



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 10:12 pm BST

PDB ID : 7R15  
EMDB ID : EMD-14231  
Title : Alpha Variant SARS-CoV-2 Spike with 2 Erect RBDs  
Authors : Benton, D.J.; Wrobel, A.G.; Gamblin, S.J.  
Deposited on : 2022-02-02  
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

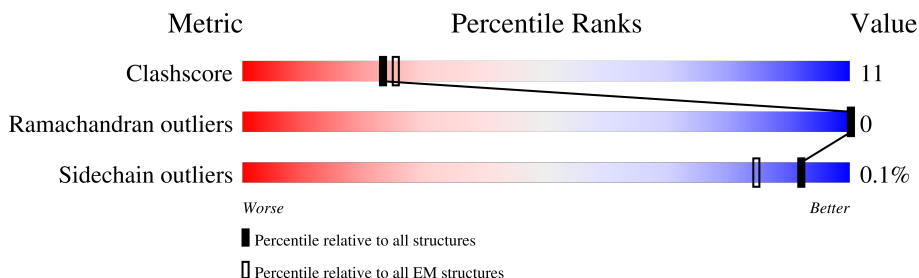
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1284	
1	B	1284	
1	C	1284	
2	D	2	
2	E	2	
2	F	2	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24100 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	983	Total	C	N	O	S	0	0
			7702	4930	1280	1459	33		
1	B	1020	Total	C	N	O	S	0	0
			7988	5106	1331	1515	36		
1	C	997	Total	C	N	O	S	0	0
			7808	4997	1296	1480	35		

There are 249 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP A0A7T8R415
A	-29	GLY	-	expression tag	UNP A0A7T8R415
A	-28	ILE	-	expression tag	UNP A0A7T8R415
A	-27	LEU	-	expression tag	UNP A0A7T8R415
A	-26	PRO	-	expression tag	UNP A0A7T8R415
A	-25	SER	-	expression tag	UNP A0A7T8R415
A	-24	PRO	-	expression tag	UNP A0A7T8R415
A	-23	GLY	-	expression tag	UNP A0A7T8R415
A	-22	MET	-	expression tag	UNP A0A7T8R415
A	-21	PRO	-	expression tag	UNP A0A7T8R415
A	-20	ALA	-	expression tag	UNP A0A7T8R415
A	-19	LEU	-	expression tag	UNP A0A7T8R415
A	-18	LEU	-	expression tag	UNP A0A7T8R415
A	-17	SER	-	expression tag	UNP A0A7T8R415
A	-16	LEU	-	expression tag	UNP A0A7T8R415
A	-15	VAL	-	expression tag	UNP A0A7T8R415
A	-14	SER	-	expression tag	UNP A0A7T8R415
A	-13	LEU	-	expression tag	UNP A0A7T8R415
A	-12	LEU	-	expression tag	UNP A0A7T8R415
A	-11	SER	-	expression tag	UNP A0A7T8R415
A	-10	VAL	-	expression tag	UNP A0A7T8R415
A	-9	LEU	-	expression tag	UNP A0A7T8R415
A	-8	LEU	-	expression tag	UNP A0A7T8R415
A	-7	MET	-	expression tag	UNP A0A7T8R415

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A0A7T8R415
A	-5	CYS	-	expression tag	UNP A0A7T8R415
A	-4	VAL	-	expression tag	UNP A0A7T8R415
A	-3	ALA	-	expression tag	UNP A0A7T8R415
A	-2	GLU	-	expression tag	UNP A0A7T8R415
A	-1	THR	-	expression tag	UNP A0A7T8R415
A	0	GLY	-	expression tag	UNP A0A7T8R415
A	682	SER	ARG	variant	UNP A0A7T8R415
A	685	SER	ARG	variant	UNP A0A7T8R415
A	986	PRO	LYS	variant	UNP A0A7T8R415
A	987	PRO	VAL	variant	UNP A0A7T8R415
A	1209	SER	-	expression tag	UNP A0A7T8R415
A	1210	GLY	-	expression tag	UNP A0A7T8R415
A	1211	ARG	-	expression tag	UNP A0A7T8R415
A	1212	GLU	-	expression tag	UNP A0A7T8R415
A	1213	ASN	-	expression tag	UNP A0A7T8R415
A	1214	LEU	-	expression tag	UNP A0A7T8R415
A	1215	TYR	-	expression tag	UNP A0A7T8R415
A	1216	PHE	-	expression tag	UNP A0A7T8R415
A	1217	GLN	-	expression tag	UNP A0A7T8R415
A	1218	GLY	-	expression tag	UNP A0A7T8R415
A	1219	GLY	-	expression tag	UNP A0A7T8R415
A	1220	GLY	-	expression tag	UNP A0A7T8R415
A	1221	GLY	-	expression tag	UNP A0A7T8R415
A	1222	SER	-	expression tag	UNP A0A7T8R415
A	1223	GLY	-	expression tag	UNP A0A7T8R415
A	1224	TYR	-	expression tag	UNP A0A7T8R415
A	1225	ILE	-	expression tag	UNP A0A7T8R415
A	1226	PRO	-	expression tag	UNP A0A7T8R415
A	1227	GLU	-	expression tag	UNP A0A7T8R415
A	1228	ALA	-	expression tag	UNP A0A7T8R415
A	1229	PRO	-	expression tag	UNP A0A7T8R415
A	1230	ARG	-	expression tag	UNP A0A7T8R415
A	1231	ASP	-	expression tag	UNP A0A7T8R415
A	1232	GLY	-	expression tag	UNP A0A7T8R415
A	1233	GLN	-	expression tag	UNP A0A7T8R415
A	1234	ALA	-	expression tag	UNP A0A7T8R415
A	1235	TYR	-	expression tag	UNP A0A7T8R415
A	1236	VAL	-	expression tag	UNP A0A7T8R415
A	1237	ARG	-	expression tag	UNP A0A7T8R415
A	1238	LYS	-	expression tag	UNP A0A7T8R415
A	1239	ASP	-	expression tag	UNP A0A7T8R415

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	GLY	-	expression tag	UNP A0A7T8R415
A	1241	GLU	-	expression tag	UNP A0A7T8R415
A	1242	TRP	-	expression tag	UNP A0A7T8R415
A	1243	VAL	-	expression tag	UNP A0A7T8R415
A	1244	LEU	-	expression tag	UNP A0A7T8R415
A	1245	LEU	-	expression tag	UNP A0A7T8R415
A	1246	SER	-	expression tag	UNP A0A7T8R415
A	1247	THR	-	expression tag	UNP A0A7T8R415
A	1248	PHE	-	expression tag	UNP A0A7T8R415
A	1249	LEU	-	expression tag	UNP A0A7T8R415
A	1250	GLY	-	expression tag	UNP A0A7T8R415
A	1251	HIS	-	expression tag	UNP A0A7T8R415
A	1252	HIS	-	expression tag	UNP A0A7T8R415
A	1253	HIS	-	expression tag	UNP A0A7T8R415
A	1254	HIS	-	expression tag	UNP A0A7T8R415
A	1255	HIS	-	expression tag	UNP A0A7T8R415
A	1256	HIS	-	expression tag	UNP A0A7T8R415
B	-30	MET	-	initiating methionine	UNP A0A7T8R415
B	-29	GLY	-	expression tag	UNP A0A7T8R415
B	-28	ILE	-	expression tag	UNP A0A7T8R415
B	-27	LEU	-	expression tag	UNP A0A7T8R415
B	-26	PRO	-	expression tag	UNP A0A7T8R415
B	-25	SER	-	expression tag	UNP A0A7T8R415
B	-24	PRO	-	expression tag	UNP A0A7T8R415
B	-23	GLY	-	expression tag	UNP A0A7T8R415
B	-22	MET	-	expression tag	UNP A0A7T8R415
B	-21	PRO	-	expression tag	UNP A0A7T8R415
B	-20	ALA	-	expression tag	UNP A0A7T8R415
B	-19	LEU	-	expression tag	UNP A0A7T8R415
B	-18	LEU	-	expression tag	UNP A0A7T8R415
B	-17	SER	-	expression tag	UNP A0A7T8R415
B	-16	LEU	-	expression tag	UNP A0A7T8R415
B	-15	VAL	-	expression tag	UNP A0A7T8R415
B	-14	SER	-	expression tag	UNP A0A7T8R415
B	-13	LEU	-	expression tag	UNP A0A7T8R415
B	-12	LEU	-	expression tag	UNP A0A7T8R415
B	-11	SER	-	expression tag	UNP A0A7T8R415
B	-10	VAL	-	expression tag	UNP A0A7T8R415
B	-9	LEU	-	expression tag	UNP A0A7T8R415
B	-8	LEU	-	expression tag	UNP A0A7T8R415
B	-7	MET	-	expression tag	UNP A0A7T8R415
B	-6	GLY	-	expression tag	UNP A0A7T8R415

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	CYS	-	expression tag	UNP A0A7T8R415
B	-4	VAL	-	expression tag	UNP A0A7T8R415
B	-3	ALA	-	expression tag	UNP A0A7T8R415
B	-2	GLU	-	expression tag	UNP A0A7T8R415
B	-1	THR	-	expression tag	UNP A0A7T8R415
B	0	GLY	-	expression tag	UNP A0A7T8R415
B	682	SER	ARG	variant	UNP A0A7T8R415
B	685	SER	ARG	variant	UNP A0A7T8R415
B	986	PRO	LYS	variant	UNP A0A7T8R415
B	987	PRO	VAL	variant	UNP A0A7T8R415
B	1209	SER	-	expression tag	UNP A0A7T8R415
B	1210	GLY	-	expression tag	UNP A0A7T8R415
B	1211	ARG	-	expression tag	UNP A0A7T8R415
B	1212	GLU	-	expression tag	UNP A0A7T8R415
B	1213	ASN	-	expression tag	UNP A0A7T8R415
B	1214	LEU	-	expression tag	UNP A0A7T8R415
B	1215	TYR	-	expression tag	UNP A0A7T8R415
B	1216	PHE	-	expression tag	UNP A0A7T8R415
B	1217	GLN	-	expression tag	UNP A0A7T8R415
B	1218	GLY	-	expression tag	UNP A0A7T8R415
B	1219	GLY	-	expression tag	UNP A0A7T8R415
B	1220	GLY	-	expression tag	UNP A0A7T8R415
B	1221	GLY	-	expression tag	UNP A0A7T8R415
B	1222	SER	-	expression tag	UNP A0A7T8R415
B	1223	GLY	-	expression tag	UNP A0A7T8R415
B	1224	TYR	-	expression tag	UNP A0A7T8R415
B	1225	ILE	-	expression tag	UNP A0A7T8R415
B	1226	PRO	-	expression tag	UNP A0A7T8R415
B	1227	GLU	-	expression tag	UNP A0A7T8R415
B	1228	ALA	-	expression tag	UNP A0A7T8R415
B	1229	PRO	-	expression tag	UNP A0A7T8R415
B	1230	ARG	-	expression tag	UNP A0A7T8R415
B	1231	ASP	-	expression tag	UNP A0A7T8R415
B	1232	GLY	-	expression tag	UNP A0A7T8R415
B	1233	GLN	-	expression tag	UNP A0A7T8R415
B	1234	ALA	-	expression tag	UNP A0A7T8R415
B	1235	TYR	-	expression tag	UNP A0A7T8R415
B	1236	VAL	-	expression tag	UNP A0A7T8R415
B	1237	ARG	-	expression tag	UNP A0A7T8R415
B	1238	LYS	-	expression tag	UNP A0A7T8R415
B	1239	ASP	-	expression tag	UNP A0A7T8R415
B	1240	GLY	-	expression tag	UNP A0A7T8R415

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1241	GLU	-	expression tag	UNP A0A7T8R415
B	1242	TRP	-	expression tag	UNP A0A7T8R415
B	1243	VAL	-	expression tag	UNP A0A7T8R415
B	1244	LEU	-	expression tag	UNP A0A7T8R415
B	1245	LEU	-	expression tag	UNP A0A7T8R415
B	1246	SER	-	expression tag	UNP A0A7T8R415
B	1247	THR	-	expression tag	UNP A0A7T8R415
B	1248	PHE	-	expression tag	UNP A0A7T8R415
B	1249	LEU	-	expression tag	UNP A0A7T8R415
B	1250	GLY	-	expression tag	UNP A0A7T8R415
B	1251	HIS	-	expression tag	UNP A0A7T8R415
B	1252	HIS	-	expression tag	UNP A0A7T8R415
B	1253	HIS	-	expression tag	UNP A0A7T8R415
B	1254	HIS	-	expression tag	UNP A0A7T8R415
B	1255	HIS	-	expression tag	UNP A0A7T8R415
B	1256	HIS	-	expression tag	UNP A0A7T8R415
C	-30	MET	-	initiating methionine	UNP A0A7T8R415
C	-29	GLY	-	expression tag	UNP A0A7T8R415
C	-28	ILE	-	expression tag	UNP A0A7T8R415
C	-27	LEU	-	expression tag	UNP A0A7T8R415
C	-26	PRO	-	expression tag	UNP A0A7T8R415
C	-25	SER	-	expression tag	UNP A0A7T8R415
C	-24	PRO	-	expression tag	UNP A0A7T8R415
C	-23	GLY	-	expression tag	UNP A0A7T8R415
C	-22	MET	-	expression tag	UNP A0A7T8R415
C	-21	PRO	-	expression tag	UNP A0A7T8R415
C	-20	ALA	-	expression tag	UNP A0A7T8R415
C	-19	LEU	-	expression tag	UNP A0A7T8R415
C	-18	LEU	-	expression tag	UNP A0A7T8R415
C	-17	SER	-	expression tag	UNP A0A7T8R415
C	-16	LEU	-	expression tag	UNP A0A7T8R415
C	-15	VAL	-	expression tag	UNP A0A7T8R415
C	-14	SER	-	expression tag	UNP A0A7T8R415
C	-13	LEU	-	expression tag	UNP A0A7T8R415
C	-12	LEU	-	expression tag	UNP A0A7T8R415
C	-11	SER	-	expression tag	UNP A0A7T8R415
C	-10	VAL	-	expression tag	UNP A0A7T8R415
C	-9	LEU	-	expression tag	UNP A0A7T8R415
C	-8	LEU	-	expression tag	UNP A0A7T8R415
C	-7	MET	-	expression tag	UNP A0A7T8R415
C	-6	GLY	-	expression tag	UNP A0A7T8R415
C	-5	CYS	-	expression tag	UNP A0A7T8R415

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	VAL	-	expression tag	UNP A0A7T8R415
C	-3	ALA	-	expression tag	UNP A0A7T8R415
C	-2	GLU	-	expression tag	UNP A0A7T8R415
C	-1	THR	-	expression tag	UNP A0A7T8R415
C	0	GLY	-	expression tag	UNP A0A7T8R415
C	682	SER	ARG	variant	UNP A0A7T8R415
C	685	SER	ARG	variant	UNP A0A7T8R415
C	986	PRO	LYS	variant	UNP A0A7T8R415
C	987	PRO	VAL	variant	UNP A0A7T8R415
C	1209	SER	-	expression tag	UNP A0A7T8R415
C	1210	GLY	-	expression tag	UNP A0A7T8R415
C	1211	ARG	-	expression tag	UNP A0A7T8R415
C	1212	GLU	-	expression tag	UNP A0A7T8R415
C	1213	ASN	-	expression tag	UNP A0A7T8R415
C	1214	LEU	-	expression tag	UNP A0A7T8R415
C	1215	TYR	-	expression tag	UNP A0A7T8R415
C	1216	PHE	-	expression tag	UNP A0A7T8R415
C	1217	GLN	-	expression tag	UNP A0A7T8R415
C	1218	GLY	-	expression tag	UNP A0A7T8R415
C	1219	GLY	-	expression tag	UNP A0A7T8R415
C	1220	GLY	-	expression tag	UNP A0A7T8R415
C	1221	GLY	-	expression tag	UNP A0A7T8R415
C	1222	SER	-	expression tag	UNP A0A7T8R415
C	1223	GLY	-	expression tag	UNP A0A7T8R415
C	1224	TYR	-	expression tag	UNP A0A7T8R415
C	1225	ILE	-	expression tag	UNP A0A7T8R415
C	1226	PRO	-	expression tag	UNP A0A7T8R415
C	1227	GLU	-	expression tag	UNP A0A7T8R415
C	1228	ALA	-	expression tag	UNP A0A7T8R415
C	1229	PRO	-	expression tag	UNP A0A7T8R415
C	1230	ARG	-	expression tag	UNP A0A7T8R415
C	1231	ASP	-	expression tag	UNP A0A7T8R415
C	1232	GLY	-	expression tag	UNP A0A7T8R415
C	1233	GLN	-	expression tag	UNP A0A7T8R415
C	1234	ALA	-	expression tag	UNP A0A7T8R415
C	1235	TYR	-	expression tag	UNP A0A7T8R415
C	1236	VAL	-	expression tag	UNP A0A7T8R415
C	1237	ARG	-	expression tag	UNP A0A7T8R415
C	1238	LYS	-	expression tag	UNP A0A7T8R415
C	1239	ASP	-	expression tag	UNP A0A7T8R415
C	1240	GLY	-	expression tag	UNP A0A7T8R415
C	1241	GLU	-	expression tag	UNP A0A7T8R415

