



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:56 PM JST

PDB ID : 9XI3 / pdb_00009xi3
EMDB ID : EMD-66895
Title : SARS-CoV-2 Omicron BA.4/5 spike trimer in complex with C807 Fab and ACE2 (3 RBD up)
Authors : Niu, C.; Liu, B.; Gao, X.; Li, Z.; He, J.; Xiong, X.
Deposited on : 2025-11-02
Resolution : 4.74 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

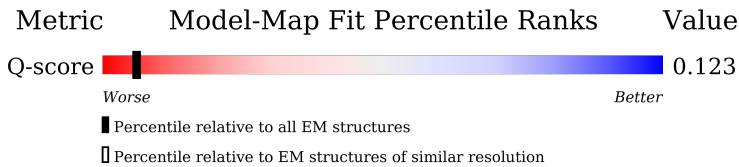
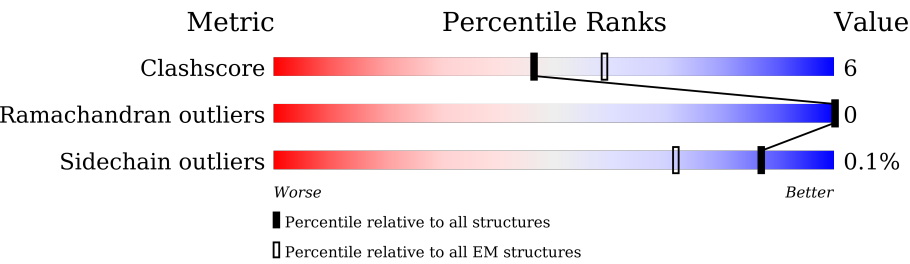
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.74 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1628 (4.24 - 5.23)

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

Mol	Chain	Length	Quality of chain
1	D	602	23% 87% 11% .
1	E	602	38% 84% 15% .
1	F	602	. 85% 14% .
2	G	228	34% 82% 15% .

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Mol	Chain	Length	Quality of chain
2	H	228	
2	I	228	
3	J	217	
3	K	217	
3	L	217	
4	A	1247	
4	B	1247	
4	C	1247	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	Q	2	
5	R	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49623 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	596	Total	C	N	O	S	0	0
			4864	3112	805	918	29		
1	F	596	Total	C	N	O	S	0	0
			4864	3112	805	918	29		
1	E	596	Total	C	N	O	S	0	0
			4864	3112	805	918	29		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	PRO	-	expression tag	UNP Q9BYF1
D	617	LEU	-	expression tag	UNP Q9BYF1
D	618	VAL	-	expression tag	UNP Q9BYF1
D	619	PRO	-	expression tag	UNP Q9BYF1
D	620	ARG	-	expression tag	UNP Q9BYF1
F	616	PRO	-	expression tag	UNP Q9BYF1
F	617	LEU	-	expression tag	UNP Q9BYF1
F	618	VAL	-	expression tag	UNP Q9BYF1
F	619	PRO	-	expression tag	UNP Q9BYF1
F	620	ARG	-	expression tag	UNP Q9BYF1
E	616	PRO	-	expression tag	UNP Q9BYF1
E	617	LEU	-	expression tag	UNP Q9BYF1
E	618	VAL	-	expression tag	UNP Q9BYF1
E	619	PRO	-	expression tag	UNP Q9BYF1
E	620	ARG	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Heavy chain of C807 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	222	Total	C	N	O	S	2	0
			1650	1045	271	328	6		
2	I	222	Total	C	N	O	S	2	0
			1650	1045	271	328	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	222	Total	C	N	O	S	2	0
			1650	1045	271	328	6		

- Molecule 3 is a protein called Light chain of C807 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	213	Total	C	N	O	S	0	0
			1558	972	262	320	4		
3	K	213	Total	C	N	O	S	0	0
			1558	972	262	320	4		
3	J	213	Total	C	N	O	S	0	0
			1558	972	262	320	4		

- Molecule 4 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1051	Total	C	N	O	S	0	0
			8244	5273	1376	1558	37		
4	B	1051	Total	C	N	O	S	0	0
			8244	5273	1376	1558	37		
4	C	1051	Total	C	N	O	S	0	0
			8244	5273	1376	1558	37		

There are 249 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2

- Molecule 5 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
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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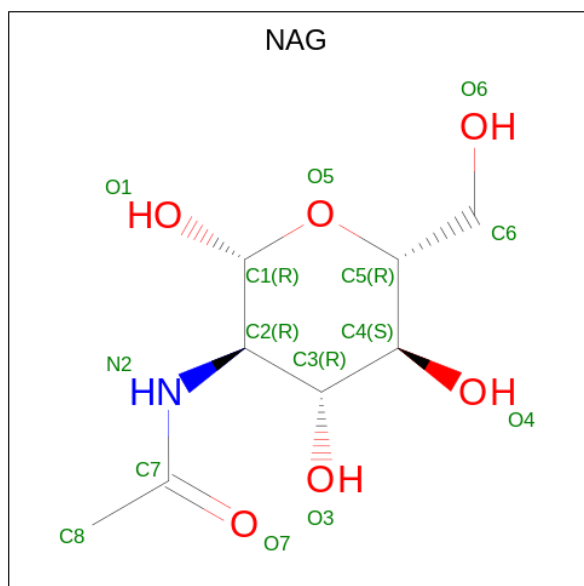
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Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Zn	0
			1	1	
6	F	1	Total	Zn	0
			1	1	
6	E	1	Total	Zn	0
			1	1	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	F	1	Total	C	N	O	0
			14	8	1	5	

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

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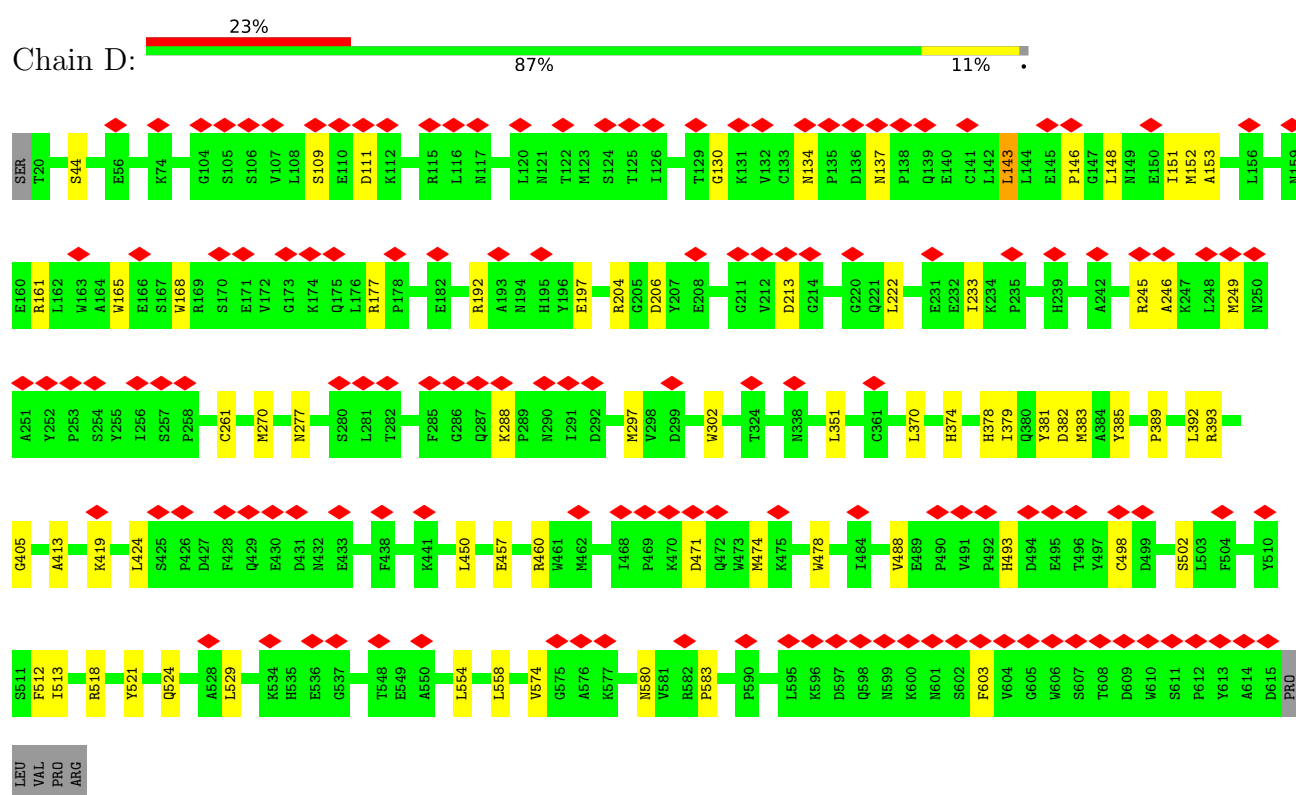
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Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total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

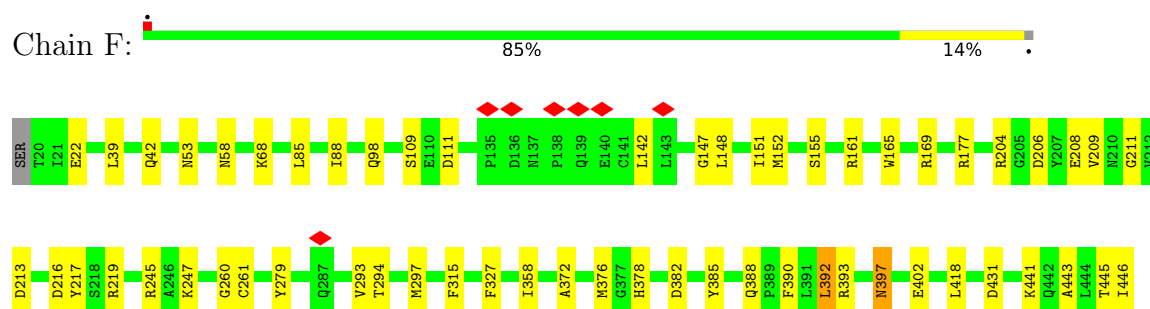
3 Residue-property plots

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

- Molecule 1: Processed angiotensin-converting enzyme 2

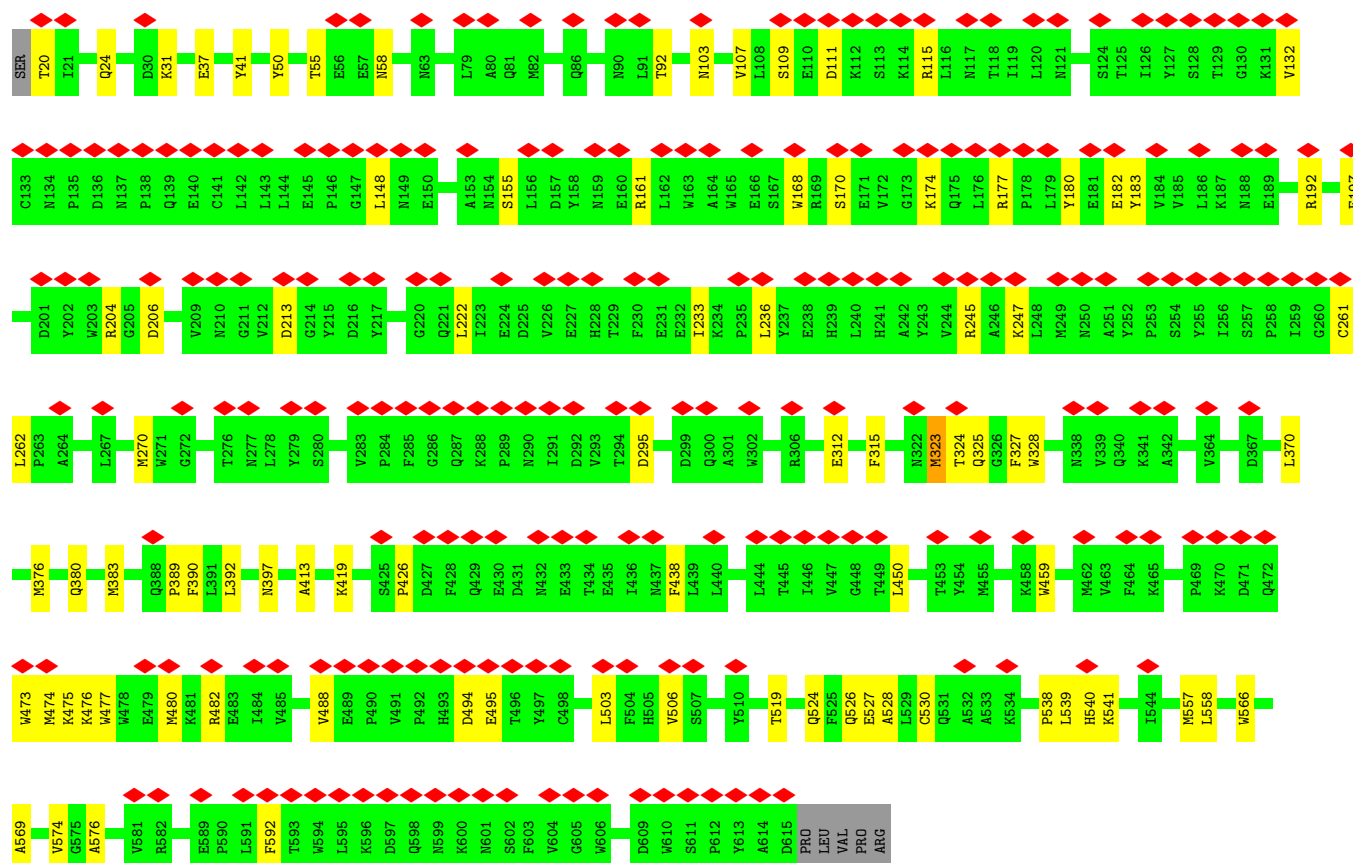
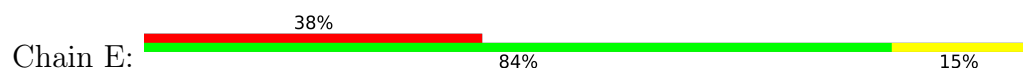


- Molecule 1: Processed angiotensin-converting enzyme 2

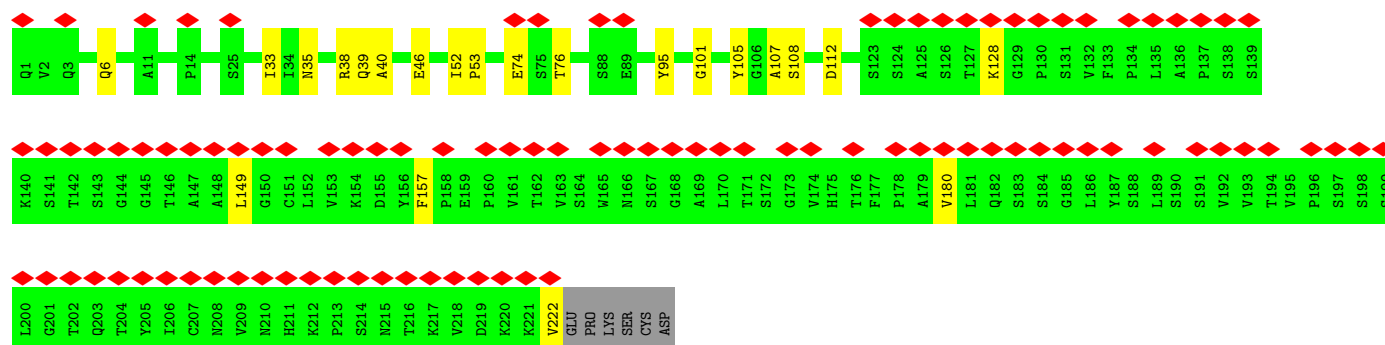
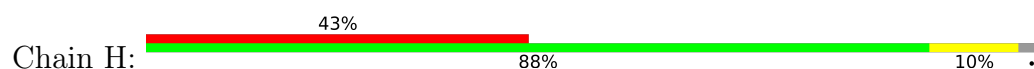




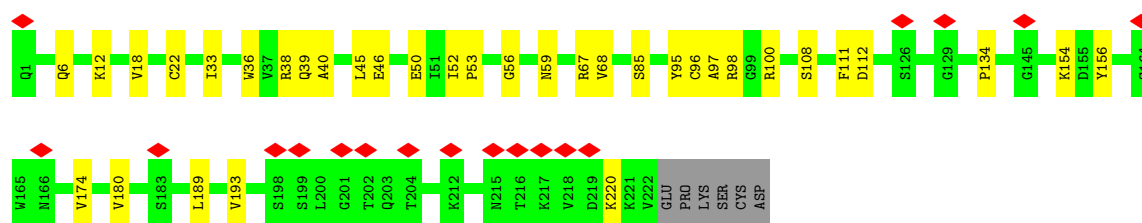
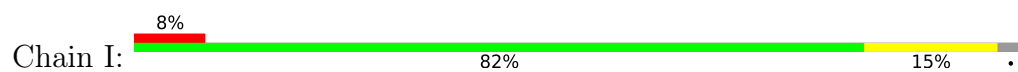
• Molecule 1: Processed angiotensin-converting enzyme 2



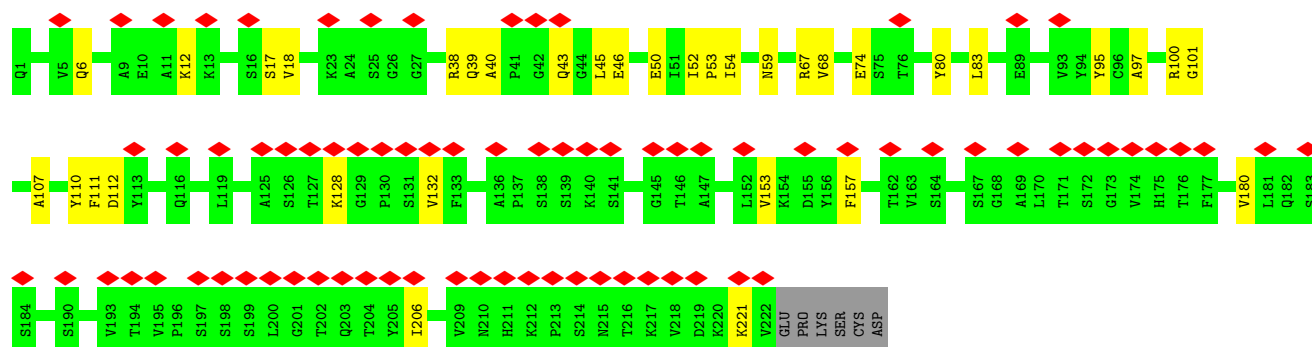
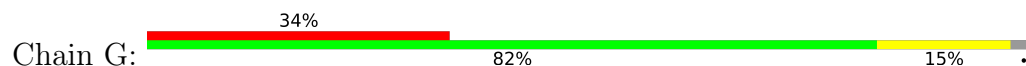
• Molecule 2: Heavy chain of C807 Fab



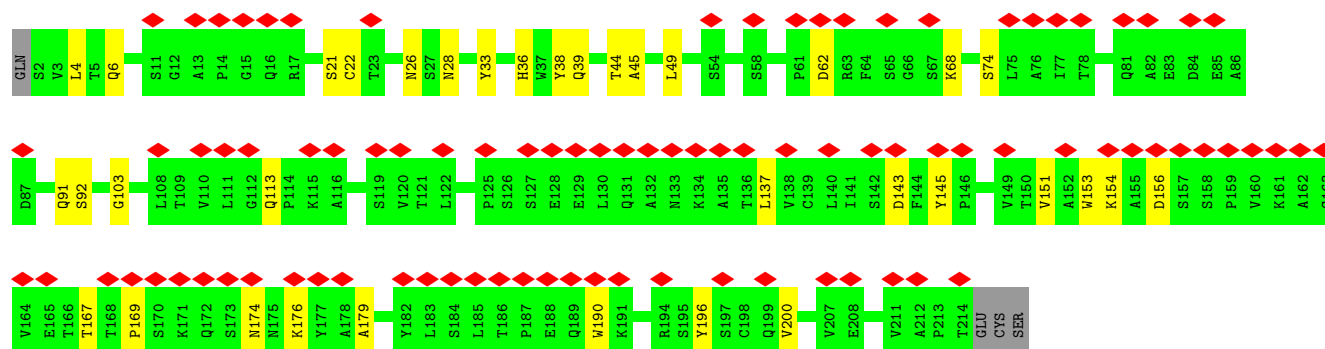
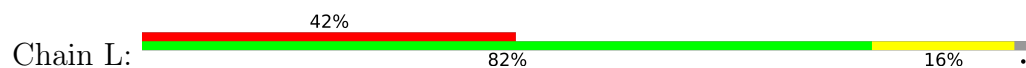
• Molecule 2: Heavy chain of C807 Fab



