Full wwPDB EM Validation Report (i)

Nov 23, 2022 – 07:29 AM JST

PDB ID	:	7FJN
EMDB ID	:	EMD-31624
Title	:	Cryo-EM structure of South African (B.1.351) SARS-CoV-2 spike glycoprotein in complex with two T6 Fab
Authors	:	Wang, X.; Zhang, L.; Zhang, S.; Liang, Q.
Deposited on	:	2021-08-04
Resolution	:	3.25 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 (i) 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 (i)) were used in the production of this report:

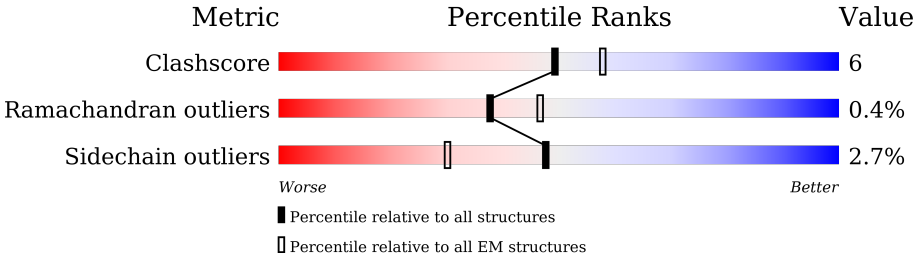
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.25 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	1280	6% 71% 6% 22%
1	B	1280	• 72% 5% 22%
1	C	1280	5% 72% 5% 22%
2	H	117	61% 59% 30% • 9%
2	I	117	86% 61% 30% • 9%
3	J	113	84% 65% 30% • •
3	L	113	52% 66% 29% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26824 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,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	993	7687	4917	1277	1458	35	0	0
1	B	993	7691	4921	1277	1458	35	0	0
1	C	992	7678	4916	1279	1448	35	0	0

There are 237 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
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	305	THR	SER	engineered mutation	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	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP M1E1E4
A	1240	SER	-	expression tag	UNP M1E1E4
A	1241	LEU	-	expression tag	UNP M1E1E4
A	1242	GLU	-	expression tag	UNP M1E1E4
A	1243	VAL	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1244	LEU	-	expression tag	UNP M1E1E4
A	1245	PHE	-	expression tag	UNP M1E1E4
A	1246	GLN	-	expression tag	UNP M1E1E4
A	1247	GLY	-	expression tag	UNP M1E1E4
A	1248	PRO	-	expression tag	UNP M1E1E4
A	1249	GLY	-	expression tag	UNP M1E1E4
A	1250	HIS	-	expression tag	UNP M1E1E4
A	1251	HIS	-	expression tag	UNP M1E1E4
A	1252	HIS	-	expression tag	UNP M1E1E4
A	1253	HIS	-	expression tag	UNP M1E1E4
A	1254	HIS	-	expression tag	UNP M1E1E4
A	1255	HIS	-	expression tag	UNP M1E1E4
A	1256	HIS	-	expression tag	UNP M1E1E4
A	1257	HIS	-	expression tag	UNP M1E1E4
A	1258	SER	-	expression tag	UNP M1E1E4
A	1259	ALA	-	expression tag	UNP M1E1E4
A	1260	TRP	-	expression tag	UNP M1E1E4
A	1261	SER	-	expression tag	UNP M1E1E4
A	1262	HIS	-	expression tag	UNP M1E1E4
A	1263	PRO	-	expression tag	UNP M1E1E4
A	1264	GLN	-	expression tag	UNP M1E1E4
A	1265	PHE	-	expression tag	UNP M1E1E4
A	1266	GLU	-	expression tag	UNP M1E1E4
A	1267	LYS	-	expression tag	UNP M1E1E4
A	1268	GLY	-	expression tag	UNP M1E1E4
A	1269	GLY	-	expression tag	UNP M1E1E4
A	1270	GLY	-	expression tag	UNP M1E1E4
A	1271	SER	-	expression tag	UNP M1E1E4
A	1272	GLY	-	expression tag	UNP M1E1E4
A	1273	GLY	-	expression tag	UNP M1E1E4
A	1274	GLY	-	expression tag	UNP M1E1E4
A	1275	GLY	-	expression tag	UNP M1E1E4
A	1276	SER	-	expression tag	UNP M1E1E4
A	1277	GLY	-	expression tag	UNP M1E1E4
A	1278	GLY	-	expression tag	UNP M1E1E4
A	1279	SER	-	expression tag	UNP M1E1E4
A	1280	ALA	-	expression tag	UNP M1E1E4
A	1281	TRP	-	expression tag	UNP M1E1E4
A	1282	SER	-	expression tag	UNP M1E1E4
A	1283	HIS	-	expression tag	UNP M1E1E4
A	1284	PRO	-	expression tag	UNP M1E1E4
A	1285	GLN	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1286	PHE	-	expression tag	UNP M1E1E4
A	1287	GLU	-	expression tag	UNP M1E1E4
A	1288	LYS	-	expression tag	UNP M1E1E4
A	1289	GLY	-	expression tag	UNP M1E1E4
A	1290	SER	-	expression tag	UNP M1E1E4
A	1291	ASP	-	expression tag	UNP M1E1E4
A	1292	TYR	-	expression tag	UNP M1E1E4
A	1293	LYS	-	expression tag	UNP M1E1E4
A	1294	ASP	-	expression tag	UNP M1E1E4
A	1295	ASP	-	expression tag	UNP M1E1E4
A	1296	ASP	-	expression tag	UNP M1E1E4
A	1297	ASP	-	expression tag	UNP M1E1E4
A	1298	LYS	-	expression tag	UNP M1E1E4
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	engineered mutation	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	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP M1E1E4
B	1240	SER	-	expression tag	UNP M1E1E4
B	1241	LEU	-	expression tag	UNP M1E1E4
B	1242	GLU	-	expression tag	UNP M1E1E4
B	1243	VAL	-	expression tag	UNP M1E1E4
B	1244	LEU	-	expression tag	UNP M1E1E4
B	1245	PHE	-	expression tag	UNP M1E1E4
B	1246	GLN	-	expression tag	UNP M1E1E4
B	1247	GLY	-	expression tag	UNP M1E1E4
B	1248	PRO	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	GLY	-	expression tag	UNP M1E1E4
B	1250	HIS	-	expression tag	UNP M1E1E4
B	1251	HIS	-	expression tag	UNP M1E1E4
B	1252	HIS	-	expression tag	UNP M1E1E4
B	1253	HIS	-	expression tag	UNP M1E1E4
B	1254	HIS	-	expression tag	UNP M1E1E4
B	1255	HIS	-	expression tag	UNP M1E1E4
B	1256	HIS	-	expression tag	UNP M1E1E4
B	1257	HIS	-	expression tag	UNP M1E1E4
B	1258	SER	-	expression tag	UNP M1E1E4
B	1259	ALA	-	expression tag	UNP M1E1E4
B	1260	TRP	-	expression tag	UNP M1E1E4
B	1261	SER	-	expression tag	UNP M1E1E4
B	1262	HIS	-	expression tag	UNP M1E1E4
B	1263	PRO	-	expression tag	UNP M1E1E4
B	1264	GLN	-	expression tag	UNP M1E1E4
B	1265	PHE	-	expression tag	UNP M1E1E4
B	1266	GLU	-	expression tag	UNP M1E1E4
B	1267	LYS	-	expression tag	UNP M1E1E4
B	1268	GLY	-	expression tag	UNP M1E1E4
B	1269	GLY	-	expression tag	UNP M1E1E4
B	1270	GLY	-	expression tag	UNP M1E1E4
B	1271	SER	-	expression tag	UNP M1E1E4
B	1272	GLY	-	expression tag	UNP M1E1E4
B	1273	GLY	-	expression tag	UNP M1E1E4
B	1274	GLY	-	expression tag	UNP M1E1E4
B	1275	GLY	-	expression tag	UNP M1E1E4
B	1276	SER	-	expression tag	UNP M1E1E4
B	1277	GLY	-	expression tag	UNP M1E1E4
B	1278	GLY	-	expression tag	UNP M1E1E4
B	1279	SER	-	expression tag	UNP M1E1E4
B	1280	ALA	-	expression tag	UNP M1E1E4
B	1281	TRP	-	expression tag	UNP M1E1E4
B	1282	SER	-	expression tag	UNP M1E1E4
B	1283	HIS	-	expression tag	UNP M1E1E4
B	1284	PRO	-	expression tag	UNP M1E1E4
B	1285	GLN	-	expression tag	UNP M1E1E4
B	1286	PHE	-	expression tag	UNP M1E1E4
B	1287	GLU	-	expression tag	UNP M1E1E4
B	1288	LYS	-	expression tag	UNP M1E1E4
B	1289	GLY	-	expression tag	UNP M1E1E4
B	1290	SER	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1291	ASP	-	expression tag	UNP M1E1E4
B	1292	TYR	-	expression tag	UNP M1E1E4
B	1293	LYS	-	expression tag	UNP M1E1E4
B	1294	ASP	-	expression tag	UNP M1E1E4
B	1295	ASP	-	expression tag	UNP M1E1E4
B	1296	ASP	-	expression tag	UNP M1E1E4
B	1297	ASP	-	expression tag	UNP M1E1E4
B	1298	LYS	-	expression tag	UNP M1E1E4
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	engineered mutation	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	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP M1E1E4
C	1240	SER	-	expression tag	UNP M1E1E4
C	1241	LEU	-	expression tag	UNP M1E1E4
C	1242	GLU	-	expression tag	UNP M1E1E4
C	1243	VAL	-	expression tag	UNP M1E1E4
C	1244	LEU	-	expression tag	UNP M1E1E4
C	1245	PHE	-	expression tag	UNP M1E1E4
C	1246	GLN	-	expression tag	UNP M1E1E4
C	1247	GLY	-	expression tag	UNP M1E1E4
C	1248	PRO	-	expression tag	UNP M1E1E4
C	1249	GLY	-	expression tag	UNP M1E1E4
C	1250	HIS	-	expression tag	UNP M1E1E4
C	1251	HIS	-	expression tag	UNP M1E1E4
C	1252	HIS	-	expression tag	UNP M1E1E4
C	1253	HIS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1254	HIS	-	expression tag	UNP M1E1E4
C	1255	HIS	-	expression tag	UNP M1E1E4
C	1256	HIS	-	expression tag	UNP M1E1E4
C	1257	HIS	-	expression tag	UNP M1E1E4
C	1258	SER	-	expression tag	UNP M1E1E4
C	1259	ALA	-	expression tag	UNP M1E1E4
C	1260	TRP	-	expression tag	UNP M1E1E4
C	1261	SER	-	expression tag	UNP M1E1E4
C	1262	HIS	-	expression tag	UNP M1E1E4
C	1263	PRO	-	expression tag	UNP M1E1E4
C	1264	GLN	-	expression tag	UNP M1E1E4
C	1265	PHE	-	expression tag	UNP M1E1E4
C	1266	GLU	-	expression tag	UNP M1E1E4
C	1267	LYS	-	expression tag	UNP M1E1E4
C	1268	GLY	-	expression tag	UNP M1E1E4
C	1269	GLY	-	expression tag	UNP M1E1E4
C	1270	GLY	-	expression tag	UNP M1E1E4
C	1271	SER	-	expression tag	UNP M1E1E4
C	1272	GLY	-	expression tag	UNP M1E1E4
C	1273	GLY	-	expression tag	UNP M1E1E4
C	1274	GLY	-	expression tag	UNP M1E1E4
C	1275	GLY	-	expression tag	UNP M1E1E4
C	1276	SER	-	expression tag	UNP M1E1E4
C	1277	GLY	-	expression tag	UNP M1E1E4
C	1278	GLY	-	expression tag	UNP M1E1E4
C	1279	SER	-	expression tag	UNP M1E1E4
C	1280	ALA	-	expression tag	UNP M1E1E4
C	1281	TRP	-	expression tag	UNP M1E1E4
C	1282	SER	-	expression tag	UNP M1E1E4
C	1283	HIS	-	expression tag	UNP M1E1E4
C	1284	PRO	-	expression tag	UNP M1E1E4
C	1285	GLN	-	expression tag	UNP M1E1E4
C	1286	PHE	-	expression tag	UNP M1E1E4
C	1287	GLU	-	expression tag	UNP M1E1E4
C	1288	LYS	-	expression tag	UNP M1E1E4
C	1289	GLY	-	expression tag	UNP M1E1E4
C	1290	SER	-	expression tag	UNP M1E1E4
C	1291	ASP	-	expression tag	UNP M1E1E4
C	1292	TYR	-	expression tag	UNP M1E1E4
C	1293	LYS	-	expression tag	UNP M1E1E4
C	1294	ASP	-	expression tag	UNP M1E1E4
C	1295	ASP	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1296	ASP	-	expression tag	UNP M1E1E4
C	1297	ASP	-	expression tag	UNP M1E1E4
C	1298	LYS	-	expression tag	UNP M1E1E4