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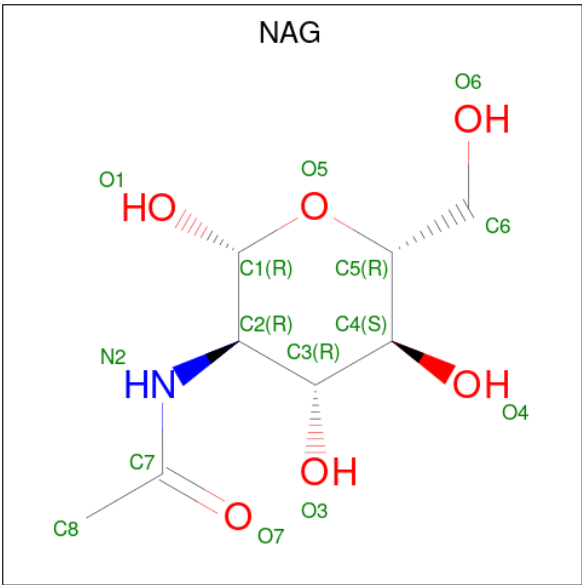
Chain	Residue	Modelled	Actual	Comment	Reference
C	1242	TRP	-	expression tag	UNP A0A7T8R415
C	1243	VAL	-	expression tag	UNP A0A7T8R415
C	1244	LEU	-	expression tag	UNP A0A7T8R415
C	1245	LEU	-	expression tag	UNP A0A7T8R415
C	1246	SER	-	expression tag	UNP A0A7T8R415
C	1247	THR	-	expression tag	UNP A0A7T8R415
C	1248	PHE	-	expression tag	UNP A0A7T8R415
C	1249	LEU	-	expression tag	UNP A0A7T8R415
C	1250	GLY	-	expression tag	UNP A0A7T8R415
C	1251	HIS	-	expression tag	UNP A0A7T8R415
C	1252	HIS	-	expression tag	UNP A0A7T8R415
C	1253	HIS	-	expression tag	UNP A0A7T8R415
C	1254	HIS	-	expression tag	UNP A0A7T8R415
C	1255	HIS	-	expression tag	UNP A0A7T8R415
C	1256	HIS	-	expression tag	UNP A0A7T8R415

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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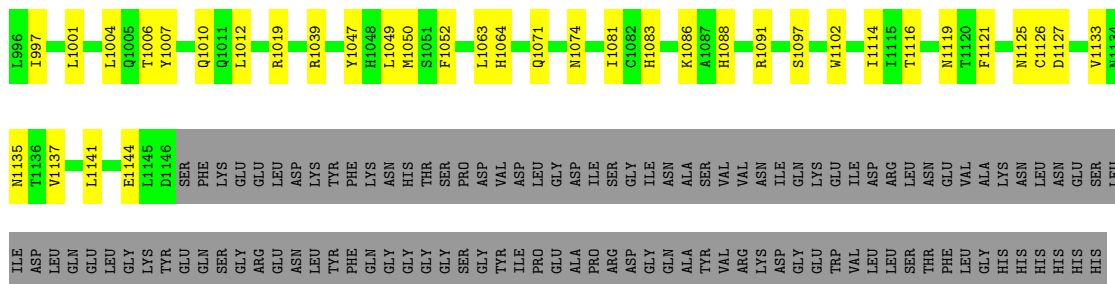
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3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

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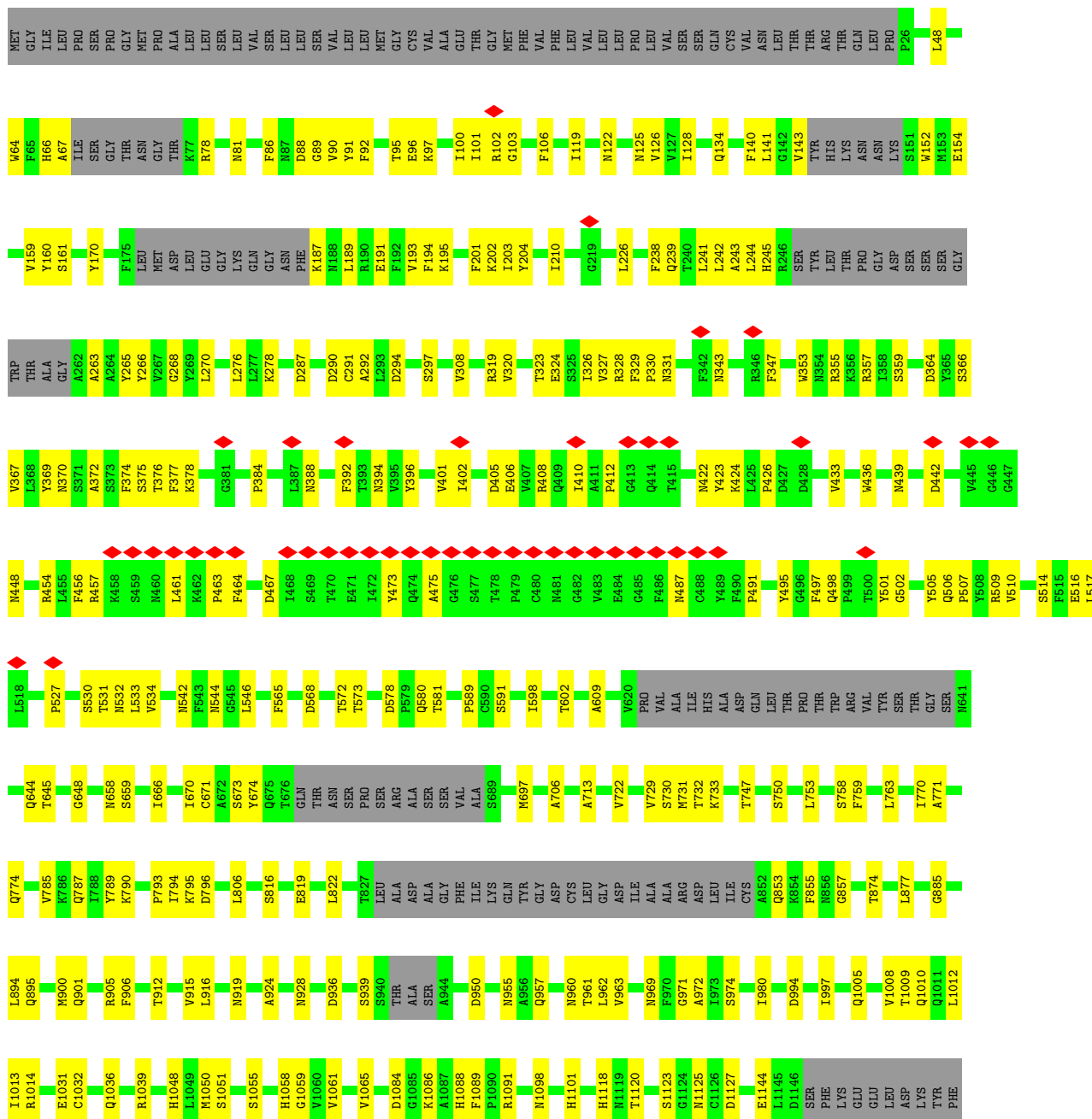
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	





• Molecule 1: Spike glycoprotein

Chain B: 59% 21% 21%



GLN  
GLY  
GLY  
GLY  
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  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 1: Spike glycoprotein

Chain C:  57% 20% 22%

MET	GLY	ILE	LEU	PRO	SER	PRO	GLY	LEU	SER	VAL	SER	VAL	LEU	SER	GLY	CYS	VAL	ALA	GLU	THR	GLY	MET	PHE	VAL	PHE	LEU	VAL	LEU	PRO	VAL	SER	SER	GLN	CYS	VAL	ASN	LEU	THR	THR	ARG	THR	GLN	LEU	<b>F25</b>	<b>N30</b>	<b>163</b>
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L48	Q52	F59	A67	I1E	SER	GLY	THR	ASN	GLY	THR	LYS	ARG	F79	P82	F86	H87	D88	A93	S94	THR	GLU	LYS	SER	H99	I100	I101	R102	F106	L110	V120	M121	M122	A123	T124	H125	V126	V127	I128	V129	K130	C131	F132	F133	Q134	F135	L141	GLY	ASN
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TVR	HIS	LYS	ASN	ASN	LYS	TRP	GLU	GLU	F157	F158	V159	I160	I161	I162	E169	V170	V171	F175	LEU	MET	ASP	LEU	GLU	GLY	GLY	ASN	PHE	LYS	GLN	GLY	ASN	ASP	LYS	M188	I189	R190	E191	M196	F201	K202	L203	T204	S205	K206	H207	T208	P209	L212	V213	R214	D215	L216	P217
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L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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R328	R329	R330	R340	R343	R353	R354	R355	R365	R366	R367	R368	R369	R370	R371	R374	R375	R379	R382	R383	R384	R403	R404	R405	R409	R410	R411	R414	R415	R416	R417	R418	R419	R420	R421	R424	R425	R426	R427	R428	R433	R436
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R437	R438	R439	R440	R441	R442	R443	R448	R451	R456	R457	R463	R466	R467	R468	R473	R474	R475	R480	R481	R485	R486	R487	R488	R489	R490	R491	R497	R504	R505	R506	R512	R516	R517	R518	R519	R523	R524	R525	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000
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C538	N542	F543	N544	C566	R567	D568	I569	D570	D571	A575	V576	R577	O580	I584	S591	E619	VAL	PRO	PRO	VAL	ALA	ALA	ILE	HIS	ALA	ASP	ASP	GLN	LEU	THR	THR	PRO	THR	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	I641	G644	T645	V656	N657	N658	S659	V660	E661	C662	D663	I664
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A672	T676	GLN	THR	ASN	SER	PRO	ARG	ARG	ALA	SER	SER	VAL	ALA	ALA	P689
M697	S698														K699
A713	M717	F718	I726	V729	G730	M731	T732	K733	M751	L764	Q755	F759	L763	H764	R765
I770	Q774	D775	K786	I791	L806	K811	P812	S813	N814						

R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000
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Q914	Q915	Q916	Q919	Q922	Q923	Q926	Q939	SER	THR	ALA	SER	A944	Q954	Q962	Q965	Q976	Q979	Q985	Q986	Q987	Q988	Q991	Q992	Q993	Q996	Q997	Q1002	Q1005	Q1006	Q1007	Q1008	Q1009	Q1010	Q1011	Q1012	Q1013	Q1014	Q1029	Q1030	Q1031	Q1032	Q1033	Q1034	Q1035	Q1036	Q1037	Q1038	Q1039	Q1040	Q1041	Q1042	Q1043	Q1044	Q1045	Q1046	Q1047	Q1048	Q1049	Q1050	Q1051	Q1052	Q1053	Q1054	Q1055	Q1056	Q1057	Q1058	Q1059	Q1060	Q1061	Q1062	Q1063	Q1064	Q1065	Q1066	Q1067	Q1068	Q1069	Q1070	Q1071	Q1072	Q1073	Q1074	Q1075	Q1076	Q1077	Q1078	Q1079	Q1080	Q1081	Q1082	Q1083	Q1084	Q1085	Q1086	Q1087	Q1088	Q1089	Q1090	Q1091	Q1092	Q1093	Q1094	Q1095	Q1096	Q1097	Q1098	Q1099	Q1100	Q1101	Q1102	Q1103	Q1104	Q1105	Q1106	Q1107	Q1108	Q1109	Q1110	Q1111	Q1112	Q1113	Q1114	Q1115	Q1116	Q1117	Q1118	Q1119	Q1120	Q1121	Q1122	Q1123	Q1124	Q1125	Q1126	Q1127	Q1128	Q1129	Q1130	Q1131	Q1132	Q1133	Q1134	Q1135	Q1136	Q1137	Q1138	Q1139	Q1140	Q1141	Q1142	Q1143	Q1144	Q1145	Q1146	Q1147	Q1148	Q1149	Q1150	Q1151	Q1152	Q1153	Q1154	Q1155	Q1156	Q1157	Q1158	Q1159	Q1160	Q1161	Q1162	Q1163	Q1164	Q1165	Q1166	Q1167	Q1168	Q1169	Q1170	Q1171	Q1172	Q1173	Q1174	Q1175	Q1176	Q1177	Q1178	Q1179	Q1180	Q1181	Q1182	Q1183	Q1184	Q1185	Q1186	Q1187	Q1188	Q1189	Q1190	Q1191	Q1192	Q1193	Q1194	Q1195	Q1196	Q1197	Q1198	Q1199	Q1200	Q1201	Q1202	Q1203	Q1204	Q1205	Q1206	Q1207	Q1208	Q1209	Q1210	Q1211	Q1212	Q1213	Q1214	Q1215	Q1216	Q1217	Q1218	Q1219	Q1220	Q1221	Q1222	Q1223	Q1224	Q1225	Q1226	Q1227	Q1228	Q1229	Q1230	Q1231	Q1232	Q1233	Q1234	Q1235	Q1236	Q1237	Q1238	Q1239	Q1240	Q1241	Q1242	Q1243	Q1244	Q1245	Q1246	Q1247	Q1248	Q1249	Q1250	Q1251	Q1252	Q1253	Q1254	Q1255	Q1256	Q1257	Q1258	Q1259	Q1260	Q1261	Q1262	Q1263	Q1264	Q1265	Q1266	Q1267	Q1268	Q1269	Q1270	Q1271	Q1272	Q1273	Q1274	Q1275	Q1276	Q1277	Q1278	Q1279	Q1280	Q1281	Q1282	Q1283	Q1284	Q1285	Q1286	Q1287	Q1288	Q1289	Q1290	Q1291	Q1292	Q1293	Q1294	Q1295	Q1296	Q1297	Q1298	Q1299	Q1300	Q1301	Q1302	Q1303	Q1304	Q1305	Q1306	Q1307	Q1308	Q1309	Q1310	Q1311	Q1312	Q1313	Q1314	Q1315	Q1316	Q1317	Q1318	Q1319	Q1320	Q1321	Q1322	Q1323	Q1324	Q1325	Q1326	Q1327	Q1328	Q1329	Q1330	Q1331	Q1332	Q1333	Q1334	Q1335	Q1336	Q1337	Q1338	Q1339	Q1340	Q1341	Q1342	Q1343	Q1344	Q1345	Q1346	Q1347	Q1348	Q1349	Q1350	Q1351	Q1352	Q1353	Q1354	Q1355	Q1356	Q1357	Q1358	Q1359	Q1360	Q1361	Q1362	Q1363	Q1364	Q1365	Q1366	Q1367	Q1368	Q1369	Q1370	Q1371	Q1372	Q1373	Q1374	Q1375	Q1376	Q1377	Q1378	Q1379	Q1380	Q1381	Q1382	Q1383	Q1384	Q1385	Q1386	Q1387	Q1388	Q1389	Q1390	Q1391	Q1392	Q1393	Q1394	Q1395	Q1396	Q1397	Q1398	Q1399	Q1400	Q1401	Q1402	Q1403
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[illegible]

VAL	ASP	LEU	GLY	ASP	ASP	ILE	SER	GLY	ILE	ILE	ASN	ALA	SER	VAL	ASN	ASN	GLN	LYS	GLU	ILE	ASP	ASP	LEU	LEU	ASN	ASN	GLU	VAL	ALA	LYS	ASN	ASN	LEU	LEU	GLU	GLU	SER	SER	LEU	LEU	GLN	GLU	GLN	GLN	GLY	ARG	GLY	LYS	TTR	TTR	LEU	LEU	ASN	ASN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	SER	SER	GLY	GLY
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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 HIS HIS HIS HIS HIS HIS

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.346	Depositor
Minimum map value	-1.757	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	0.29	0/7877	0.48	0/10717
1	B	0.29	0/8171	0.48	0/11113
1	C	0.29	0/7988	0.48	0/10868
All	All	0.29	0/24036	0.48	0/32698

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7702	0	7524	176	0
1	B	7988	0	7784	179	0
1	C	7808	0	7601	185	0
2	D	28	0	25	3	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
3	A	154	0	143	2	0
3	B	182	0	169	2	0
3	C	182	0	169	3	0
All	All	24100	0	23465	516	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 11.