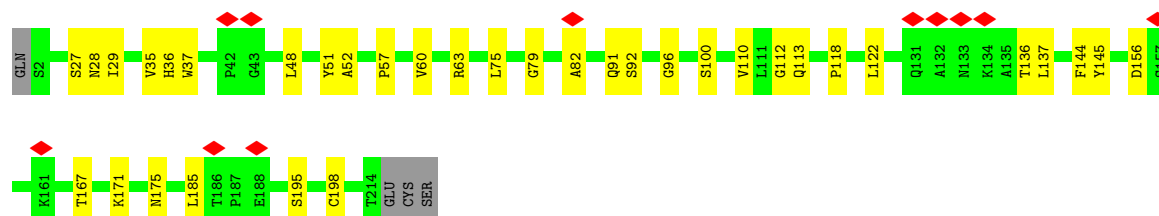
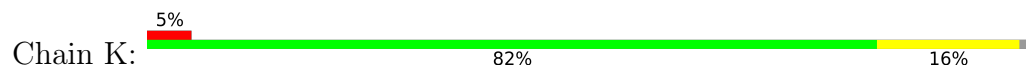
• Molecule 2: Heavy chain of C807 Fab



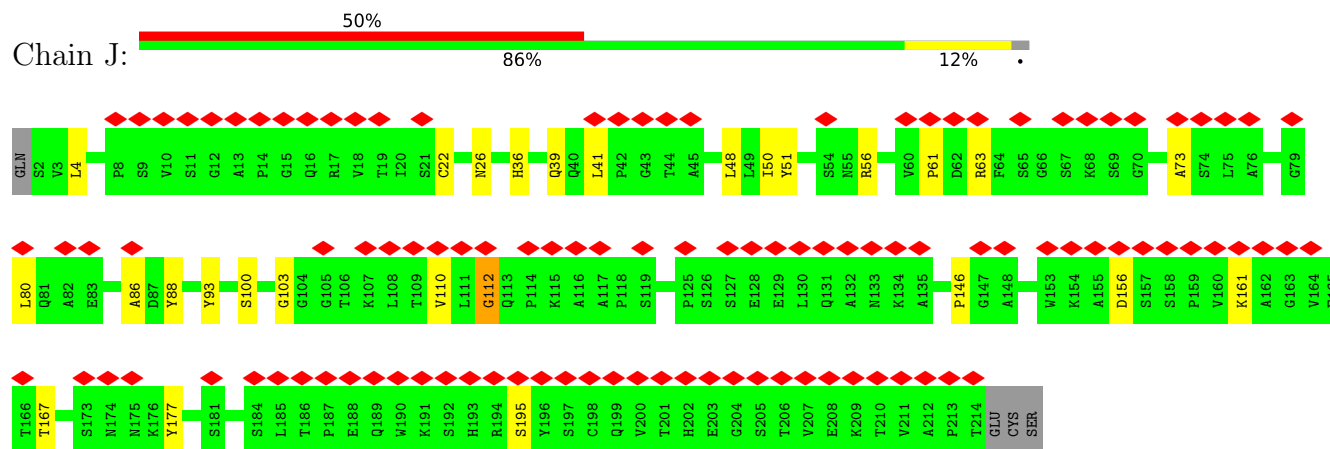
• Molecule 3: Light chain of C807 Fab



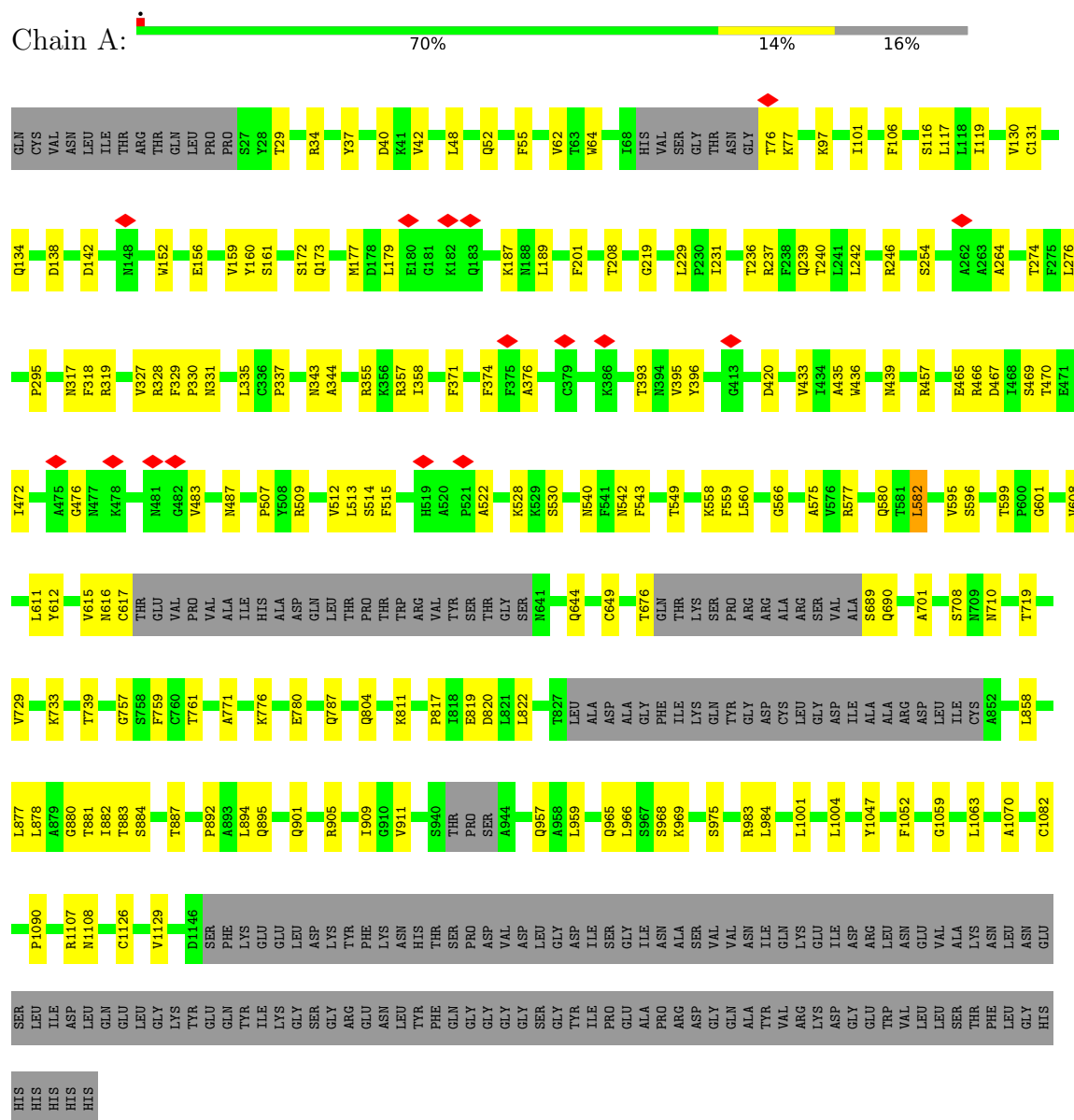
• Molecule 3: Light chain of C807 Fab



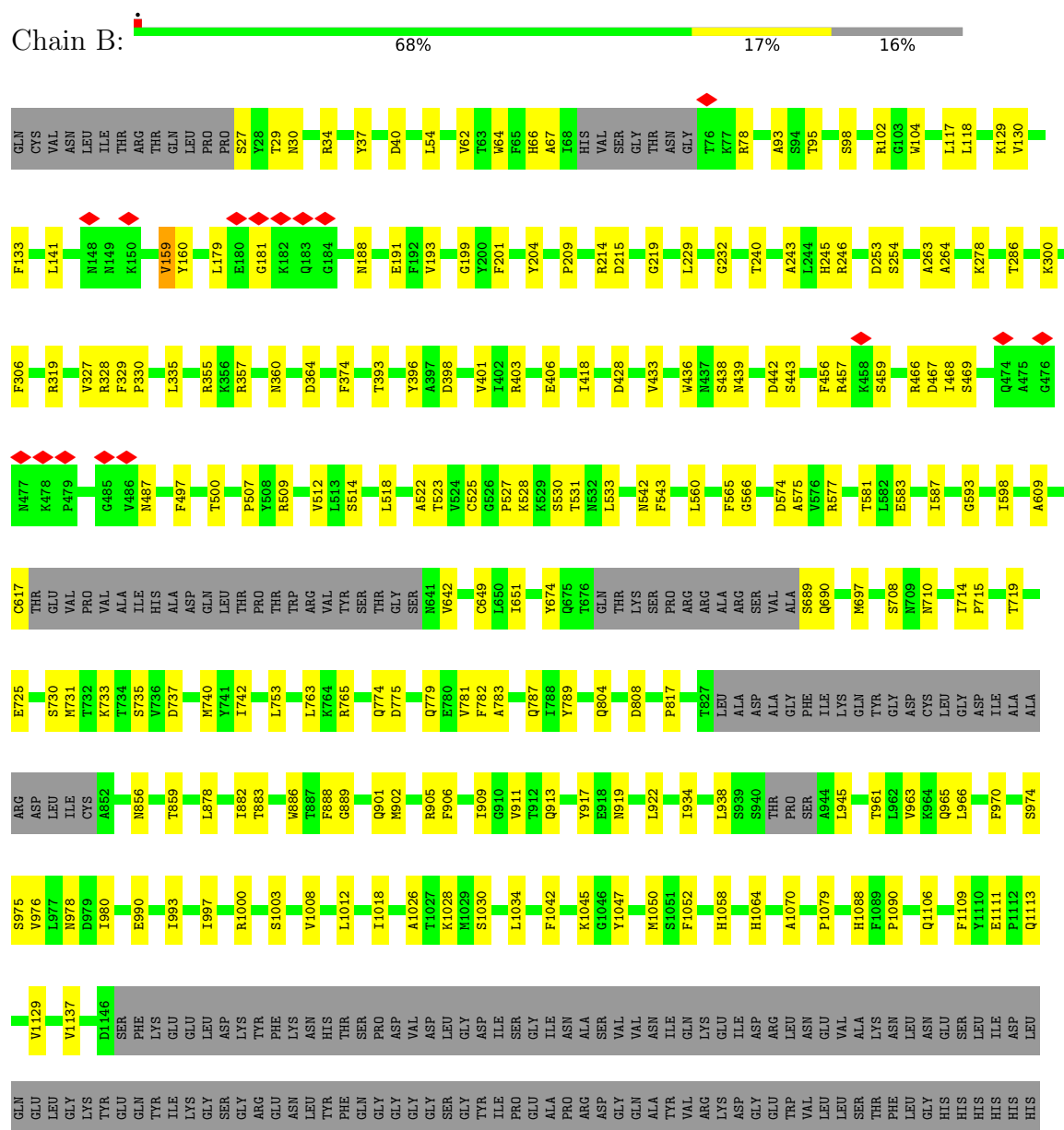
Chain J:



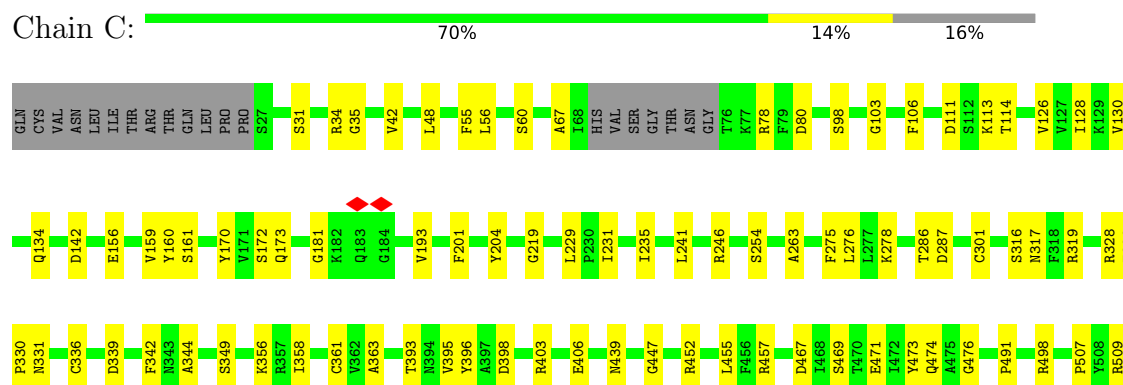
Chain A:

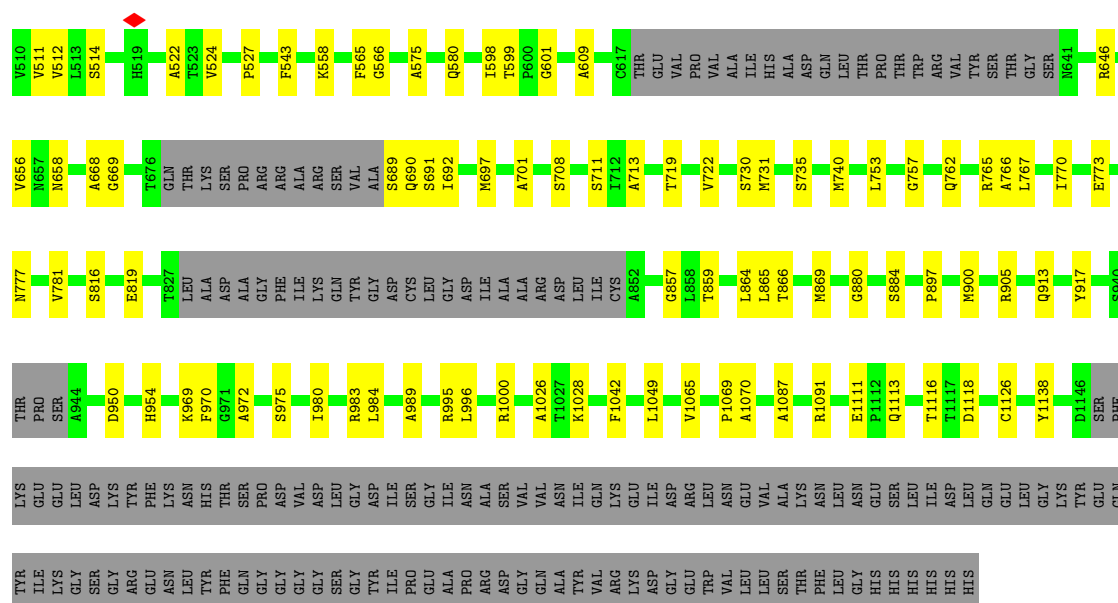


• Molecule 4: Spike glycoprotein



• Molecule 4: Spike glycoprotein





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

MG1
MG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

MG1
MG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15224	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	421.632, 421.632, 421.632	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	Depositor