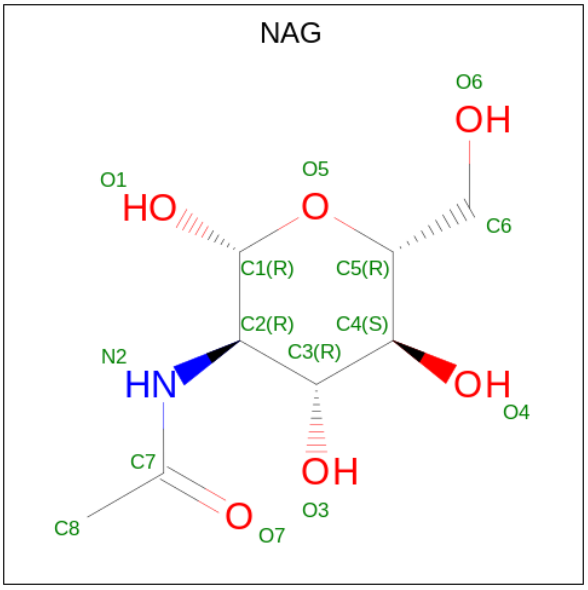
- Molecule 2 is a protein called T6 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	107	823	517	132	170	4	0	0
2	I	107	823	517	132	170	4	0	0

- Molecule 3 is a protein called T6 light chain.

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

- 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
			Total	C	N	O	
4	A	1	112	64	8	40	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	C	1	126	72	9	45	0
4	C	1	126	72	9	45	0
4	C	1	126	72	9	45	0
4	C	1	126	72	9	45	0
4	C	1	126	72	9	45	0
4	C	1	126	72	9	45	0

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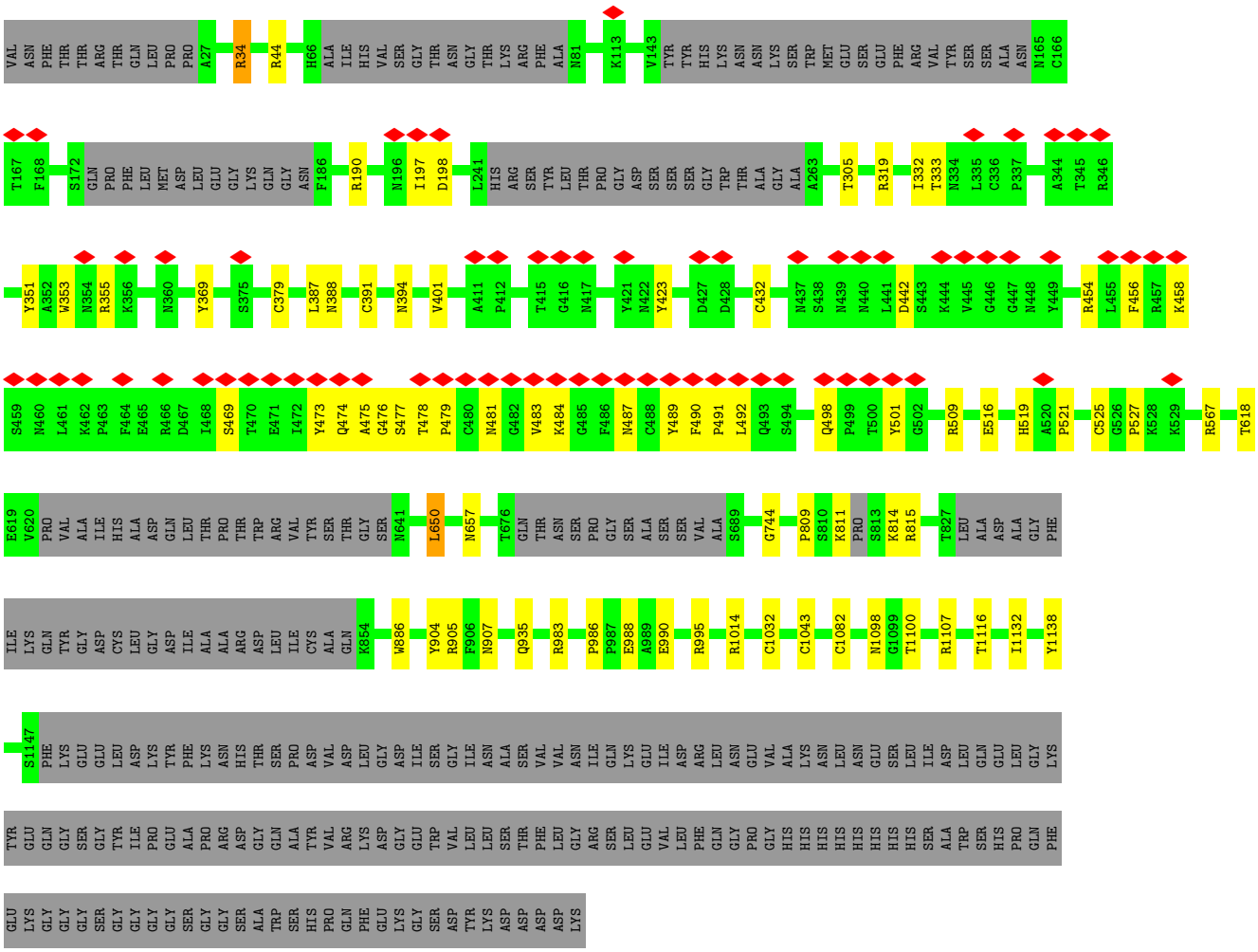
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	C	1	126	72	9	45	0
			Total	C	N	O	
4	C	1	126	72	9	45	0
			Total	C	N	O	
4	C	1	126	72	9	45	0

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.

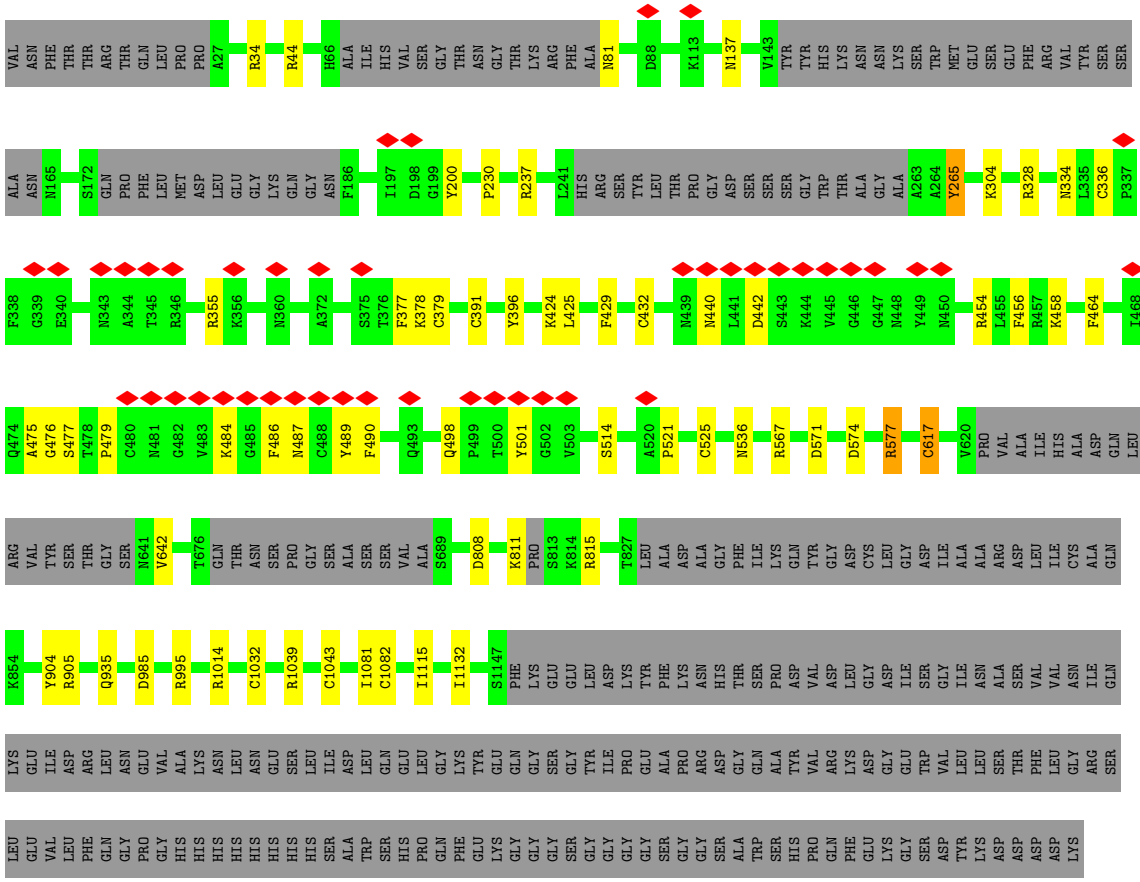
• Molecule 1: Spike glycoprotein,Envelope glycoprotein

Chain A:



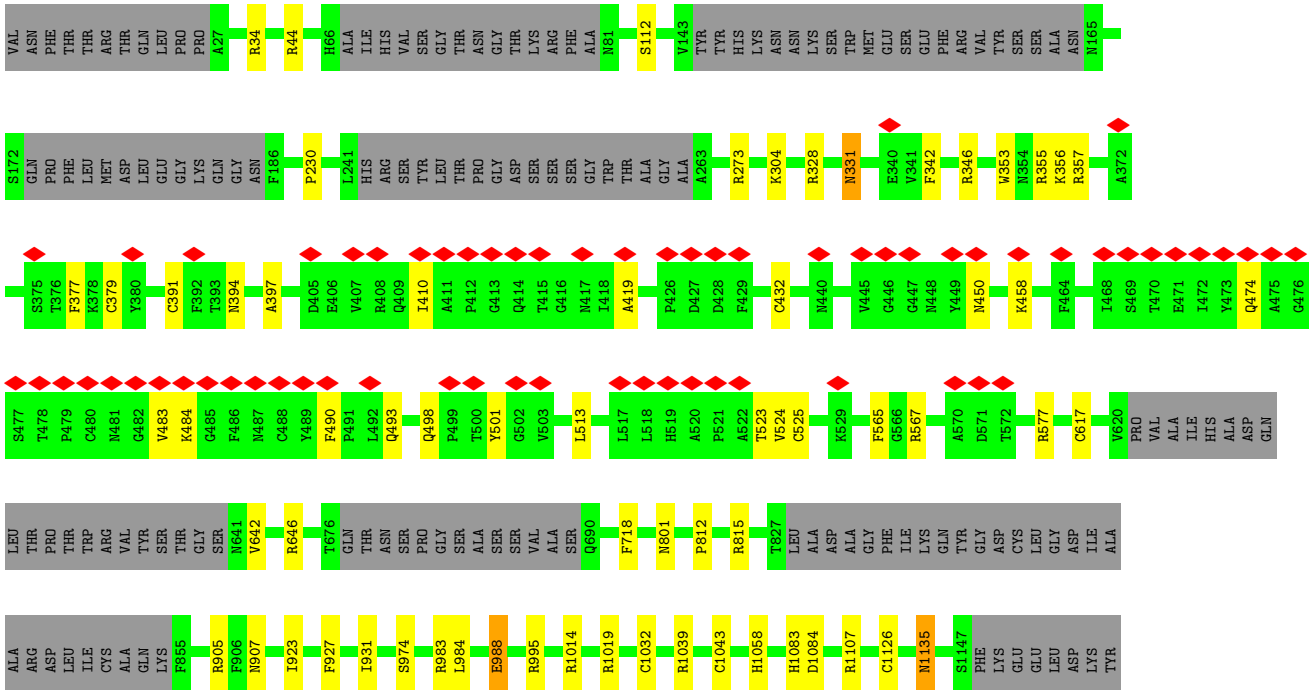
• Molecule 1: Spike glycoprotein,Envelope glycoprotein

Chain B:



- Molecule 1: Spike glycoprotein,Envelope glycoprotein

Chain C:



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 ALA TRP SER HIS PRO GLN PHE GLU LYS GLY 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 ASP LYS

- Molecule 2: T6 heavy chain

Chain H: 61% 59% 30% • 9%

GLN VAL GLN LEU GLN GLN PRO GLY THR GLU L11 V12 N13 P14 G15 A16 S17 L18 K19 M20 S21 C22 Y32 I33 I34 H35 W36 V37 K38 Q39 T40 P41 G42 Q43 G44 L45 E46 W47 I48 G49 A50 I51 F52 P53 E54 N55 D56 D57 T58 S59 Y60 S61 Q62 K63 F64 K65 G66 K67 A68

T69 L70 T71 T72 D73 T74 S75 S76 S77 T78 A79 Y80 M81 Q82 L83 S84 S85 L86 T87 S88 E89 D90 S91 A92 V93 Y94 Y95 C96 A97 R98 N102 V103 L104 D105 Y106 W107 G108 Q109 G110 T111 S112 V113 T114 V115 S116 S117

- Molecule 2: T6 heavy chain

Chain I: 86% 61% 30% • 9%

GLN VAL GLN LEU GLN GLN PRO GLY THR GLU L11 V12 N13 P14 G15 A16 S17 L18 K19 M20 S21 C22 K23 T24 S25 G26 Y27 R28 F29 T30 S31 Y32 I33 I34 H35 W36 V37 K38 Q39 T40 P41 G42 Q43 G44 L45 I48 G49 A50 I51 F52 P53 E54 N55 D56 D57 T58 S59 Y60 S61

Q62 K63 F64 K65 G66 K67 A68 T69 L70 T71 T72 D73 T74 S75 S76 S77 T78 A79 Y80 M81 Q82 L83 S84 S85 L86 T87 S88 E89 D90 S91 A92 V93 Y94 Y95 C96 A97 R98 D99 G100 E101 N102 V103 L104 D105 Y106 W107 G108 Q109 G110 T111 S112 V113 T114 V115 S116 S117

- Molecule 3: T6 light chain

Chain J: 84% 65% 30% • •

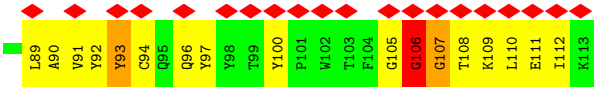
Q1 I2 V3 L4 T5 Q6 S7 P8 S9 S10 L11 A12 V13 S14 V15 G16 E17 K18 V19 T20 L21 S22 C23 K24 S25 S26 Q27 S28 L29 L30 Y31 S32 N33 N34 Q35 K36 N37 Y38 Q43 Q44 K45 S46 G47 R48 S49 P50 K51 L52 L53 L54 H55 W56 T57 S58 T59 R60 E61 S62 G63

V64 P65 D66 R67 F68 T69 G70 S71 G72 S73 G74 T75 D76 F77 T78 L79 T80 I81 S82 S83 V84 K85 A86 E87 D88 L89 A90 V91 Y92 Y93 C94 Q95 Q96 Y97 Y98 T99 Y100 P101 F104 G105 G106 G107 T108 K109 L110 E111 I112 K113

- Molecule 3: T6 light chain

Chain L: 52% 66% 29% • •

Q1 I2 V3 L4 T5 Q6 S7 P8 S9 S10 L11 A12 V13 S14 V15 G16 E17 K18 V19 T20 L21 S22 C23 K24 S25 S26 Q27 S28 L29 L30 Y31 S32 N33 N34 Q35 Y38 Q43 Q44 K45 S46 G47 R48 L53 L54 H55 W56 T57 S73 G74 T75 D76 F77 S83 A86


