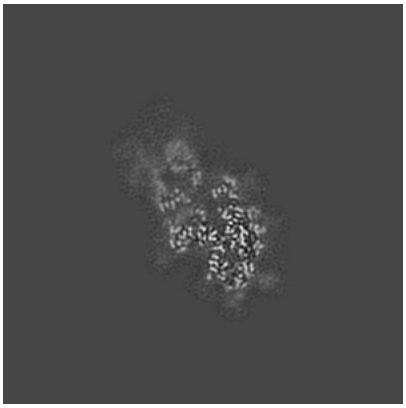
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

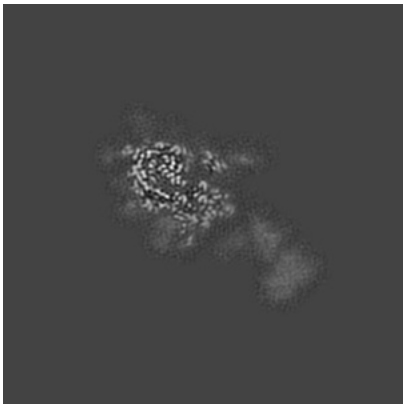
6.3.1 Primary map



X Index: 136



Y Index: 182

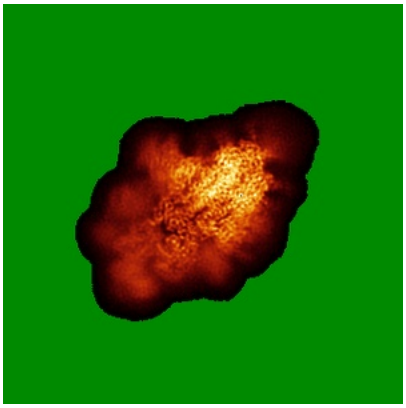


Z Index: 166

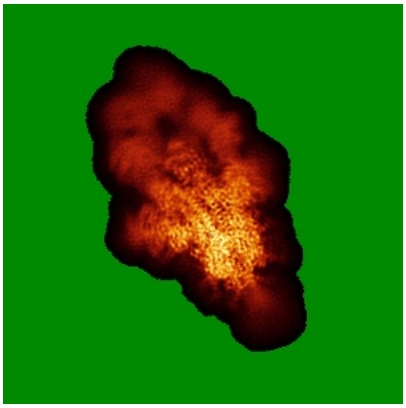
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

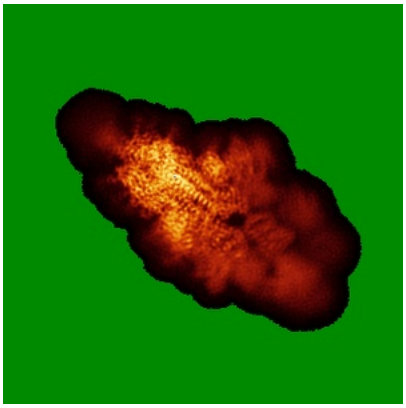
6.4.1 Primary map



X



Y

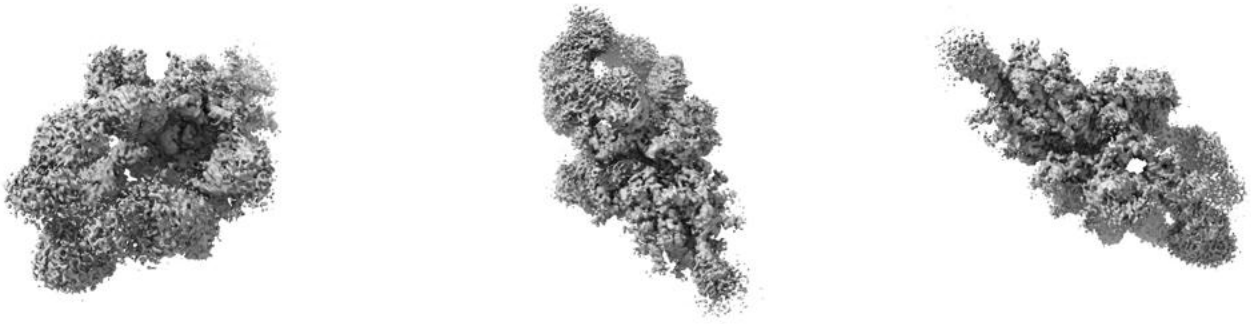


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0083. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