5 Model quality

5.1 Standard geometry

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

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	D	0.10	0/5001	0.26	0/6795
1	E	0.10	0/5001	0.27	0/6795
1	F	0.12	0/5001	0.32	0/6795
2	G	0.11	0/1698	0.30	0/2311
2	H	0.10	0/1698	0.29	0/2311
2	I	0.11	0/1698	0.32	0/2311
3	J	0.09	0/1596	0.36	1/2183 (0.0%)
3	K	0.09	0/1596	0.29	0/2183
3	L	0.09	0/1596	0.26	0/2183
4	A	0.11	0/8442	0.29	0/11484
4	B	0.11	0/8442	0.31	0/11484
4	C	0.12	0/8442	0.32	0/11484
All	All	0.11	0/50211	0.30	1/68319 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
3	K	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	112	GLY	O-C-N	-10.26	109.36	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	112	GLY	Mainchain
3	K	112	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4864	0	4634	44	0
1	E	4864	0	4634	57	0
1	F	4864	0	4634	60	0
2	G	1650	0	1611	24	0
2	H	1650	0	1611	15	0
2	I	1650	0	1611	25	0
3	J	1558	0	1499	15	0
3	K	1558	0	1499	21	0
3	L	1558	0	1499	20	0
4	A	8244	0	8039	113	0
4	B	8244	0	8039	132	0
4	C	8244	0	8039	105	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	1	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	112	0	104	0	0
7	B	112	0	104	0	0
7	C	112	0	104	0	0
7	D	56	0	52	0	0
7	E	56	0	52	1	0
7	F	56	0	52	0	0
All	All	49623	0	47967	591	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 (591) 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:F:148:LEU:HD12	1:F:151:ILE:HD11	1.18	1.16
1:F:148:LEU:CD1	1:F:151:ILE:HD11	2.03	0.86
4:B:214:ARG:HE	4:B:215:ASP:H	1.35	0.73
1:D:143:LEU:HB3	1:D:146:PRO:HD2	1.73	0.71
4:A:152:TRP:HB2	4:A:179:LEU:HB3	1.72	0.70
4:C:1091:ARG:NH2	4:C:1118:ASP:O	2.25	0.69
4:C:246:ARG:HH22	4:C:254:SER:HB3	1.58	0.68
2:G:6:GLN:HE22	2:G:95:TYR:HA	1.60	0.66
4:B:335:LEU:HD13	4:B:364:ASP:HB3	1.77	0.65
1:E:323:MET:HE1	1:E:327:PHE:CB	2.28	0.64
4:C:358:ILE:HB	4:C:395:VAL:HB	1.80	0.64
3:L:143:ASP:H	3:L:176:LYS:HE2	1.63	0.64
3:J:41:LEU:HD13	3:J:86:ALA:HB2	1.80	0.64
4:C:1111:GLU:OE1	4:C:1113:GLN:NE2	2.31	0.64
4:C:329:PHE:HB2	4:C:330:PRO:HD3	1.80	0.63
2:I:6:GLN:HE22	2:I:95:TYR:HA	1.64	0.63
4:C:599:THR:HG22	4:C:601:GLY:H	1.63	0.63
4:A:393:THR:HA	4:A:522:ALA:HA	1.80	0.63
2:G:50:GLU:H	2:G:59:ASN:HB2	1.65	0.62
4:B:401:VAL:HG22	4:B:509:ARG:HG2	1.82	0.62
4:C:331:ASN:HB3	4:C:580:GLN:HA	1.80	0.62
4:A:236:THR:HG23	4:A:237:ARG:HG3	1.80	0.61
4:B:1079:PRO:HB3	4:C:900:MET:HE1	1.82	0.61
4:A:64:TRP:HE1	4:A:264:ALA:HB1	1.66	0.61
4:B:593:GLY:H	4:C:859:THR:HG21	1.64	0.61
4:A:787:GLN:HG2	4:C:701:ALA:HB3	1.82	0.61
4:B:133:PHE:HB3	4:B:160:TYR:CD2	2.35	0.61
4:B:965:GLN:HB3	4:B:970:PHE:HZ	1.65	0.61
1:D:524:GLN:NE2	1:D:580:ASN:OD1	2.34	0.60
4:A:582:LEU:HD12	4:A:582:LEU:O	2.02	0.60
4:C:142:ASP:HB2	4:C:156:GLU:HB2	1.84	0.60
2:I:39:GLN:NE2	2:I:40:ALA:O	2.35	0.60
4:C:669:GLY:HA2	4:C:697:MET:HE3	1.84	0.60
1:D:261:CYS:HB2	1:D:488:VAL:HG23	1.84	0.60
1:D:524:GLN:HB3	1:D:574:VAL:HG11	1.83	0.59
4:A:97:LYS:HD3	4:A:187:LYS:H	1.67	0.59
4:C:905:ARG:NH1	4:C:1049:LEU:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:617:CYS:N	4:A:649:CYS:SG	2.74	0.59
3:J:4:LEU:HB2	3:J:103:GLY:HA2	1.84	0.59
2:H:6:GLN:HE22	2:H:95:TYR:HA	1.68	0.59
4:C:201:PHE:HB3	4:C:229:LEU:HB2	1.83	0.59
3:L:26:ASN:HB3	4:A:357:ARG:HB3	1.84	0.58
4:A:246:ARG:HH22	4:A:254:SER:HB3	1.68	0.58
4:B:66:HIS:HB2	4:B:78:ARG:HG2	1.84	0.58
4:A:327:VAL:HG22	4:A:542:ASN:HB3	1.84	0.58
1:F:39:LEU:O	1:F:68:LYS:NZ	2.37	0.58
4:A:1090:PRO:O	4:B:913:GLN:NE2	2.36	0.58
1:E:323:MET:O	7:E:904:NAG:H82	2.04	0.58
4:A:909:ILE:HD12	4:A:1047:TYR:HB3	1.85	0.58
1:F:245:ARG:NH1	1:F:260:GLY:O	2.37	0.58
1:D:385:TYR:O	1:D:393:ARG:NH1	2.36	0.58
4:A:396:TYR:HB2	4:A:514:SER:HB3	1.86	0.58
4:C:78:ARG:HE	4:C:80:ASP:HB2	1.68	0.57
2:H:39:GLN:NE2	2:H:40:ALA:O	2.36	0.57
2:I:67:ARG:HG3	2:I:68:VAL:HG23	1.86	0.57
4:A:729:VAL:H	4:A:1059:GLY:HA2	1.69	0.57
4:A:895:GLN:H	4:C:713:ALA:HB3	1.69	0.57
4:B:393:THR:HG21	4:B:518:LEU:HB2	1.86	0.57
4:A:689:SER:OG	4:A:690:GLN:N	2.38	0.57
4:A:901:GLN:HG2	4:A:905:ARG:HH12	1.68	0.57
4:B:64:TRP:HE1	4:B:264:ALA:HB1	1.69	0.57
1:F:447:VAL:HA	1:F:450:LEU:HD12	1.87	0.57
4:A:159:VAL:HG23	4:A:160:TYR:HD1	1.69	0.57
4:A:1129:VAL:HG22	4:B:917:TYR:HB3	1.85	0.57
4:C:773:GLU:O	4:C:777:ASN:N	2.37	0.57
4:C:722:VAL:HG22	4:C:1065:VAL:HG12	1.85	0.57
4:C:753:LEU:O	4:C:757:GLY:N	2.37	0.57
4:B:246:ARG:HH22	4:B:254:SER:HB3	1.70	0.56
1:F:155:SER:HB3	1:F:161:ARG:HH11	1.71	0.56
1:F:453:THR:HA	1:F:512:PHE:HE2	1.70	0.56
4:B:781:VAL:HG23	4:B:782:PHE:HD1	1.69	0.56
4:A:317:ASN:ND2	4:B:737:ASP:OD2	2.37	0.56
4:B:617:CYS:N	4:B:649:CYS:SG	2.79	0.56
4:A:1107:ARG:HH22	4:B:886:TRP:HE1	1.53	0.56
4:C:689:SER:OG	4:C:690:GLN:N	2.39	0.56
1:E:526:GLN:NE2	1:E:530:CYS:SG	2.79	0.55
1:F:148:LEU:O	1:F:151:ILE:CG1	2.55	0.55
4:B:731:MET:HG3	4:B:774:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:50:GLU:HB3	2:I:59:ASN:HB2	1.88	0.55
3:K:118:PRO:HB3	3:K:144:PHE:HB3	1.89	0.55
4:A:596:SER:HB3	4:A:611:LEU:HB3	1.89	0.55
4:C:398:ASP:HB2	4:C:512:VAL:HB	1.88	0.55
2:G:206:ILE:HG22	2:G:221:LYS:HG2	1.89	0.55
4:A:34:ARG:NH2	4:A:219:GLY:O	2.40	0.55
1:E:261:CYS:HB2	1:E:488:VAL:HG23	1.89	0.55
1:D:379:ILE:HG22	1:D:383:MET:HE1	1.89	0.55
4:B:1028:LYS:NZ	4:B:1042:PHE:O	2.40	0.55
4:B:1129:VAL:HG23	4:C:917:TYR:HB3	1.88	0.55
4:C:880:GLY:O	4:C:884:SER:OG	2.25	0.55
1:D:152:MET:O	1:D:161:ARG:NH1	2.40	0.54
4:A:117:LEU:HG	4:A:130:VAL:HG22	1.89	0.54
2:H:108:SER:OG	3:L:36:HIS:NE2	2.41	0.54
3:K:63:ARG:NH1	3:K:79:GLY:O	2.38	0.54
4:A:328:ARG:HG2	4:A:530:SER:HA	1.90	0.54
3:J:50:ILE:HG12	3:J:56:ARG:HG2	1.90	0.54
2:I:67:ARG:NH2	2:I:85:SER:O	2.40	0.54
4:C:735:SER:HA	4:C:767:LEU:HD21	1.88	0.54
1:E:524:GLN:HB3	1:E:574:VAL:HG11	1.89	0.54
1:F:315:PHE:HE2	1:F:376:MET:HE3	1.73	0.54
4:C:344:ALA:O	4:C:509:ARG:NH2	2.41	0.54
1:D:168:TRP:HE1	1:D:502:SER:HB2	1.73	0.53
4:A:739:THR:HG22	4:C:319:ARG:HH22	1.73	0.53
4:C:866:THR:H	4:C:869:MET:HE2	1.72	0.53
2:G:38:ARG:HH22	2:G:83:LEU:HD13	1.72	0.53
1:F:397:ASN:C	1:F:397:ASN:HD22	2.16	0.53
1:F:524:GLN:HE22	1:F:579:MET:HG3	1.72	0.53
4:A:344:ALA:O	4:A:509:ARG:NH2	2.42	0.53
1:E:323:MET:HE1	1:E:327:PHE:CG	2.43	0.53
4:C:396:TYR:HB2	4:C:514:SER:HB3	1.91	0.53
2:I:134:PRO:HD3	2:I:220:LYS:HD2	1.90	0.53
1:D:474:MET:HE3	1:D:498:CYS:HA	1.91	0.53
4:A:101:ILE:HG13	4:A:242:LEU:HD13	1.90	0.53
1:F:524:GLN:HB3	1:F:574:VAL:HG11	1.90	0.53
4:A:337:PRO:HD2	4:A:358:ILE:HG12	1.91	0.53
2:G:12:LYS:HE2	2:G:18:VAL:HG22	1.89	0.53
3:L:6:GLN:HE21	3:L:22:CYS:HB2	1.72	0.53
1:F:526:GLN:NE2	1:F:530:CYS:SG	2.82	0.53
4:A:759:PHE:HD2	4:A:1001:LEU:HD21	1.73	0.53
1:D:148:LEU:HD12	1:D:151:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:180:VAL:HB	3:L:167:THR:HG22	1.90	0.53
4:A:201:PHE:HB3	4:A:229:LEU:HB2	1.90	0.53
4:A:887:THR:HG21	4:A:894:LEU:HD12	1.91	0.53
4:C:393:THR:HA	4:C:522:ALA:HA	1.91	0.53
2:I:108:SER:OG	3:K:36:HIS:NE2	2.36	0.52
4:A:616:ASN:OD1	4:A:644:GLN:NE2	2.43	0.52
4:C:983:ARG:HG3	4:C:984:LEU:HG	1.90	0.52
4:C:1116:THR:HG22	4:C:1138:TYR:HB3	1.91	0.52
1:D:165:TRP:HA	1:D:270:MET:HE1	1.90	0.52
4:A:439:ASN:HA	4:A:507:PRO:HG2	1.91	0.52
3:J:48:LEU:HD21	3:J:51:TYR:HB3	1.90	0.52
1:E:170:SER:OG	1:E:174:LYS:NZ	2.42	0.52
1:D:233:ILE:HD13	1:D:450:LEU:HD13	1.91	0.52
4:C:34:ARG:NH2	4:C:219:GLY:O	2.43	0.52
4:C:708:SER:HB3	4:C:711:SER:HB3	1.91	0.52
4:C:1028:LYS:NZ	4:C:1042:PHE:O	2.38	0.52
4:B:360:ASN:H	4:B:523:THR:HB	1.74	0.52
4:A:881:THR:O	4:A:901:GLN:NE2	2.42	0.52
4:B:456:PHE:HZ	1:E:31:LYS:HB2	1.74	0.52
4:A:117:LEU:HD23	4:A:119:ILE:HD11	1.90	0.51
4:A:969:LYS:HZ1	4:A:975:SER:HB2	1.76	0.51
4:B:253:ASP:OD1	4:B:253:ASP:N	2.44	0.51
4:B:374:PHE:HD1	4:B:436:TRP:HB3	1.75	0.51
4:B:188:ASN:HA	4:B:209:PRO:HA	1.92	0.51
4:B:714:ILE:HD12	4:B:715:PRO:HD2	1.91	0.51
2:I:52:ILE:HD12	2:I:53:PRO:HD2	1.92	0.51
4:A:134:GLN:HB2	4:A:161:SER:HB2	1.92	0.51
1:E:527:GLU:HA	1:E:539:LEU:HD11	1.92	0.51
4:A:566:GLY:N	4:A:575:ALA:O	2.43	0.51
4:B:974:SER:HB3	4:B:980:ILE:HG23	1.91	0.51
1:D:177:ARG:HH11	1:D:474:MET:HE2	1.75	0.51
3:L:4:LEU:HB2	3:L:103:GLY:HA2	1.90	0.51
4:B:689:SER:OG	4:B:690:GLN:N	2.43	0.51
2:H:105:TYR:HA	4:A:465:GLU:HA	1.93	0.51
3:K:171:LYS:NZ	3:K:175:ASN:OD1	2.40	0.51
4:B:406:GLU:HG2	4:B:418:ILE:HG12	1.93	0.51
1:F:206:ASP:OD1	1:F:206:ASP:N	2.44	0.51
4:A:106:PHE:HB2	4:A:117:LEU:HB2	1.93	0.51
4:B:328:ARG:HH12	4:B:533:LEU:HB2	1.75	0.51
1:D:192:ARG:NH1	1:D:197:GLU:O	2.44	0.51
1:F:490:PRO:HA	1:F:612:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:35:GLY:HA3	4:C:56:LEU:HB3	1.92	0.51
1:D:153:ALA:HA	1:D:277:ASN:HB3	1.92	0.51
4:A:319:ARG:HH22	4:B:740:MET:HB3	1.76	0.51
1:F:148:LEU:O	1:F:151:ILE:HG13	2.11	0.50
1:E:37:GLU:HG3	1:E:390:PHE:HB2	1.92	0.50
1:D:297:MET:HB3	1:D:302:TRP:HB2	1.93	0.50
1:D:518:ARG:HA	1:D:521:TYR:HB2	1.91	0.50
1:F:213:ASP:OD1	1:F:213:ASP:N	2.43	0.50
2:H:74:GLU:HB3	2:H:76:THR:HG22	1.93	0.50
1:D:206:ASP:OD1	1:D:206:ASP:N	2.45	0.50
4:B:201:PHE:HB3	4:B:229:LEU:HB2	1.94	0.50
4:B:393:THR:HA	4:B:522:ALA:HA	1.92	0.50
4:C:316:SER:OG	4:C:317:ASN:N	2.42	0.50
2:H:107:ALA:H	4:A:466:ARG:HH11	1.57	0.50
4:B:961:THR:HG22	4:B:965:GLN:HE22	1.75	0.50
4:C:403:ARG:NH2	4:C:406:GLU:OE2	2.45	0.50
1:D:213:ASP:N	1:D:213:ASP:OD1	2.42	0.50
4:B:906:PHE:HB3	4:B:911:VAL:HB	1.93	0.50
1:E:370:LEU:HD11	1:E:413:ALA:HB2	1.92	0.50
2:I:39:GLN:HB2	2:I:45:LEU:HD23	1.93	0.50
4:C:126:VAL:HB	4:C:172:SER:HB3	1.94	0.50
4:C:457:ARG:NE	4:C:467:ASP:OD2	2.38	0.50
1:F:148:LEU:HG	1:F:152:MET:HE1	1.94	0.50
4:C:762:GLN:HA	4:C:765:ARG:HG2	1.94	0.50
4:A:331:ASN:HB3	4:A:580:GLN:HA	1.93	0.50
4:B:319:ARG:HE	4:C:740:MET:HE3	1.76	0.50
4:A:29:THR:HG23	4:A:62:VAL:HG13	1.93	0.49
4:B:1030:SER:HA	4:B:1034:LEU:HD12	1.94	0.49
4:C:972:ALA:HB2	4:C:995:ARG:HH12	1.76	0.49
1:E:103:ASN:HB3	1:E:107:VAL:HB	1.94	0.49
4:B:102:ARG:HD3	4:B:243:ALA:HB2	1.94	0.49
1:F:152:MET:O	1:F:161:ARG:NH1	2.44	0.49
3:K:48:LEU:HD21	3:K:51:TYR:HB3	1.93	0.49
4:A:239:GLN:NE2	4:A:240:THR:O	2.46	0.49
4:C:970:PHE:O	4:C:995:ARG:NH1	2.44	0.49
4:B:581:THR:HG23	4:B:583:GLU:HB2	1.93	0.49
4:C:598:ILE:HB	4:C:609:ALA:HB3	1.93	0.49
1:E:109:SER:OG	1:E:111:ASP:OD1	2.29	0.49
1:D:370:LEU:HD11	1:D:413:ALA:HB2	1.95	0.49
4:B:67:ALA:HB3	4:B:263:ALA:HB3	1.93	0.49
4:B:278:LYS:HD3	4:B:286:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:487:ASN:ND2	1:E:24:GLN:OE1	2.45	0.49
4:B:742:ILE:HD11	4:B:997:ILE:HA	1.95	0.49
4:B:976:VAL:HG22	4:B:978:ASN:H	1.78	0.49
1:F:42:GLN:HG2	4:C:498:ARG:HH22	1.77	0.49
4:A:374:PHE:HD1	4:A:436:TRP:HB3	1.78	0.49
4:B:439:ASN:HA	4:B:507:PRO:HG2	1.94	0.49
4:C:740:MET:HB3	4:C:857:GLY:HA3	1.94	0.49
1:E:177:ARG:HH22	1:E:473:TRP:HB2	1.77	0.49
4:A:911:VAL:HG22	4:A:1108:ASN:HB2	1.95	0.49
1:E:438:PHE:HE2	1:E:540:HIS:HB2	1.78	0.49
2:G:52:ILE:HD12	2:G:53:PRO:HD2	1.94	0.49
1:F:443:ALA:O	1:F:448:GLY:N	2.45	0.49
4:C:130:VAL:HG21	4:C:231:ILE:HG12	1.95	0.49
4:C:474:GLN:NE2	4:C:476:GLY:O	2.44	0.49
2:I:38:ARG:NH1	2:I:46:GLU:OE1	2.46	0.48
4:B:398:ASP:HB2	4:B:512:VAL:HB	1.94	0.48
4:B:804:GLN:HA	4:B:817:PRO:HG2	1.94	0.48
2:G:97:ALA:HB1	2:G:111:PHE:HB3	1.95	0.48
2:H:38:ARG:NH1	2:H:46:GLU:OE1	2.45	0.48
4:C:113:LYS:HG3	4:C:114:THR:HG23	1.95	0.48
1:E:132:VAL:HG11	1:E:148:LEU:HD13	1.95	0.48
4:A:1052:PHE:HB2	4:A:1063:LEU:HB2	1.96	0.48
4:C:106:PHE:HB3	4:C:235:ILE:HD13	1.94	0.48
4:C:469:SER:HB2	4:C:471:GLU:HG2	1.93	0.48
1:D:246:ALA:HA	1:D:249:MET:HE2	1.96	0.48
1:F:151:ILE:O	1:F:155:SER:HB2	2.13	0.48
4:C:975:SER:O	4:C:1000:ARG:NH2	2.47	0.48
1:D:374:HIS:ND1	1:D:405:GLY:O	2.46	0.48
3:L:33:TYR:O	3:L:68:LYS:NZ	2.39	0.48
4:B:29:THR:HG23	4:B:62:VAL:HG13	1.96	0.48
2:H:33:ILE:HG22	2:H:35:ASN:HD21	1.78	0.48
1:F:142:LEU:HD11	1:F:147:GLY:HA3	1.96	0.48
4:A:957:GLN:OE1	4:B:765:ARG:NH1	2.45	0.48
4:B:457:ARG:NH1	4:B:459:SER:O	2.41	0.48
4:B:1111:GLU:OE1	4:B:1113:GLN:NE2	2.44	0.48
4:C:864:LEU:HG	4:C:865:LEU:HG	1.95	0.48
1:E:557:MET:HE3	1:E:558:LEU:HD23	1.96	0.48
4:C:328:ARG:NH1	4:C:580:GLN:HG3	2.28	0.48
4:A:560:LEU:O	4:A:577:ARG:NH2	2.43	0.48
4:A:901:GLN:HE21	4:A:905:ARG:HH22	1.62	0.48
1:F:204:ARG:HE	1:F:219:ARG:HG2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:36:HIS:HD1	3:K:52:ALA:H	1.62	0.47
4:C:996:LEU:HG	4:C:1000:ARG:HE	1.79	0.47
1:E:20:THR:HG22	1:E:24:GLN:HE21	1.79	0.47
1:D:478:TRP:HE1	1:D:493:HIS:HB2	1.79	0.47
3:L:190:TRP:O	3:L:196:TYR:OH	2.32	0.47
1:F:111:ASP:OD1	1:F:111:ASP:N	2.47	0.47
4:C:656:VAL:HG22	4:C:658:ASN:H	1.79	0.47
1:E:213:ASP:OD1	1:E:213:ASP:N	2.44	0.47
3:L:28:ASN:O	3:L:92:SER:OG	2.29	0.47
2:G:128:LYS:HG2	2:G:157:PHE:HE2	1.80	0.47
4:A:612:TYR:HB3	4:A:615:VAL:HB	1.96	0.47
4:B:500:THR:OG1	1:E:41:TYR:OH	2.30	0.47
2:G:39:GLN:HB3	2:G:45:LEU:HA	1.97	0.47
4:A:877:LEU:O	4:A:881:THR:OG1	2.28	0.47
4:B:328:ARG:HD3	4:B:531:THR:H	1.80	0.47
1:E:192:ARG:NH1	1:E:197:GLU:O	2.48	0.47
2:G:74:GLU:HG2	2:G:80:TYR:HE2	1.79	0.47
1:F:460:ARG:HH22	1:F:512:PHE:HB3	1.79	0.47
4:A:376:ALA:HB3	4:A:435:ALA:HB3	1.95	0.47
4:B:27:SER:N	4:B:64:TRP:O	2.47	0.47
4:B:300:LYS:NZ	4:B:306:PHE:O	2.40	0.47
1:E:155:SER:HB3	1:E:161:ARG:HH11	1.80	0.47
1:E:233:ILE:HD13	1:E:450:LEU:HD13	1.96	0.47
1:D:130:GLY:HA3	1:D:168:TRP:HZ3	1.80	0.47
2:H:52:ILE:HD12	2:H:53:PRO:HD2	1.97	0.47
2:I:12:LYS:HE2	2:I:18:VAL:HG22	1.97	0.47
2:I:100:ARG:NH2	2:I:112:ASP:OD2	2.48	0.47
4:A:172:SER:OG	4:A:173:GLN:N	2.47	0.47
4:A:327:VAL:H	4:A:528:LYS:HZ2	1.63	0.47
4:C:134:GLN:HB2	4:C:161:SER:HB2	1.97	0.47
4:C:358:ILE:HG22	4:C:524:VAL:HG21	1.97	0.47
1:E:538:PRO:HG2	1:E:541:LYS:HD3	1.97	0.47
2:I:180:VAL:HB	3:K:167:THR:HG22	1.97	0.47
4:A:811:LYS:NZ	4:A:820:ASP:OD2	2.41	0.47
4:B:1106:GLN:HE21	4:B:1109:PHE:HB3	1.79	0.47
1:E:476:LYS:HG3	1:E:480:MET:HE2	1.97	0.47
4:B:118:LEU:N	4:B:129:LYS:O	2.46	0.47
1:D:389:PRO:HD2	1:D:392:LEU:HB2	1.95	0.47
1:D:524:GLN:HG2	1:D:583:PRO:HG2	1.97	0.47
1:D:529:LEU:HD21	1:D:554:LEU:HB2	1.96	0.47
4:B:730:SER:HB3	4:B:1058:HIS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:892:PRO:HD2	4:C:1069:PRO:HG2	1.97	0.46
4:B:598:ILE:HB	4:B:609:ALA:HB3	1.97	0.46
4:B:708:SER:OG	4:B:710:ASN:OD1	2.33	0.46
3:L:62:ASP:OD1	3:L:62:ASP:N	2.48	0.46
1:F:148:LEU:O	1:F:151:ILE:HG12	2.16	0.46
2:I:97:ALA:HB1	2:I:111:PHE:HB3	1.97	0.46
4:A:757:GLY:O	4:A:761:THR:N	2.45	0.46
1:D:245:ARG:NH2	1:D:603:PHE:O	2.48	0.46
2:I:52:ILE:HG23	2:I:56:GLY:H	1.81	0.46
4:C:439:ASN:HA	4:C:507:PRO:HG2	1.97	0.46
4:A:116:SER:N	4:A:131:CYS:O	2.48	0.46
4:B:428:ASP:OD1	4:B:428:ASP:N	2.48	0.46
4:C:816:SER:HB2	4:C:819:GLU:OE1	2.15	0.46
4:A:138:ASP:N	4:A:138:ASP:OD1	2.49	0.46
4:B:98:SER:HB3	4:B:181:GLY:HA2	1.97	0.46
4:B:882:ILE:HG13	4:B:883:THR:HG23	1.97	0.46
3:K:57:PRO:HD2	3:K:60:VAL:HG21	1.98	0.46
4:A:48:LEU:HB3	4:A:276:LEU:HD11	1.98	0.46