All (516) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:PHE:HB3	1:B:436:TRP:HB3	1.54	0.89
1:A:706:ALA:H	1:B:895:GLN:HE21	1.24	0.84
1:B:753:LEU:HD13	1:B:997:ILE:HD11	1.65	0.77
1:B:974:SER:HB2	1:B:980:ILE:HD11	1.66	0.76
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.69	0.74
1:A:375:SER:H	1:A:436:TRP:HA	1.53	0.74
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.71	0.73
1:A:716:ILE:HG22	1:A:1071:GLN:HB2	1.71	0.73
1:C:48:LEU:HB3	1:C:276:LEU:HD11	1.72	0.72
1:B:763:LEU:HD12	1:B:1008:VAL:HG21	1.70	0.71
1:A:725:GLU:OE2	1:A:1064:HIS:NE2	2.23	0.71
1:A:298:GLU:HG3	1:A:315:THR:HG21	1.73	0.70
1:C:537:LYS:NZ	1:C:538:CYS:O	2.23	0.69
1:A:188:ASN:HA	1:A:210:ILE:H	1.57	0.69
1:B:644:GLN:NE2	1:B:645:THR:O	2.19	0.69
1:B:331:ASN:HA	1:B:580:GLN:HG2	1.74	0.68
1:A:210:ILE:HG23	1:A:212:LEU:HD23	1.75	0.68
1:B:1098:ASN:HB3	1:B:1101:HIS:H	1.58	0.68
1:B:732:THR:OG1	1:B:955:ASN:ND2	2.27	0.67
1:B:92:PHE:HE1	1:B:265:TYR:HB2	1.60	0.67
1:C:330:PRO:O	1:C:580:GLN:NE2	2.26	0.67
1:B:969:ASN:HB3	1:C:755:GLN:HG3	1.76	0.67
1:B:376:THR:OG1	1:B:378:LYS:NZ	2.17	0.66
1:B:439:ASN:ND2	1:B:506:GLN:OE1	2.29	0.66
1:A:1081:ILE:HD11	1:A:1135:ASN:HB3	1.76	0.66
1:A:328:ARG:HB3	1:A:580:GLN:HG2	1.78	0.66
1:B:102:ARG:HE	1:B:243:ALA:HB2	1.62	0.65
1:A:206:LYS:NZ	1:A:207:HIS:O	2.28	0.65
1:A:965:GLN:O	1:A:968:SER:OG	2.14	0.64
1:A:366:SER:H	1:A:388:ASN:HD21	1.46	0.64
1:A:971:GLY:O	1:A:995:ARG:NH1	2.26	0.64
1:A:294:ASP:O	1:A:297:SER:OG	2.10	0.64
1:B:578:ASP:OD2	1:B:581:THR:N	2.26	0.64
1:B:456:PHE:H	1:B:491:PRO:HB3	1.62	0.64
1:B:81:ASN:O	1:B:239:GLN:NE2	2.30	0.63
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.32	0.63
1:C:763:LEU:HD12	1:C:1008:VAL:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:HD22	2:D:1:NAG:H82	1.63	0.63
1:A:985:ASP:HB3	1:A:987:PRO:HD2	1.80	0.63
1:B:134:GLN:HB3	1:B:161:SER:HB2	1.80	0.63
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.81	0.63
1:C:206:LYS:NZ	1:C:207:HIS:O	2.29	0.63
1:A:327:VAL:HG22	1:A:542:ASN:HB3	1.81	0.62
1:C:367:VAL:O	1:C:371:SER:OG	2.17	0.62
1:C:82:PRO:O	1:C:239:GLN:NE2	2.31	0.62
1:C:854:LYS:NZ	1:C:858:LEU:O	2.33	0.62
1:C:475:ALA:HB3	1:C:487:ASN:HB3	1.81	0.62
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.82	0.62
1:A:983:ARG:HB2	1:C:382:VAL:HG22	1.82	0.62
1:A:570:ASP:HB2	1:B:963:VAL:HG11	1.82	0.62
1:A:976:VAL:HG12	1:A:979:ASP:H	1.64	0.61
1:C:1029:MET:HE1	1:C:1053:PRO:HG3	1.81	0.61
1:C:141:LEU:HB2	1:C:243:ALA:HA	1.82	0.61
1:A:473:TYR:HB2	1:A:491:PRO:HG3	1.82	0.61
1:B:822:LEU:HD21	1:B:1061:VAL:HG21	1.82	0.61
1:C:280:ASN:OD1	1:C:284:THR:N	2.33	0.61
1:A:82:PRO:O	1:A:239:GLN:NE2	2.33	0.61
1:C:226:LEU:HD23	1:C:227:VAL:HG23	1.83	0.61
1:C:52:GLN:OE1	1:C:274:THR:OG1	2.19	0.61
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.34	0.61
1:A:448:ASN:HB2	1:A:497:PHE:HB2	1.82	0.61
1:C:662:CYS:HB2	1:C:697:MET:HG3	1.83	0.61
1:B:473:TYR:HB2	1:B:491:PRO:HG3	1.83	0.60
1:B:731:MET:N	1:B:774:GLN:OE1	2.29	0.60
1:A:456:PHE:H	1:A:491:PRO:HB3	1.64	0.60
1:A:592:PHE:HE2	1:B:857:GLY:H	1.49	0.60
1:B:501:TYR:O	1:B:506:GLN:NE2	2.35	0.60
1:B:278:LYS:HE3	1:B:287:ASP:HB3	1.84	0.60
1:C:328:ARG:NH1	1:C:531:THR:O	2.34	0.60
1:C:991:VAL:HG23	1:C:992:GLN:HE21	1.67	0.59
1:A:65:PHE:HE2	1:A:84:LEU:HD21	1.66	0.59
1:A:376:THR:HB	1:A:435:ALA:HB3	1.84	0.59
1:A:773:GLU:OE2	1:A:1019:ARG:NH1	2.35	0.59
1:A:1086:LYS:HG3	1:A:1088:HIS:HE1	1.66	0.59
1:C:644:GLN:NE2	1:C:645:THR:O	2.36	0.59
1:C:537:LYS:NZ	1:C:538:CYS:SG	2.76	0.59
1:A:1091:ARG:HE	1:A:1121:PHE:HB3	1.67	0.59
1:B:957:GLN:OE1	1:C:765:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:OD1	1:C:288:ALA:N	2.36	0.58
1:A:1141:LEU:HD11	1:B:1144:GLU:HG2	1.85	0.58
1:B:1125:ASN:ND2	1:B:1127:ASP:OD2	2.36	0.58
1:C:567:ARG:NH1	1:C:571:ASP:OD1	2.35	0.58
1:B:448:ASN:H	1:B:497:PHE:H	1.52	0.58
1:C:365:TYR:HD1	1:C:388:ASN:HB2	1.68	0.58
1:B:189:LEU:HB2	1:B:210:ILE:HD13	1.86	0.57
1:B:193:VAL:HB	1:B:204:TYR:HB2	1.86	0.57
1:B:369:TYR:HA	1:B:372:ALA:HB2	1.85	0.57
1:C:791:THR:HG21	1:C:806:LEU:HD21	1.84	0.57
1:A:329:PHE:HB2	1:A:330:PRO:HD3	1.87	0.57
1:B:319:ARG:HG3	1:B:591:SER:HB3	1.86	0.57
1:B:706:ALA:O	1:C:895:GLN:NE2	2.33	0.57
1:B:1010:GLN:HB3	1:B:1014:ARG:HH21	1.68	0.57
1:A:808:ASP:OD2	1:A:810:SER:OG	2.21	0.57
1:B:915:VAL:O	1:B:919:ASN:ND2	2.38	0.57
1:B:475:ALA:HB3	1:B:487:ASN:HB3	1.85	0.57
1:C:905:ARG:NH1	1:C:1050:MET:HG2	2.19	0.57
1:A:291:CYS:HB2	1:A:298:GLU:HA	1.87	0.57
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.87	0.57
1:B:290:ASP:OD1	1:B:292:ALA:N	2.29	0.57
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.86	0.57
1:A:231:ILE:HG23	1:A:233:ILE:HG12	1.86	0.56
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.87	0.56
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.86	0.56
1:C:328:ARG:HE	1:C:533:LEU:HB2	1.70	0.56
1:A:330:PRO:O	1:A:580:GLN:NE2	2.33	0.56
1:A:816:SER:OG	1:A:819:GLU:OE1	2.14	0.56
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.88	0.56
1:A:454:ARG:HH22	1:A:471:GLU:H	1.54	0.56
1:A:756:TYR:O	1:C:965:GLN:NE2	2.37	0.56
1:A:422:ASN:OD1	1:A:454:ARG:N	2.38	0.56
1:A:1039:ARG:NE	1:B:1031:GLU:OE2	2.32	0.55
1:A:433:VAL:HG22	1:A:512:VAL:HG23	1.88	0.55
1:C:121:ASN:HA	1:C:126:VAL:HG22	1.89	0.55
1:A:589:PRO:HD3	1:B:855:PHE:CZ	2.41	0.55
1:B:366:SER:HA	1:B:369:TYR:CZ	2.41	0.55
1:A:1144:GLU:N	1:A:1144:GLU:OE1	2.38	0.55
1:B:66:HIS:HB2	1:B:78:ARG:HG2	1.87	0.55
1:B:357:ARG:NH2	1:B:394:ASN:OD1	2.39	0.55
1:B:424:LYS:HB2	1:B:461:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLU:HA	1:A:343:ASN:HB2	1.89	0.55
1:B:159:VAL:HG23	1:B:160:TYR:HD1	1.72	0.55
1:B:722:VAL:HG22	1:B:1065:VAL:HG12	1.88	0.55
1:A:474:GLN:NE2	1:A:488:CYS:SG	2.80	0.55
1:C:188:ASN:HA	1:C:209:PRO:HA	1.88	0.54
1:C:442:ASP:HB3	1:C:451:TYR:HE2	1.73	0.54
1:C:94:SER:OG	1:C:190:ARG:O	2.21	0.54
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.88	0.54
1:C:330:PRO:HD2	1:C:530:SER:HB2	1.88	0.54
1:B:410:ILE:HG13	1:B:510:VAL:HG11	1.90	0.54
1:A:273:ARG:HE	1:A:292:ALA:HB3	1.73	0.54
1:B:328:ARG:NH2	1:B:531:THR:O	2.39	0.54
1:B:378:LYS:HB2	1:B:433:VAL:HB	1.89	0.54
1:B:406:GLU:OE1	1:B:495:TYR:OH	2.17	0.53
1:B:1009:THR:O	1:B:1013:ILE:HG12	2.08	0.53
1:C:566:GLY:HA3	1:C:575:ALA:HB3	1.89	0.53
1:B:666:ILE:HD13	1:B:670:ILE:HG22	1.90	0.53
1:C:816:SER:N	1:C:819:GLU:OE2	2.42	0.53
1:A:759:PHE:HD2	1:A:1001:LEU:HD21	1.74	0.53
1:A:962:LEU:HD11	1:A:1007:TYR:CG	2.43	0.53
1:C:365:TYR:N	1:C:388:ASN:OD1	2.41	0.53
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.24	0.53
1:C:134:GLN:HB3	1:C:161:SER:HB2	1.89	0.53
1:B:568:ASP:OD1	1:B:572:THR:N	2.32	0.53
1:C:273:ARG:HH21	1:C:292:ALA:HB3	1.74	0.53
1:A:81:ASN:OD1	1:A:239:GLN:NE2	2.42	0.52
1:A:353:TRP:O	1:A:466:ARG:NH1	2.42	0.52
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.42	0.52
1:C:202:LYS:HB3	1:C:204:TYR:HE1	1.74	0.52
1:C:819:GLU:HA	1:C:822:LEU:HD12	1.91	0.52
1:A:33:THR:HG22	1:A:58:PHE:HD2	1.74	0.52
1:A:993:ILE:O	1:A:997:ILE:HG12	2.09	0.52
1:C:102:ARG:HH11	1:C:243:ALA:HB2	1.75	0.52
1:A:965:GLN:OE1	1:B:758:SER:OG	2.28	0.52
1:B:320:VAL:H	1:B:591:SER:HA	1.75	0.52
1:B:64:TRP:CD1	1:B:266:TYR:HE1	2.28	0.52
1:C:374:PHE:HB3	1:C:436:TRP:HB3	1.92	0.52
1:A:116:SER:OG	1:A:131:CYS:O	2.27	0.51
1:B:900:MET:SD	1:B:900:MET:N	2.83	0.51
1:C:86:PHE:HB2	1:C:238:PHE:CD1	2.45	0.51
1:A:1125:ASN:OD1	1:A:1126:CYS:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASP:O	1:B:408:ARG:NH1	2.43	0.51
1:B:816:SER:N	1:B:819:GLU:OE2	2.43	0.51
1:A:448:ASN:O	1:A:494:SER:OG	2.26	0.51
1:B:454:ARG:HD2	1:B:491:PRO:HB2	1.92	0.51
1:C:102:ARG:O	1:C:121:ASN:N	2.37	0.51
1:C:976:VAL:HG12	1:C:979:ASP:H	1.75	0.51
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.46	0.51
1:A:458:LYS:NZ	1:A:472:ILE:O	2.44	0.51
1:A:280:ASN:HD21	1:A:282:ASN:HB2	1.75	0.51
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.93	0.51
1:B:88:ASP:OD1	1:B:88:ASP:N	2.44	0.51
1:B:320:VAL:O	1:B:591:SER:OG	2.27	0.51
1:B:924:ALA:O	1:B:928:ASN:ND2	2.44	0.51
1:C:522:ALA:HB2	1:C:544:ASN:HB3	1.93	0.51
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.42	0.51
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.11	0.51
1:C:365:TYR:O	1:C:369:TYR:N	2.37	0.51
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.93	0.51
1:A:702:GLU:OE1	1:B:790:LYS:NZ	2.35	0.51
1:B:565:PHE:HB2	1:C:42:VAL:HG22	1.91	0.51
1:B:969:ASN:OD1	1:B:972:ALA:N	2.44	0.51
1:C:1054:GLN:HB2	1:C:1061:VAL:HB	1.93	0.51
1:B:936:ASP:O	1:B:939:SER:OG	2.24	0.50
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.93	0.50
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.92	0.50
1:C:421:TYR:CG	1:C:457:ARG:HB2	2.46	0.50
1:C:854:LYS:HD2	1:C:858:LEU:HB2	1.92	0.50
1:A:295:PRO:HA	1:A:298:GLU:CD	2.31	0.50
1:A:642:VAL:HG22	1:A:651:ILE:HG22	1.94	0.50
1:A:127:VAL:HG21	3:A:1311:NAG:H61	1.91	0.50
1:C:664:ILE:HD11	1:C:672:ALA:HB3	1.93	0.50
1:C:731:MET:H	1:C:774:GLN:NE2	2.10	0.50
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.92	0.50
1:B:343:ASN:HB2	3:B:1311:NAG:C7	2.41	0.50
1:C:93:ALA:HA	1:C:191:GLU:HG3	1.93	0.50
1:A:299:THR:OG1	1:A:597:VAL:HG11	2.12	0.50
1:B:326:ILE:HD13	1:B:534:VAL:HG12	1.93	0.50
1:C:811:LYS:HD2	1:C:812:PRO:HD2	1.92	0.50
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.93	0.50
1:A:393:THR:HG21	1:A:518:LEU:HB2	1.93	0.50
1:B:1032:CYS:O	1:B:1051:SER:OG	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:ILE:HD11	1:C:1012:LEU:HD13	1.94	0.49
1:A:330:PRO:HG3	1:A:528:LYS:HB3	1.94	0.49
1:A:1086:LYS:HG3	1:A:1088:HIS:CE1	2.46	0.49
1:B:377:PHE:CD2	1:B:384:PRO:HB3	2.48	0.49
1:C:905:ARG:CZ	1:C:1050:MET:HG2	2.43	0.49
1:A:1125:ASN:ND2	1:A:1127:ASP:OD2	2.45	0.49
1:C:86:PHE:HB2	1:C:238:PHE:HD1	1.76	0.49
1:C:110:LEU:HB2	1:C:237:ARG:HH21	1.78	0.49
1:C:884:SER:OG	1:C:887:THR:OG1	2.24	0.49
1:C:1091:ARG:NH1	1:C:1118:HIS:O	2.40	0.49
1:A:280:ASN:OD1	1:A:284:THR:N	2.33	0.49
1:A:357:ARG:NH2	1:A:394:ASN:OD1	2.46	0.49
1:C:159:VAL:HG23	1:C:160:TYR:CD2	2.48	0.49
1:A:969:ASN:OD1	1:A:972:ALA:N	2.32	0.49
1:C:1083:HIS:CG	1:C:1137:VAL:HG12	2.46	0.49
1:B:327:VAL:N	1:B:531:THR:OG1	2.45	0.49
1:A:807:PRO:HA	1:A:816:SER:HB3	1.94	0.49
1:A:1116:THR:H	1:A:1119:ASN:HD21	1.60	0.49
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.22	0.49
1:C:1002:GLN:O	1:C:1006:THR:HG23	2.13	0.49
1:B:1123:SER:OG	1:C:914:ASN:OD1	2.22	0.49
1:A:815:ARG:HB3	1:A:819:GLU:HB2	1.94	0.49
1:B:589:PRO:HG3	1:C:855:PHE:HA	1.95	0.49
1:B:1089:PHE:HE2	1:C:914:ASN:HA	1.78	0.49
1:C:759:PHE:O	1:C:763:LEU:HD23	2.12	0.49
1:A:676:THR:N	1:A:690:GLN:OE1	2.39	0.48
1:B:426:PRO:HG3	1:B:463:PRO:HB3	1.94	0.48
1:B:498:GLN:OE1	1:B:501:TYR:N	2.46	0.48
1:C:867:ASP:N	1:C:867:ASP:OD1	2.46	0.48
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.95	0.48
1:B:328:ARG:HH12	1:B:533:LEU:HB2	1.78	0.48
1:C:962:LEU:HD11	1:C:1007:TYR:CG	2.48	0.48
1:A:1074:ASN:HB2	3:A:1308:NAG:O5	2.12	0.48
1:B:140:PHE:HB2	1:B:244:LEU:HD13	1.95	0.48
1:B:874:THR:HG1	1:B:1055:SER:HG	1.61	0.48
1:A:280:ASN:ND2	1:A:282:ASN:H	2.12	0.48
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.95	0.48
1:A:553:THR:HG23	1:A:586:ASP:HB2	1.95	0.48
1:C:201:PHE:HD2	1:C:203:ILE:HD11	1.78	0.48
1:C:569:ILE:H	1:C:569:ILE:HD12	1.78	0.48
1:C:985:ASP:OD2	1:C:987:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ALA:HB2	1:A:354:ASN:HD22	1.78	0.48
1:B:401:VAL:HG22	1:B:509:ARG:HD3	1.96	0.48
1:C:577:ARG:HD3	1:C:584:ILE:HD13	1.96	0.48
1:C:962:LEU:HD21	1:C:1007:TYR:HB2	1.95	0.48
1:A:104:TRP:H	1:A:119:ILE:HG23	1.79	0.48
1:B:658:ASN:OD1	1:B:659:SER:N	2.42	0.48
1:B:785:VAL:HG22	1:B:787:GLN:H	1.79	0.47
1:B:67:ALA:HB3	1:B:263:ALA:H	1.79	0.47
1:B:497:PHE:HB3	1:B:507:PRO:HD3	1.96	0.47
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.47
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	1.96	0.47
1:B:90:VAL:HG22	1:B:194:PHE:HB2	1.97	0.47
1:B:103:GLY:H	1:B:241:LEU:HB2	1.79	0.47
1:C:365:TYR:CD1	1:C:388:ASN:HB2	2.49	0.47
1:B:366:SER:N	1:B:388:ASN:HD21	2.11	0.47
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.96	0.47
1:B:793:PRO:O	1:B:795:LYS:NZ	2.46	0.47
1:C:329:PHE:CZ	1:C:391:CYS:HB2	2.49	0.47
1:C:343:ASN:HB2	3:C:1312:NAG:H83	1.96	0.47
1:C:88:ASP:N	1:C:88:ASP:OD1	2.44	0.47