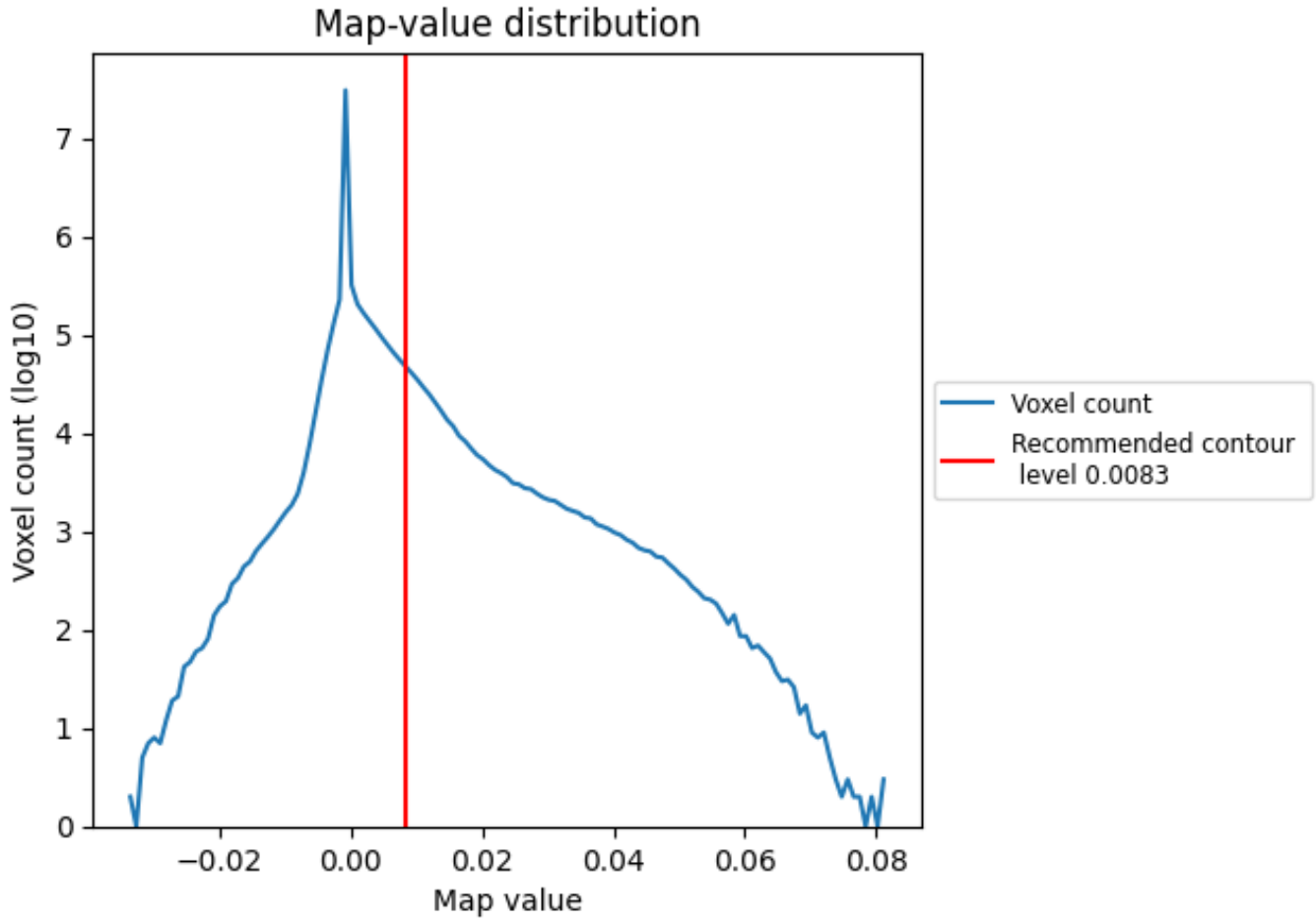
6.6 Mask visualisation (i)