L89
A90
V91
Y92
Y93
C94
Q95
Q96
Y97
Y98
T99
Y100
P101
W102
T103
F104
G105
G106
G107
T108
K109
L110
E111
I112
K113

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	286245	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	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 (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	0.58	0/7858	0.81	11/10696 (0.1%)
1	B	0.59	0/7864	0.84	13/10706 (0.1%)
1	C	0.57	0/7853	0.82	14/10696 (0.1%)
2	H	0.66	0/842	0.65	0/1144
2	I	0.66	0/842	0.65	0/1144
3	J	0.70	1/907 (0.1%)	0.65	0/1231
3	L	0.70	1/907 (0.1%)	0.65	0/1231
All	All	0.59	2/27073 (0.0%)	0.80	38/36848 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	106	GLY	CA-C	6.98	1.63	1.51
3	J	106	GLY	CA-C	6.96	1.62	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	273	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	904	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	C	1014	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	1014	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	34	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	C	577	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	904	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	C	328	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	1014	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	1107	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	905	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	C	905	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	C	815	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	577	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	C	995	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	995	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	319	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	815	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	567	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	34	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	567	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	905	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	567	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	237	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	1039	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	44	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	C	646	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	815	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	1039	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	1039	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	995	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	44	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	34	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	1019	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	1107	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	190	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	44	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	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
1	A	332	ILE	Peptide
1	A	34	ARG	Sidechain
1	B	577	ARG	Sidechain
3	J	106	GLY	Mainchain
3	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	A	7687	0	7472	86	0
1	B	7691	0	7484	90	0
1	C	7678	0	7478	50	0
2	H	823	0	779	43	0
2	I	823	0	779	33	0
3	J	886	0	872	57	0
3	L	886	0	872	57	0
4	A	112	0	104	0	0
4	B	112	0	104	0	0
4	C	126	0	117	0	0
All	All	26824	0	26061	321	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 6.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PRO:CG	1:B:230:PRO:HB2	1.18	1.62
1:C:498:GLN:CB	1:C:501:TYR:CE2	1.75	1.60
1:B:456:PHE:CZ	2:H:54:GLU:HG2	1.32	1.59
1:A:521:PRO:HG2	1:B:230:PRO:CB	1.14	1.58
1:A:498:GLN:HB2	1:A:501:TYR:CE2	1.42	1.52
1:C:498:GLN:HB2	1:C:501:TYR:CE2	1.01	1.51
1:A:498:GLN:CG	1:A:501:TYR:HE2	1.23	1.49
1:A:498:GLN:HB2	1:A:501:TYR:CD2	1.46	1.48
1:C:498:GLN:CB	1:C:501:TYR:HE2	1.10	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLN:CB	1:A:501:TYR:CE2	2.06	1.35
1:A:475:ALA:HB1	2:I:52:PHE:CE1	1.60	1.35
1:A:498:GLN:CG	1:A:501:TYR:CE2	2.15	1.29
1:A:498:GLN:CB	1:A:501:TYR:HE2	1.42	1.28
1:B:498:GLN:HB2	1:B:501:TYR:CD2	1.70	1.27
3:J:94:CYS:H	3:J:106:GLY:CA	1.47	1.27
1:A:475:ALA:CB	2:I:52:PHE:CE1	2.14	1.27
3:L:94:CYS:H	3:L:106:GLY:CA	1.47	1.25
1:B:456:PHE:CZ	2:H:54:GLU:CG	2.19	1.25
1:B:498:GLN:HB2	1:B:501:TYR:CE2	1.75	1.20
1:A:521:PRO:HG3	1:B:200:TYR:CE2	1.76	1.19
1:B:486:PHE:CE1	2:H:59:SER:HB2	1.77	1.19
1:B:486:PHE:HE1	2:H:59:SER:CB	1.56	1.18
1:C:498:GLN:HB2	1:C:501:TYR:CD2	1.78	1.17
1:A:476:GLY:CA	2:I:33:ILE:HD11	1.76	1.15
1:B:456:PHE:HZ	2:H:54:GLU:CG	1.54	1.15
1:A:473:TYR:OH	2:I:32:TYR:CE1	1.99	1.15
1:B:475:ALA:HB1	2:H:52:PHE:CE1	1.82	1.15
1:B:486:PHE:HE1	2:H:59:SER:HB2	1.00	1.12
1:B:473:TYR:OH	2:H:32:TYR:CE1	2.04	1.10
1:B:486:PHE:CE1	2:H:59:SER:CB	2.34	1.10
1:B:521:PRO:HG2	1:C:230:PRO:O	1.51	1.10
1:B:456:PHE:CE1	2:H:54:GLU:HG2	1.87	1.09
1:A:476:GLY:HA2	2:I:33:ILE:HD11	1.18	1.08
3:L:94:CYS:H	3:L:106:GLY:HA2	0.94	1.08
1:A:498:GLN:HG3	1:A:501:TYR:HE2	1.18	1.08
1:B:475:ALA:HB1	2:H:52:PHE:HE1	1.16	1.08
1:A:475:ALA:CB	2:I:52:PHE:HE1	1.56	1.07
1:C:483:VAL:O	1:C:484:LYS:HG3	1.53	1.06
1:B:484:LYS:NZ	1:B:490:PHE:HD1	1.54	1.06
1:C:498:GLN:CA	1:C:501:TYR:HE2	1.67	1.06
3:L:4:LEU:HB2	3:L:105:GLY:HA3	1.34	1.06
1:C:498:GLN:CG	1:C:501:TYR:CE2	2.38	1.05
3:L:94:CYS:N	3:L:106:GLY:CA	2.20	1.05
3:L:94:CYS:N	3:L:106:GLY:HA2	1.70	1.05
1:A:498:GLN:HG3	1:A:501:TYR:CE2	1.84	1.04
3:J:94:CYS:H	3:J:106:GLY:HA2	0.94	1.04
3:J:94:CYS:N	3:J:106:GLY:HA2	1.70	1.04
3:L:93:TYR:CD2	3:L:106:GLY:CA	2.40	1.04
3:J:93:TYR:CD2	3:J:106:GLY:CA	2.40	1.04
3:J:4:LEU:HB2	3:J:105:GLY:HA3	1.34	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:CYS:N	3:J:106:GLY:CA	2.20	1.03
3:J:93:TYR:CG	3:J:106:GLY:HA3	1.97	1.00
1:A:521:PRO:CD	1:B:230:PRO:O	2.08	1.00
1:B:498:GLN:CB	1:B:501:TYR:CE2	2.42	0.99
3:L:93:TYR:CD2	3:L:106:GLY:HA3	1.98	0.98
3:J:93:TYR:CD2	3:J:106:GLY:HA3	1.98	0.98
3:L:93:TYR:CG	3:L:106:GLY:HA3	1.97	0.98
1:A:521:PRO:HG2	1:B:230:PRO:HB3	1.45	0.97
1:B:475:ALA:CB	2:H:52:PHE:CE1	2.48	0.97
1:A:475:ALA:HB2	2:I:52:PHE:CE1	1.95	0.97
1:C:498:GLN:O	1:C:501:TYR:HD2	1.46	0.97
3:J:6:GLN:OE1	3:J:106:GLY:HA2	1.65	0.97
1:A:521:PRO:CD	1:B:230:PRO:HB2	1.95	0.95
3:L:93:TYR:CA	3:L:106:GLY:HA3	1.97	0.95
3:L:6:GLN:OE1	3:L:106:GLY:HA2	1.65	0.95
1:B:486:PHE:CE1	2:H:59:SER:OG	2.20	0.94
1:C:498:GLN:HB2	1:C:501:TYR:CZ	2.01	0.94
3:J:93:TYR:CA	3:J:106:GLY:HA3	1.97	0.93
1:A:476:GLY:HA2	2:I:33:ILE:CD1	1.99	0.93
1:B:479:PRO:HB2	3:L:31:TYR:CE2	2.03	0.92
1:C:498:GLN:CA	1:C:501:TYR:CE2	2.45	0.91
1:C:498:GLN:CG	1:C:501:TYR:OH	2.18	0.91
1:B:1082:CYS:SG	1:B:1132:ILE:CD1	2.58	0.91
1:A:498:GLN:CB	1:A:501:TYR:CD2	2.42	0.91
1:A:475:ALA:HB1	2:I:52:PHE:CD1	2.05	0.89
3:J:93:TYR:CB	3:J:106:GLY:HA3	2.01	0.89
1:C:498:GLN:CG	1:C:501:TYR:HE2	1.77	0.89
3:L:93:TYR:CB	3:L:106:GLY:HA3	2.02	0.89
1:A:521:PRO:HD2	1:B:230:PRO:O	1.69	0.89
1:C:498:GLN:HG3	1:C:501:TYR:OH	1.72	0.88
1:A:498:GLN:HB2	1:A:501:TYR:HD2	1.32	0.87
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.16	0.86
3:J:6:GLN:OE1	3:J:106:GLY:CA	2.24	0.85
3:L:6:GLN:OE1	3:L:106:GLY:CA	2.24	0.85
1:C:498:GLN:CG	1:C:501:TYR:CZ	2.60	0.85
1:B:498:GLN:HB2	1:B:501:TYR:HD2	1.32	0.85
1:B:484:LYS:HZ3	1:B:490:PHE:HD1	1.21	0.84
1:C:498:GLN:N	1:C:501:TYR:CE2	2.45	0.84
1:B:1082:CYS:SG	1:B:1132:ILE:HD11	2.18	0.83
3:J:93:TYR:HA	3:J:106:GLY:CA	2.09	0.82
3:L:93:TYR:HA	3:L:106:GLY:CA	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:CYS:SG	1:B:642:VAL:HG11	2.18	0.82
1:B:487:ASN:ND2	3:L:100:TYR:HE2	1.78	0.82
3:L:16:GLY:HA2	3:L:83:SER:HA	1.62	0.81
1:B:484:LYS:NZ	1:B:490:PHE:CD1	2.46	0.81
3:J:16:GLY:HA2	3:J:83:SER:HA	1.62	0.81
1:A:521:PRO:HD3	1:B:230:PRO:O	1.81	0.81
1:A:521:PRO:CB	1:B:230:PRO:HB2	2.11	0.81
1:A:489:TYR:OH	2:I:57:ASP:OD1	2.00	0.80
1:B:475:ALA:CB	2:H:52:PHE:HE1	1.87	0.80
1:A:473:TYR:OH	2:I:32:TYR:CZ	2.35	0.80
1:A:475:ALA:HB1	2:I:52:PHE:HE1	1.02	0.79
1:B:487:ASN:ND2	3:L:100:TYR:CE2	2.50	0.79
1:B:476:GLY:HA2	2:H:33:ILE:HD11	1.64	0.79
3:L:93:TYR:CG	3:L:106:GLY:CA	2.64	0.79
1:A:521:PRO:HG3	1:B:200:TYR:HE2	1.43	0.78
2:H:98:ARG:HB2	2:H:106:TYR:HB3	1.65	0.78
1:C:483:VAL:O	1:C:484:LYS:CG	2.32	0.77
2:I:98:ARG:HB2	2:I:106:TYR:HB3	1.65	0.77
1:B:456:PHE:CZ	2:H:54:GLU:CB	2.68	0.77
3:L:93:TYR:CA	3:L:106:GLY:CA	2.63	0.76
1:A:476:GLY:CA	2:I:33:ILE:CD1	2.62	0.76
3:J:93:TYR:CA	3:J:106:GLY:CA	2.63	0.76
1:A:521:PRO:CG	1:B:200:TYR:CE2	2.65	0.76
3:J:93:TYR:CG	3:J:106:GLY:CA	2.64	0.76
1:A:479:PRO:HD2	3:J:98:TYR:O	1.87	0.74
1:B:479:PRO:CB	3:L:31:TYR:CE2	2.70	0.74
1:A:1082:CYS:SG	1:A:1132:ILE:CD1	2.76	0.73
1:A:521:PRO:HG2	1:B:230:PRO:CA	2.16	0.73
3:L:38:TYR:HB3	3:L:97:TYR:HB3	1.71	0.72
1:B:479:PRO:HG2	3:L:31:TYR:CD2	2.25	0.72
1:C:498:GLN:O	1:C:501:TYR:CD2	2.37	0.72
3:J:93:TYR:CD2	3:J:106:GLY:C	2.63	0.72
3:L:6:GLN:OE1	3:L:106:GLY:C	2.28	0.71