1:C:718:PHE:HZ	1:C:923:ILE:HD11	1.78	0.47
1:C:884:SER:OG	1:C:894:LEU:N	2.40	0.47
1:B:1091:ARG:NE	1:B:1118:HIS:O	2.47	0.47
1:A:128:ILE:O	1:A:170:TYR:N	2.48	0.47
1:A:357:ARG:NH1	1:A:396:TYR:OH	2.48	0.47
1:A:741:TYR:CE2	1:A:966:LEU:HD21	2.49	0.47
1:A:787:GLN:HB2	1:A:789:TYR:CZ	2.49	0.47
1:A:882:ILE:HG23	1:A:883:THR:HG23	1.96	0.47
1:B:97:LYS:HE2	1:B:187:LYS:HB2	1.97	0.47
1:B:308:VAL:HB	1:B:602:THR:HB	1.97	0.47
1:B:343:ASN:HB2	3:B:1311:NAG:N2	2.29	0.47
1:C:954:GLN:HG2	1:C:1014:ARG:CZ	2.45	0.47
1:C:988:GLU:OE1	1:C:988:GLU:N	2.48	0.47
1:A:125:ASN:HA	1:A:173:GLN:O	2.14	0.47
1:B:101:ILE:HA	1:B:242:LEU:HD13	1.97	0.47
1:B:960:ASN:OD1	1:B:961:THR:N	2.47	0.47
1:C:656:VAL:HG22	1:C:658:ASN:H	1.80	0.47
1:C:751:ASN:HA	1:C:754:LEU:HD23	1.97	0.47
1:A:347:PHE:CE2	1:A:509:ARG:HB3	2.50	0.47
1:A:578:ASP:HB3	1:A:583:GLU:H	1.80	0.47
1:A:737:ASP:OD2	1:C:317:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:HB2	1:B:238:PHE:HB2	1.97	0.46
1:B:355:ARG:NH2	1:B:516:GLU:OE2	2.48	0.46
2:F:1:NAG:H4	2:F:2:NAG:H2	1.75	0.46
1:B:347:PHE:CD2	1:B:509:ARG:HD2	2.50	0.46
1:B:372:ALA:HB1	1:B:377:PHE:HB2	1.98	0.46
1:C:298:GLU:O	1:C:302:THR:OG1	2.27	0.46
1:A:457:ARG:HE	1:A:467:ASP:HA	1.81	0.46
1:B:194:PHE:HD2	1:B:201:PHE:HZ	1.62	0.46
1:C:731:MET:HG2	1:C:774:GLN:HE21	1.81	0.46
1:A:360:ASN:H	1:A:523:THR:HG23	1.80	0.46
1:A:905:ARG:CZ	1:A:1050:MET:HB2	2.46	0.46
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.51	0.46
1:C:128:ILE:HD13	1:C:170:TYR:HD2	1.79	0.46
1:C:993:ILE:O	1:C:997:ILE:HG12	2.15	0.46
1:C:1010:GLN:HE22	1:C:1014:ARG:NH1	2.14	0.46
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.97	0.46
1:B:95:THR:HG22	1:B:189:LEU:HD13	1.98	0.46
1:B:357:ARG:NH1	1:B:359:SER:OG	2.49	0.46
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.96	0.46
1:A:312:ILE:HD12	1:A:598:ILE:HG12	1.98	0.46
1:B:971:GLY:H	1:C:755:GLN:HG2	1.80	0.46
1:A:454:ARG:HD2	1:A:491:PRO:HB2	1.97	0.46
1:C:516:GLU:HB3	1:C:519:HIS:ND1	2.30	0.46
1:A:233:ILE:HG13	1:A:235:ILE:HD11	1.96	0.46
1:C:1081:ILE:HG23	1:C:1088:HIS:HB2	1.97	0.46
1:B:442:ASP:OD1	1:B:442:ASP:N	2.49	0.46
1:C:676:THR:OG1	1:C:690:GLN:OE1	2.34	0.46
1:C:524:VAL:HG23	1:C:524:VAL:O	2.16	0.45
1:A:453:TYR:CZ	1:A:493:GLN:HB2	2.51	0.45
1:B:423:TYR:HE1	1:B:464:PHE:HA	1.80	0.45
1:C:124:THR:O	1:C:175:PHE:N	2.35	0.45
1:C:280:ASN:HD21	1:C:282:ASN:HB2	1.80	0.45
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG11	2.51	0.45
1:C:1010:GLN:HE22	1:C:1014:ARG:NH2	2.13	0.45
1:B:91:TYR:HB3	1:B:268:GLY:HA3	1.98	0.45
1:B:377:PHE:HD2	1:B:384:PRO:HB3	1.80	0.45
1:C:440:ASN:HA	1:C:443:SER:HB2	1.98	0.45
1:C:731:MET:HG2	1:C:774:GLN:NE2	2.31	0.45
1:B:367:VAL:HA	1:B:370:ASN:HB2	1.99	0.45
1:B:422:ASN:HA	1:B:467:ASP:HB2	1.98	0.45
1:A:962:LEU:HD11	1:A:1007:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ASP:O	1:C:448:ASN:ND2	2.44	0.45
1:B:364:ASP:HA	1:B:527:PRO:HD3	1.99	0.45
1:C:1083:HIS:HD2	1:C:1136:THR:HA	1.81	0.45
1:A:617:CYS:HB2	1:A:649:CYS:HB3	1.90	0.45
1:B:327:VAL:HG13	1:B:542:ASN:HB3	1.97	0.45
1:C:329:PHE:CE2	1:C:525:CYS:HB3	2.52	0.45
1:C:403:ARG:HD3	1:C:505:TYR:HD1	1.81	0.45
1:B:422:ASN:O	1:B:457:ARG:NH1	2.50	0.45
1:C:101:ILE:HA	1:C:242:LEU:HD13	1.98	0.45
1:C:733:LYS:HZ3	1:C:775:ASP:CG	2.20	0.45
1:C:922:LEU:HG	1:C:926:GLN:HE22	1.81	0.45
1:B:542:ASN:HA	1:B:546:LEU:O	2.17	0.45
1:C:763:LEU:HD21	1:C:1005:GLN:OE1	2.17	0.44
1:A:188:ASN:HA	1:A:209:PRO:HA	1.99	0.44
1:A:540:ASN:OD1	1:A:541:PHE:N	2.49	0.44
1:B:392:PHE:HA	1:B:517:LEU:HD21	2.00	0.44
1:C:1097:SER:HB2	1:C:1102:TRP:CE3	2.52	0.44
1:A:80:ASP:OD1	1:A:80:ASP:N	2.49	0.44
1:C:411:ALA:HB3	1:C:414:GLN:HB3	1.99	0.44
1:A:281:GLU:OE1	1:A:281:GLU:N	2.44	0.44
1:B:375:SER:HB3	1:B:436:TRP:HA	1.99	0.44
1:B:412:PRO:HG2	1:B:426:PRO:O	2.17	0.44
1:A:811:LYS:HZ2	1:A:812:PRO:HD2	1.81	0.44
1:A:281:GLU:OE2	2:D:1:NAG:N2	2.35	0.44
1:B:673:SER:OG	1:B:674:TYR:N	2.51	0.44
1:C:354:ASN:OD1	1:C:355:ARG:N	2.50	0.44
1:C:906:PHE:CD2	1:C:916:LEU:HD12	2.52	0.44
1:A:53:ASP:OD2	1:A:195:LYS:NZ	2.47	0.44
1:B:329:PHE:HD1	1:B:544:ASN:HA	1.81	0.44
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.99	0.44
1:A:455:LEU:N	1:A:491:PRO:O	2.51	0.44
1:A:718:PHE:HE2	1:A:923:ILE:HD13	1.83	0.44
1:B:733:LYS:HD2	1:B:771:ALA:HB1	1.99	0.44
1:C:473:TYR:N	1:C:489:TYR:O	2.47	0.43
1:C:874:THR:HG21	1:C:1055:SER:HB3	1.99	0.43
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	2.00	0.43
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.53	0.43
1:C:353:TRP:NE1	1:C:466:ARG:HG2	2.32	0.43
1:A:53:ASP:HB3	1:A:55:PHE:CE1	2.53	0.43
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.52	0.43
1:C:403:ARG:HE	1:C:497:PHE:HE1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:SER:OG	1:C:531:THR:N	2.51	0.43
1:C:1010:GLN:HE22	1:C:1014:ARG:HH22	1.66	0.43
1:A:205:SER:HA	1:A:223:LEU:HD23	2.01	0.43
1:A:936:ASP:O	1:A:939:SER:OG	2.28	0.43
1:C:280:ASN:OD1	1:C:283:GLY:N	2.52	0.43
1:C:1094:VAL:HG23	1:C:1096:VAL:HG13	2.00	0.43
1:A:616:ASN:O	1:A:618:THR:N	2.51	0.43
1:C:127:VAL:HG22	1:C:171:VAL:HA	1.99	0.43
1:A:57:PRO:HB3	1:A:273:ARG:NH1	2.34	0.43
1:A:220:PHE:HD2	1:A:287:ASP:HA	1.84	0.43
1:B:102:ARG:NE	1:B:243:ALA:HB2	2.31	0.43
1:B:994:ASP:O	1:B:997:ILE:HG22	2.19	0.43
1:C:814:LYS:HA	1:C:814:LYS:HD3	1.64	0.43
1:C:379:CYS:SG	1:C:384:PRO:HB3	2.58	0.43
1:C:122:ASN:OD1	1:C:123:ALA:N	2.52	0.43
2:D:1:NAG:H4	2:D:2:NAG:H2	1.73	0.43
1:A:901:GLN:HE22	1:A:905:ARG:NH2	2.17	0.43
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.43
1:B:402:ILE:HG12	1:B:510:VAL:HG21	2.00	0.43
1:B:644:GLN:NE2	1:B:648:GLY:O	2.52	0.43
1:B:787:GLN:HB2	1:B:789:TYR:CZ	2.54	0.43
1:A:316:SER:OG	1:A:317:ASN:N	2.50	0.43
1:A:741:TYR:CE1	1:A:1004:LEU:HD21	2.54	0.43
1:C:212:LEU:HD12	1:C:213:VAL:O	2.19	0.43
1:C:403:ARG:HD3	1:C:505:TYR:CD1	2.54	0.43
1:A:644:GLN:NE2	1:A:645:THR:O	2.46	0.42
1:C:367:VAL:HG11	3:C:1312:NAG:H61	2.00	0.42
1:C:818:ILE:HG13	1:C:819:GLU:N	2.34	0.42
1:C:1089:PHE:N	1:C:1120:THR:OG1	2.52	0.42
1:A:130:VAL:N	1:A:168:PHE:O	2.51	0.42
1:A:386:LYS:O	1:A:386:LYS:HG3	2.20	0.42
1:B:442:ASP:O	1:B:507:PRO:HG3	2.19	0.42
1:A:351:TYR:HB2	1:A:467:ASP:HB3	2.01	0.42
1:A:592:PHE:H	1:B:853:GLN:NE2	2.18	0.42
1:B:532:ASN:OD1	1:B:532:ASN:N	2.52	0.42
1:C:30:ASN:HD21	1:C:59:PHE:HB3	1.83	0.42
1:C:922:LEU:O	1:C:926:GLN:OE1	2.37	0.42
1:A:189:LEU:N	1:A:208:THR:O	2.53	0.42
1:A:281:GLU:HG2	1:A:282:ASN:OD1	2.19	0.42
1:C:120:VAL:O	1:C:126:VAL:HG13	2.20	0.42
1:C:427:ASP:OD1	1:C:428:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ASN:ND2	1:C:506:GLN:OE1	2.33	0.42
1:A:295:PRO:HA	1:A:298:GLU:OE2	2.18	0.42
1:A:379:CYS:HB3	1:A:382:VAL:HG23	2.00	0.42
1:B:731:MET:HG2	1:B:774:GLN:OE1	2.19	0.42
1:C:134:GLN:N	1:C:162:SER:OG	2.53	0.42
1:C:433:VAL:HG12	1:C:512:VAL:HG22	2.01	0.42
1:C:490:PHE:CD1	1:C:491:PRO:HD2	2.55	0.42
1:B:203:ILE:HG22	1:B:226:LEU:HB3	2.01	0.42
1:C:659:SER:HB3	1:C:698:SER:OG	2.19	0.42
1:B:141:LEU:O	1:B:244:LEU:N	2.51	0.42
1:B:502:GLY:O	1:B:506:GLN:HG2	2.20	0.42
1:A:290:ASP:O	1:A:297:SER:HB2	2.19	0.42
1:A:418:ILE:HG23	1:A:422:ASN:HB2	2.02	0.42
1:B:501:TYR:CD2	1:B:505:TYR:HB2	2.55	0.42
1:A:124:THR:C	1:A:174:PRO:HA	2.40	0.42
1:A:316:SER:O	1:A:595:VAL:N	2.46	0.42
1:A:666:ILE:HD12	1:A:670:ILE:HG22	2.01	0.42
1:A:920:GLN:O	1:A:923:ILE:HG22	2.20	0.42
1:A:1083:HIS:CE1	1:A:1137:VAL:H	2.37	0.42
1:B:950:ASP:OD1	1:B:950:ASP:N	2.52	0.42
1:C:134:GLN:O	1:C:161:SER:N	2.53	0.42
1:C:456:PHE:HB3	1:C:473:TYR:CG	2.55	0.42
1:A:334:ASN:O	1:A:362:VAL:N	2.53	0.42
1:B:48:LEU:HB3	1:B:276:LEU:HD11	2.01	0.42
1:B:203:ILE:HD13	1:B:203:ILE:HA	1.86	0.42
1:B:794:ILE:HG22	1:B:796:ASP:H	1.85	0.42
1:B:994:ASP:HA	1:B:997:ILE:HG22	2.01	0.42
1:C:986:PRO:HB2	1:C:987:PRO:HD3	2.01	0.42
1:A:193:VAL:HG22	1:A:204:TYR:HB2	2.02	0.41
1:A:879:ALA:HA	1:A:882:ILE:HG22	2.02	0.41
1:B:152:TRP:CH2	1:B:245:HIS:HB3	2.55	0.41
1:B:195:LYS:O	1:B:202:LYS:N	2.44	0.41
1:B:747:THR:O	1:B:750:SER:OG	2.27	0.41
1:B:1084:ASP:HB2	1:B:1086:LYS:NZ	2.35	0.41
1:C:1010:GLN:HE22	1:C:1014:ARG:HH12	1.66	0.41
1:A:206:LYS:HZ2	1:A:208:THR:HG22	1.85	0.41
1:A:291:CYS:HB3	1:A:301:CYS:HB2	1.30	0.41
1:A:537:LYS:HD3	1:A:537:LYS:HA	1.78	0.41
1:A:581:THR:OG1	1:A:583:GLU:OE1	2.36	0.41
1:B:327:VAL:HG22	1:B:542:ASN:HB3	2.02	0.41
1:B:671:CYS:SG	1:B:697:MET:HE2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:996:LEU:HD23	1:C:996:LEU:HA	1.90	0.41
1:A:47:VAL:HG12	1:C:569:ILE:HG13	2.01	0.41
1:A:91:TYR:HE1	1:A:191:GLU:HB3	1.85	0.41
1:B:89:GLY:C	1:B:270:LEU:HD13	2.41	0.41
1:B:294:ASP:O	1:B:297:SER:OG	2.21	0.41
1:C:327:VAL:N	1:C:531:THR:OG1	2.36	0.41
1:A:339:GLY:O	1:A:343:ASN:N	2.53	0.41
1:A:909:ILE:HG12	1:A:1047:TYR:HB3	2.01	0.41
1:C:1080:ALA:O	1:C:1132:ILE:HG13	2.21	0.41
1:A:128:ILE:HD13	1:A:170:TYR:CD2	2.55	0.41
1:B:143:VAL:HG22	1:B:154:GLU:HG2	2.02	0.41
1:C:196:ASN:OD1	1:C:196:ASN:O	2.38	0.41
1:C:327:VAL:HB	1:C:531:THR:HG23	2.01	0.41
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.21	0.41
1:A:950:ASP:OD1	1:A:950:ASP:N	2.54	0.41
1:B:1036:GLN:HA	1:B:1048:HIS:CE1	2.56	0.41
1:C:106:PHE:HB3	1:C:235:ILE:HG21	2.02	0.41
1:C:227:VAL:HG12	1:C:229:LEU:HD22	2.02	0.41
1:C:409:GLN:OE1	1:C:418:ILE:HG12	2.21	0.41
1:C:580:GLN:O	3:C:1311:NAG:O6	2.36	0.41
1:A:904:TYR:CE2	1:C:1107:ARG:HD3	2.56	0.41
1:B:328:ARG:HG3	1:B:530:SER:HB2	2.02	0.41
1:C:135:PHE:CD1	1:C:160:TYR:HB3	2.56	0.41
1:C:919:ASN:O	1:C:923:ILE:HD12	2.20	0.41
1:A:287:ASP:OD1	1:A:288:ALA:N	2.53	0.41
1:A:346:ARG:HA	1:A:509:ARG:HH22	1.86	0.41
1:A:438:SER:O	1:A:507:PRO:HG2	2.20	0.41
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.49	0.41
1:A:1114:ILE:O	1:A:1116:THR:HG23	2.21	0.41
1:C:280:ASN:ND2	1:C:282:ASN:HB2	2.36	0.41
1:A:280:ASN:OD1	1:A:283:GLY:N	2.54	0.41
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.55	0.41
1:B:763:LEU:HD21	1:B:1005:GLN:OE1	2.20	0.41
1:B:912:THR:O	1:B:915:VAL:HG12	2.20	0.41
1:C:424:LYS:HZ1	1:C:463:PRO:HD3	1.86	0.41
1:C:717:ASN:HB2	1:C:1070:ALA:HB3	2.03	0.41
1:B:189:LEU:HG	1:B:191:GLU:OE1	2.21	0.41
1:C:416:GLY:O	1:C:420:ASP:N	2.54	0.41
1:C:866:THR:H	1:C:869:MET:HE3	1.85	0.41
1:B:122:ASN:HB3	1:B:125:ASN:O	2.20	0.40
1:B:759:PHE:O	1:B:763:LEU:HD23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1088:HIS:HD1	1:B:1120:THR:HG21	1.86	0.40
1:C:129:LYS:HG3	1:C:169:GLU:OE2	2.21	0.40
1:C:340:GLU:N	1:C:340:GLU:OE1	2.52	0.40
1:C:405:ASP:N	1:C:504:GLY:O	2.54	0.40
1:C:763:LEU:HD13	1:C:763:LEU:HA	1.90	0.40
1:C:1120:THR:OG1	1:C:1121:PHE:N	2.54	0.40
1:A:437:ASN:HA	1:A:508:TYR:CD1	2.56	0.40
1:B:125:ASN:OD1	1:B:126:VAL:N	2.54	0.40
1:B:713:ALA:HB3	1:C:894:LEU:HB3	2.03	0.40
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.90	0.40
1:A:328:ARG:HH12	1:A:533:LEU:HD12	1.86	0.40
1:A:713:ALA:HB3	1:B:894:LEU:HB3	2.03	0.40
1:B:106:PHE:HE2	1:B:119:ILE:HG13	1.86	0.40
1:B:290:ASP:OD1	1:B:291:CYS:N	2.55	0.40
1:B:497:PHE:CD2	1:B:507:PRO:HB3	2.55	0.40
1:B:730:SER:O	1:B:1058:HIS:HB3	2.21	0.40
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.92	0.40
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.54	0.40
1:A:24:LEU:HD23	1:A:25:PRO:O	2.21	0.40
1:A:96:GLU:HB2	1:A:187:LYS:HZ3	1.86	0.40
1:A:962:LEU:HD21	1:A:1007:TYR:HB2	2.03	0.40
1:B:96:GLU:OE2	1:B:100:ILE:N	2.55	0.40
1:B:905:ARG:CZ	1:B:1050:MET:HB3	2.51	0.40
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.86	0.40
1:B:962:LEU:HD23	1:B:962:LEU:HA	1.89	0.40
1:C:131:CYS:HB2	1:C:133:PHE:CE1	2.57	0.40
1:C:327:VAL:HG13	1:C:542:ASN:HD21	1.85	0.40
1:C:474:GLN:HA	1:C:480:CYS:SG	2.62	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	963/1284 (75%)	902 (94%)	61 (6%)	0	100	100
1	B	1002/1284 (78%)	945 (94%)	57 (6%)	0	100	100
1	C	977/1284 (76%)	914 (94%)	63 (6%)	0	100	100
All	All	2942/3852 (76%)	2761 (94%)	181 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	861/1112 (77%)	860 (100%)	1 (0%)	92	95
1	B	891/1112 (80%)	891 (100%)	0	100	100
1	C	872/1112 (78%)	870 (100%)	2 (0%)	92	94
All	All	2624/3336 (79%)	2621 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	921	LYS
1	C	310	LYS
1	C	786	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1083	HIS
1	B	439	ASN
1	B	506	GLN
1	B	895	GLN
1	B	955	ASN
1	C	658	ASN
1	C	955	ASN