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

7 Map analysis

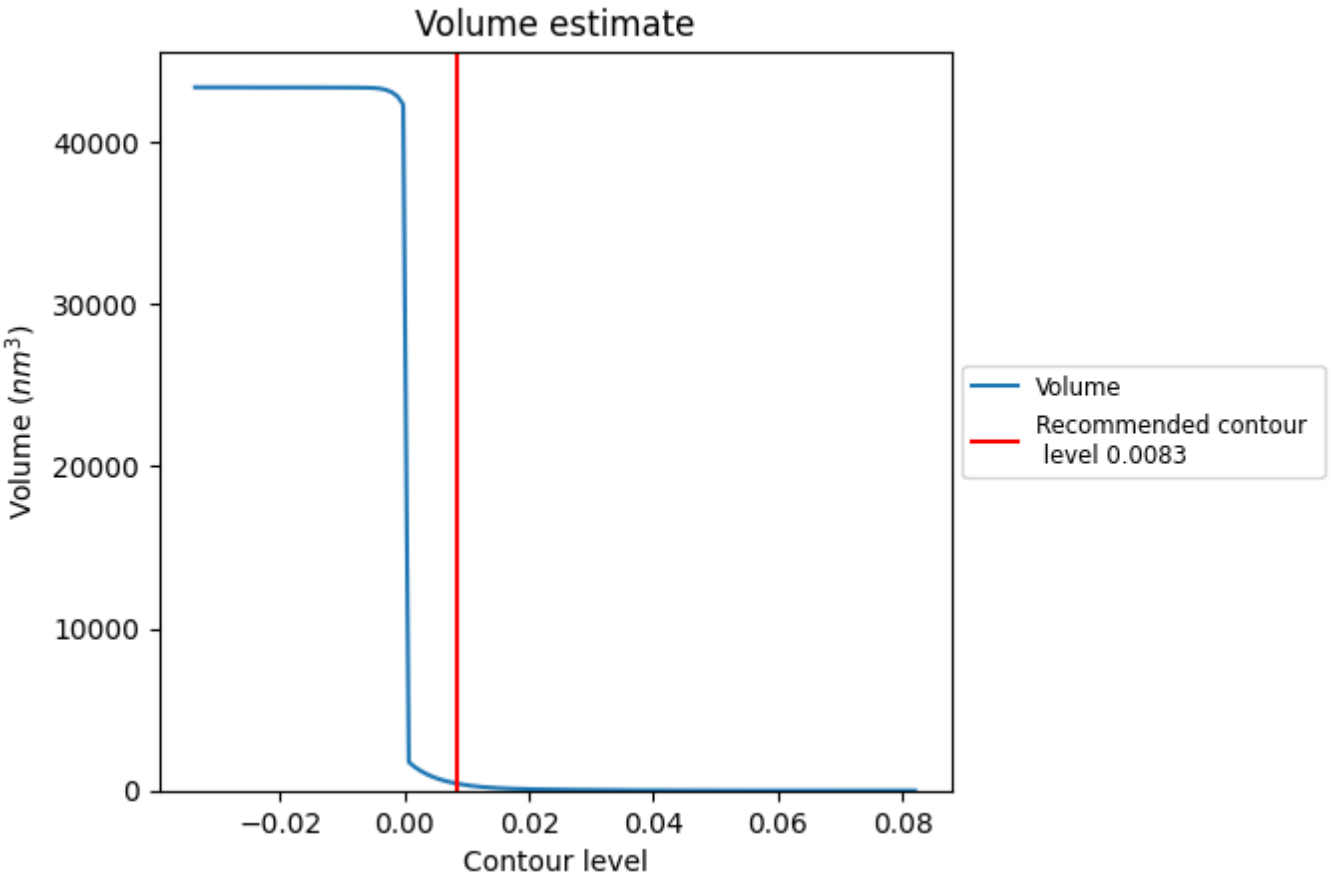
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