1:B:498:GLN:CB	1:B:501:TYR:CD2	2.64	0.71
3:L:93:TYR:CD2	3:L:106:GLY:C	2.63	0.71
3:J:6:GLN:OE1	3:J:106:GLY:C	2.28	0.71
3:J:38:TYR:HB3	3:J:97:TYR:HB3	1.71	0.71
1:C:498:GLN:N	1:C:501:TYR:HE2	1.85	0.71
3:L:93:TYR:CD2	3:L:106:GLY:N	2.59	0.70
1:A:489:TYR:OH	2:I:57:ASP:HA	1.92	0.70
3:J:93:TYR:CD2	3:J:106:GLY:N	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLN:HG3	1:A:501:TYR:CZ	2.28	0.69
1:C:498:GLN:HG2	1:C:501:TYR:OH	1.91	0.69
3:J:94:CYS:N	3:J:106:GLY:HA3	2.06	0.69
1:A:521:PRO:CG	1:B:230:PRO:CB	2.07	0.68
3:L:94:CYS:N	3:L:106:GLY:HA3	2.06	0.68
1:B:489:TYR:OH	2:H:57:ASP:OD1	2.11	0.68
3:J:6:GLN:OE1	3:J:107:GLY:N	2.27	0.68
3:J:93:TYR:HA	3:J:106:GLY:HA3	1.74	0.68
3:L:6:GLN:OE1	3:L:107:GLY:N	2.27	0.67
1:B:484:LYS:HZ1	1:B:490:PHE:HD1	1.42	0.66
1:B:617:CYS:SG	1:B:642:VAL:CG1	2.83	0.66
2:H:36:TRP:HE1	2:H:51:ILE:HD11	1.61	0.66
1:A:498:GLN:HG2	1:A:501:TYR:CE2	2.29	0.66
2:I:36:TRP:HE1	2:I:51:ILE:HD11	1.61	0.65
1:A:475:ALA:CB	2:I:52:PHE:CD1	2.72	0.65
1:C:498:GLN:HG2	1:C:501:TYR:CE2	2.31	0.65
1:B:486:PHE:CZ	2:H:59:SER:CB	2.79	0.65
1:A:479:PRO:HB3	3:J:31:TYR:CZ	2.33	0.64
1:A:456:PHE:CE1	2:I:54:GLU:OE2	2.41	0.64
1:B:479:PRO:HB2	3:L:31:TYR:CZ	2.32	0.64
3:L:89:LEU:HA	3:L:110:LEU:HD23	1.81	0.62
1:B:440:ASN:C	1:B:442:ASP:H	2.01	0.62
2:I:51:ILE:HG12	2:I:70:LEU:HD13	1.81	0.62
1:B:808:ASP:HB3	1:B:811:LYS:HE2	1.82	0.62
3:J:93:TYR:CG	3:J:106:GLY:C	2.73	0.62
3:L:93:TYR:CG	3:L:106:GLY:C	2.73	0.61
2:H:51:ILE:HG12	2:H:70:LEU:HD13	1.81	0.61
3:L:43:GLN:HB2	3:L:53:LEU:HD23	1.82	0.61
1:A:454:ARG:HG3	1:A:491:PRO:HB2	1.83	0.61
3:J:89:LEU:HA	3:J:110:LEU:HD23	1.81	0.60
1:A:476:GLY:HA3	2:I:33:ILE:HD11	1.75	0.60
1:B:476:GLY:CA	2:H:33:ILE:HD11	2.32	0.60
1:C:391:CYS:HA	1:C:525:CYS:HA	1.83	0.60
1:C:498:GLN:HG3	1:C:501:TYR:CZ	2.35	0.60
3:J:43:GLN:HB2	3:J:53:LEU:HD23	1.82	0.60
3:L:4:LEU:HD11	3:L:96:GLN:HB3	1.84	0.59
3:L:93:TYR:HA	3:L:106:GLY:HA3	1.74	0.58
1:A:391:CYS:HA	1:A:525:CYS:HA	1.83	0.58
3:J:4:LEU:HD11	3:J:96:GLN:HB3	1.84	0.58
2:H:34:ILE:HA	2:H:98:ARG:HA	1.85	0.58
2:I:87:THR:H	2:I:90:ASP:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ALA:O	2:I:32:TYR:HB3	2.03	0.58
1:B:475:ALA:HB2	2:H:52:PHE:CE1	2.36	0.57
1:A:1082:CYS:SG	1:A:1132:ILE:HD13	2.43	0.57
1:B:379:CYS:HA	1:B:432:CYS:HA	1.86	0.57
2:H:87:THR:H	2:H:90:ASP:HB2	1.68	0.57
2:I:34:ILE:HA	2:I:98:ARG:HA	1.85	0.57
1:B:456:PHE:HZ	2:H:54:GLU:CB	2.08	0.57
1:A:454:ARG:NH2	1:A:469:SER:O	2.38	0.57
1:A:442:ASP:HB3	1:A:509:ARG:HH21	1.69	0.56
1:B:477:SER:OG	3:L:97:TYR:CE2	2.57	0.56
1:C:927:PHE:CZ	1:C:931:ILE:HD11	2.40	0.56
1:A:1082:CYS:SG	1:A:1132:ILE:HD11	2.45	0.56
1:A:379:CYS:HA	1:A:432:CYS:HA	1.88	0.56
1:C:410:ILE:HD13	1:C:419:ALA:HB2	1.88	0.56
1:C:498:GLN:CA	1:C:501:TYR:CD2	2.89	0.55
1:A:1032:CYS:HG	1:A:1043:CYS:HG	1.55	0.55
1:B:391:CYS:HA	1:B:525:CYS:HA	1.88	0.55
1:A:811:LYS:HG2	1:A:814:LYS:H	1.72	0.55
1:A:1116:THR:HG22	1:A:1138:TYR:HD2	1.72	0.54
3:J:2:ILE:HG23	3:J:26:SER:HB3	1.89	0.54
3:L:2:ILE:HG23	3:L:26:SER:HB3	1.89	0.54
3:L:93:TYR:CE2	3:L:106:GLY:C	2.82	0.54
1:A:394:ASN:HB2	1:A:516:GLU:HB3	1.88	0.53
3:J:93:TYR:C	3:J:106:GLY:HA3	2.28	0.53
1:B:454:ARG:NH2	1:B:469:SER:O	2.41	0.53
1:C:379:CYS:HA	1:C:432:CYS:HA	1.89	0.53
1:C:483:VAL:C	1:C:484:LYS:HG3	2.27	0.53
3:J:94:CYS:SG	3:J:105:GLY:C	2.88	0.53
3:L:94:CYS:SG	3:L:105:GLY:C	2.88	0.53
3:J:93:TYR:CE2	3:J:106:GLY:C	2.82	0.53
3:L:93:TYR:C	3:L:106:GLY:HA3	2.28	0.52
1:A:1098:ASN:ND2	1:A:1100:THR:OG1	2.42	0.52
1:B:456:PHE:CE1	2:H:54:GLU:CG	2.69	0.52
1:B:456:PHE:HZ	2:H:54:GLU:HG2	0.77	0.52
1:B:475:ALA:HB1	2:H:52:PHE:CD1	2.42	0.52
1:C:498:GLN:CB	1:C:501:TYR:CD2	2.61	0.52
1:A:809:PRO:HA	1:A:814:LYS:HE3	1.92	0.52
1:B:440:ASN:C	1:B:442:ASP:N	2.63	0.52
1:B:489:TYR:OH	2:H:57:ASP:HA	2.09	0.51
1:B:486:PHE:HZ	2:H:50:ALA:HB3	1.74	0.51
1:B:479:PRO:HG2	3:L:31:TYR:CG	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:93:TYR:CE2	3:L:106:GLY:O	2.64	0.51
2:I:38:LYS:HB2	2:I:48:ILE:HD11	1.92	0.51
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.92	0.51
1:B:486:PHE:CZ	2:H:59:SER:OG	2.53	0.50
3:J:93:TYR:CE2	3:J:106:GLY:O	2.64	0.50
1:A:481:ASN:CG	3:J:31:TYR:OH	2.49	0.50
1:A:475:ALA:O	2:I:32:TYR:CB	2.60	0.50
1:B:473:TYR:OH	2:H:32:TYR:CZ	2.60	0.50
1:A:476:GLY:HA2	2:I:33:ILE:CG1	2.40	0.50
2:I:44:GLY:HA3	3:J:93:TYR:OH	2.12	0.50
1:B:458:LYS:NZ	1:B:471:GLU:OE1	2.45	0.49
1:C:357:ARG:NH2	1:C:394:ASN:OD1	2.45	0.49
1:A:479:PRO:CB	3:J:31:TYR:CE1	2.95	0.49
1:C:353:TRP:HZ3	1:C:355:ARG:HB2	1.78	0.49
2:H:44:GLY:HA3	3:L:93:TYR:OH	2.12	0.49
3:J:44:GLN:HB2	3:J:91:VAL:HB	1.95	0.49
3:L:93:TYR:C	3:L:106:GLY:CA	2.81	0.49
1:A:388:ASN:O	1:A:527:PRO:HD2	2.13	0.49
1:B:498:GLN:CD	1:B:501:TYR:OH	2.37	0.49
1:A:521:PRO:HG3	1:B:200:TYR:CZ	2.38	0.49
3:L:44:GLN:HB2	3:L:91:VAL:HB	1.95	0.48
1:A:498:GLN:HG3	1:A:501:TYR:OH	2.14	0.48
1:B:477:SER:HG	3:L:97:TYR:HE2	1.53	0.48
3:J:92:TYR:HE2	3:J:110:LEU:HD22	1.79	0.48
1:A:519:HIS:O	1:B:200:TYR:OH	2.32	0.48
1:C:974:SER:HB2	1:C:983:ARG:HH21	1.78	0.48
3:J:55:HIS:C	3:J:57:THR:H	2.17	0.47
3:L:92:TYR:HE2	3:L:110:LEU:HD22	1.79	0.47
1:C:617:CYS:SG	1:C:642:VAL:CG1	3.02	0.47
1:C:490:PHE:O	1:C:493:GLN:NE2	2.47	0.47
1:C:498:GLN:C	1:C:501:TYR:CD2	2.88	0.47
1:A:351:TYR:OH	1:A:469:SER:O	2.32	0.47
1:C:498:GLN:C	1:C:501:TYR:HD2	2.17	0.47
3:L:55:HIS:C	3:L:57:THR:H	2.17	0.47
1:B:1032:CYS:HG	1:B:1043:CYS:HG	1.58	0.47
2:H:104:LEU:HD13	2:H:104:LEU:HA	1.79	0.47
1:C:346:ARG:HH21	1:C:450:ASN:HB3	1.80	0.46
1:A:650:LEU:HD13	1:A:650:LEU:HA	1.77	0.46
1:B:81:ASN:N	1:B:265:TYR:HH	2.13	0.46
2:H:61:SER:HB3	2:H:64:PHE:HD2	1.81	0.46
1:A:478:THR:HG21	3:J:100:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ASN:CG	3:J:31:TYR:HH	2.18	0.45
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.99	0.45
1:A:458:LYS:HE2	1:A:474:GLN:H	1.81	0.45
3:J:11:LEU:HD11	3:J:21:LEU:HB3	1.99	0.45
1:A:479:PRO:HB2	3:J:31:TYR:CE1	2.52	0.45
1:A:479:PRO:CD	3:J:98:TYR:O	2.63	0.45
2:I:61:SER:HB3	2:I:64:PHE:HD2	1.81	0.45
3:L:11:LEU:HD11	3:L:21:LEU:HB3	1.99	0.45
1:C:498:GLN:HG2	1:C:501:TYR:CZ	2.42	0.44
1:B:486:PHE:HE2	3:L:100:TYR:HH	1.46	0.44
2:H:60:TYR:HE1	2:H:70:LEU:HG	1.83	0.44
2:I:60:TYR:HE1	2:I:70:LEU:HG	1.83	0.44
1:C:498:GLN:HG3	1:C:501:TYR:HH	1.78	0.43
1:A:353:TRP:HH2	1:A:355:ARG:HH21	1.65	0.43
1:A:521:PRO:CB	1:B:230:PRO:CB	2.85	0.43
1:A:479:PRO:CB	3:J:31:TYR:CZ	3.01	0.43
1:B:456:PHE:CE1	2:H:54:GLU:CD	2.92	0.43
3:J:93:TYR:C	3:J:106:GLY:CA	2.81	0.43
3:L:38:TYR:HD2	3:L:97:TYR:HD2	1.67	0.43
1:A:477:SER:HB3	3:J:97:TYR:CE2	2.53	0.43
1:B:424:LYS:NZ	1:B:425:LEU:O	2.51	0.43
3:J:38:TYR:HD2	3:J:97:TYR:HD2	1.67	0.43
2:I:38:LYS:NZ	2:I:90:ASP:HA	2.34	0.43
3:L:43:GLN:HG2	3:L:90:ALA:HB3	2.01	0.43
3:L:45:LYS:HB2	3:L:48:ARG:HG3	2.01	0.43
1:C:1032:CYS:HG	1:C:1043:CYS:HG	1.65	0.43
2:H:38:LYS:NZ	2:H:90:ASP:HA	2.34	0.42
1:B:479:PRO:CG	3:L:31:TYR:CD2	2.99	0.42
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.02	0.42
1:B:487:ASN:ND2	3:L:100:TYR:CZ	2.88	0.42
2:H:97:ALA:HA	2:H:107:TRP:HA	2.01	0.42
3:J:45:LYS:HB2	3:J:48:ARG:HG3	2.01	0.42
3:J:43:GLN:HG2	3:J:90:ALA:HB3	2.01	0.42
1:A:476:GLY:HA3	2:I:33:ILE:CD1	2.42	0.42
1:A:487:ASN:HB2	3:J:100:TYR:HE2	1.84	0.42
1:A:387:LEU:C	1:A:387:LEU:HD12	2.40	0.42
1:A:481:ASN:OD1	3:J:31:TYR:OH	2.37	0.41
1:C:1083:HIS:CG	1:C:1084:ASP:H	2.37	0.41
3:L:43:GLN:HG2	3:L:90:ALA:CB	2.50	0.41
3:L:94:CYS:O	3:L:106:GLY:N	2.53	0.41
1:B:1081:ILE:HD11	1:B:1115:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PHE:HZ	1:C:513:LEU:HD11	1.84	0.41
2:I:37:VAL:HG11	2:I:45:LEU:HB3	2.02	0.41
1:B:355:ARG:HH22	1:B:464:PHE:HB3	1.85	0.41
1:C:458:LYS:HE3	1:C:474:GLN:HG2	2.02	0.41
3:J:43:GLN:HG2	3:J:90:ALA:CB	2.50	0.41
1:C:356:LYS:HB3	1:C:397:ALA:HB3	2.02	0.41
1:C:1135:ASN:HD22	1:C:1135:ASN:HA	1.71	0.41
2:H:37:VAL:HG11	2:H:45:LEU:HB3	2.02	0.41
2:H:62:GLN:H	2:H:62:GLN:HG3	1.56	0.41
3:L:7:SER:HB2	3:L:8:PRO:HA	2.02	0.41
1:C:523:THR:HG23	1:C:524:VAL:HG23	2.03	0.41
2:I:97:ALA:HA	2:I:107:TRP:HA	2.01	0.41
3:J:94:CYS:O	3:J:106:GLY:N	2.53	0.41
1:C:718:PHE:HZ	1:C:923:ILE:HD11	1.86	0.41
1:B:378:LYS:HE2	1:B:378:LYS:HB2	1.90	0.41
1:C:331:ASN:OD1	1:C:331:ASN:N	2.53	0.41
1:C:984:LEU:HD13	1:C:988:GLU:HB2	2.02	0.41
3:J:7:SER:HB2	3:J:8:PRO:HA	2.03	0.41
1:A:811:LYS:HZ3	1:A:814:LYS:HG2	1.86	0.40
3:L:94:CYS:SG	3:L:105:GLY:O	2.79	0.40
1:B:521:PRO:CG	1:C:230:PRO:O	2.43	0.40
3:J:94:CYS:SG	3:J:105:GLY:O	2.79	0.40
1:A:490:PHE:HE2	1:A:492:LEU:HB2	1.86	0.40
1:A:521:PRO:HD2	1:B:230:PRO:HB2	1.95	0.40
1:B:304:LYS:HD3	1:B:304:LYS:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	975/1280 (76%)	893 (92%)	78 (8%)	4 (0%)	34 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	975/1280 (76%)	891 (91%)	80 (8%)	4 (0%)	34	67
1	C	976/1280 (76%)	899 (92%)	74 (8%)	3 (0%)	41	72
2	H	105/117 (90%)	97 (92%)	8 (8%)	0	100	100
2	I	105/117 (90%)	97 (92%)	8 (8%)	0	100	100
3	J	111/113 (98%)	108 (97%)	2 (2%)	1 (1%)	17	50
3	L	111/113 (98%)	108 (97%)	2 (2%)	1 (1%)	17	50
All	All	3358/4300 (78%)	3093 (92%)	252 (8%)	13 (0%)	38	67