1:E:50:TYR:HA	1:E:58:ASN:HB3	1.97	0.46
3:K:82:ALA:HA	3:K:110:VAL:HG11	1.98	0.46
4:A:295:PRO:HB2	4:A:608:VAL:HG21	1.97	0.46
4:A:355:ARG:HB2	4:A:466:ARG:HH22	1.81	0.46
4:A:966:LEU:O	4:A:975:SER:OG	2.31	0.46
4:B:642:VAL:HG13	4:B:651:ILE:HG22	1.98	0.46
3:L:38:TYR:OH	3:L:91:GLN:OE1	2.30	0.46
4:B:95:THR:OG1	4:B:188:ASN:O	2.27	0.46
1:E:494:ASP:OD1	1:E:495:GLU:N	2.43	0.46
1:D:460:ARG:HH22	1:D:512:PHE:H	1.64	0.46
3:L:154:LYS:HG2	3:L:156:ASP:H	1.81	0.46
1:F:53:ASN:O	1:F:58:ASN:ND2	2.49	0.46
4:A:420:ASP:OD1	4:A:420:ASP:N	2.49	0.45
4:B:574:ASP:O	4:B:587:ILE:N	2.47	0.45
1:E:206:ASP:N	1:E:206:ASP:OD1	2.50	0.45
1:F:109:SER:OG	1:F:111:ASP:OD1	2.32	0.45
1:F:460:ARG:NH2	1:F:512:PHE:HB3	2.31	0.45
3:K:35:VAL:HG22	3:K:92:SER:HB2	1.99	0.45
3:K:122:LEU:HD13	3:K:198:CYS:HB2	1.98	0.45
4:A:472:ILE:HG13	4:A:483:VAL:HA	1.99	0.45
4:B:159:VAL:HG23	4:B:160:TYR:HD1	1.81	0.45
4:B:966:LEU:O	4:B:975:SER:OG	2.31	0.45
4:A:880:GLY:O	4:A:884:SER:OG	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:98:SER:HB3	4:C:181:GLY:HA2	1.97	0.45
1:D:111:ASP:OD1	1:D:111:ASP:N	2.48	0.45
1:F:177:ARG:HH22	1:F:473:TRP:HB2	1.81	0.45
4:B:856:ASN:HD21	4:B:963:VAL:HG12	1.81	0.45
1:E:482:ARG:HG2	1:E:488:VAL:HG22	1.98	0.45
1:D:378:HIS:CE1	1:D:405:GLY:HA3	2.52	0.45
4:A:358:ILE:HB	4:A:395:VAL:HB	1.99	0.45
4:B:329:PHE:HB2	4:B:330:PRO:HD3	1.98	0.45
1:E:295:ASP:OD1	1:E:295:ASP:N	2.48	0.45
2:G:132:VAL:HG22	2:G:153:VAL:HG13	1.98	0.45
4:B:781:VAL:HG12	4:B:1026:ALA:HB2	1.99	0.45
1:E:528:ALA:HB2	1:E:574:VAL:HG12	1.97	0.45
1:D:44:SER:HB3	1:D:351:LEU:HG	1.99	0.45
1:F:294:THR:HA	1:F:297:MET:HE2	1.98	0.45
1:F:327:PHE:HE1	1:F:358:ILE:HG12	1.82	0.45
2:I:36:TRP:CE2	2:I:96:CYS:HB3	2.51	0.45
4:A:719:THR:HG23	4:A:1070:ALA:HB2	1.97	0.45
4:B:327:VAL:HG22	4:B:542:ASN:HB3	1.97	0.45
4:B:439:ASN:O	4:B:443:SER:OG	2.31	0.45
4:C:455:LEU:N	4:C:491:PRO:O	2.49	0.45
1:F:397:ASN:O	1:F:397:ASN:ND2	2.41	0.45
4:A:76:THR:HG23	4:A:77:LYS:HG3	1.99	0.45
4:C:193:VAL:HB	4:C:204:TYR:HB2	1.98	0.45
1:E:247:LYS:HD2	1:E:247:LYS:HA	1.79	0.45
4:A:40:ASP:OD1	4:A:40:ASP:N	2.50	0.45
4:A:329:PHE:HB2	4:A:330:PRO:HD3	1.99	0.45
4:A:52:GLN:HB2	4:A:274:THR:HG22	1.97	0.45
4:A:457:ARG:NE	4:A:467:ASP:OD2	2.40	0.45
4:B:327:VAL:HB	4:B:528:LYS:HE2	1.98	0.45
4:B:457:ARG:NE	4:B:467:ASP:OD2	2.43	0.45
1:E:312:GLU:HA	1:E:376:MET:HE1	1.99	0.45
3:K:27:SER:HB2	4:C:356:LYS:HD3	2.00	0.44
3:K:113:GLN:HG2	3:K:145:TYR:HD2	1.81	0.44
3:K:137:LEU:HD23	3:K:185:LEU:HD12	1.97	0.44
4:B:102:ARG:HG3	4:B:141:LEU:HD12	1.99	0.44
4:B:468:ILE:HG12	2:G:107:ALA:HB1	1.99	0.44
2:G:67:ARG:HG3	2:G:68:VAL:HG23	1.97	0.44
4:B:733:LYS:NZ	4:B:775:ASP:OD1	2.49	0.44
1:D:381:TYR:HD1	1:D:558:LEU:HD22	1.81	0.44
3:K:91:GLN:HE21	3:K:100:SER:HB2	1.81	0.44
4:C:339:ASP:OD1	4:C:339:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:LEU:HD13	1:E:592:PHE:HD1	1.81	0.44
2:I:33:ILE:HD13	2:I:52:ILE:HD13	1.99	0.44
4:B:104:TRP:HA	4:B:240:THR:HA	1.99	0.44
4:B:735:SER:O	4:B:859:THR:OG1	2.30	0.44
4:B:1008:VAL:O	4:B:1012:LEU:N	2.42	0.44
2:G:52:ILE:HG13	2:G:54:ILE:H	1.83	0.44
1:F:382:ASP:OD1	1:F:385:TYR:OH	2.32	0.44
1:F:392:LEU:N	1:F:392:LEU:HD23	2.32	0.44
4:A:42:VAL:HG12	4:C:565:PHE:HB2	1.99	0.44
4:A:395:VAL:HG22	4:A:515:PHE:HE1	1.83	0.44
4:B:117:LEU:HD22	4:B:130:VAL:HG22	1.98	0.44
4:B:355:ARG:HB2	4:B:466:ARG:HH22	1.82	0.44
4:C:336:CYS:HB2	4:C:361:CYS:HB2	1.76	0.44
2:G:39:GLN:HB3	2:G:45:LEU:HD23	1.99	0.44
1:D:457:GLU:OE2	1:D:460:ARG:NH2	2.47	0.44
1:F:261:CYS:HB2	1:F:488:VAL:HG23	1.99	0.44
2:I:6:GLN:HA	2:I:22:CYS:HA	1.98	0.44
4:B:34:ARG:NH2	4:B:219:GLY:O	2.50	0.44
4:C:691:SER:OG	4:C:692:ILE:N	2.51	0.44
4:A:558:LYS:NZ	4:A:559:PHE:O	2.50	0.44
4:A:983:ARG:HG3	4:A:984:LEU:HG	1.99	0.44
4:C:48:LEU:HB3	4:C:276:LEU:HD11	1.99	0.44
2:G:18:VAL:HB	2:G:83:LEU:HB3	1.99	0.44
3:J:61:PRO:HB2	3:J:63:ARG:HG2	1.99	0.44
4:A:130:VAL:HG11	4:A:231:ILE:HG21	1.99	0.44
4:A:1082:CYS:HB2	4:A:1126:CYS:HB2	1.93	0.44
4:C:646:ARG:HB3	4:C:668:ALA:HB1	1.98	0.44
1:E:315:PHE:CE2	1:E:380:GLN:HG3	2.53	0.44
1:D:109:SER:OG	1:D:111:ASP:OD1	2.31	0.43
2:H:101:GLY:HA3	4:A:469:SER:HA	1.99	0.43
4:B:396:TYR:HB2	4:B:514:SER:HB3	1.99	0.43
1:E:574:VAL:HG23	1:E:576:ALA:H	1.83	0.43
1:D:288:LYS:HD2	1:D:288:LYS:HA	1.85	0.43
2:I:156:TYR:CZ	2:I:189:LEU:HD23	2.53	0.43
4:B:674:TYR:CZ	4:B:690:GLN:HB2	2.53	0.43
4:C:128:ILE:HD12	4:C:170:TYR:HD2	1.82	0.43
4:C:278:LYS:HB3	4:C:287:ASP:H	1.84	0.43
4:C:358:ILE:N	4:C:395:VAL:O	2.51	0.43
3:L:44:THR:OG1	3:L:45:ALA:N	2.50	0.43
1:F:208:GLU:HA	1:F:217:TYR:HD2	1.82	0.43
1:F:247:LYS:HA	1:F:247:LYS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:189:LEU:N	4:A:208:THR:O	2.52	0.43
4:A:433:VAL:HG12	4:A:512:VAL:HG22	2.00	0.43
4:A:878:LEU:HD22	4:A:1052:PHE:HD1	1.83	0.43
4:B:40:ASP:OD1	4:B:40:ASP:N	2.50	0.43
4:B:697:MET:HG3	4:C:869:MET:HG2	1.99	0.43
4:B:905:ARG:HE	4:B:1050:MET:HB3	1.83	0.43
2:G:180:VAL:HB	3:J:167:THR:HG22	1.99	0.43
4:A:318:PHE:HB2	4:A:595:VAL:HG13	2.01	0.43
4:B:193:VAL:HB	4:B:204:TYR:HB2	2.00	0.43
4:B:357:ARG:HB3	3:J:26:ASN:HB3	2.00	0.43
4:B:808:ASP:OD1	4:B:808:ASP:N	2.51	0.43
4:B:1090:PRO:O	4:C:913:GLN:NE2	2.51	0.43
2:G:38:ARG:O	2:G:46:GLU:N	2.51	0.43
3:L:169:PRO:HA	3:L:179:ALA:HB2	2.00	0.43
2:I:100:ARG:NH1	2:I:112:ASP:OD1	2.51	0.43
3:K:156:ASP:OD1	3:K:195:SER:OG	2.36	0.43
4:C:67:ALA:HB3	4:C:263:ALA:HB3	2.01	0.43
4:C:781:VAL:HG22	4:C:1026:ALA:HB2	2.01	0.43
1:E:204:ARG:HD2	1:E:222:LEU:HD23	2.00	0.43
4:A:37:TYR:H	4:A:55:PHE:HE2	1.65	0.43
4:A:819:GLU:HA	4:A:822:LEU:HD12	2.00	0.43
4:C:447:GLY:N	4:C:498:ARG:HE	2.17	0.43
1:E:168:TRP:CD1	1:E:270:MET:HE1	2.54	0.43
1:F:372:ALA:O	1:F:376:MET:HG2	2.19	0.43
4:A:328:ARG:HH21	4:A:543:PHE:HZ	1.67	0.43
4:B:566:GLY:N	4:B:575:ALA:O	2.51	0.43
4:B:990:GLU:HA	4:B:993:ILE:HD12	2.01	0.43
1:E:474:MET:HA	1:E:474:MET:HE2	2.00	0.43
4:A:476:GLY:HA3	4:A:487:ASN:HD22	1.83	0.43
4:B:901:GLN:HG2	4:B:905:ARG:HD2	2.01	0.43
4:A:327:VAL:HB	4:A:528:LYS:HD3	2.00	0.43
4:B:469:SER:HA	2:G:101:GLY:HA3	2.00	0.43
4:C:950:ASP:O	4:C:954:HIS:N	2.50	0.43
2:H:112:ASP:OD1	2:H:112:ASP:N	2.52	0.43
1:F:22:GLU:HG2	1:F:88:ILE:HG12	2.01	0.43
1:F:565:PRO:HD2	1:F:568:LEU:HD23	1.99	0.43
4:A:130:VAL:HG21	4:A:231:ILE:HG12	2.01	0.43
4:B:466:ARG:HH11	2:G:107:ALA:H	1.65	0.43
4:B:763:LEU:HD12	4:B:1008:VAL:HG21	2.01	0.43
4:C:1087:ALA:HB2	4:C:1126:CYS:HA	1.99	0.43
1:E:323:MET:HE1	1:E:327:PHE:HB2	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:156:ASP:OD2	3:J:195:SER:OG	2.37	0.43
1:F:390:PHE:HA	1:F:393:ARG:HD3	2.01	0.42
1:F:445:THR:HG23	1:F:446:ILE:HG13	2.01	0.42
1:F:482:ARG:HG2	1:F:488:VAL:HG22	2.01	0.42
4:B:364:ASP:OD1	4:B:364:ASP:N	2.52	0.42
4:B:725:GLU:OE1	4:B:1064:HIS:NE2	2.52	0.42
4:B:878:LEU:HD22	4:B:1052:PHE:HD2	1.84	0.42
1:E:115:ARG:NH1	1:E:182:GLU:OE1	2.46	0.42
3:J:80:LEU:HD13	3:J:110:VAL:HG22	2.01	0.42
3:K:28:ASN:OD1	3:K:29:ILE:N	2.51	0.42
4:B:433:VAL:HG12	4:B:512:VAL:HG13	2.01	0.42
4:B:742:ILE:HG21	4:B:753:LEU:HD13	2.01	0.42
4:C:55:PHE:HB2	4:C:275:PHE:CE2	2.54	0.42
4:C:735:SER:N	4:C:859:THR:O	2.50	0.42
1:E:55:THR:OG1	1:E:58:ASN:ND2	2.39	0.42
2:G:12:LYS:NZ	2:G:17:SER:O	2.43	0.42
3:J:146:PRO:HD3	3:J:177:TYR:CD2	2.54	0.42
2:H:101:GLY:HA3	4:A:470:THR:H	1.84	0.42
4:B:719:THR:HG23	4:B:1070:ALA:HB2	2.00	0.42
4:B:889:GLY:HA3	4:B:1034:LEU:HD22	2.01	0.42
1:E:503:LEU:HB3	1:E:506:VAL:HG22	2.02	0.42
1:D:204:ARG:HD2	1:D:222:LEU:HD23	2.01	0.42
3:L:137:LEU:HD23	3:L:153:TRP:HZ3	1.84	0.42
1:F:454:TYR:HE2	1:F:484:ILE:HD13	1.83	0.42
4:B:922:LEU:HD11	5:O:1:NAG:H3	2.01	0.42
4:C:349:SER:OG	4:C:452:ARG:O	2.37	0.42
1:D:134:ASN:ND2	1:D:137:ASN:OD1	2.51	0.42
2:H:128:LYS:HG2	2:H:157:PHE:HE2	1.85	0.42
4:A:328:ARG:CZ	4:A:580:GLN:HG3	2.50	0.42
1:F:431:ASP:OD1	1:F:431:ASP:N	2.51	0.42
4:A:142:ASP:HB2	4:A:156:GLU:HB2	2.01	0.42
4:A:395:VAL:HG22	4:A:515:PHE:CE1	2.54	0.42
4:B:93:ALA:HA	4:B:191:GLU:HA	2.01	0.42
4:B:779:GLN:O	4:B:783:ALA:N	2.49	0.42
3:J:22:CYS:N	3:J:73:ALA:O	2.53	0.42
1:D:385:TYR:HD1	1:D:393:ARG:HH11	1.66	0.42
4:B:403:ARG:HG3	4:B:497:PHE:HE1	1.83	0.42
3:J:93:TYR:HA	3:J:100:SER:HA	2.00	0.42
1:F:211:GLY:N	1:F:216:ASP:OD1	2.52	0.42
4:B:328:ARG:HH22	4:B:533:LEU:HD13	1.83	0.42
4:B:438:SER:OG	4:B:442:ASP:OD2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:560:LEU:O	4:B:577:ARG:NH2	2.51	0.42
4:C:980:ILE:HD12	4:C:989:ALA:HB1	2.02	0.42
1:E:389:PRO:HD2	1:E:392:LEU:HB2	2.02	0.42
2:G:40:ALA:HB3	2:G:43:GLN:HB2	2.02	0.42
3:L:21:SER:HA	3:L:74:SER:HA	2.01	0.42
3:L:151:VAL:HG12	3:L:200:VAL:HG22	2.01	0.42
1:F:388:GLN:OE1	1:F:392:LEU:HD11	2.19	0.42
2:I:98:ARG:HE	2:I:100:ARG:NH1	2.18	0.42
4:A:1004:LEU:HD23	4:A:1004:LEU:HA	1.89	0.42
4:C:103:GLY:H	4:C:241:LEU:HB2	1.85	0.42
4:C:897:PRO:HB2	4:C:900:MET:HG2	2.01	0.42
1:E:380:GLN:HA	1:E:383:MET:HE2	2.01	0.42
4:C:363:ALA:O	4:C:527:PRO:HD3	2.19	0.42
1:E:450:LEU:HD21	1:E:519:THR:HG21	2.02	0.42
3:J:161:LYS:HA	3:J:161:LYS:HD3	1.90	0.42
4:A:882:ILE:HG13	4:A:883:THR:HG23	2.01	0.41
4:C:276:LEU:HD22	4:C:301:CYS:HA	2.01	0.41
4:C:328:ARG:HB2	4:C:543:PHE:HE1	1.84	0.41
4:C:558:LYS:HA	4:C:558:LYS:HD2	1.93	0.41
1:E:325:GLN:HA	1:E:328:TRP:HD1	1.84	0.41
1:D:382:ASP:OD1	1:D:385:TYR:OH	2.37	0.41
1:F:85:LEU:HD21	1:F:98:GLN:HG3	2.01	0.41
4:A:701:ALA:HB3	4:B:787:GLN:HG2	2.02	0.41
4:A:804:GLN:HA	4:A:817:PRO:HG2	2.02	0.41
4:B:902:MET:HE1	4:B:1050:MET:HE1	2.01	0.41
1:F:165:TRP:HE1	1:F:169:ARG:NH1	2.18	0.41
1:F:279:TYR:CZ	1:F:441:LYS:HB2	2.55	0.41
2:I:154:LYS:HE3	3:K:136:THR:HG21	2.02	0.41
1:E:180:TYR:HA	1:E:183:TYR:HB3	2.02	0.41
1:E:397:ASN:OD1	1:E:397:ASN:N	2.53	0.41
2:G:110:TYR:HB3	3:J:36:HIS:CD2	2.55	0.41
1:F:209:VAL:H	1:F:217:TYR:HB3	1.84	0.41
4:A:177:MET:HE3	4:A:179:LEU:HD22	2.02	0.41
4:B:565:PHE:HB2	4:C:42:VAL:HG12	2.03	0.41
4:B:1088:HIS:CE1	4:B:1137:VAL:HG21	2.55	0.41
1:E:566:TRP:HA	1:E:569:ALA:HB3	2.02	0.41
3:L:113:GLN:HG2	3:L:145:TYR:HD2	1.85	0.41
4:A:965:GLN:O	4:A:968:SER:OG	2.34	0.41
1:E:111:ASP:OD1	1:E:111:ASP:N	2.51	0.41
1:D:419:LYS:HG3	1:D:424:LEU:HD23	2.02	0.41
3:L:39:GLN:HB2	3:L:49:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:858:LEU:HD23	4:A:959:LEU:HD22	2.02	0.41
4:B:934:ILE:HD13	4:B:934:ILE:HA	1.94	0.41
4:B:1000:ARG:O	4:B:1003:SER:OG	2.37	0.41
4:C:473:TYR:H	4:C:491:PRO:HD3	1.86	0.41
4:C:969:LYS:HG3	4:C:972:ALA:H	1.85	0.41
4:C:996:LEU:HD21	4:C:1000:ARG:HH21	1.86	0.41
3:J:39:GLN:HE22	3:J:88:TYR:HE2	1.69	0.41
3:L:174:ASN:OD1	3:L:174:ASN:N	2.54	0.41
4:A:733:LYS:HD2	4:A:771:ALA:HB1	2.01	0.41
4:B:179:LEU:O	4:B:245:HIS:NE2	2.52	0.41
4:C:566:GLY:N	4:C:575:ALA:O	2.54	0.41
1:D:393:ARG:HD3	1:D:393:ARG:HA	1.77	0.41
4:A:708:SER:OG	4:A:710:ASN:OD1	2.38	0.41
4:B:328:ARG:HG2	4:B:530:SER:HA	2.02	0.41
4:C:730:SER:OG	4:C:731:MET:N	2.53	0.41
1:D:471:ASP:OD1	1:D:471:ASP:N	2.48	0.41
1:F:482:ARG:NH2	1:F:613:TYR:OH	2.54	0.41
2:I:174:VAL:HG22	2:I:193:VAL:HG12	2.03	0.41
4:A:513:LEU:HD23	4:A:513:LEU:HA	1.91	0.41
4:A:676:THR:HA	4:A:690:GLN:HA	2.02	0.41
4:B:37:TYR:OH	4:B:54:LEU:O	2.33	0.41
4:B:199:GLY:HA3	4:B:232:GLY:HA2	2.03	0.41
4:B:774:GLN:HE22	4:B:1018:ILE:HG21	1.86	0.41
4:C:31:SER:HB3	4:C:60:SER:H	1.86	0.41
4:C:719:THR:HG23	4:C:1070:ALA:HB2	2.03	0.41
1:E:419:LYS:HE3	1:E:426:PRO:HA	2.03	0.41
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.56	0.41
3:K:122:LEU:HD12	3:K:122:LEU:HA	1.92	0.41
4:A:599:THR:HG22	4:A:601:GLY:H	1.86	0.41
4:B:328:ARG:HH21	4:B:543:PHE:HZ	1.68	0.41
1:F:378:HIS:HE1	1:F:402:GLU:HA	1.85	0.40
1:F:457:GLU:OE2	1:F:460:ARG:NH2	2.55	0.40
2:I:220:LYS:HE3	2:I:220:LYS:HB3	1.92	0.40
4:B:29:THR:OG1	4:B:30:ASN:N	2.55	0.40
4:B:909:ILE:HG21	4:B:1047:TYR:HB3	2.03	0.40
4:C:172:SER:OG	4:C:173:GLN:N	2.55	0.40
4:C:766:ALA:O	4:C:770:ILE:N	2.45	0.40
1:E:245:ARG:HA	1:E:262:LEU:HD21	2.03	0.40
1:D:513:ILE:HD12	1:D:513:ILE:HA	1.98	0.40
2:I:6:GLN:NE2	2:I:95:TYR:HA	2.33	0.40
3:K:27:SER:OG	3:K:96:GLY:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:938:LEU:HD22	4:B:945:LEU:HD11	2.03	0.40
4:C:342:PHE:HE1	4:C:511:VAL:HG11	1.86	0.40
2:H:149:LEU:HD21	2:H:222:VAL:HG11	2.04	0.40
1:F:293:VAL:HG21	1:F:418:LEU:HD22	2.03	0.40
4:A:343:ASN:HB2	4:A:371:PHE:HE1	1.87	0.40
4:A:540:ASN:HB3	4:A:549:THR:HG22	2.02	0.40
4:B:789:TYR:HE2	4:B:888:PHE:HB2	1.86	0.40
4:B:1045:LYS:HE2	4:B:1045:LYS:HB3	1.95	0.40
4:C:111:ASP:N	4:C:111:ASP:OD1	2.55	0.40
4:C:159:VAL:HG23	4:C:160:TYR:CD2	2.56	0.40
4:C:278:LYS:HD3	4:C:286:THR:HB	2.03	0.40
1:E:92:THR:HG23	1:E:392:LEU:HD21	2.03	0.40
1:E:475:LYS:HD2	1:E:475:LYS:HA	1.83	0.40
1:F:245:ARG:NH2	1:F:605:GLY:O	2.48	0.40
1:F:455:MET:SD	1:F:456:LEU:N	2.95	0.40
1:F:599:ASN:HB3	1:F:602:SER:HB3	2.03	0.40
4:A:776:LYS:NZ	4:A:780:GLU:OE2	2.50	0.40
4:B:525:CYS:HB3	4:B:527:PRO:HD3	2.04	0.40
1:E:459:TRP:NE1	1:E:477:TRP:HB2	2.37	0.40
4:B:919:ASN:HB2	4:B:922:LEU:HB3	2.04	0.40
2:G:100:ARG:NH2	2:G:112:ASP:OD2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	594/602 (99%)	580 (98%)	14 (2%)	0	100	100
1	E	594/602 (99%)	582 (98%)	12 (2%)	0	100	100
1	F	594/602 (99%)	581 (98%)	13 (2%)	0	100	100
2	G	222/228 (97%)	215 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	222/228 (97%)	216 (97%)	6 (3%)	0	100	100
2	I	222/228 (97%)	210 (95%)	12 (5%)	0	100	100
3	J	211/217 (97%)	201 (95%)	10 (5%)	0	100	100
3	K	211/217 (97%)	201 (95%)	10 (5%)	0	100	100
3	L	211/217 (97%)	203 (96%)	8 (4%)	0	100	100
4	A	1039/1247 (83%)	989 (95%)	50 (5%)	0	100	100
4	B	1039/1247 (83%)	999 (96%)	40 (4%)	0	100	100
4	C	1039/1247 (83%)	996 (96%)	43 (4%)	0	100	100
All	All	6198/6882 (90%)	5973 (96%)	225 (4%)	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	D	526/532 (99%)	525 (100%)	1 (0%)	87	86
1	E	526/532 (99%)	524 (100%)	2 (0%)	84	83
1	F	526/532 (99%)	524 (100%)	2 (0%)	84	83
2	G	183/188 (97%)	183 (100%)	0	100	100
2	H	183/188 (97%)	183 (100%)	0	100	100
2	I	183/188 (97%)	183 (100%)	0	100	100
3	J	173/179 (97%)	173 (100%)	0	100	100
3	K	173/179 (97%)	173 (100%)	0	100	100
3	L	173/179 (97%)	173 (100%)	0	100	100
4	A	918/1083 (85%)	916 (100%)	2 (0%)	87	86
4	B	918/1083 (85%)	917 (100%)	1 (0%)	88	88
4	C	918/1083 (85%)	918 (100%)	0	100	100
All	All	5400/5946 (91%)	5392 (100%)	8 (0%)	87	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	143	LEU
1	F	392	LEU
1	F	397	ASN
4	A	335	LEU
4	A	582	LEU
4	B	159	VAL
1	E	323	MET
1	E	324	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	330	ASN
1	D	373	HIS
1	D	417	HIS
1	D	472	GLN
1	D	522	GLN
1	D	524	GLN
1	D	526	GLN
1	D	531	GLN
2	H	6	GLN
2	H	166	ASN
2	H	210	ASN
2	H	211	HIS
3	L	16	GLN
1	F	51	ASN
1	F	76	GLN
1	F	81	GLN
1	F	102	GLN
1	F	159	ASN
1	F	277	ASN
1	F	300	GLN
1	F	373	HIS
1	F	397	ASN
1	F	437	ASN
1	F	442	GLN
1	F	531	GLN
2	I	3	GLN
2	I	6	GLN
2	I	215	ASN
3	K	39	GLN