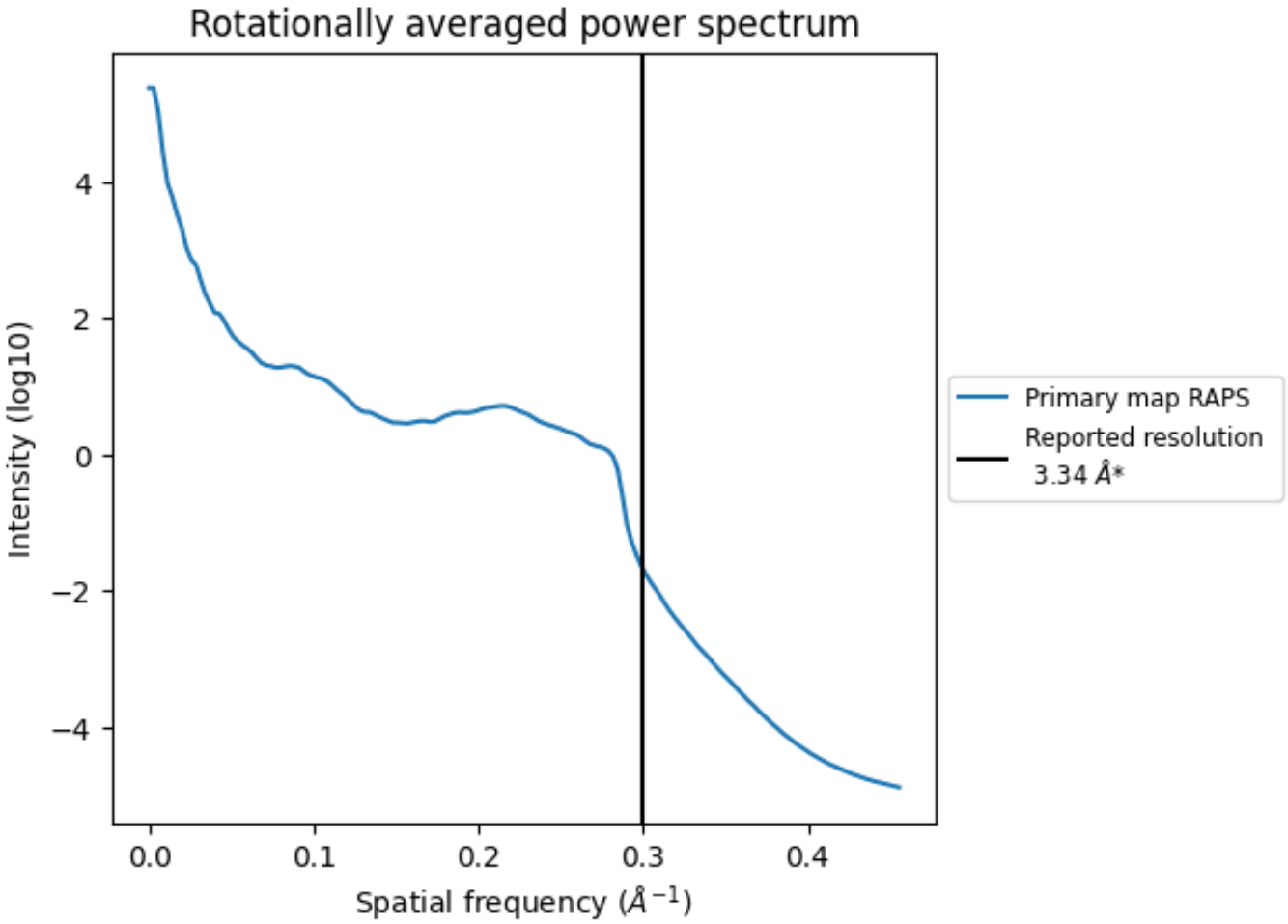
7.2 Volume estimate



The volume at the recommended contour level is 445 nm^3; this corresponds to an approximate mass of 402 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 (i)



*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

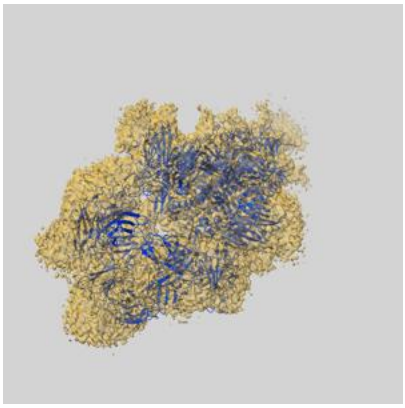
8 Fourier-Shell correlation

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

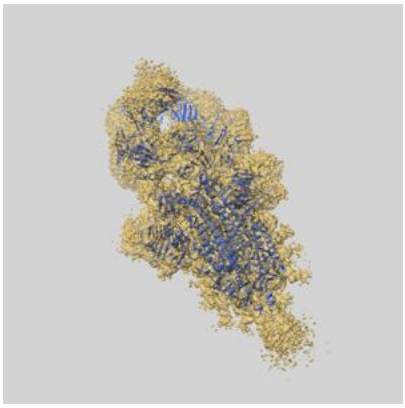
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31625 and PDB model 7FJO. Per-residue inclusion information can be found in section 3 on page 15.