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	986	PRO
1	A	197	ILE
1	C	112	SER
1	B	137	ASN
1	B	334	ASN
3	J	107	GLY
3	L	107	GLY
1	A	198	ASP
1	C	801	ASN
1	B	536	ASN
1	B	571	ASP
1	C	812	PRO
1	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	A	849/1103 (77%)	834 (98%)	15 (2%)	59	77
1	B	851/1103 (77%)	843 (99%)	8 (1%)	78	87
1	C	848/1103 (77%)	839 (99%)	9 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	92/101 (91%)	78 (85%)	14 (15%)	3	12
2	I	92/101 (91%)	78 (85%)	14 (15%)	3	12
3	J	100/100 (100%)	91 (91%)	9 (9%)	9	32
3	L	100/100 (100%)	91 (91%)	9 (9%)	9	32
All	All	2932/3711 (79%)	2854 (97%)	78 (3%)	48	70

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	THR
1	A	333	THR
1	A	369	TYR
1	A	423	TYR
1	A	483	VAL
1	A	484	LYS
1	A	618	THR
1	A	650	LEU
1	A	657	ASN
1	A	886	TRP
1	A	907	ASN
1	A	935	GLN
1	A	983	ARG
1	A	988	GLU
1	A	990	GLU
1	B	265	TYR
1	B	336	CYS
1	B	377	PHE
1	B	429	PHE
1	B	574	ASP
1	B	617	CYS
1	B	935	GLN
1	B	985	ASP
1	C	304	LYS
1	C	331	ASN
1	C	377	PHE
1	C	565	PHE
1	C	907	ASN
1	C	988	GLU
1	C	1058	HIS
1	C	1126	CYS
1	C	1135	ASN

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

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Mol	Chain	Res	Type
3	L	108	THR
3	L	109	LYS
3	L	111	GLU
3	L	112	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	409	GLN
1	A	414	GLN
1	A	474	GLN
1	B	414	GLN
1	B	487	ASN
1	B	498	GLN
1	C	334	ASN
1	C	414	GLN
1	C	474	GLN
1	C	498	GLN
1	C	1135	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1305	1	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.69	0
4	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.81	1 (5%)
4	NAG	B	1308	1	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	B	1304	1	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	C	1306	1	14,14,15	0.25	0	17,19,21	1.00	1 (5%)
4	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
4	NAG	A	1306	1	14,14,15	0.28	0	17,19,21	0.69	0
4	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	1.10	2 (11%)
4	NAG	C	1308	1	14,14,15	0.29	0	17,19,21	1.15	2 (11%)
4	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.62	0
4	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	A	1307	1	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.94	1 (5%)
4	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.72	0
4	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.95	0
4	NAG	C	1309	1	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	B	1306	1	14,14,15	0.25	0	17,19,21	0.98	1 (5%)
4	NAG	A	1303	1	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	A	1308	1	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
4	NAG	B	1301	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.76	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	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	1/6/23/26	0/1/1/1

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

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Mol	Chain	Res	Type	Atoms
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.

No monomer is involved in short contacts.

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.

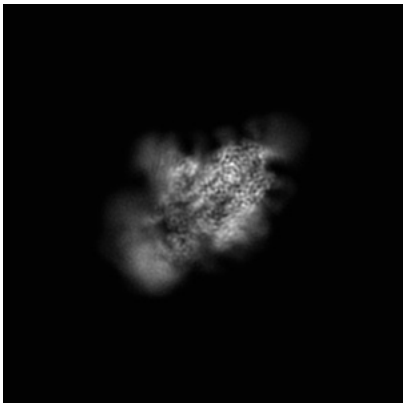
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31624. These allow visual inspection of the internal detail of the map and identification of artifacts.

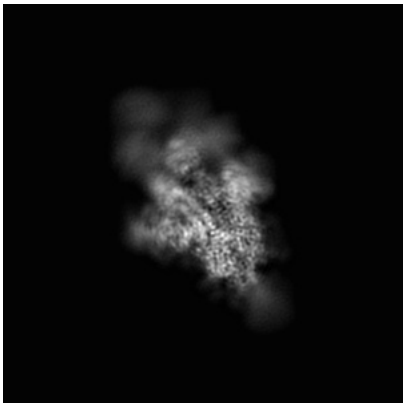
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

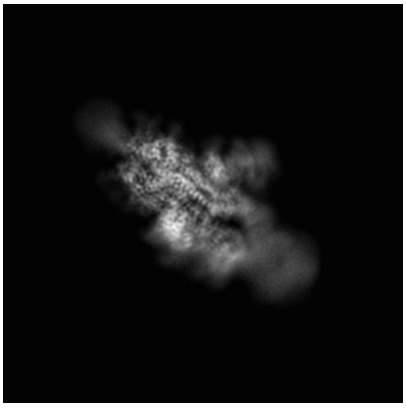
6.1.1 Primary map



X



Y

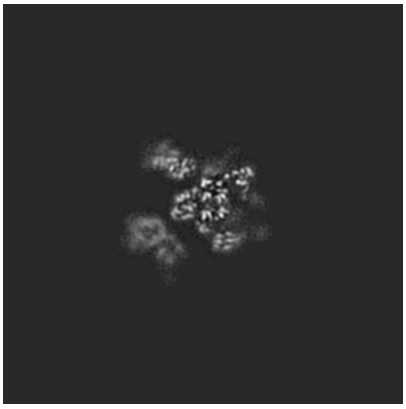


Z

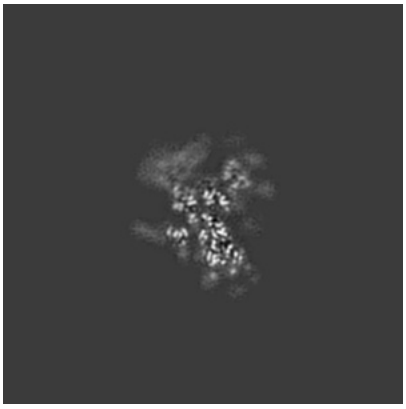
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

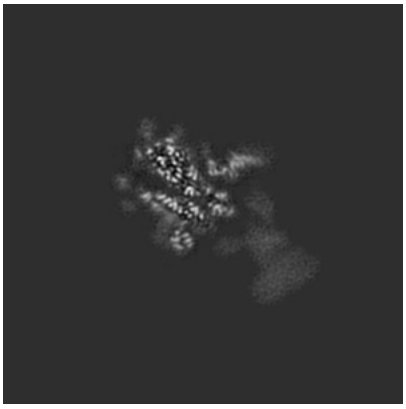
6.2.1 Primary map



X Index: 160



Y Index: 160

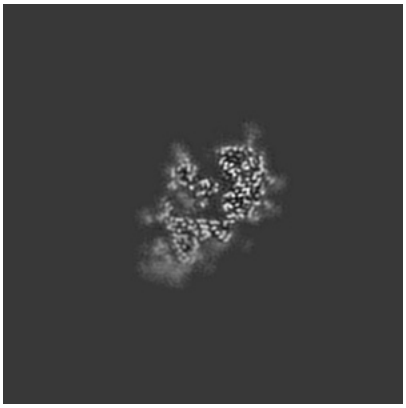


Z Index: 160

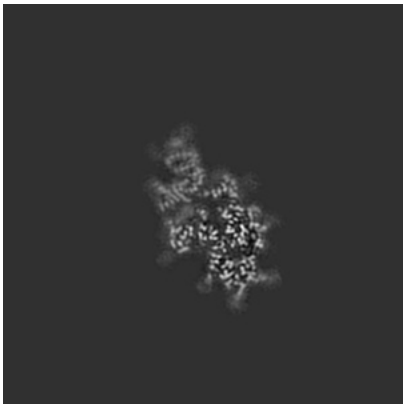
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