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Mol	Chain	Res	Type
1	C	992	GLN
1	C	1083	HIS

### 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 ⓘ

6 monosaccharides 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	$\# Z  > 2$
2	NAG	D	1	1,2	14,14,15	0.18	0	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.53	0	17,19,21	0.43	0
2	NAG	E	1	1,2	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	E	2	2	14,14,15	0.25	0	17,19,21	0.53	0
2	NAG	F	1	1,2	14,14,15	0.20	0	17,19,21	0.56	0
2	NAG	F	2	2	14,14,15	0.51	0	17,19,21	0.42	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

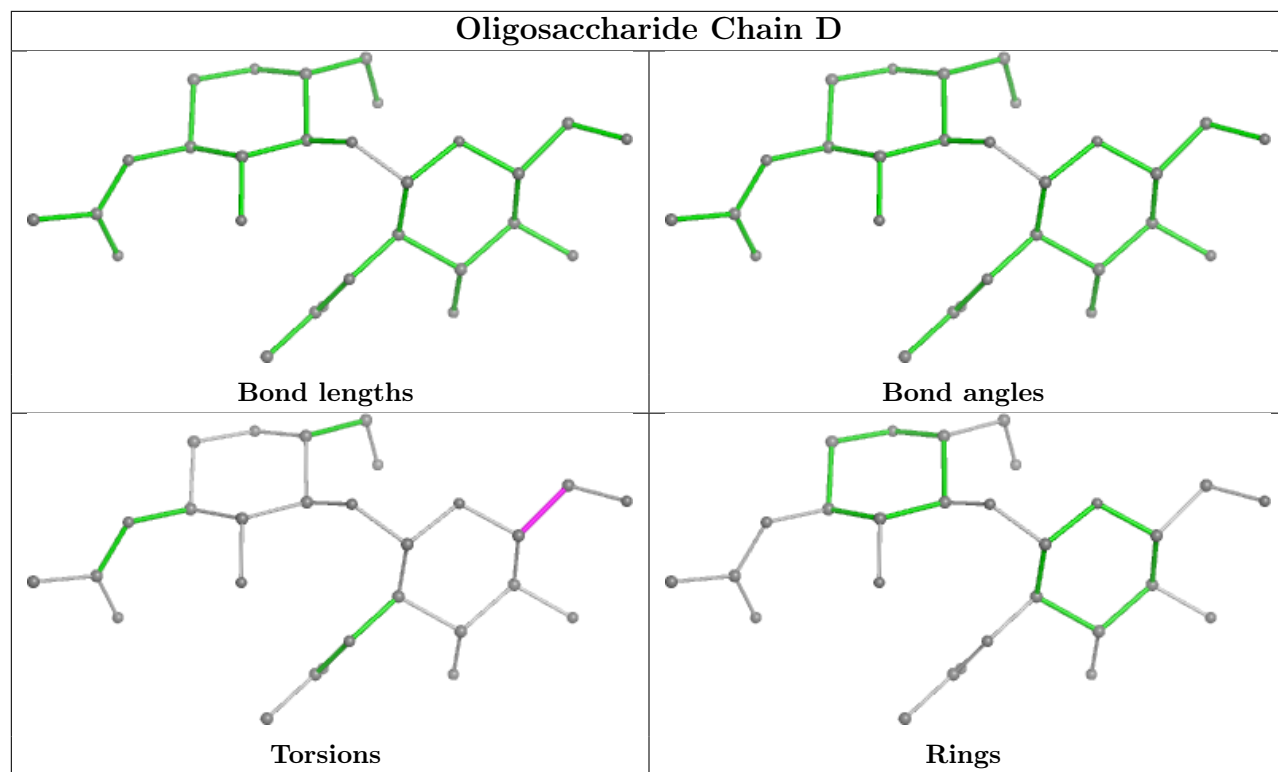
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6

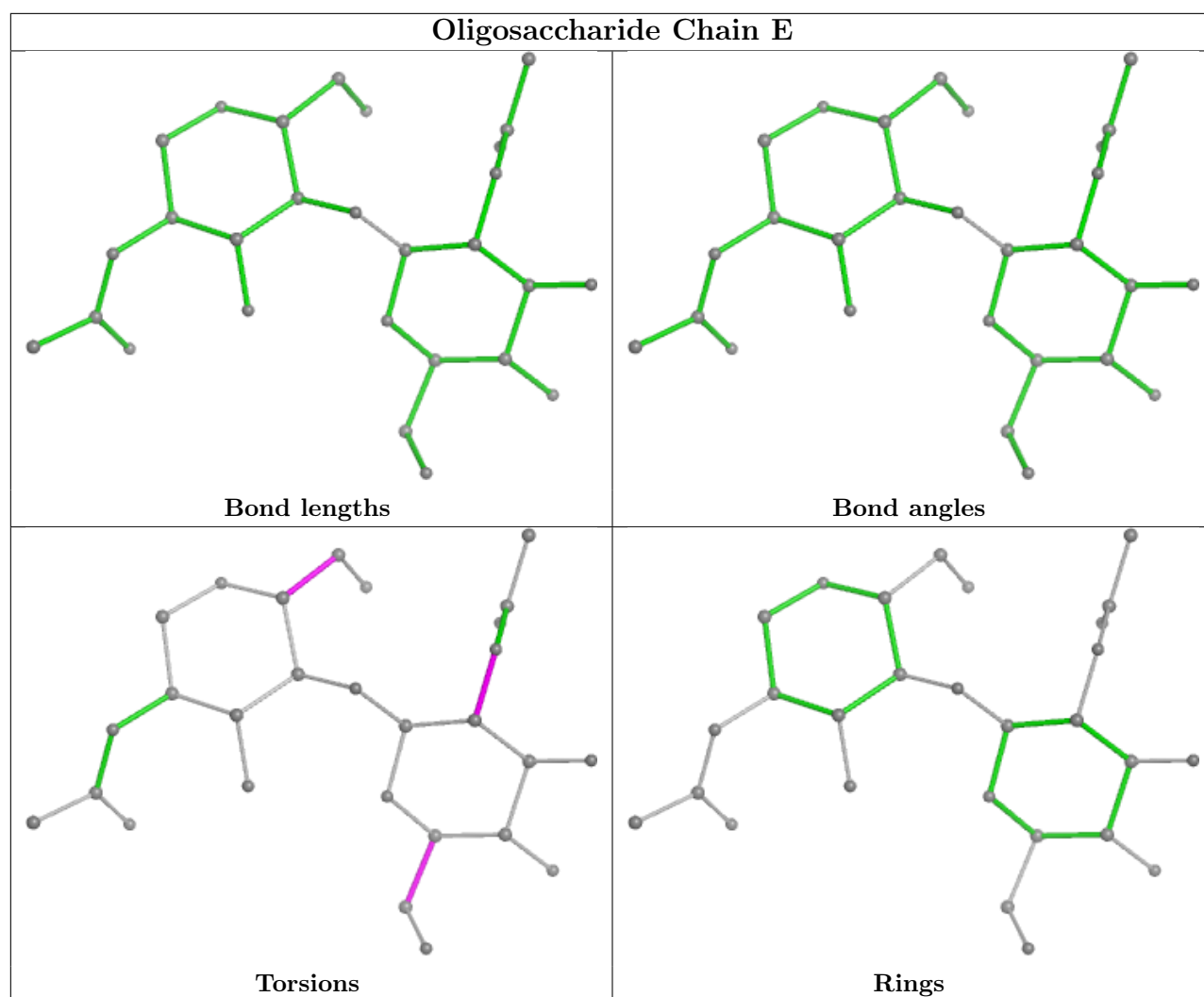
There are no ring outliers.