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Mol	Chain	Res	Type
4	A	121	ASN
4	A	207	HIS
4	A	314	GLN
4	A	448	ASN
4	A	450	ASN
4	A	487	ASN
4	A	506	GLN
4	A	901	GLN
4	A	1048	HIS
4	A	1108	ASN
4	B	99	ASN
4	B	121	ASN
4	B	188	ASN
4	B	394	ASN
4	B	481	ASN
4	B	774	GLN
4	B	953	ASN
4	B	960	ASN
4	B	1023	ASN
4	B	1054	GLN
4	B	1108	ASN
4	C	121	ASN
4	C	314	GLN
4	C	405	ASN
4	C	448	ASN
4	C	481	ASN
4	C	580	GLN
4	C	762	GLN
4	C	955	ASN
4	C	1135	ASN
1	E	58	ASN
1	E	63	ASN
1	E	102	GLN
1	E	241	HIS
1	E	277	ASN
1	E	508	ASN
1	E	531	GLN
1	E	552	GLN
2	G	3	GLN
2	G	6	GLN
2	G	65	GLN
2	G	208	ASN

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Mol	Chain	Res	Type
2	G	210	ASN
2	G	215	ASN
3	J	28	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	$\# Z > 2$
5	NAG	M	1	5,4	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	M	2	5	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	N	1	5,4	14,14,15	0.29	0	17,19,21	0.51	0
5	NAG	N	2	5	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	O	1	5,4	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	O	2	5	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	P	1	5,4	14,14,15	0.28	0	17,19,21	0.53	0
5	NAG	P	2	5	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	Q	1	5,4	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	Q	2	5	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	R	1	5,4	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	R	2	5	14,14,15	0.28	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
5	NAG	M	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	NAG	P	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	NAG	Q	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	1/6/23/26	0/1/1/1
5	NAG	R	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

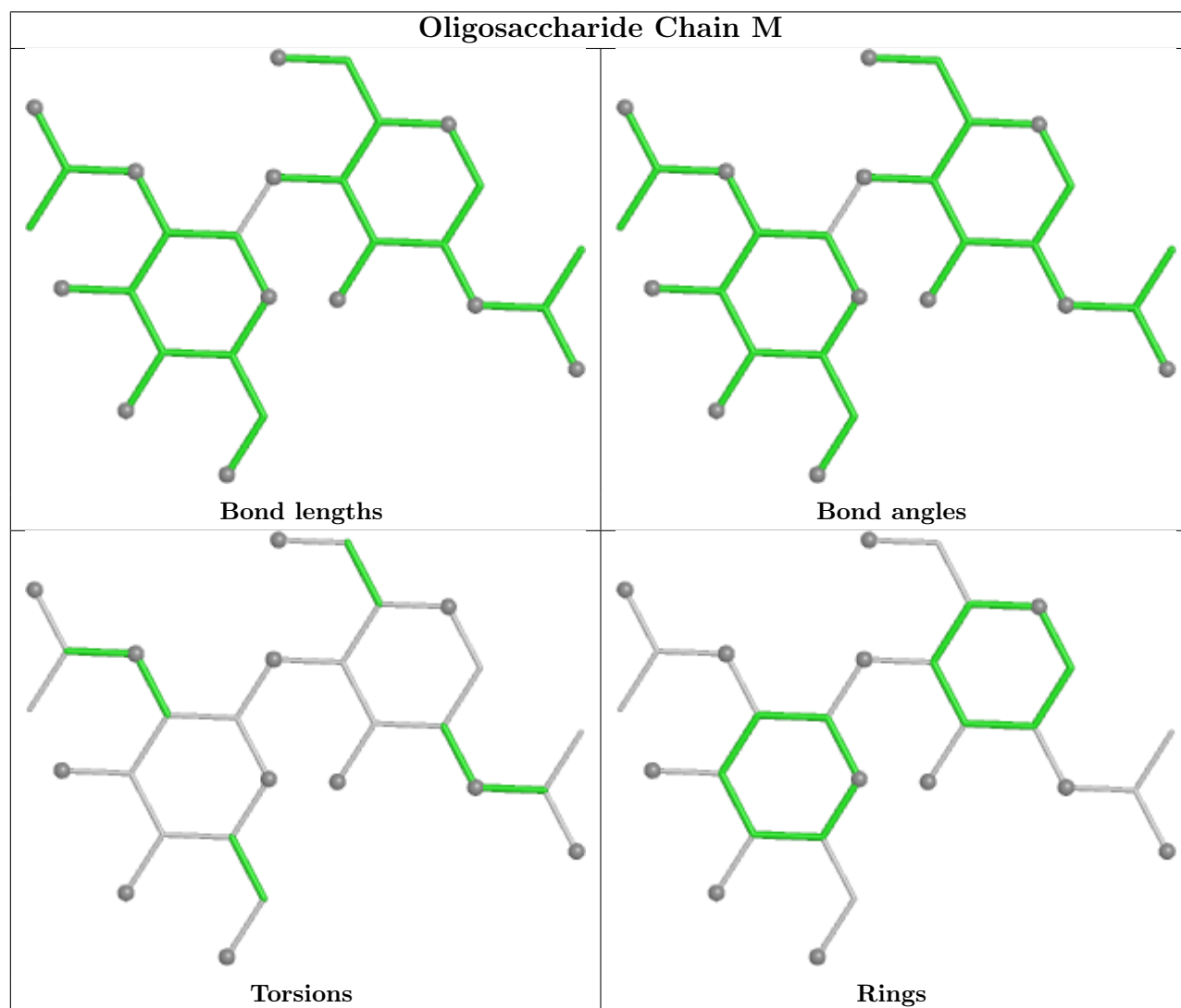
Mol	Chain	Res	Type	Atoms
5	N	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6

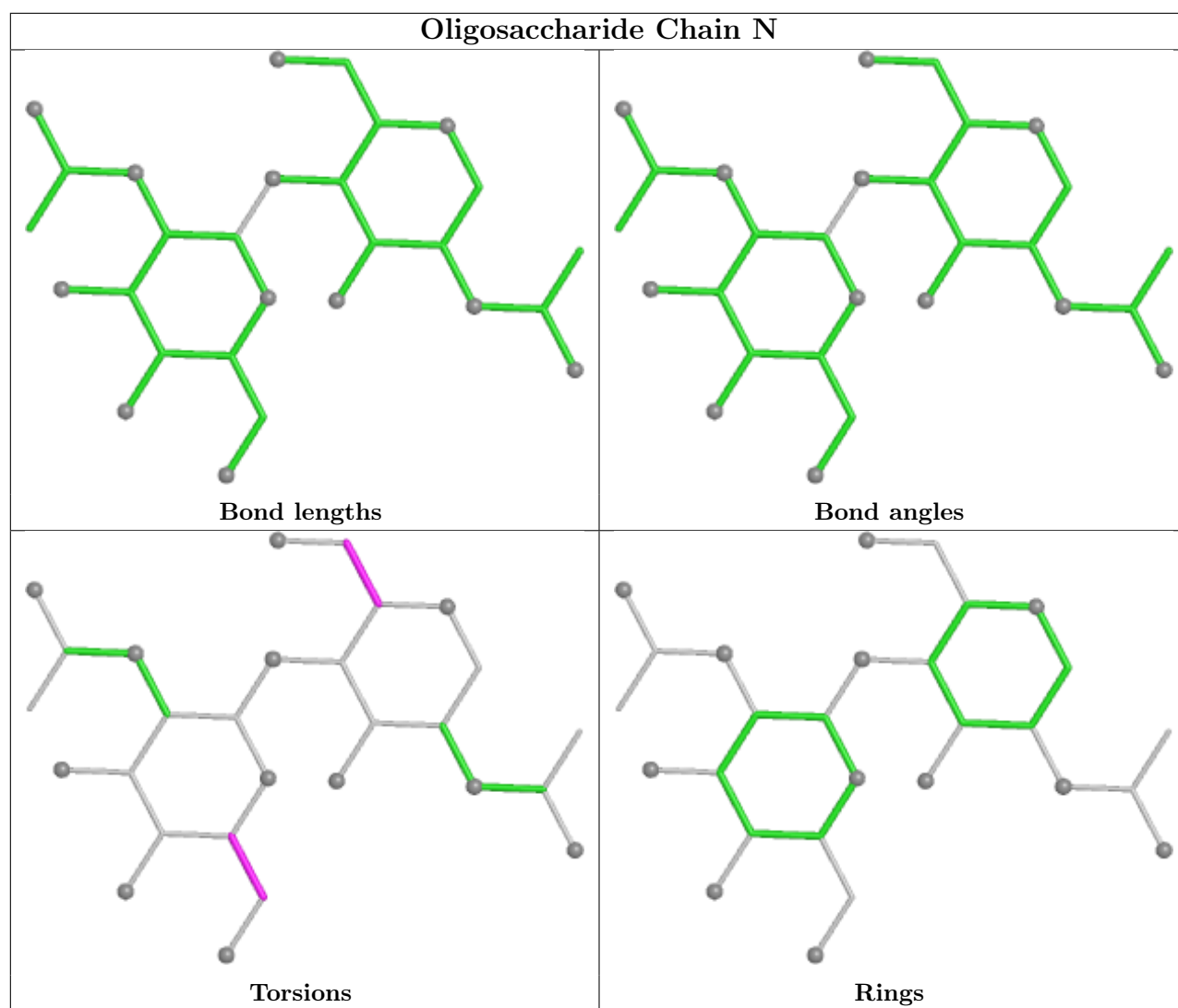
There are no ring outliers.

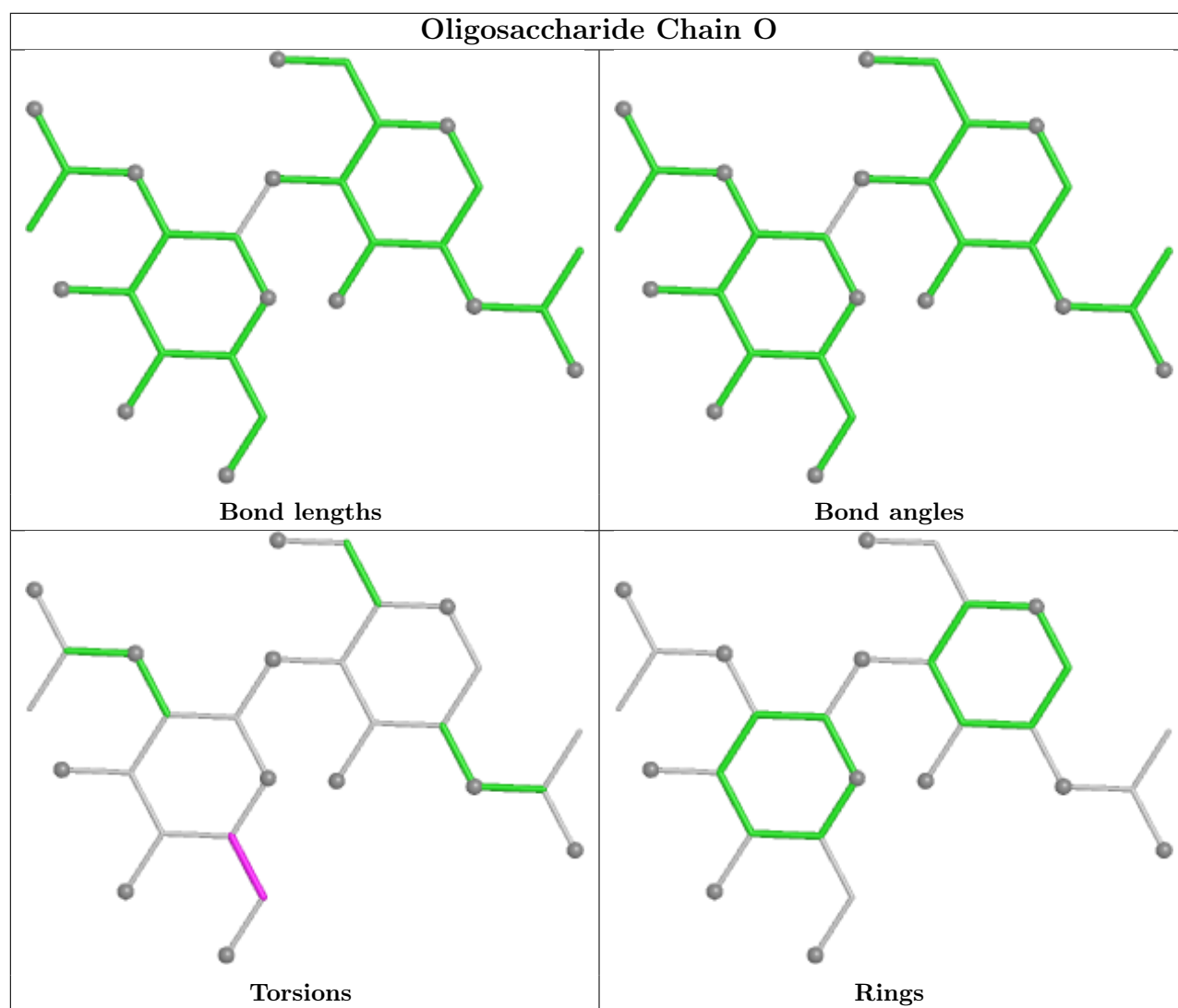
1 monomer is involved in 1 short contact:

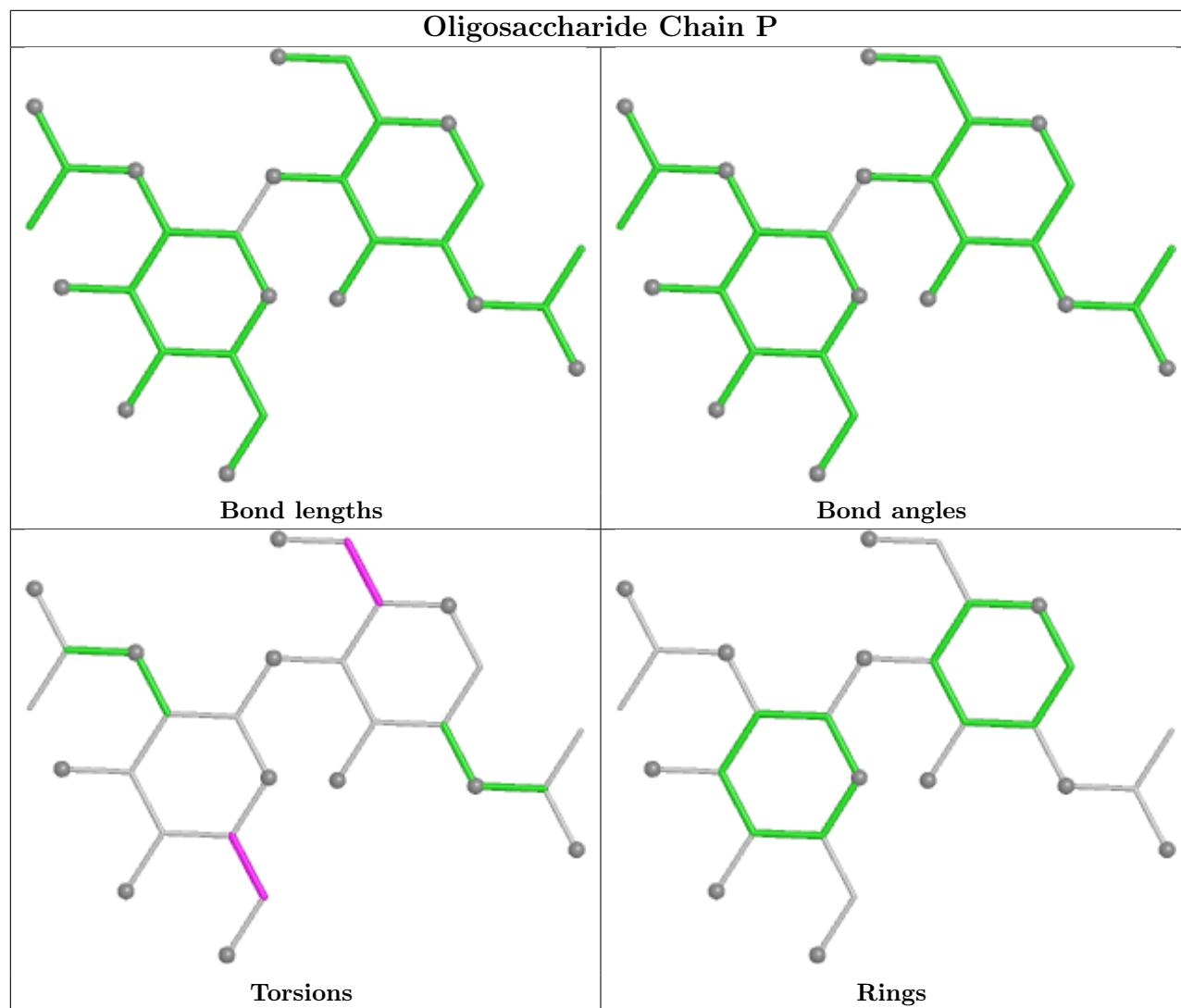
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	1	0

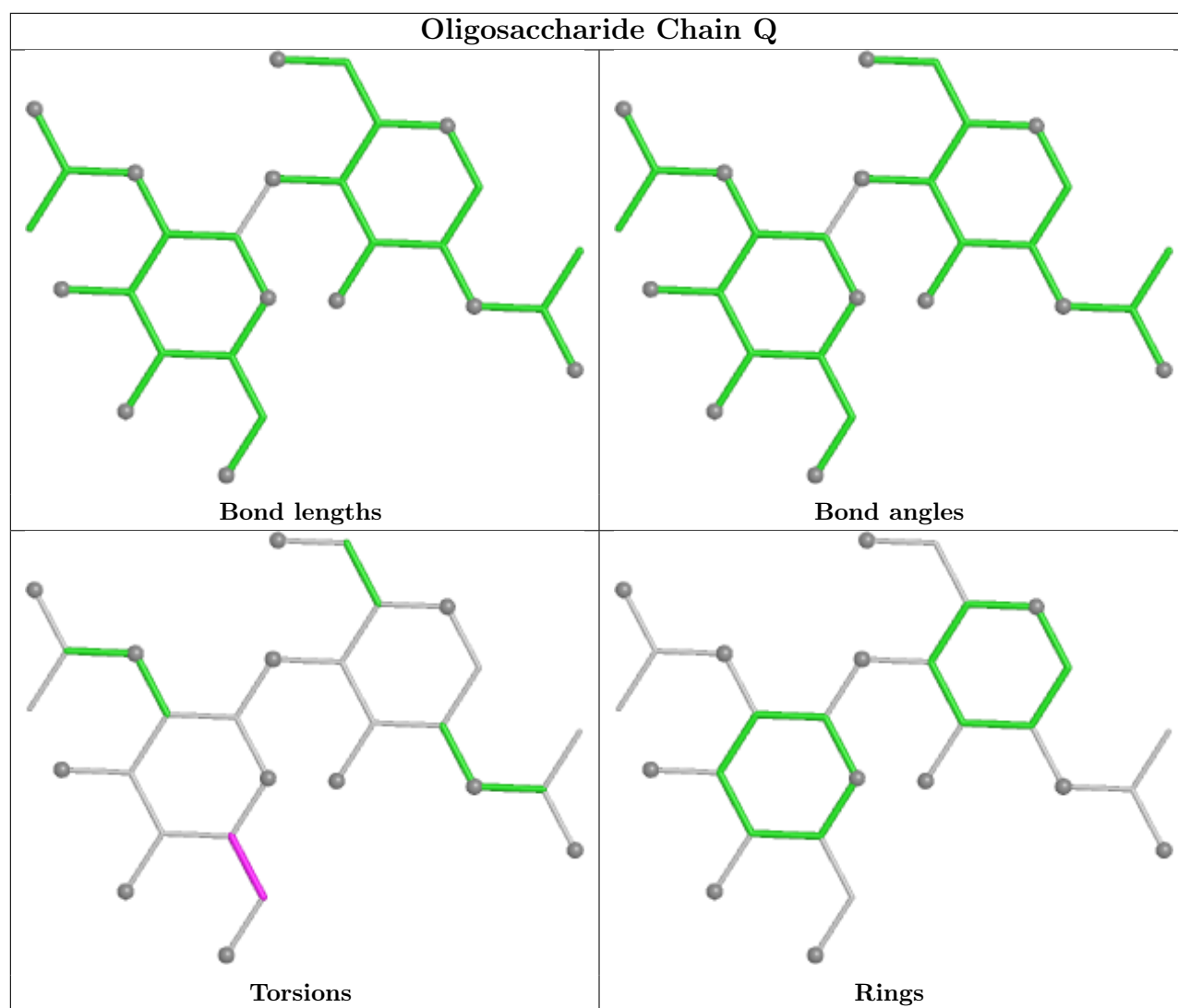
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

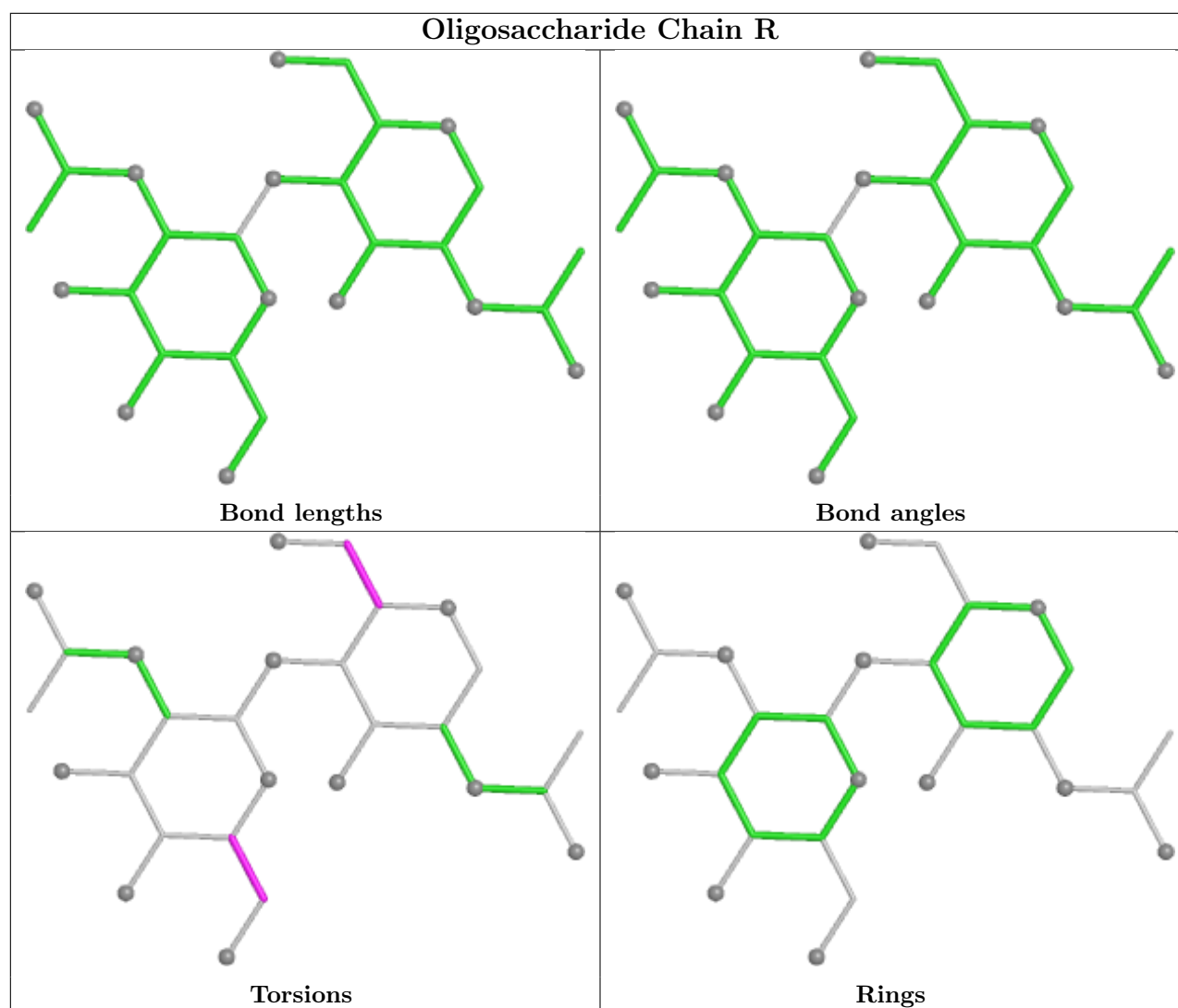












5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 3 are monoatomic - leaving 36 for Mogul analysis.

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	$\# Z > 2$
7	NAG	E	904	1	14,14,15	0.26	0	17,19,21	0.41	0
7	NAG	D	904	1	14,14,15	0.28	0	17,19,21	0.47	0
7	NAG	C	1305	4	14,14,15	0.26	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	F	902	1	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	D	902	1	14,14,15	0.25	0	17,19,21	0.44	0
7	NAG	A	1305	4	14,14,15	0.26	0	17,19,21	0.42	0
7	NAG	B	1307	4	14,14,15	0.30	0	17,19,21	0.33	0
7	NAG	E	903	1	14,14,15	0.31	0	17,19,21	0.45	0
7	NAG	A	1302	4	14,14,15	0.27	0	17,19,21	0.37	0
7	NAG	F	903	1	14,14,15	0.36	0	17,19,21	0.49	0
7	NAG	F	904	1	14,14,15	0.60	0	17,19,21	0.64	1 (5%)
7	NAG	B	1302	4	14,14,15	0.31	0	17,19,21	0.35	0
7	NAG	A	1307	4	14,14,15	0.30	0	17,19,21	0.35	0
7	NAG	D	905	1	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	C	1308	4	14,14,15	0.28	0	17,19,21	0.41	0
7	NAG	C	1304	4	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	A	1306	4	14,14,15	0.26	0	17,19,21	0.46	0
7	NAG	B	1304	4	14,14,15	0.31	0	17,19,21	0.46	0
7	NAG	B	1308	4	14,14,15	0.29	0	17,19,21	0.41	0
7	NAG	E	905	1	14,14,15	0.29	0	17,19,21	0.46	0
7	NAG	C	1307	4	14,14,15	0.33	0	17,19,21	0.34	0
7	NAG	E	902	1	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	C	1303	4	14,14,15	0.46	0	17,19,21	0.43	0
7	NAG	A	1301	4	14,14,15	0.23	0	17,19,21	0.40	0
7	NAG	C	1301	4	14,14,15	0.28	0	17,19,21	0.47	0
7	NAG	C	1302	4	14,14,15	0.21	0	17,19,21	0.51	0
7	NAG	C	1306	4	14,14,15	0.27	0	17,19,21	0.47	0
7	NAG	B	1306	4	14,14,15	0.27	0	17,19,21	0.42	0
7	NAG	B	1303	4	14,14,15	0.46	0	17,19,21	0.43	0
7	NAG	A	1304	4	14,14,15	0.26	0	17,19,21	0.44	0
7	NAG	A	1308	4	14,14,15	0.28	0	17,19,21	0.41	0
7	NAG	D	903	1	14,14,15	0.38	0	17,19,21	0.49	0
7	NAG	A	1303	4	14,14,15	0.40	0	17,19,21	0.37	0
7	NAG	B	1305	4	14,14,15	0.25	0	17,19,21	0.43	0
7	NAG	B	1301	4	14,14,15	0.29	0	17,19,21	0.47	0
7	NAG	F	905	1	14,14,15	0.26	0	17,19,21	0.45	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
7	NAG	E	904	1	-	2/6/23/26	0/1/1/1
7	NAG	D	904	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1305	4	-	2/6/23/26	0/1/1/1
7	NAG	F	902	1	-	2/6/23/26	0/1/1/1
7	NAG	D	902	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1305	4	-	1/6/23/26	0/1/1/1
7	NAG	B	1307	4	-	2/6/23/26	0/1/1/1
7	NAG	E	903	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1302	4	-	2/6/23/26	0/1/1/1
7	NAG	F	903	1	-	0/6/23/26	0/1/1/1
7	NAG	F	904	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	4	-	2/6/23/26	0/1/1/1
7	NAG	A	1307	4	-	2/6/23/26	0/1/1/1
7	NAG	D	905	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1308	4	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	4	-	2/6/23/26	0/1/1/1
7	NAG	A	1306	4	-	2/6/23/26	0/1/1/1
7	NAG	B	1304	4	-	2/6/23/26	0/1/1/1
7	NAG	B	1308	4	-	2/6/23/26	0/1/1/1
7	NAG	E	905	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1307	4	-	2/6/23/26	0/1/1/1
7	NAG	E	902	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	4	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	4	-	0/6/23/26	0/1/1/1
7	NAG	C	1301	4	-	2/6/23/26	0/1/1/1
7	NAG	C	1302	4	-	4/6/23/26	0/1/1/1
7	NAG	C	1306	4	-	2/6/23/26	0/1/1/1
7	NAG	B	1306	4	-	2/6/23/26	0/1/1/1
7	NAG	B	1303	4	-	0/6/23/26	0/1/1/1
7	NAG	A	1304	4	-	2/6/23/26	0/1/1/1
7	NAG	A	1308	4	-	2/6/23/26	0/1/1/1
7	NAG	D	903	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	4	-	1/6/23/26	0/1/1/1
7	NAG	B	1305	4	-	2/6/23/26	0/1/1/1
7	NAG	B	1301	4	-	0/6/23/26	0/1/1/1
7	NAG	F	905	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	904	NAG	C1-O5-C5	2.17	115.14	112.19

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1307	NAG	C4-C5-C6-O6
7	A	1307	NAG	C4-C5-C6-O6
7	A	1306	NAG	C4-C5-C6-O6
7	C	1302	NAG	O5-C5-C6-O6
7	E	904	NAG	O5-C5-C6-O6
7	C	1307	NAG	C4-C5-C6-O6
7	B	1307	NAG	O5-C5-C6-O6
7	D	903	NAG	C4-C5-C6-O6
7	F	902	NAG	C4-C5-C6-O6
7	D	904	NAG	O5-C5-C6-O6
7	A	1304	NAG	O5-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6
7	F	905	NAG	O5-C5-C6-O6
7	A	1307	NAG	O5-C5-C6-O6
7	C	1301	NAG	O5-C5-C6-O6
7	C	1303	NAG	O5-C5-C6-O6
7	E	902	NAG	O5-C5-C6-O6
7	E	903	NAG	O5-C5-C6-O6
7	C	1302	NAG	C4-C5-C6-O6
7	E	904	NAG	C4-C5-C6-O6
7	F	904	NAG	O5-C5-C6-O6
7	C	1307	NAG	O5-C5-C6-O6
7	D	904	NAG	C4-C5-C6-O6
7	A	1306	NAG	O5-C5-C6-O6
7	C	1305	NAG	O5-C5-C6-O6
7	D	903	NAG	O5-C5-C6-O6
7	D	905	NAG	O5-C5-C6-O6
7	A	1304	NAG	C4-C5-C6-O6
7	B	1304	NAG	C4-C5-C6-O6
7	E	903	NAG	C4-C5-C6-O6
7	D	905	NAG	C4-C5-C6-O6
7	F	904	NAG	C4-C5-C6-O6
7	C	1303	NAG	C4-C5-C6-O6
7	C	1305	NAG	C4-C5-C6-O6
7	A	1302	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	1302	NAG	O7-C7-N2-C2
7	B	1302	NAG	C8-C7-N2-C2
7	B	1302	NAG	O7-C7-N2-C2
7	C	1302	NAG	C8-C7-N2-C2
7	C	1302	NAG	O7-C7-N2-C2
7	C	1301	NAG	C4-C5-C6-O6
7	C	1304	NAG	O5-C5-C6-O6
7	F	905	NAG	C4-C5-C6-O6
7	F	902	NAG	O5-C5-C6-O6
7	A	1308	NAG	O5-C5-C6-O6
7	B	1308	NAG	O5-C5-C6-O6
7	E	902	NAG	C4-C5-C6-O6
7	C	1308	NAG	O5-C5-C6-O6
7	A	1303	NAG	O5-C5-C6-O6
7	B	1305	NAG	C4-C5-C6-O6
7	B	1306	NAG	C4-C5-C6-O6
7	D	902	NAG	O5-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6
7	B	1305	NAG	O5-C5-C6-O6
7	A	1308	NAG	C4-C5-C6-O6
7	C	1306	NAG	C4-C5-C6-O6
7	B	1306	NAG	O5-C5-C6-O6
7	A	1305	NAG	C4-C5-C6-O6
7	B	1308	NAG	C4-C5-C6-O6
7	C	1306	NAG	O5-C5-C6-O6
7	C	1308	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	904	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

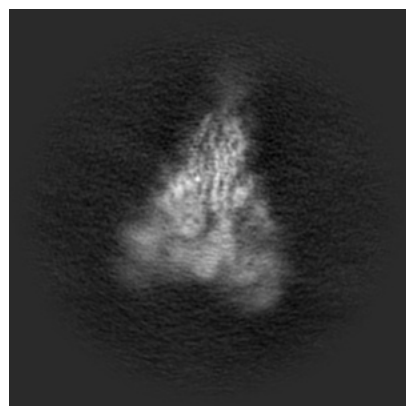
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66895. These allow visual inspection of the internal detail of the map and identification of artifacts.