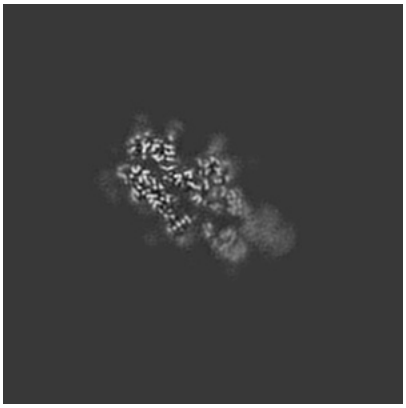
6.3.1 Primary map



X Index: 135



Y Index: 182



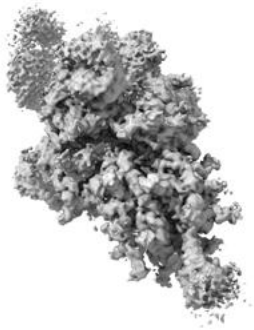
Z Index: 180

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

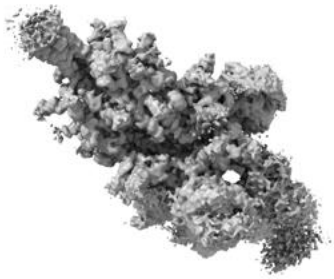
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

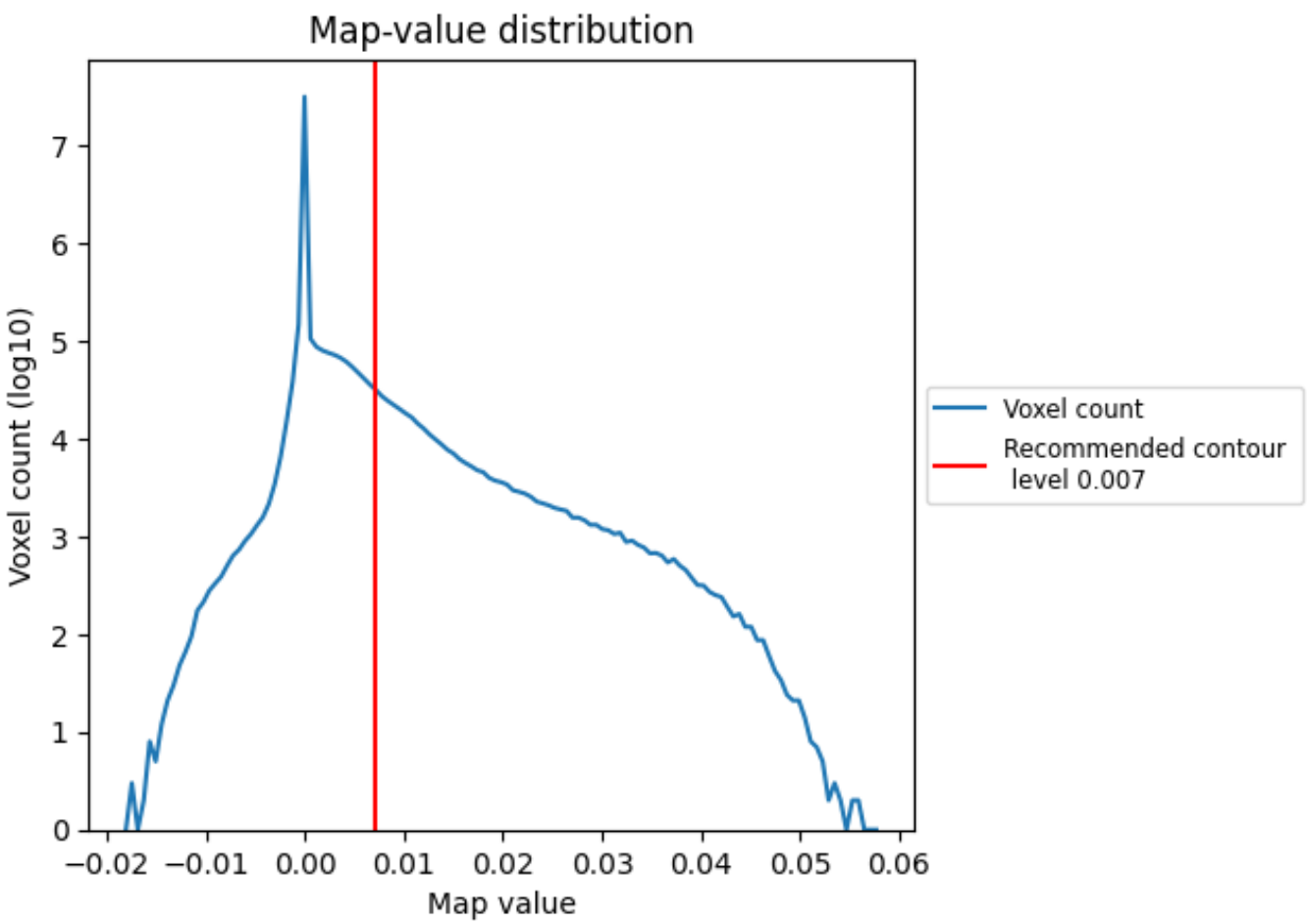
6.5 Mask visualisation (i)

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

7 Map analysis (i)

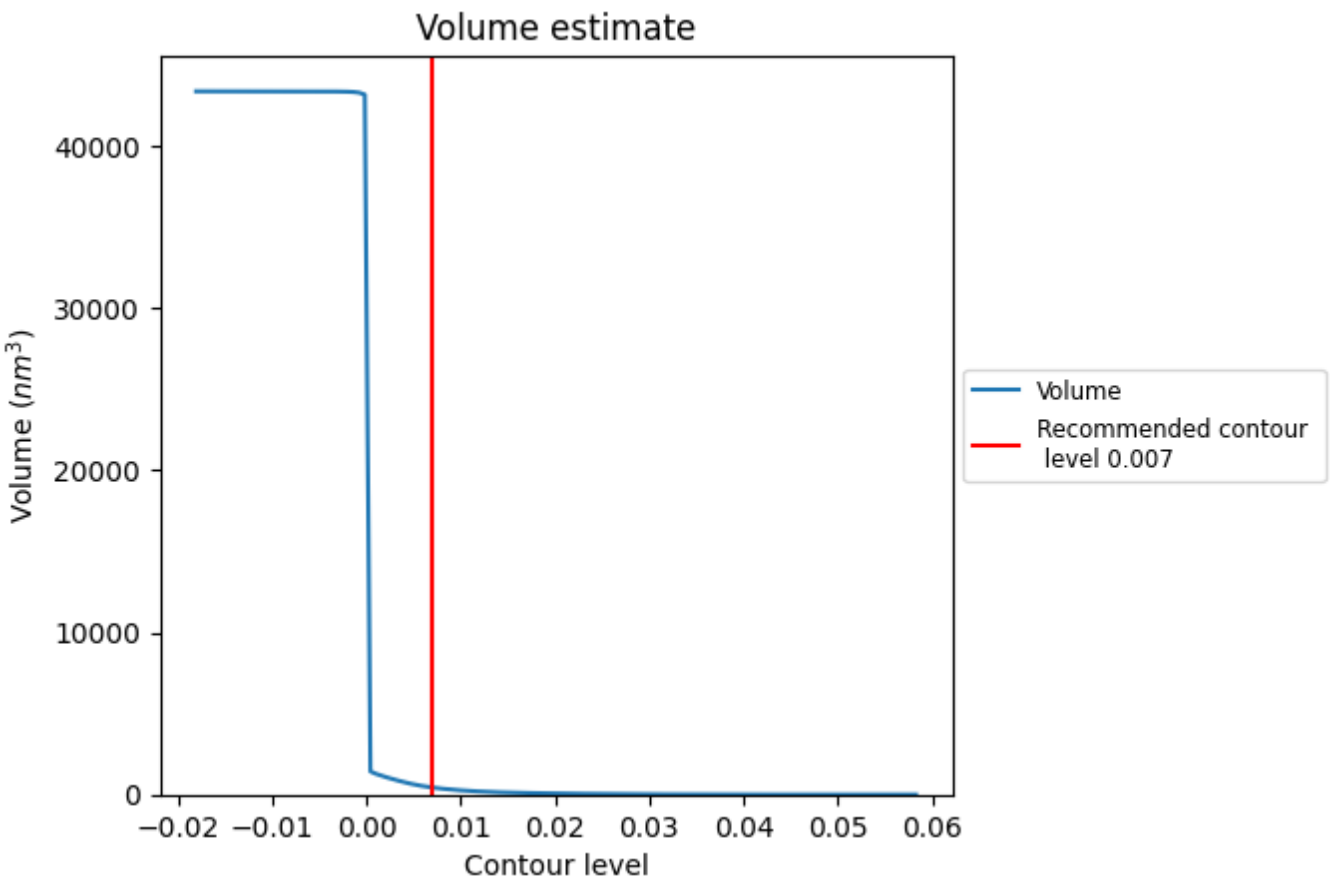
This section contains the results of statistical analysis of the map.

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.

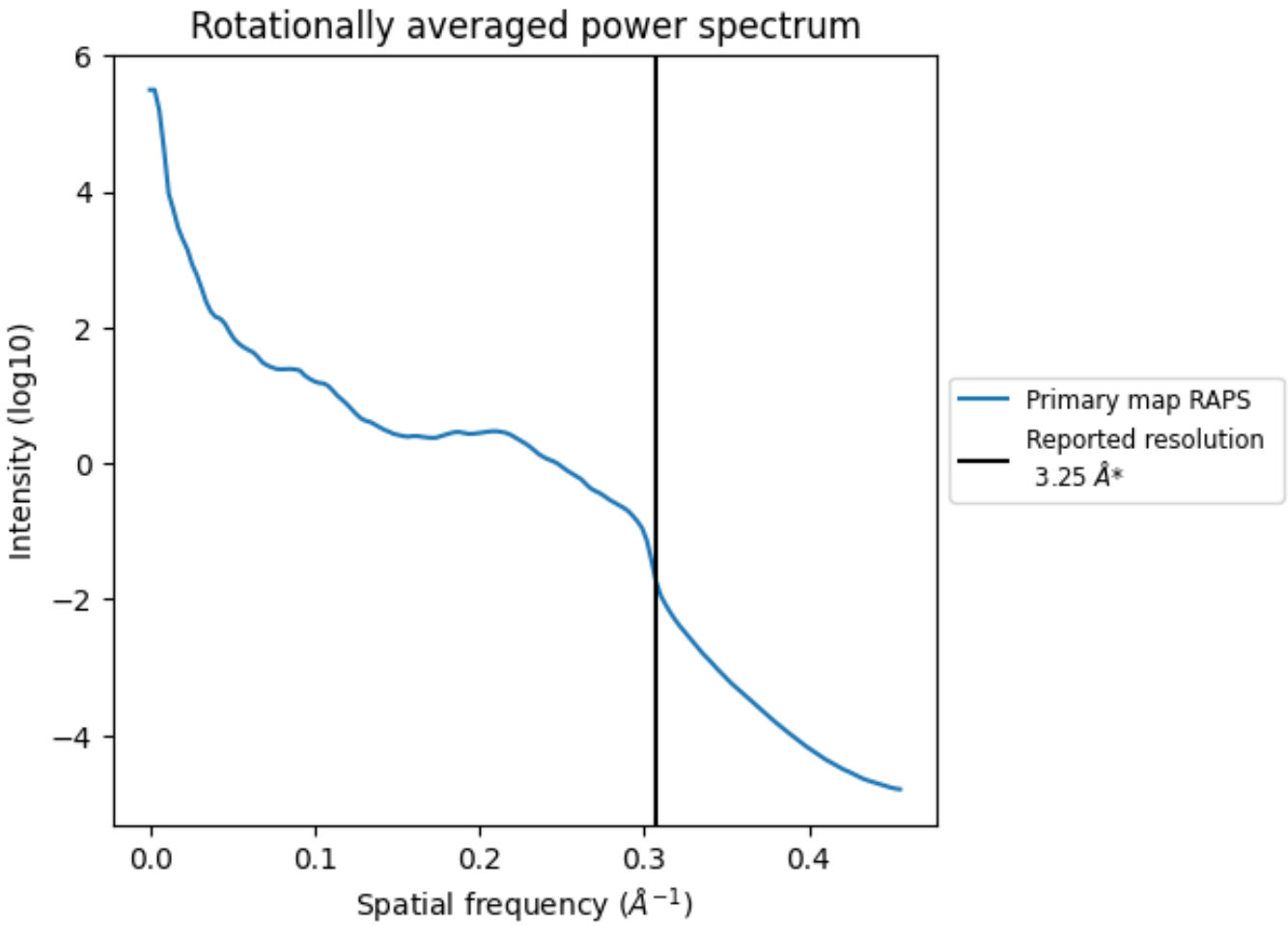
7.2 Volume estimate (i)