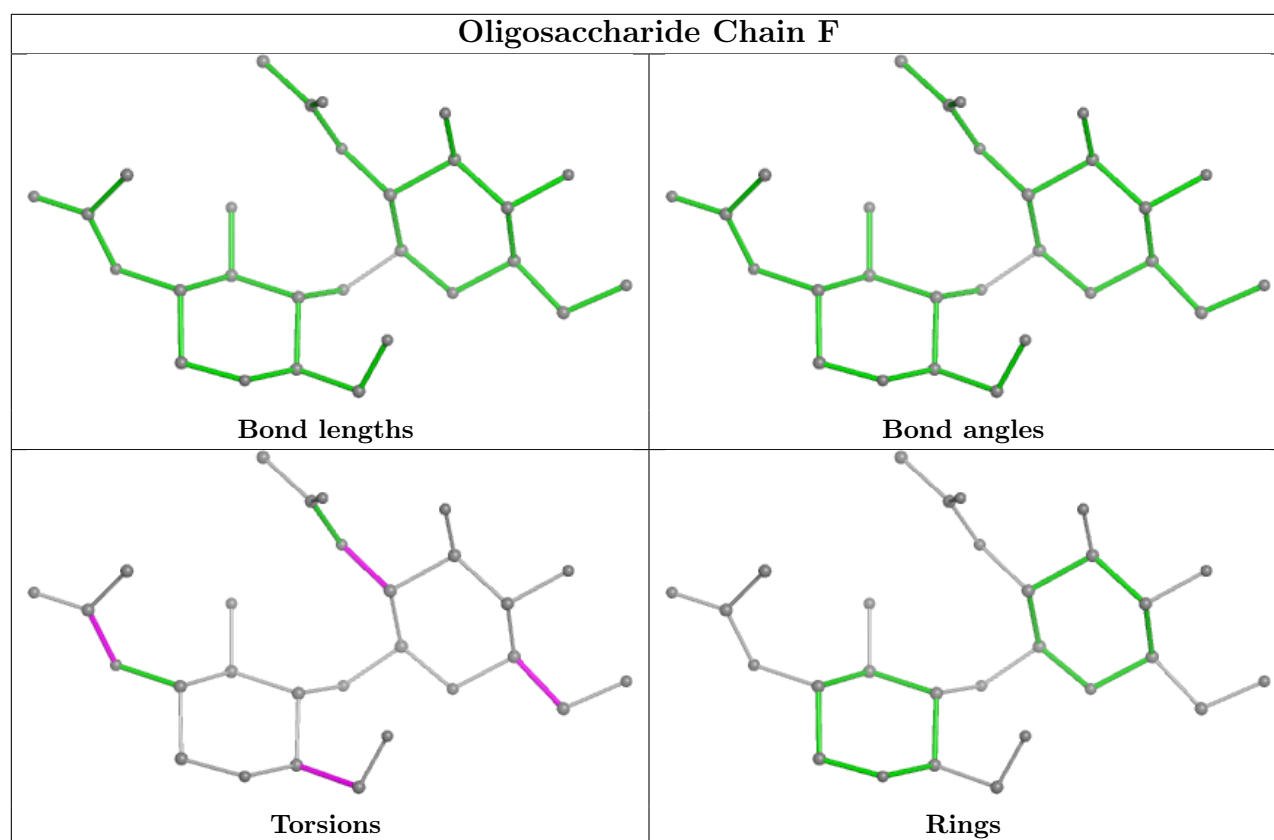
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	0
2	D	2	NAG	1	0
2	F	1	NAG	1	0
2	F	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

37 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	$\# Z  > 2$
3	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	A	1305	1	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	C	1311	1	14,14,15	0.23	0	17,19,21	0.35	0
3	NAG	C	1305	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	B	1310	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	A	1311	1	14,14,15	0.17	0	17,19,21	0.44	0
3	NAG	C	1308	1	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	C	1309	1	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	A	1307	1	14,14,15	0.18	0	17,19,21	0.42	0
3	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.34	0
3	NAG	C	1303	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	C	1312	1	14,14,15	0.42	0	17,19,21	0.37	0
3	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.51	0
3	NAG	C	1304	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	B	1301	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	A	1302	1	14,14,15	0.20	0	17,19,21	0.49	0
3	NAG	C	1313	1	14,14,15	0.30	0	17,19,21	0.36	0
3	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	B	1311	1	14,14,15	0.73	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	B	1308	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	B	1303	1	14,14,15	0.19	0	17,19,21	0.45	0
3	NAG	C	1306	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	A	1309	1	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	B	1313	1	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	B	1307	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	B	1312	1	14,14,15	0.26	0	17,19,21	0.59	1 (5%)
3	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	C	1307	1	14,14,15	0.90	1 (7%)	17,19,21	1.31	1 (5%)
3	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	A	1303	1	14,14,15	0.17	0	17,19,21	0.39	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
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1307	NAG	O5-C1	3.25	1.48	1.43
3	B	1311	NAG	C1-C2	2.41	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1307	NAG	C1-O5-C5	5.12	119.13	112.19
3	B	1311	NAG	C1-O5-C5	2.72	115.88	112.19
3	B	1312	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1310	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1313	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	C	1312	NAG	O5-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1313	NAG	O5-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	B	1313	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1312	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	B	1312	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1311	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1302	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	A	1303	NAG	C8-C7-N2-C2
3	A	1303	NAG	O7-C7-N2-C2
3	A	1309	NAG	C8-C7-N2-C2
3	A	1309	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1313	NAG	C8-C7-N2-C2
3	B	1313	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	C	1312	NAG	C8-C7-N2-C2
3	C	1312	NAG	O7-C7-N2-C2
3	A	1308	NAG	C4-C5-C6-O6
3	B	1312	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	C	1313	NAG	C4-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1313	NAG	C1-C2-N2-C7
3	A	1309	NAG	O5-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	A	1310	NAG	C3-C2-N2-C7
3	B	1311	NAG	C3-C2-N2-C7
3	C	1305	NAG	C4-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	C	1313	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1311	NAG	1	0
3	A	1311	NAG	1	0
3	A	1308	NAG	1	0
3	C	1312	NAG	2	0
3	B	1311	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.

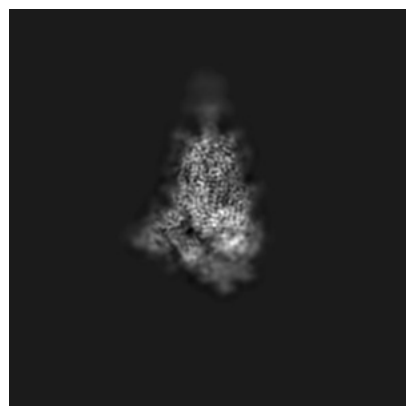
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14231. These allow visual inspection of the internal detail of the map and identification of artifacts.

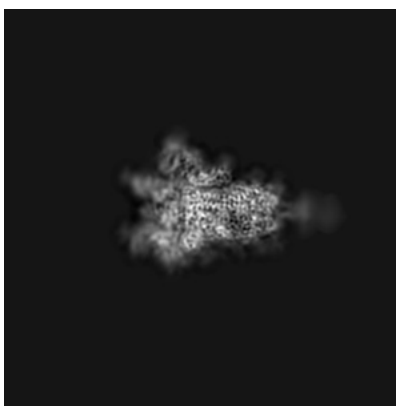
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

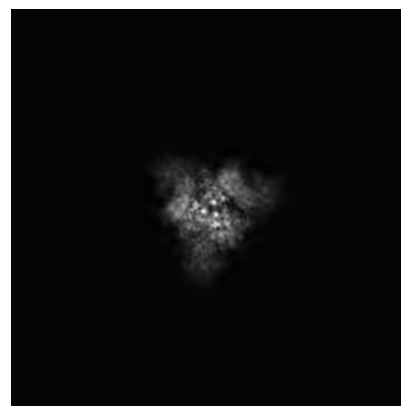
#### 6.1.1 Primary map



X

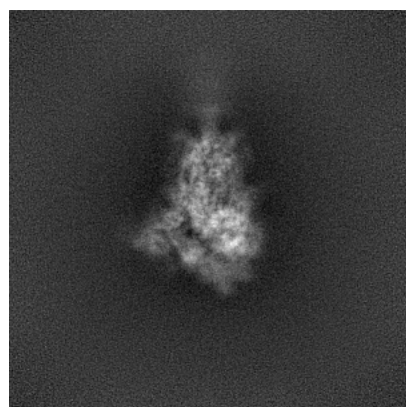


Y

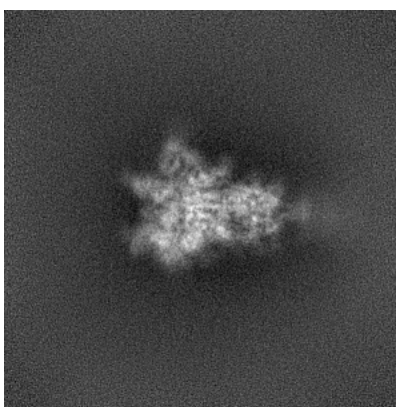


Z

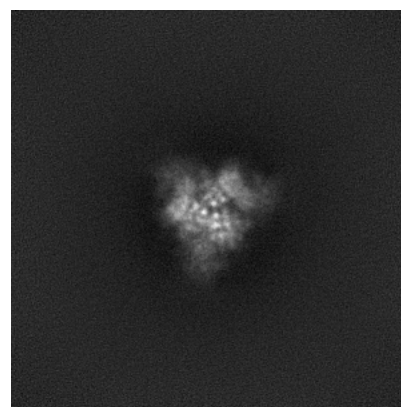
#### 6.1.2 Raw map



X



Y

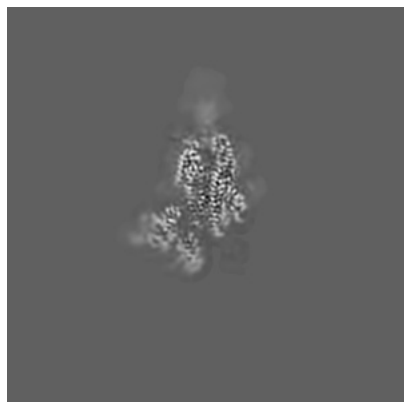


Z

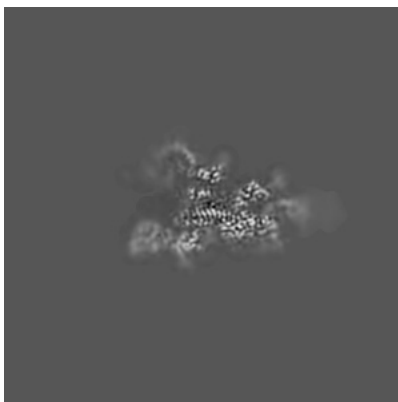
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

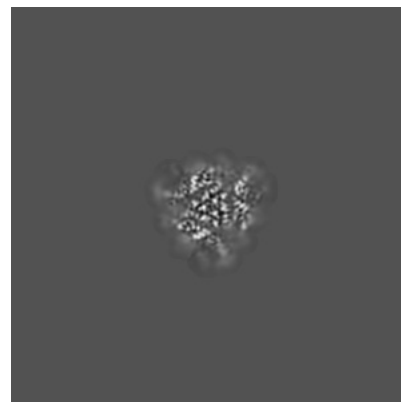
### 6.2.1 Primary map



X Index: 200

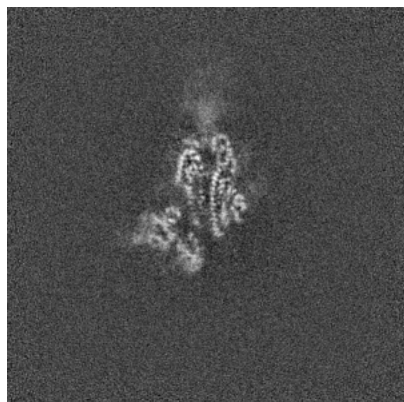


Y Index: 200

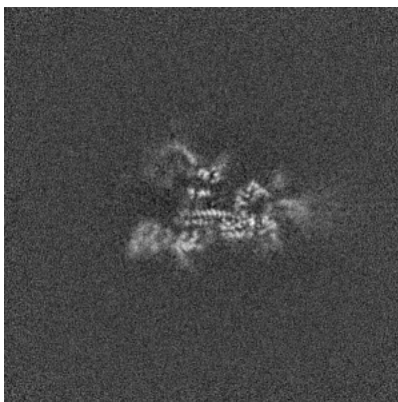


Z Index: 200

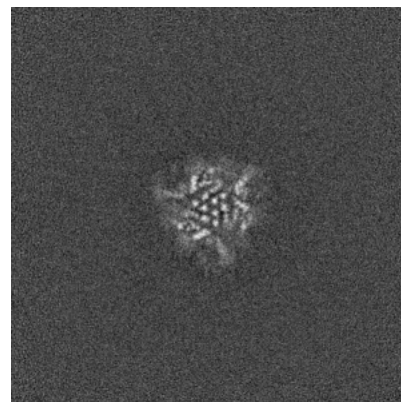
### 6.2.2 Raw map



X Index: 200



Y Index: 200

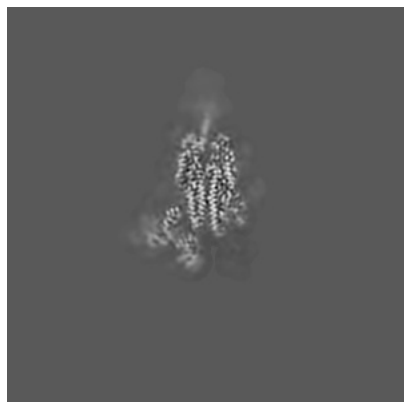


Z Index: 200

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

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

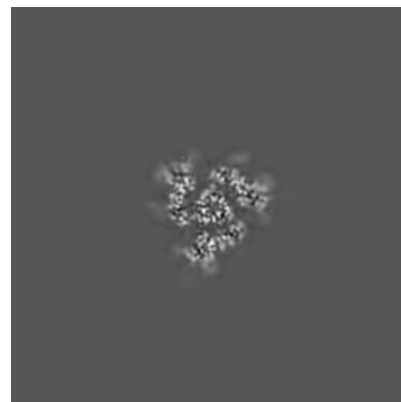
### 6.3.1 Primary map



X Index: 203

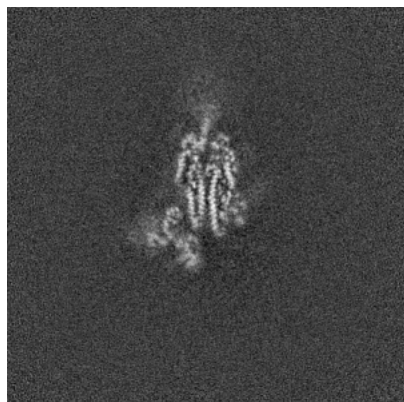


Y Index: 193



Z Index: 186

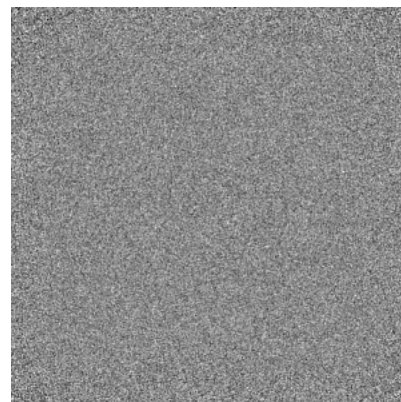
### 6.3.2 Raw map



X Index: 203



Y Index: 194

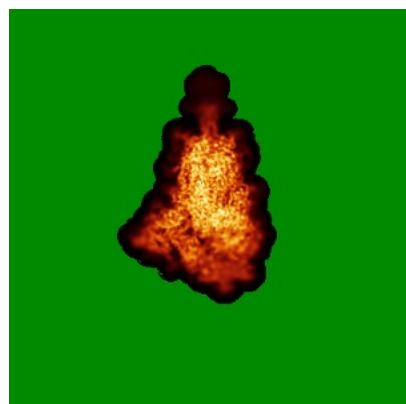


Z Index: 0

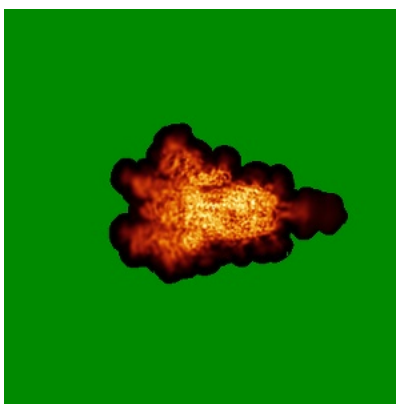
The images above show the largest variance slices of the map in three orthogonal directions.