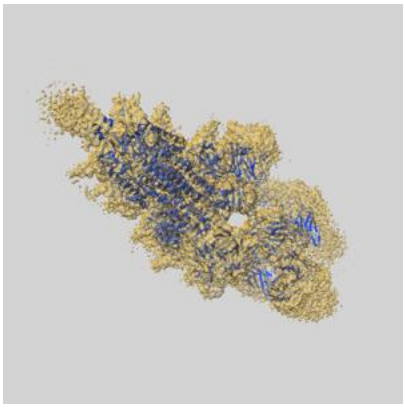
9.1 Map-model overlay



X



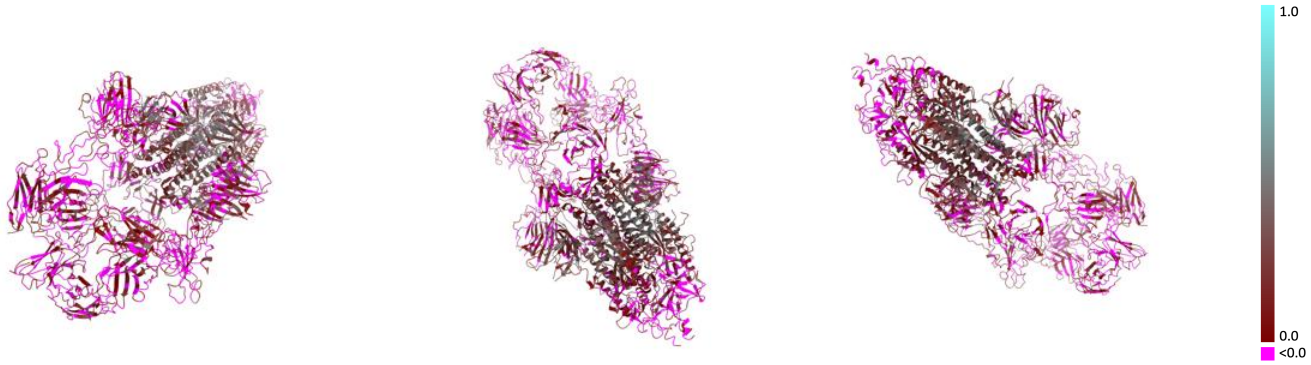
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0083 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.

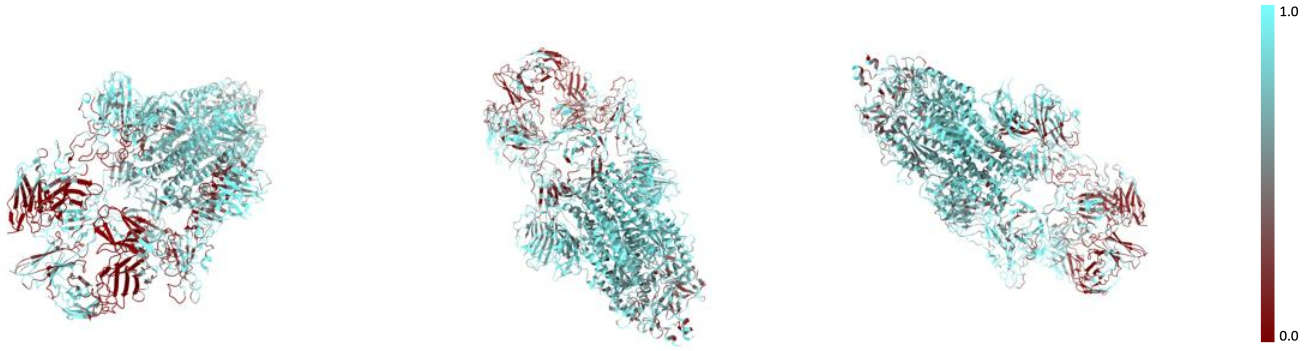
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