The volume at the recommended contour level is 433 nm^3; this corresponds to an approximate mass of 391 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 0.308 Å^{-1}

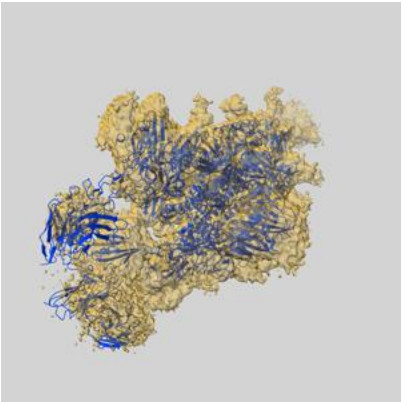
8 Fourier-Shell correlation (i)

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

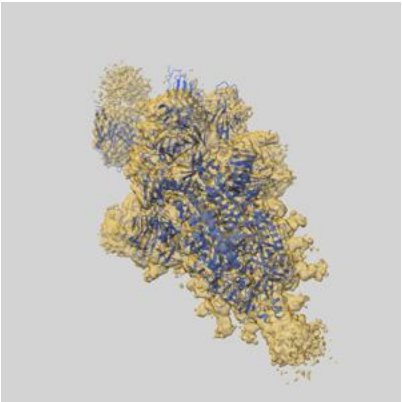
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31624 and PDB model 7FJN. Per-residue inclusion information can be found in section 3 on page 12.

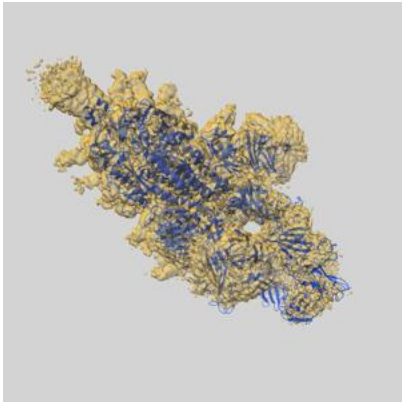
9.1 Map-model overlay (i)



X



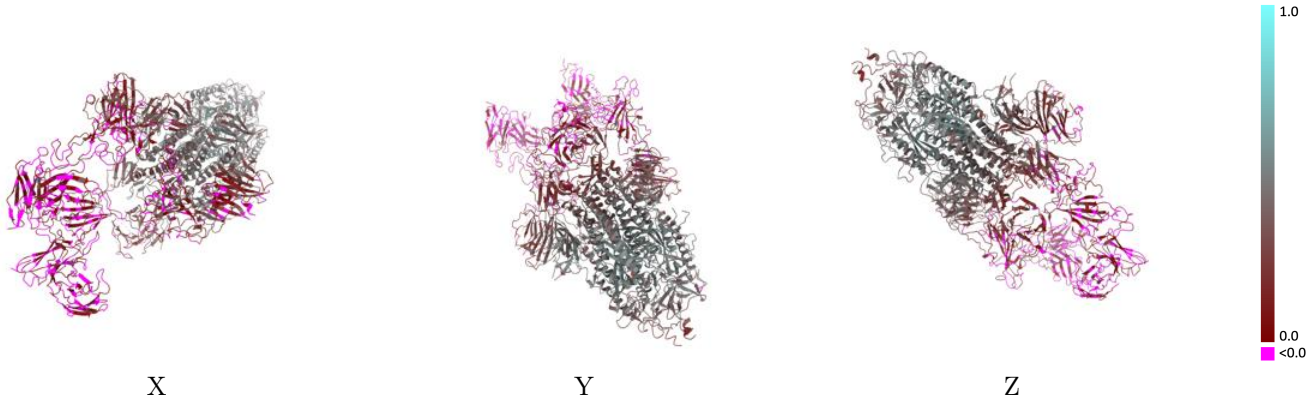
Y



Z

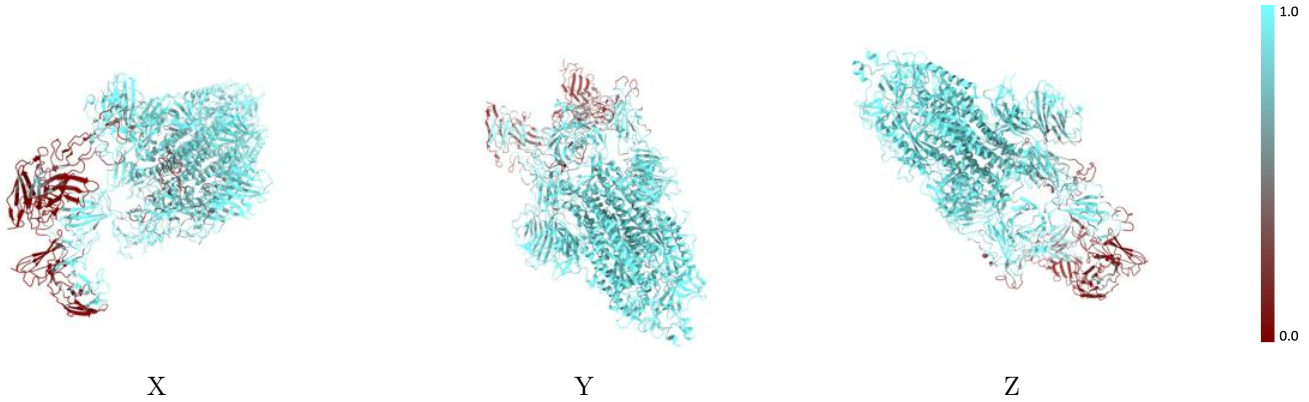
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



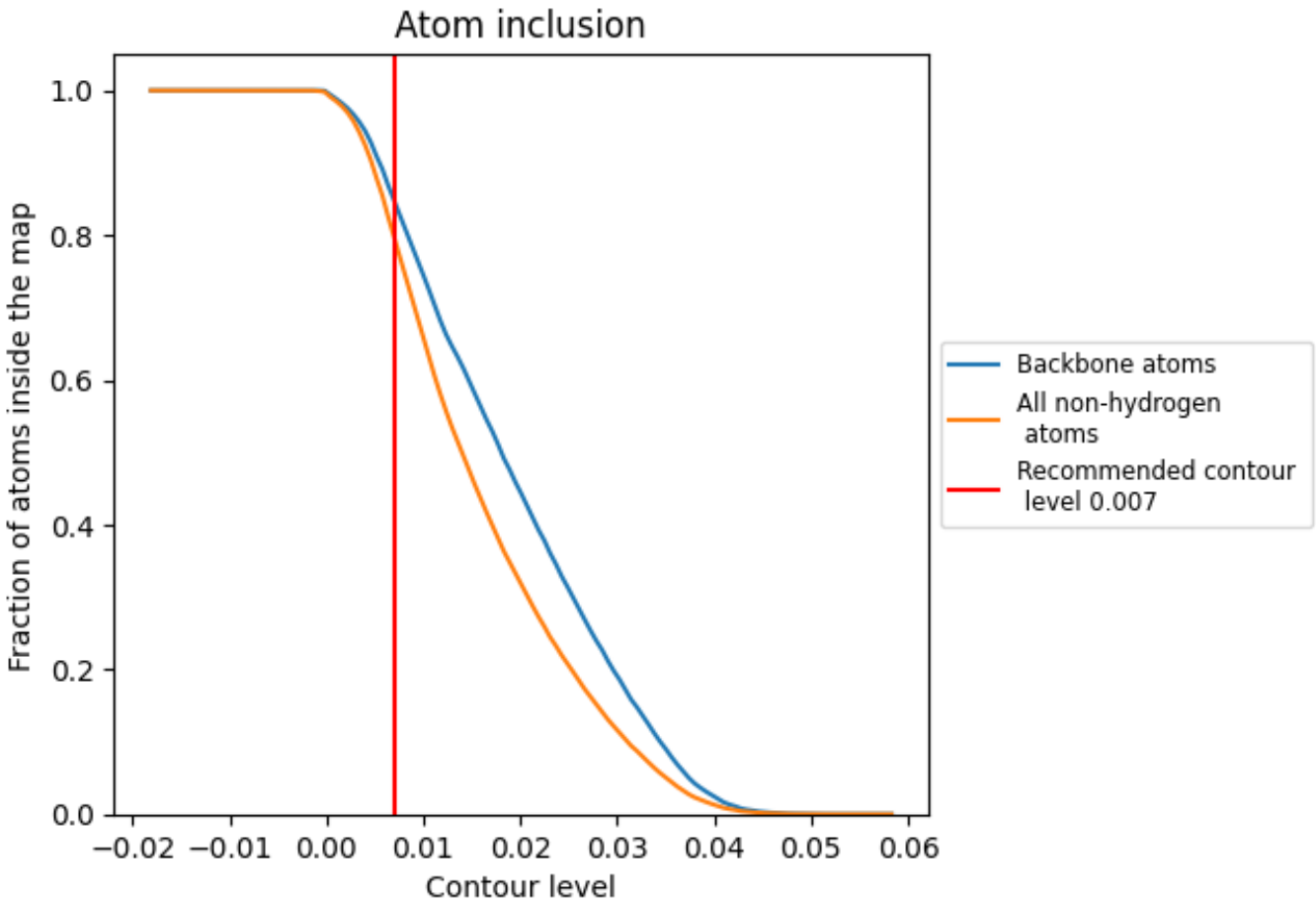
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion (i)



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 (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7969	0.2700
A	0.8616	0.2910
B	0.8878	0.3010
C	0.8717	0.3260
H	0.3473	0.0260
I	0.0952	0.0320
J	0.1484	0.0060
L	0.4776	0.0100