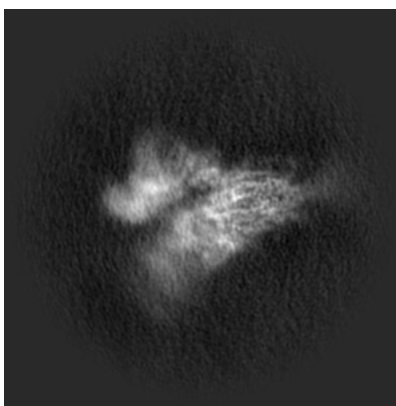
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

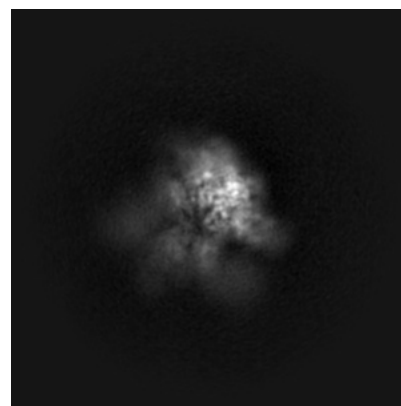
6.1.1 Primary map



X

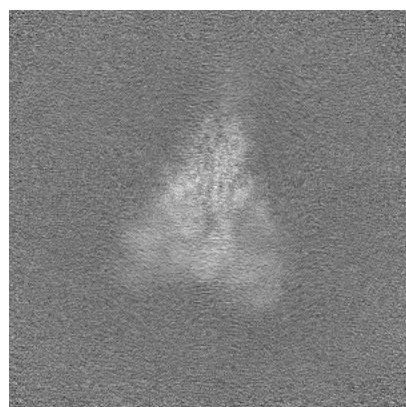


Y

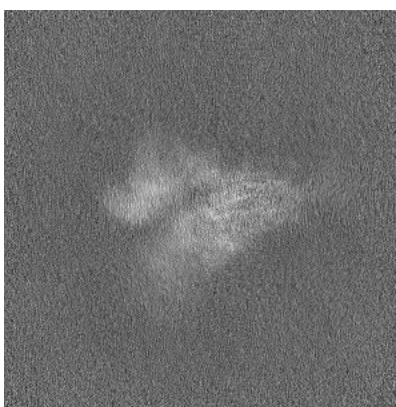


Z

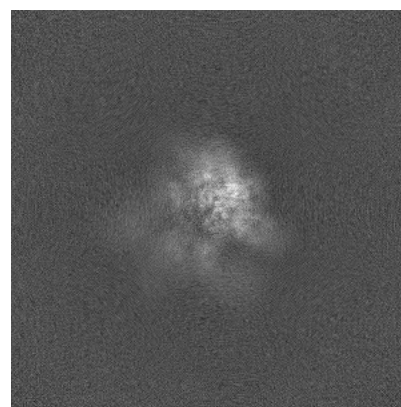
6.1.2 Raw map



X



Y

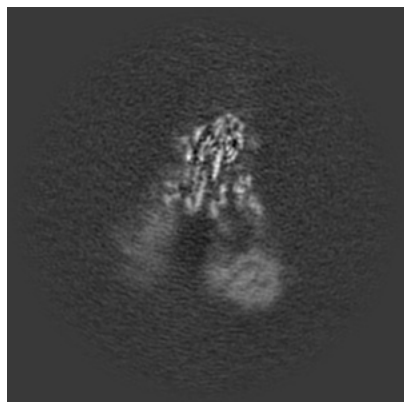


Z

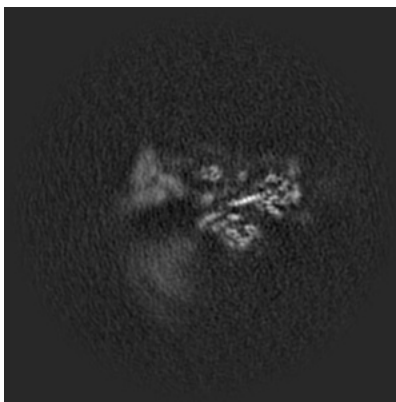
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

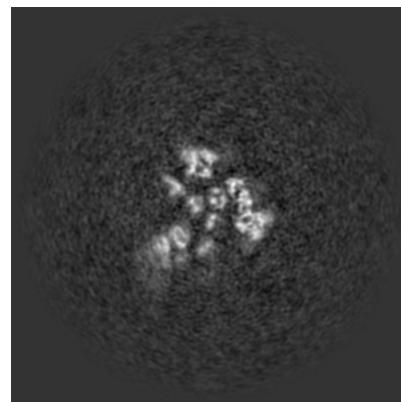
6.2.1 Primary map



X Index: 288

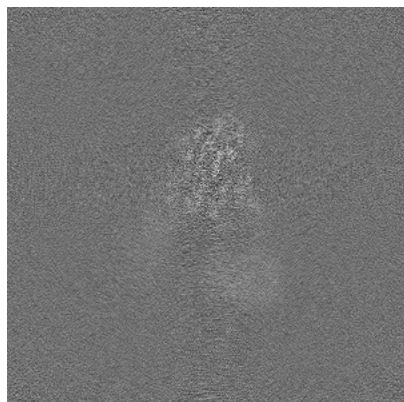


Y Index: 288

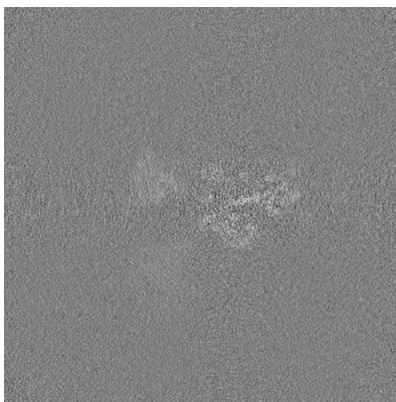


Z Index: 288

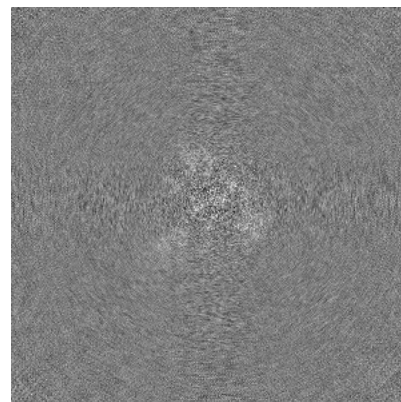
6.2.2 Raw map



X Index: 288



Y Index: 288

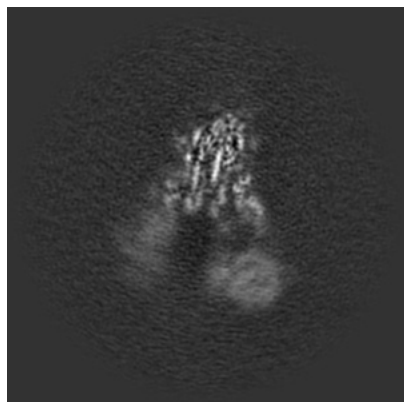


Z Index: 288

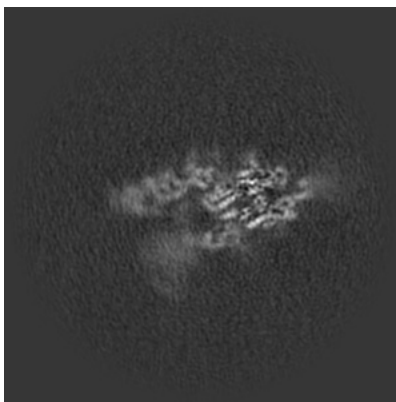
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

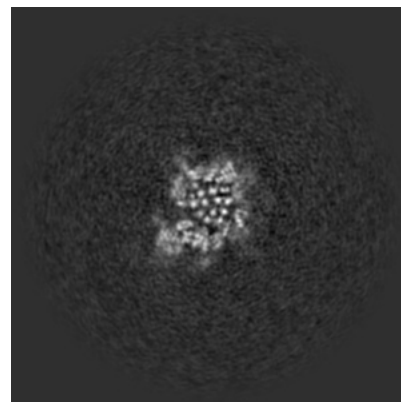
6.3.1 Primary map



X Index: 286

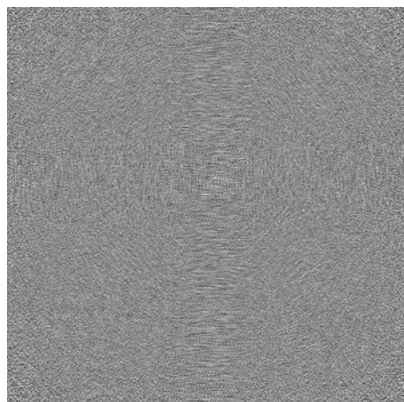


Y Index: 311

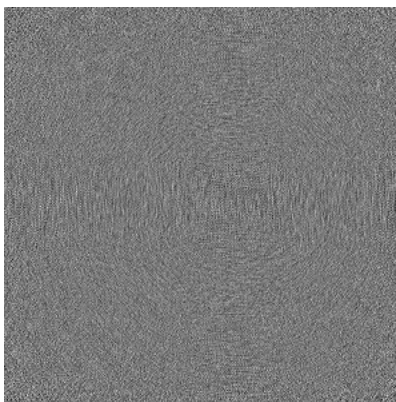


Z Index: 314

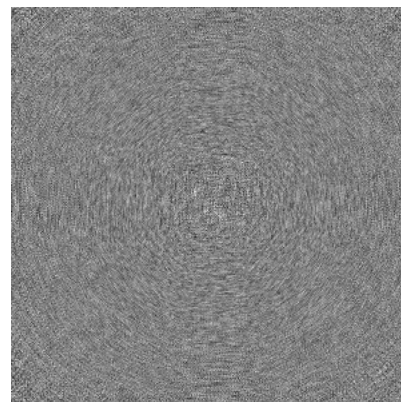
6.3.2 Raw map



X Index: 0



Y Index: 0

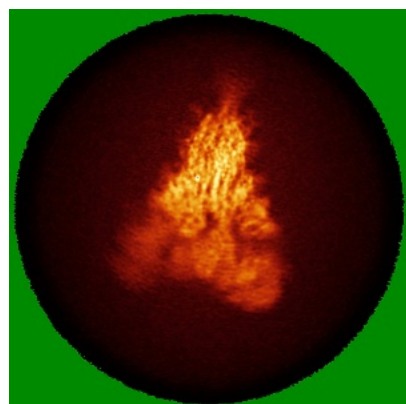


Z Index: 575

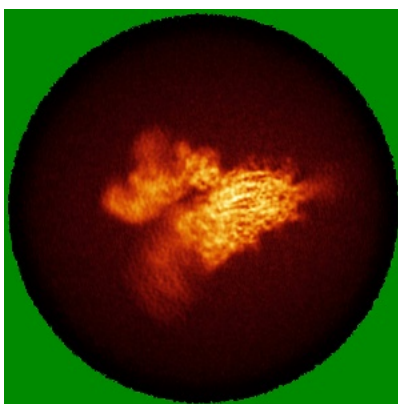
The images above show the largest variance slices of the map in three orthogonal directions.

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

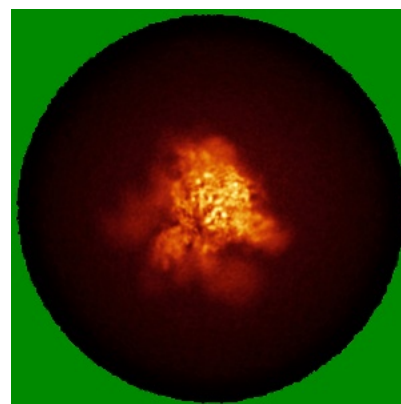
6.4.1 Primary map



X

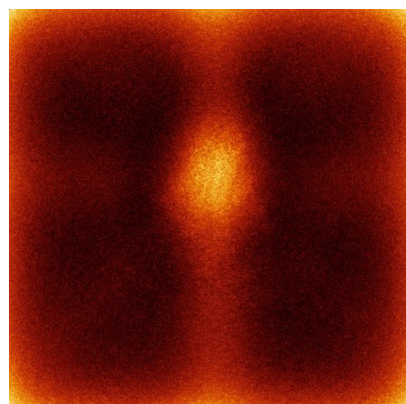


Y

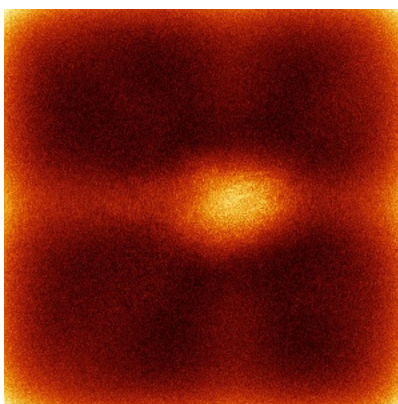


Z

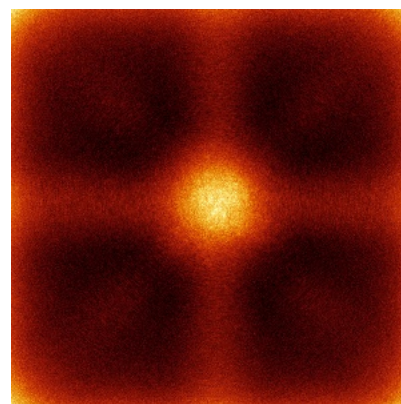
6.4.2 Raw map



X



Y

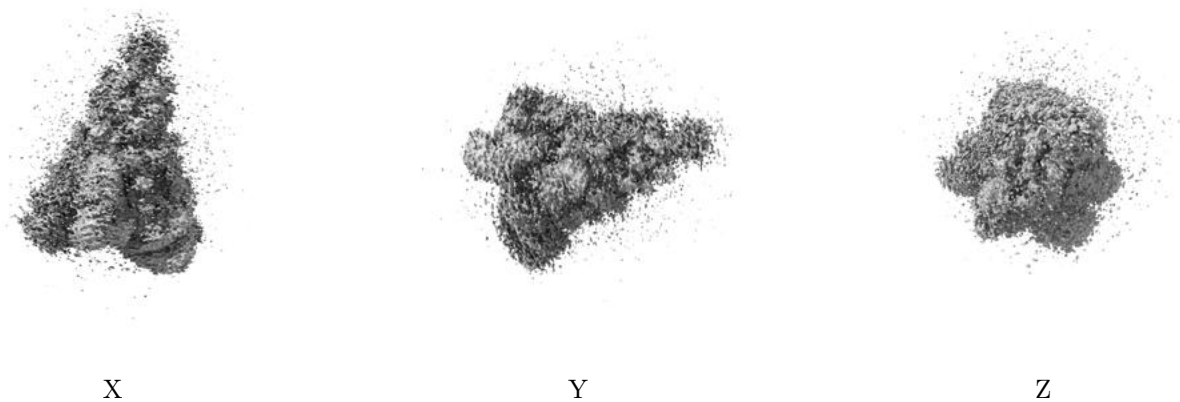


Z

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.

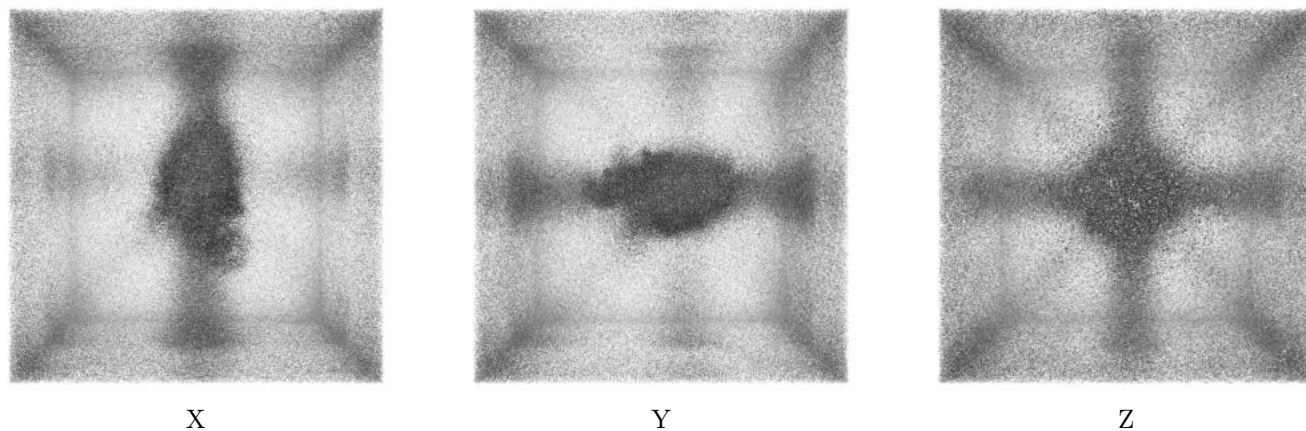
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

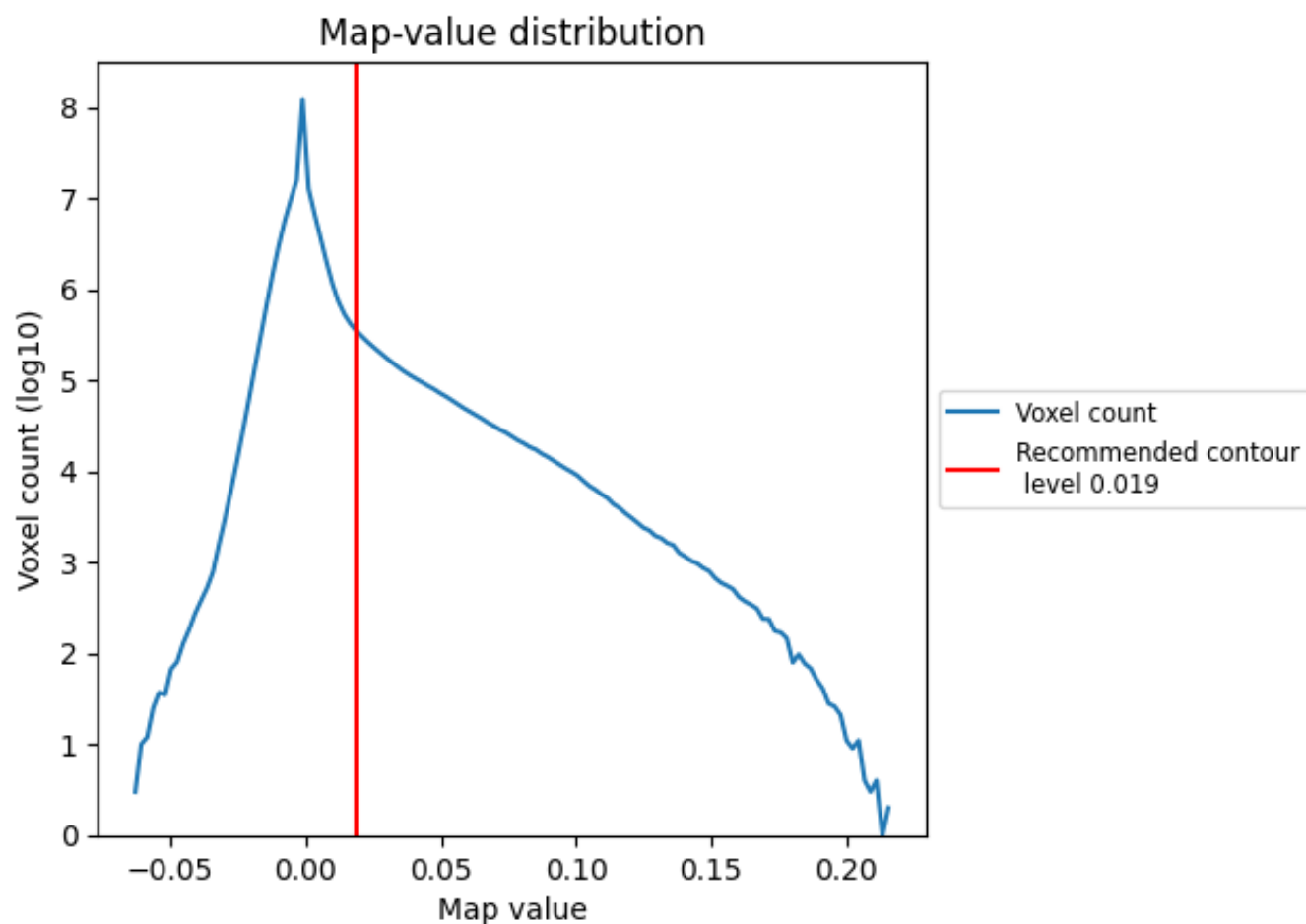
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