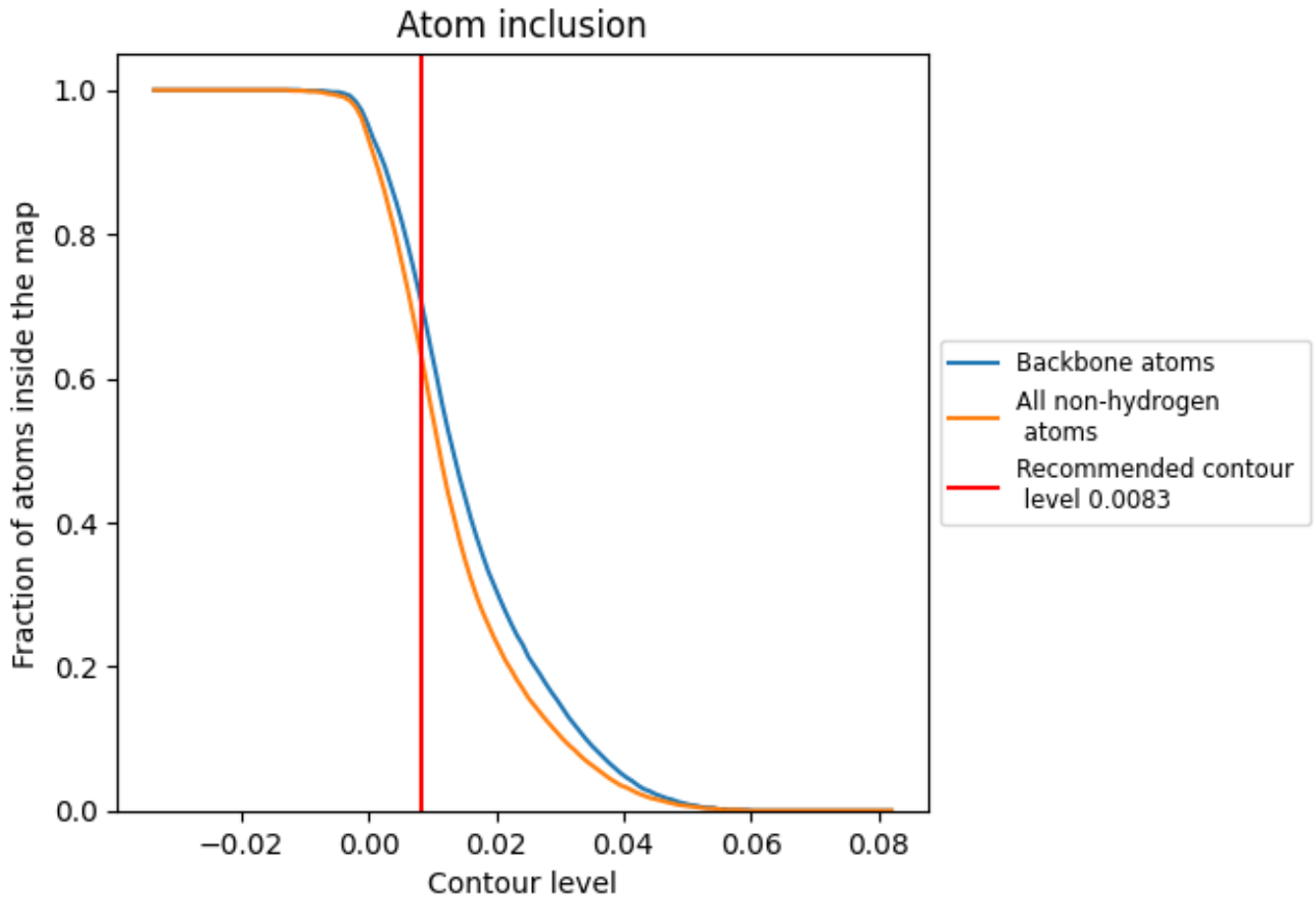
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0083).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 63% 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 (0.0083) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6300	0.1060
A	0.6800	0.1300
B	0.7510	0.1440
C	0.6600	0.0960
F	0.0730	-0.0010
G	0.2450	0.0460
H	0.1790	-0.0030
J	0.5400	0.0010
K	0.6270	0.0490
L	0.2520	0.0550