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

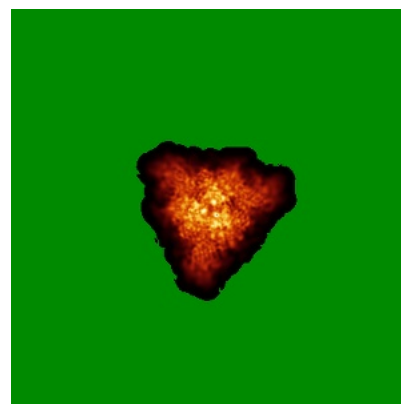
### 6.4.1 Primary map



X

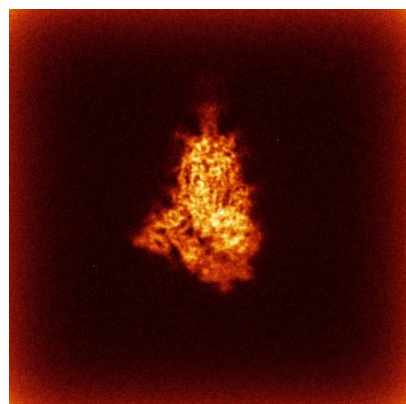


Y

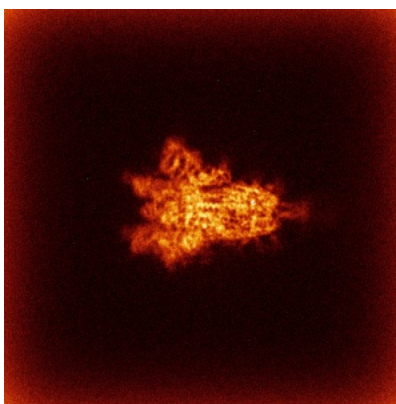


Z

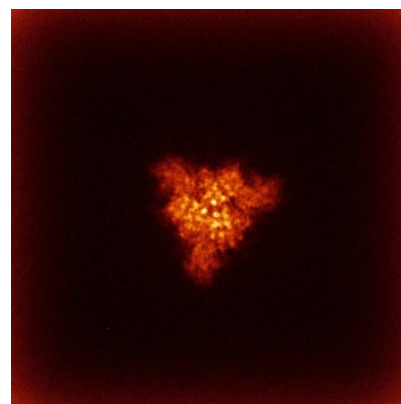
### 6.4.2 Raw map



X



Y



Z

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

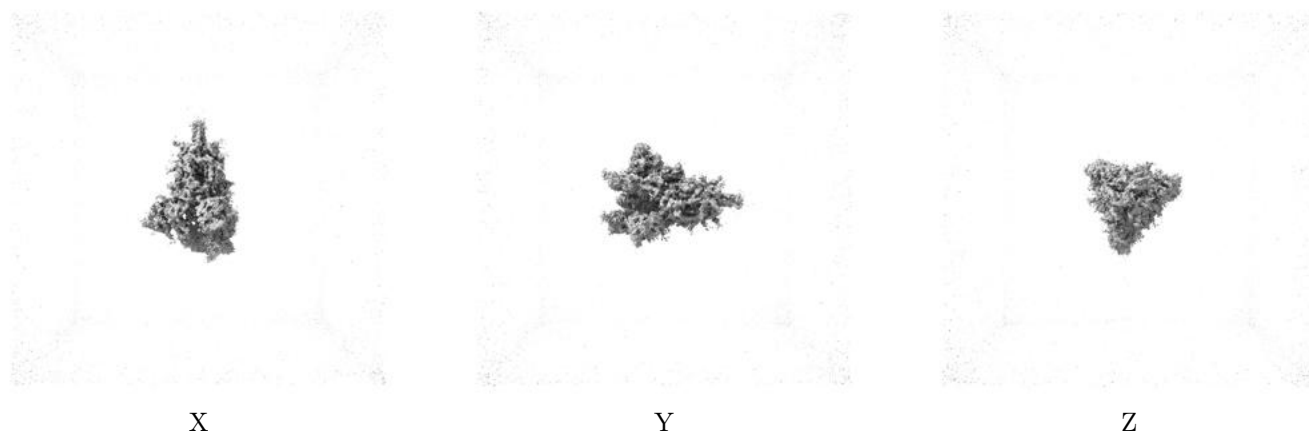
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

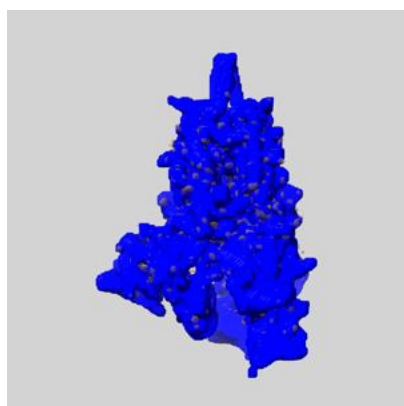
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

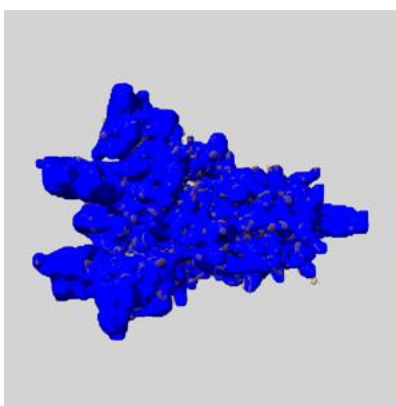
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

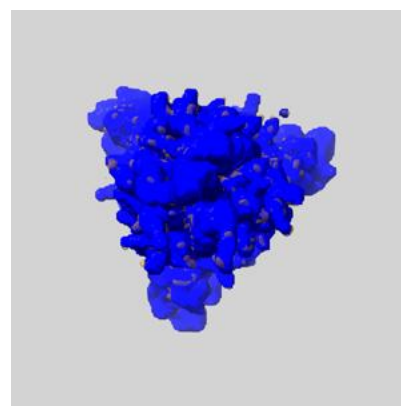
### 6.6.1 emd\_14231\_msk\_1.map [i](#)



X



Y

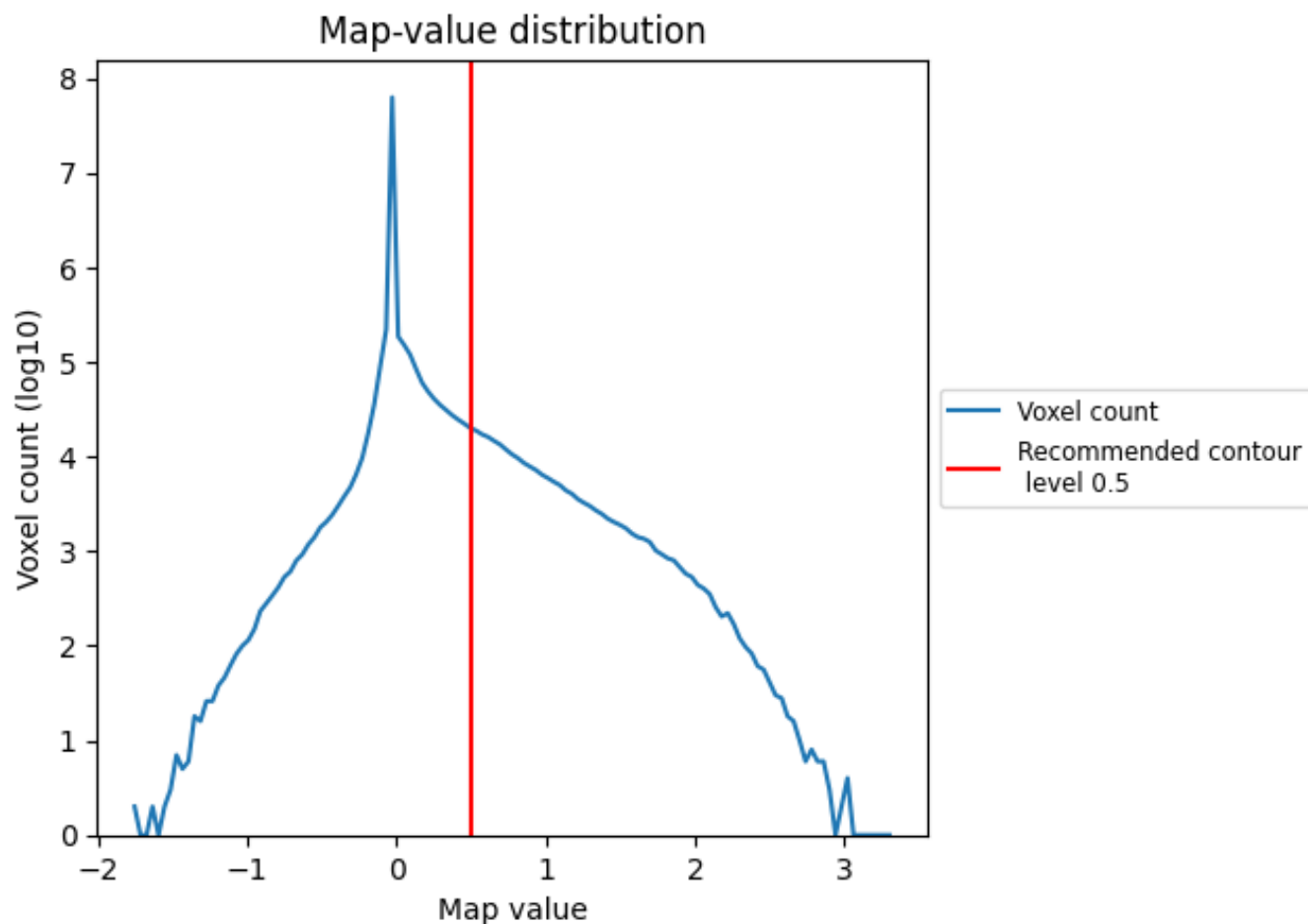


Z

## 7 Map analysis [i](#)

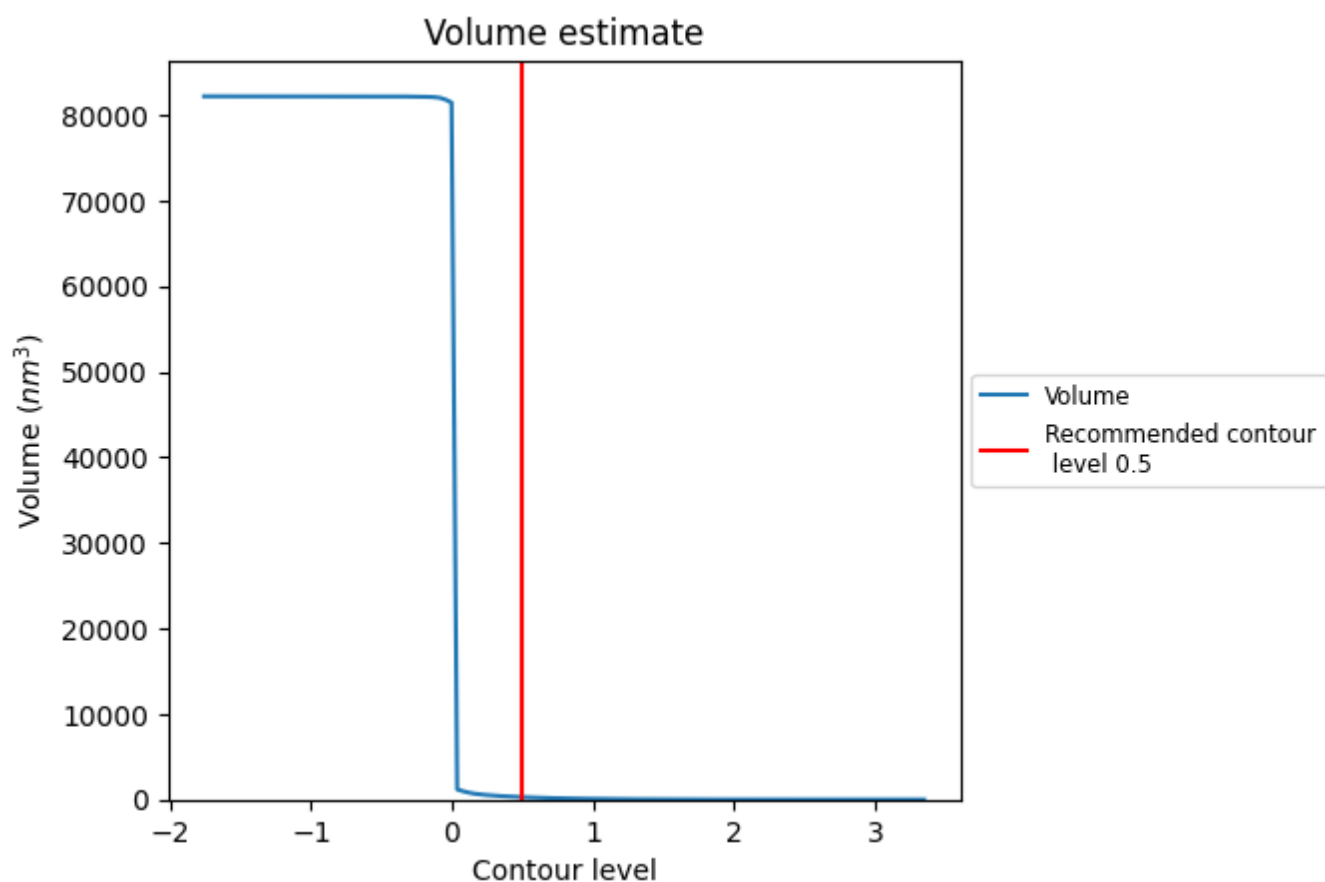
This section contains the results of statistical analysis of the map.