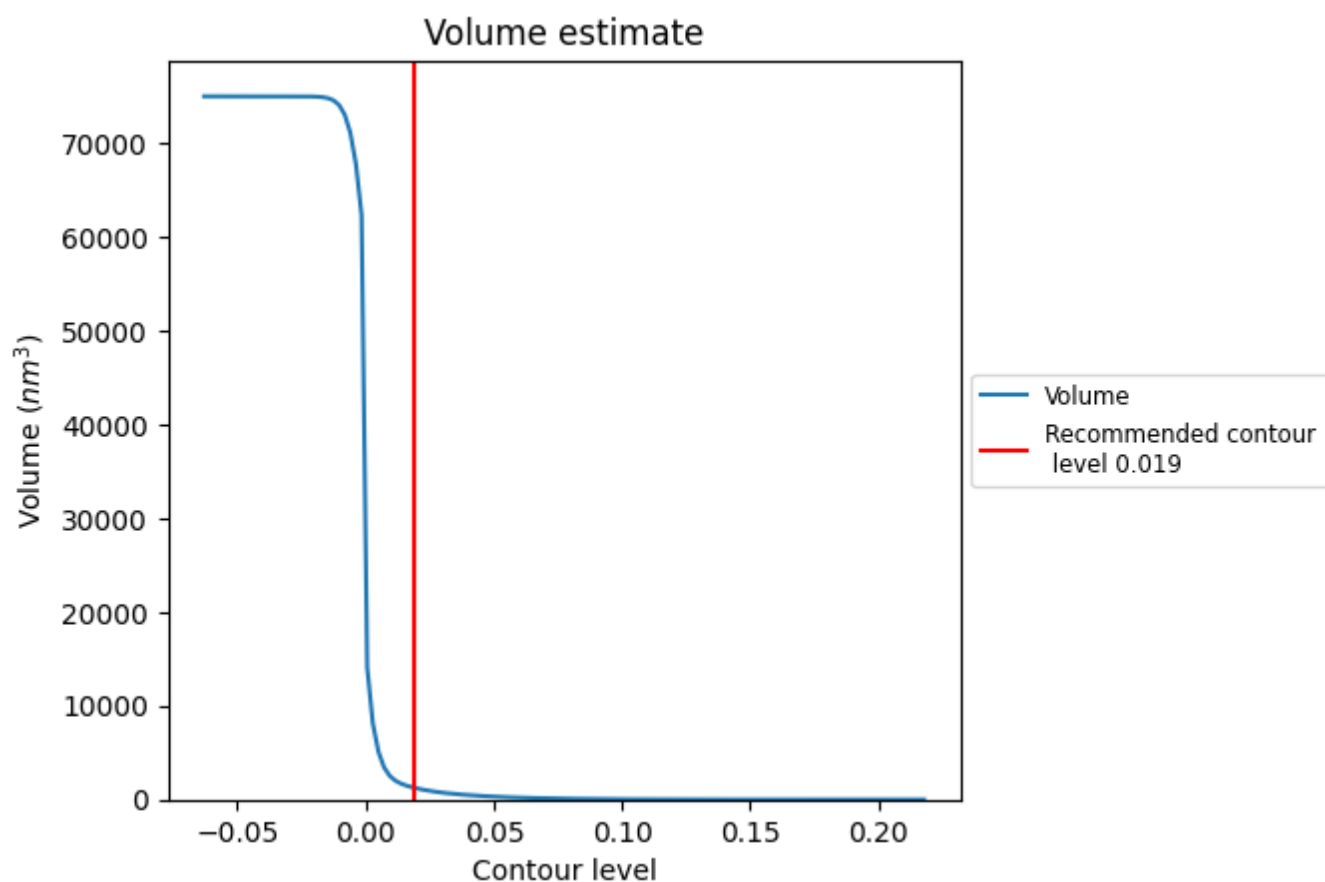
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

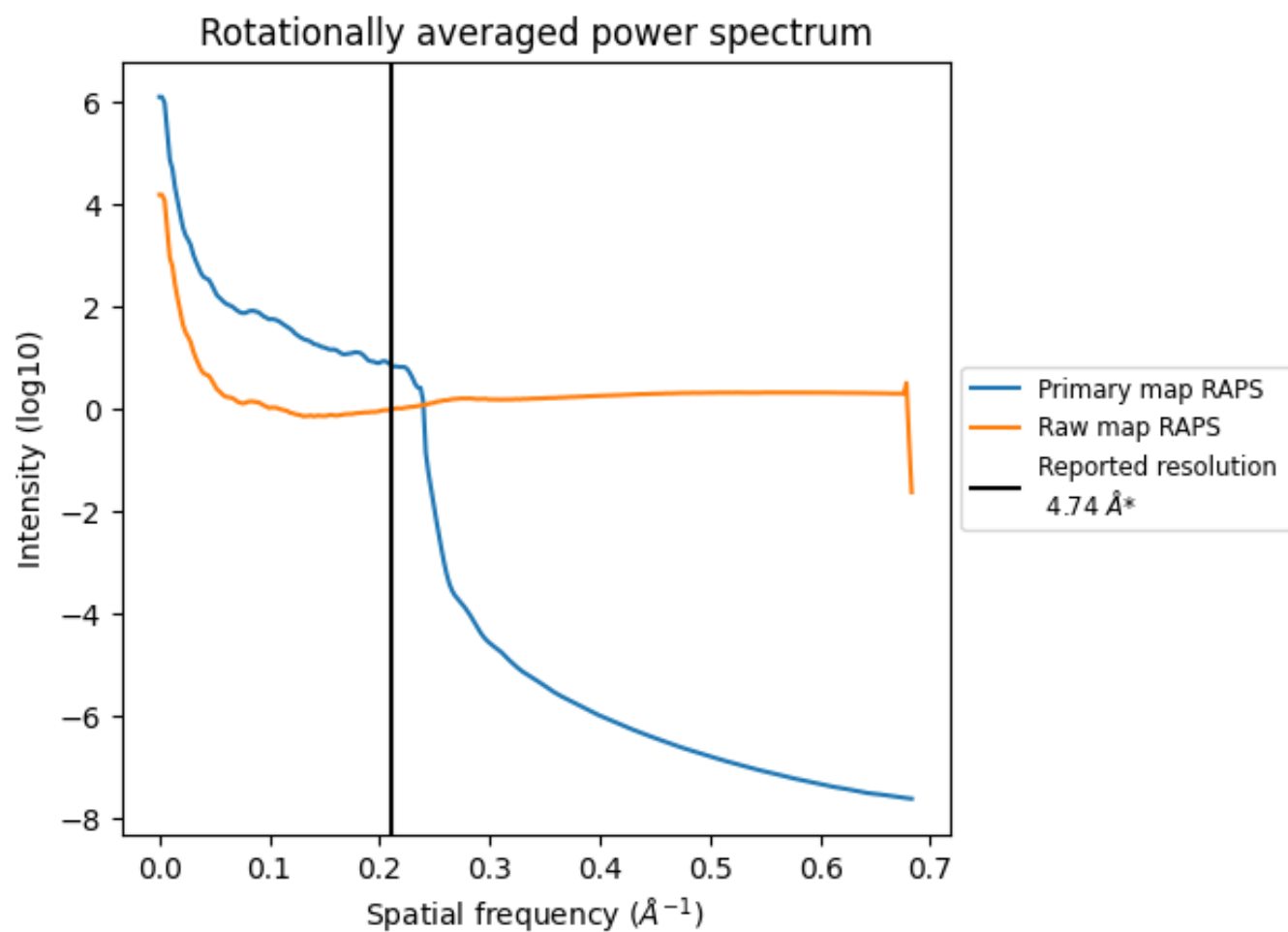
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1253 nm³; this corresponds to an approximate mass of 1132 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 ⓘ

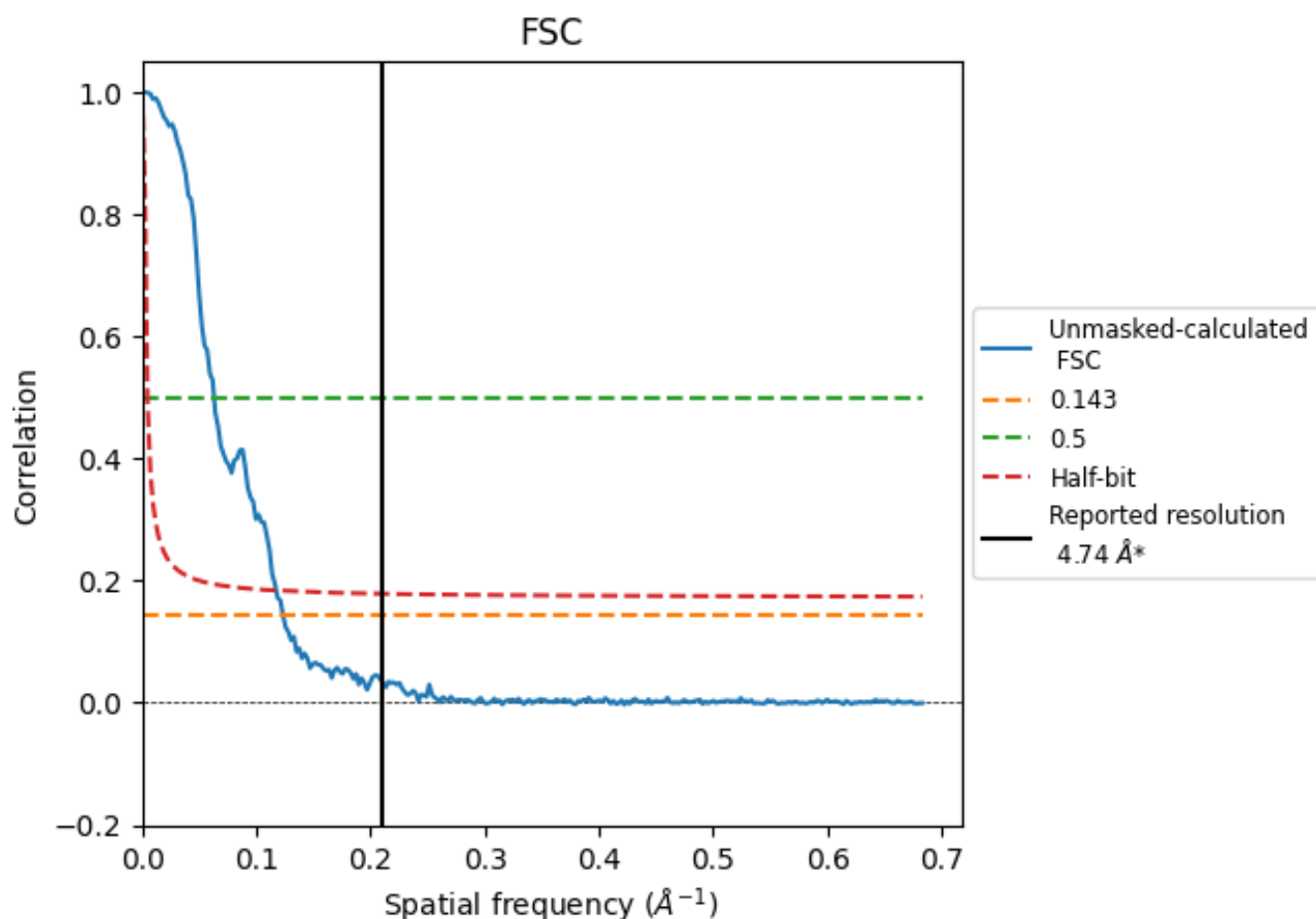


*Reported resolution corresponds to spatial frequency of 0.211 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.211 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

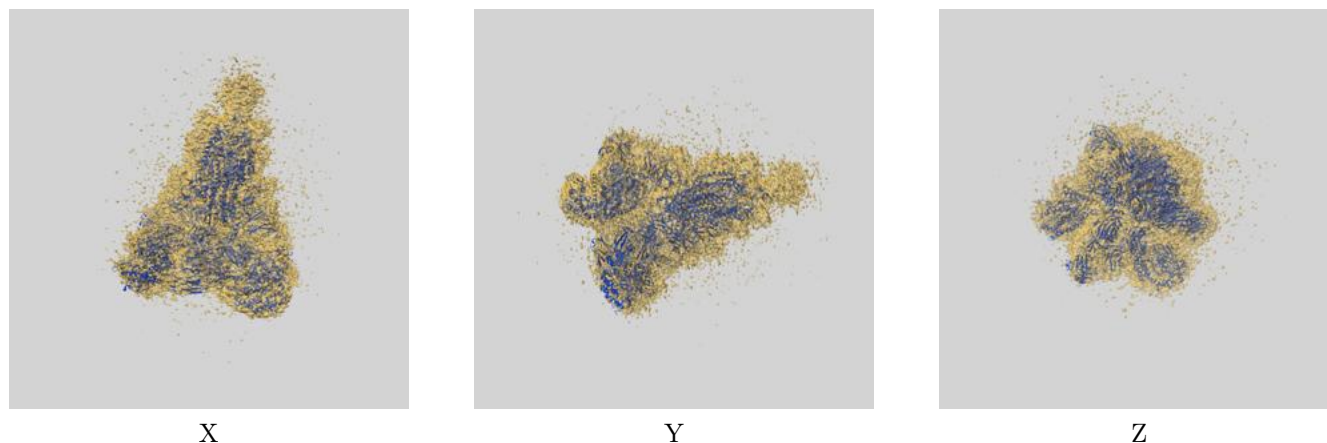
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.11	15.90	8.52

*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 8.11 differs from the reported value 4.74 by more than 10 %

9 Map-model fit [i](#)

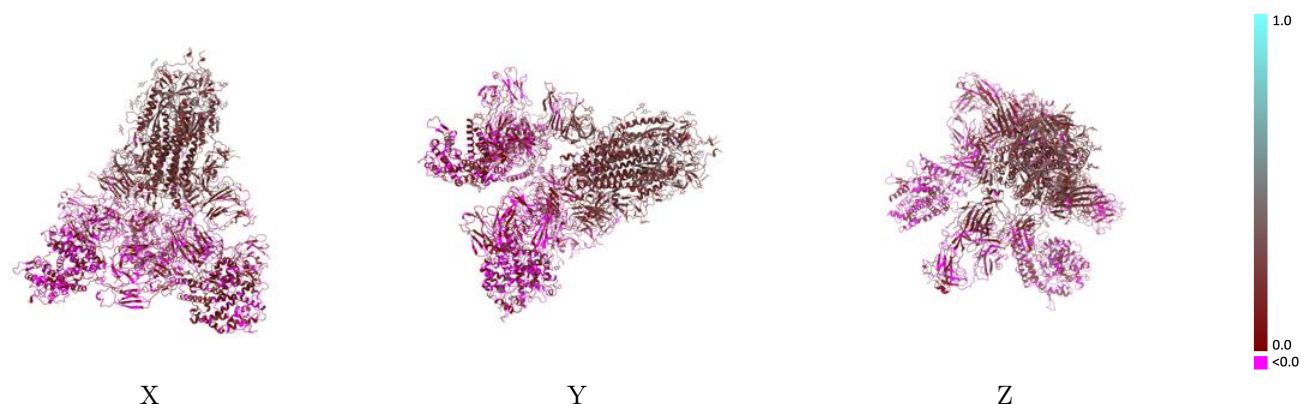
This section contains information regarding the fit between EMDB map EMD-66895 and PDB model 9XI3. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



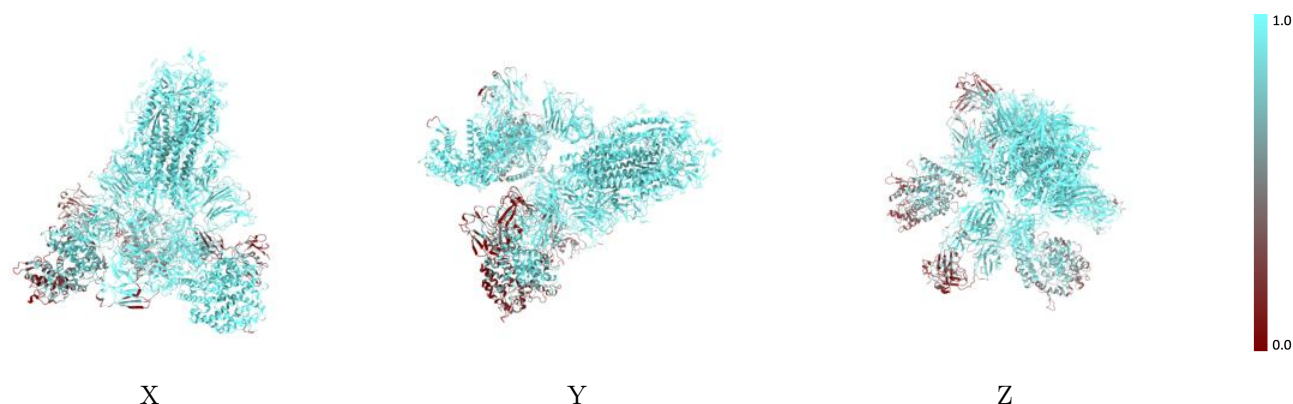
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



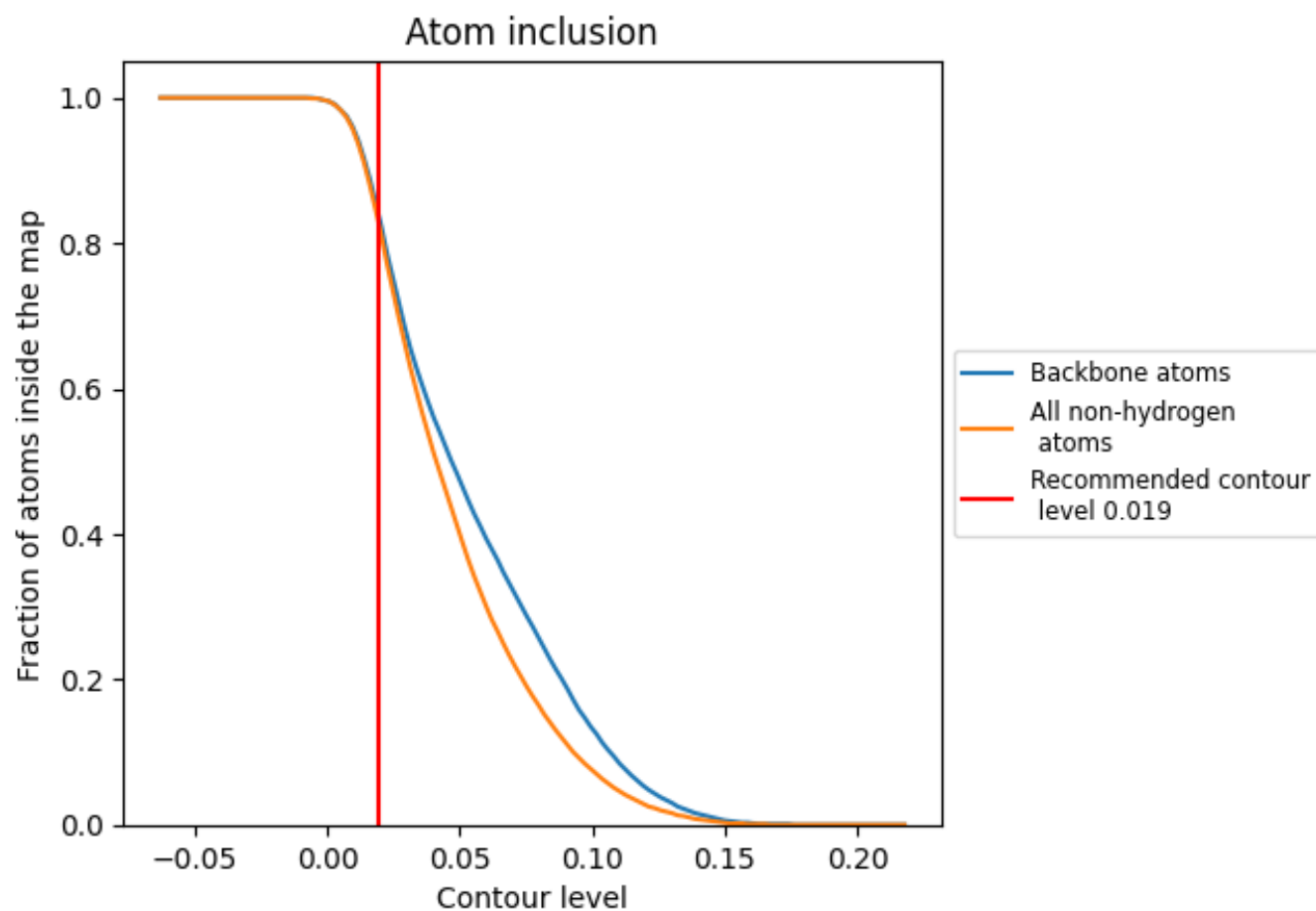
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.1230
A	 0.9610	 0.1930
B	 0.9570	 0.1930
C	 0.9760	 0.2020
D	 0.6610	 0.0340
E	 0.5390	 0.0140
F	 0.9760	 0.0800
G	 0.5860	 0.0690
H	 0.5380	 0.0300
I	 0.8900	 0.0680
J	 0.4410	 0.0420
K	 0.9170	 0.0690
L	 0.5430	 0.0440
M	 1.0000	 0.3180
N	 1.0000	 0.2690
O	 1.0000	 0.3970
P	 0.9640	 0.3070
Q	 1.0000	 0.3790
R	 1.0000	 0.2920