### 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.

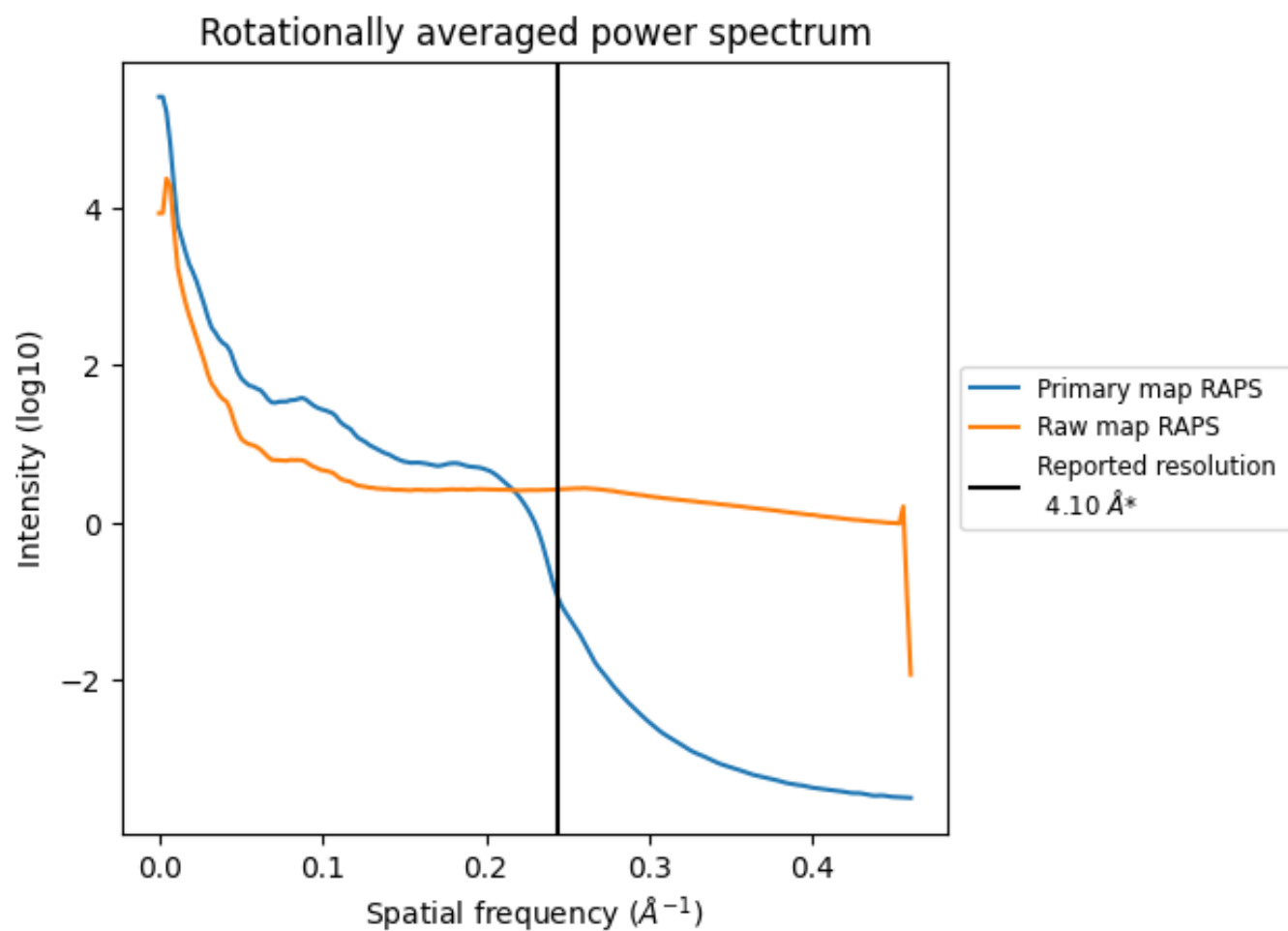
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283  $\text{nm}^3$ ; this corresponds to an approximate mass of 255 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

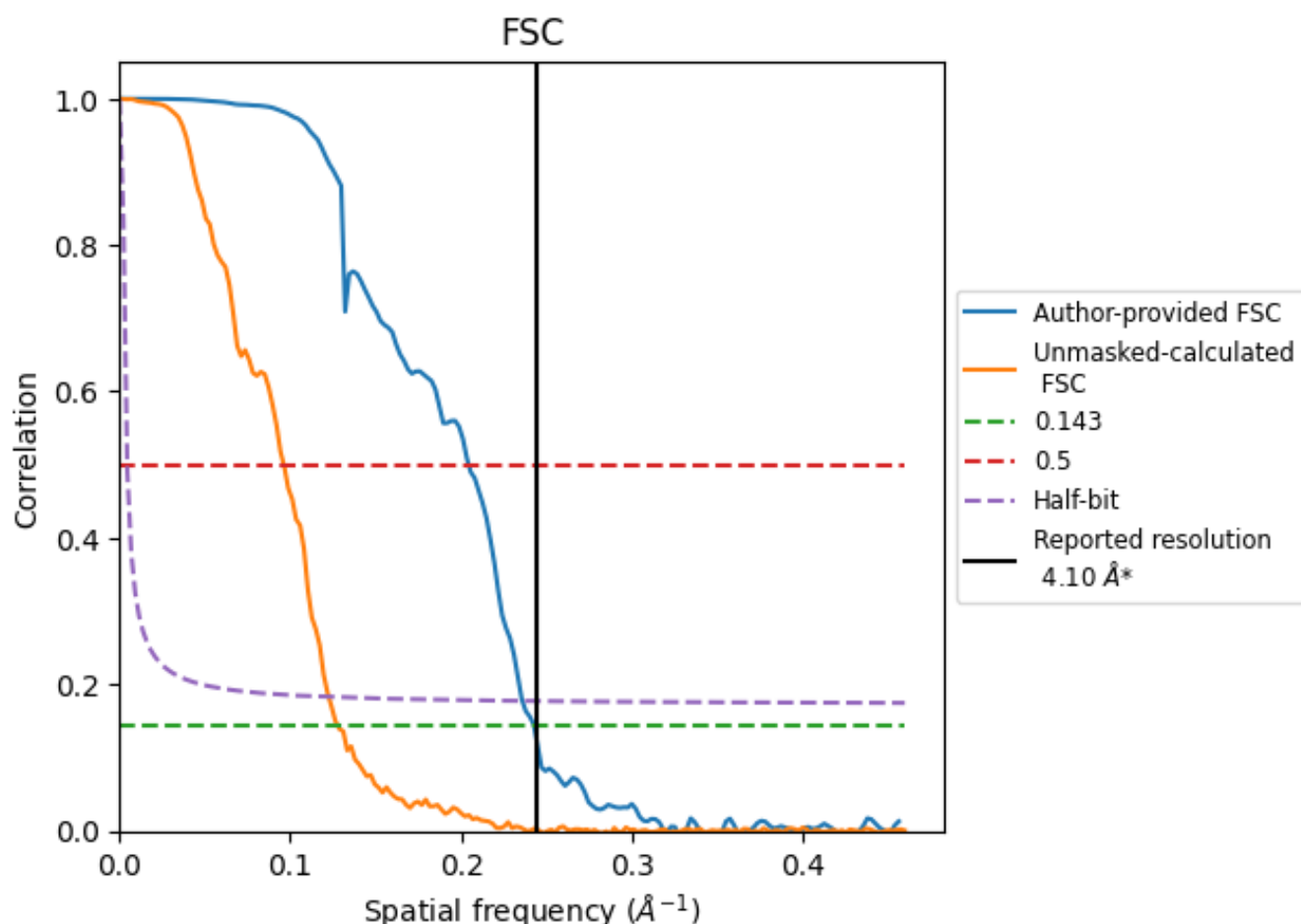


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

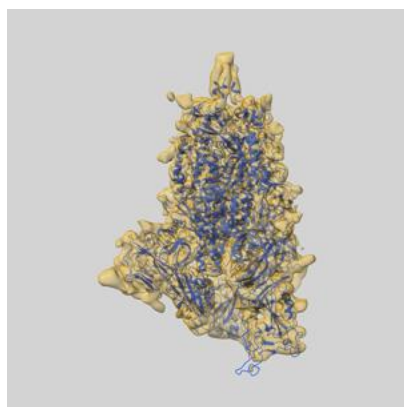
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	4.89	4.24
Unmasked-calculated*	7.82	10.38	8.16

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.82 differs from the reported value 4.1 by more than 10 %

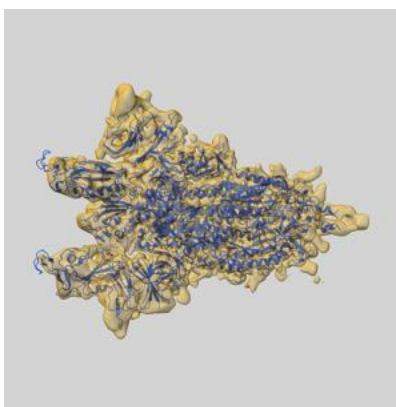
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14231 and PDB model 7R15. Per-residue inclusion information can be found in section [3](#) on page [13](#).

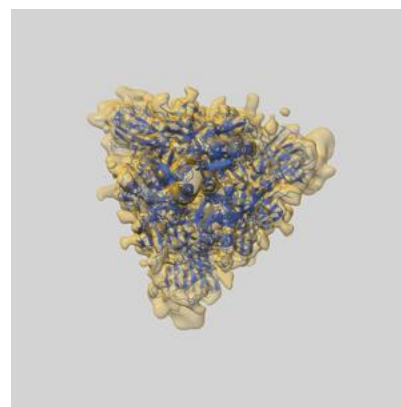
### 9.1 Map-model overlay [i](#)



X



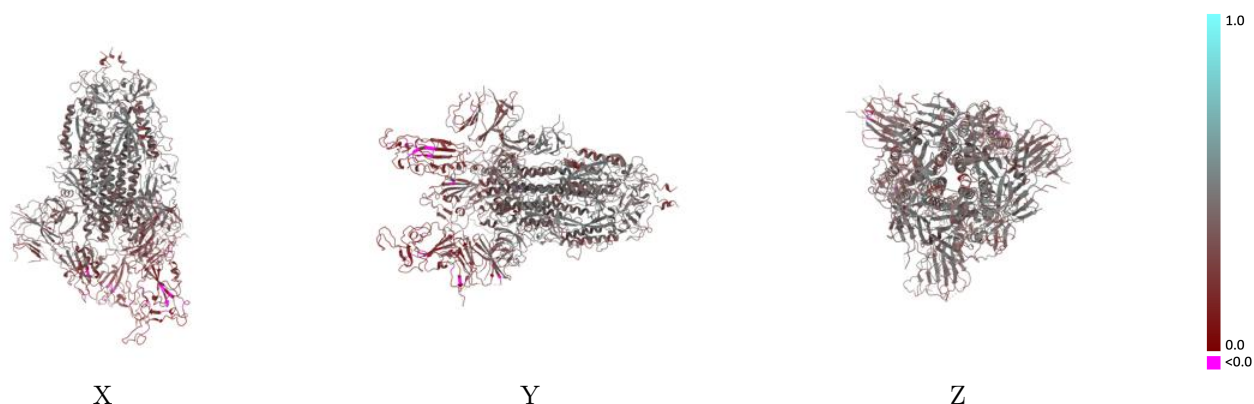
Y



Z

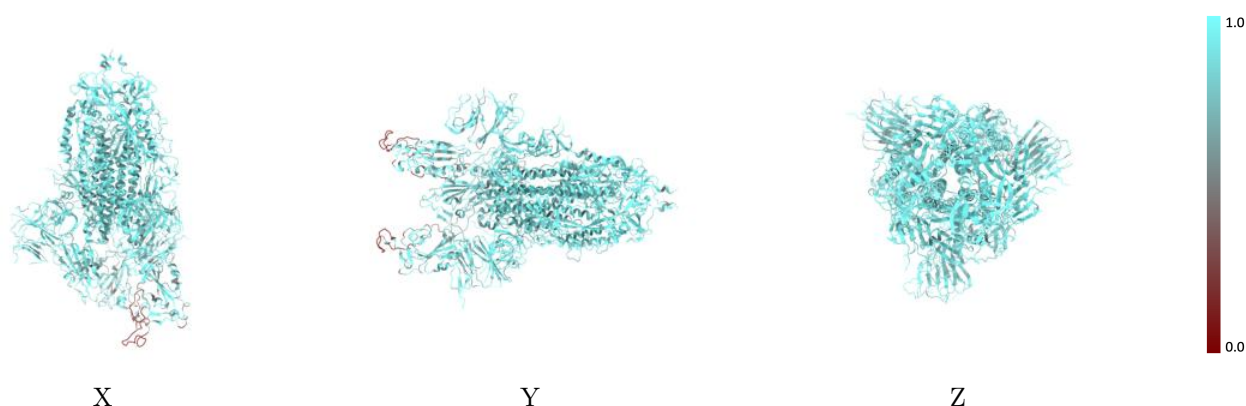
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



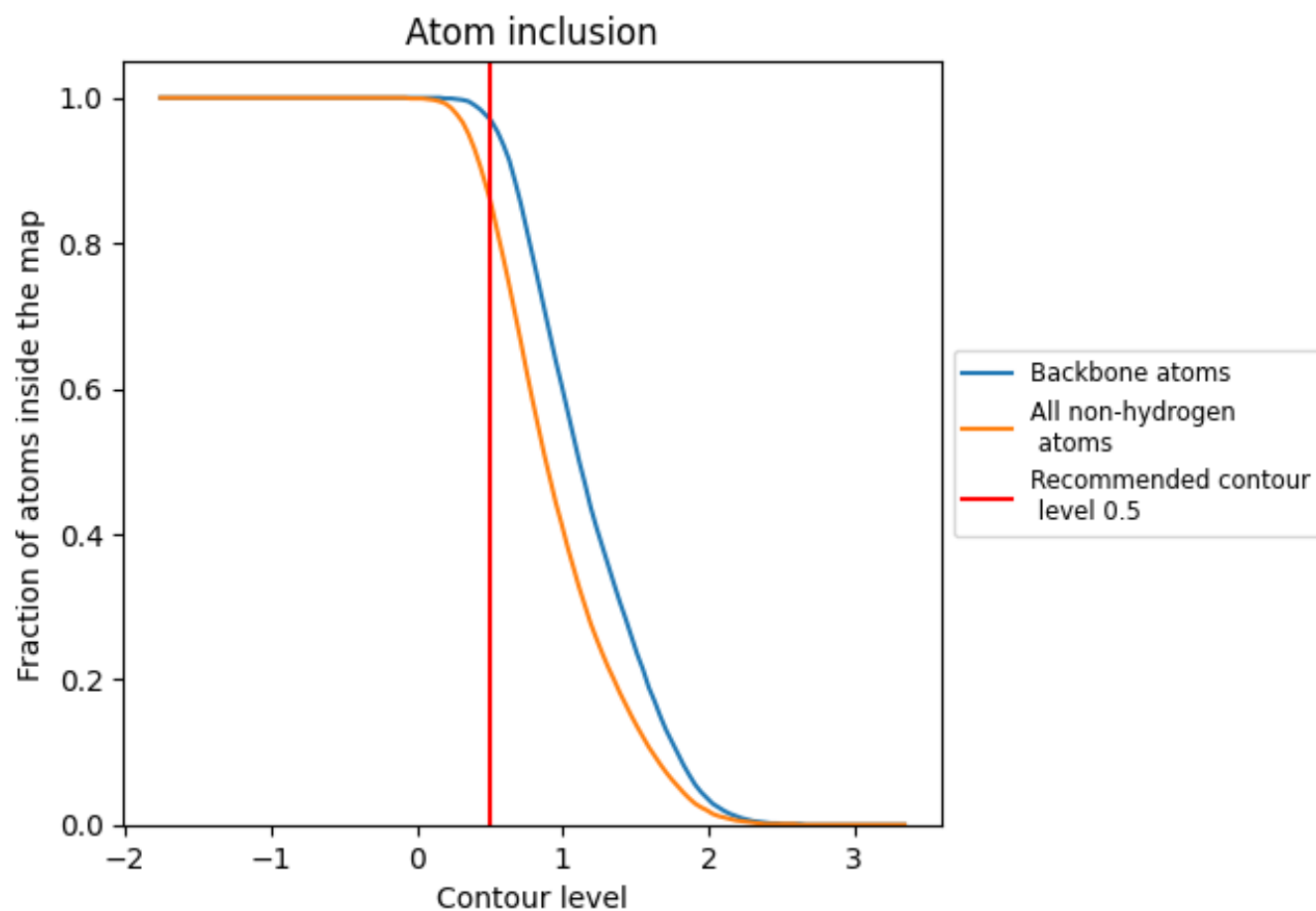
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 86% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8620</div>	<div><div></div>0.3580</div>
A	<div><div></div>0.8610</div>	<div><div></div>0.3610</div>
B	<div><div></div>0.8430</div>	<div><div></div>0.3410</div>
C	<div><div></div>0.8830</div>	<div><div></div>0.3720</div>
D	<div><div></div>0.7500</div>	<div><div></div>0.3190</div>
E	<div><div></div>0.6430</div>	<div><div></div>0.4120</div>
F	<div><div></div>1.0000</div>	<div><div></div>0.3690</div>

1.0

0.0

<0.0