



Full wwPDB EM Validation Report ⓘ

Apr 12, 2026 – 07:54 PM JST

PDB ID : 9VLT / pdb_00009vlt
EMDB ID : EMD-65168
Title : Cryo-EM structure of SARS-CoV-2 XBB.1.5 S trimer in the early fusion intermediate conformation (E-FIC) complexed with ACE2 and 76E1-Fab
Authors : Liu, Z.M.; Bao, Z.H.; Sun, X.Y.; Sun, L.
Deposited on : 2025-06-26
Resolution : 5.65 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.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

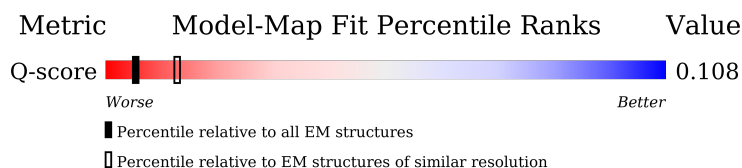
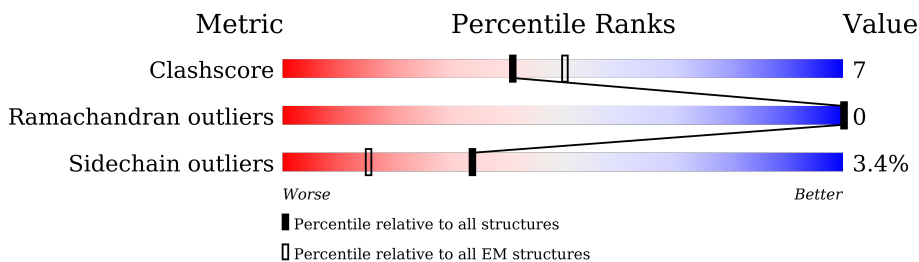
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.65 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	476 (5.15 - 6.15)

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	A	1284	
1	B	1284	
1	C	1284	
2	D	631	

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Mol	Chain	Length	Quality of chain
2	E	631	
2	F	631	
3	G	221	
3	I	221	
3	K	221	
4	H	216	
4	J	216	
4	L	216	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	Q	2	
5	R	2	
5	S	2	
5	T	2	
5	U	2	
5	V	2	
5	W	2	
5	X	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 50040 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	1073	Total	C	N	O	S	0	0
			8393	5360	1404	1590	39		
1	B	1073	Total	C	N	O	S	0	0
			8393	5360	1404	1590	39		
1	C	1073	Total	C	N	O	S	0	0
			8393	5360	1404	1590	39		

There are 366 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	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	445	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	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	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	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	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	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	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	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	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	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	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	E	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	F	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	LEU	-	expression tag	UNP Q9BYF1
D	617	GLU	-	expression tag	UNP Q9BYF1
D	618	VAL	-	expression tag	UNP Q9BYF1
D	619	LEU	-	expression tag	UNP Q9BYF1
D	620	PHE	-	expression tag	UNP Q9BYF1
D	621	GLN	-	expression tag	UNP Q9BYF1
D	622	GLY	-	expression tag	UNP Q9BYF1
D	623	PRO	-	expression tag	UNP Q9BYF1
D	624	HIS	-	expression tag	UNP Q9BYF1
D	625	HIS	-	expression tag	UNP Q9BYF1
D	626	HIS	-	expression tag	UNP Q9BYF1
D	627	HIS	-	expression tag	UNP Q9BYF1
D	628	HIS	-	expression tag	UNP Q9BYF1
D	629	HIS	-	expression tag	UNP Q9BYF1
D	630	HIS	-	expression tag	UNP Q9BYF1
D	631	HIS	-	expression tag	UNP Q9BYF1
E	616	LEU	-	expression tag	UNP Q9BYF1
E	617	GLU	-	expression tag	UNP Q9BYF1
E	618	VAL	-	expression tag	UNP Q9BYF1
E	619	LEU	-	expression tag	UNP Q9BYF1
E	620	PHE	-	expression tag	UNP Q9BYF1
E	621	GLN	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	622	GLY	-	expression tag	UNP Q9BYF1
E	623	PRO	-	expression tag	UNP Q9BYF1
E	624	HIS	-	expression tag	UNP Q9BYF1
E	625	HIS	-	expression tag	UNP Q9BYF1
E	626	HIS	-	expression tag	UNP Q9BYF1
E	627	HIS	-	expression tag	UNP Q9BYF1
E	628	HIS	-	expression tag	UNP Q9BYF1
E	629	HIS	-	expression tag	UNP Q9BYF1
E	630	HIS	-	expression tag	UNP Q9BYF1
E	631	HIS	-	expression tag	UNP Q9BYF1
F	616	LEU	-	expression tag	UNP Q9BYF1
F	617	GLU	-	expression tag	UNP Q9BYF1
F	618	VAL	-	expression tag	UNP Q9BYF1
F	619	LEU	-	expression tag	UNP Q9BYF1
F	620	PHE	-	expression tag	UNP Q9BYF1
F	621	GLN	-	expression tag	UNP Q9BYF1
F	622	GLY	-	expression tag	UNP Q9BYF1
F	623	PRO	-	expression tag	UNP Q9BYF1
F	624	HIS	-	expression tag	UNP Q9BYF1
F	625	HIS	-	expression tag	UNP Q9BYF1
F	626	HIS	-	expression tag	UNP Q9BYF1
F	627	HIS	-	expression tag	UNP Q9BYF1
F	628	HIS	-	expression tag	UNP Q9BYF1
F	629	HIS	-	expression tag	UNP Q9BYF1
F	630	HIS	-	expression tag	UNP Q9BYF1
F	631	HIS	-	expression tag	UNP Q9BYF1

- Molecule 3 is a protein called heavy chain of 76E1 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	213	Total	C	N	O	S	0	0
			1590	1003	270	311	6		
3	I	213	Total	C	N	O	S	0	0
			1590	1003	270	311	6		
3	K	213	Total	C	N	O	S	0	0
			1590	1003	270	311	6		

- Molecule 4 is a protein called light chain of 76E1 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	211	Total	C	N	O	S	0	0
			1574	986	265	317	6		

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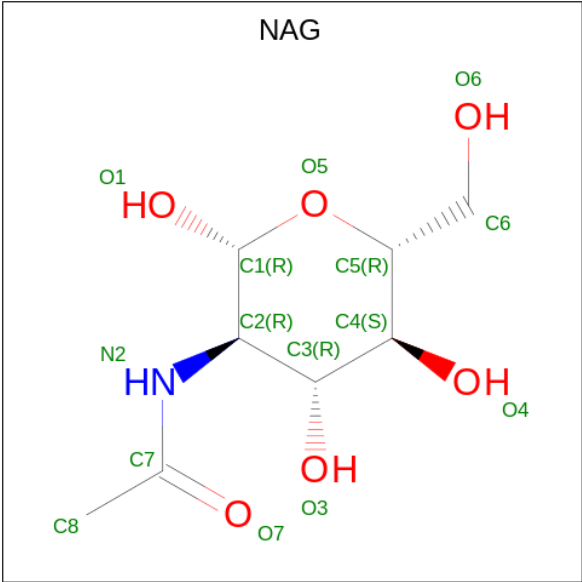
Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	211	Total	C	N	O	S	0	0
			1574	986	265	317	6		
4	L	211	Total	C	N	O	S	0	0
			1574	986	265	317	6		

- 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		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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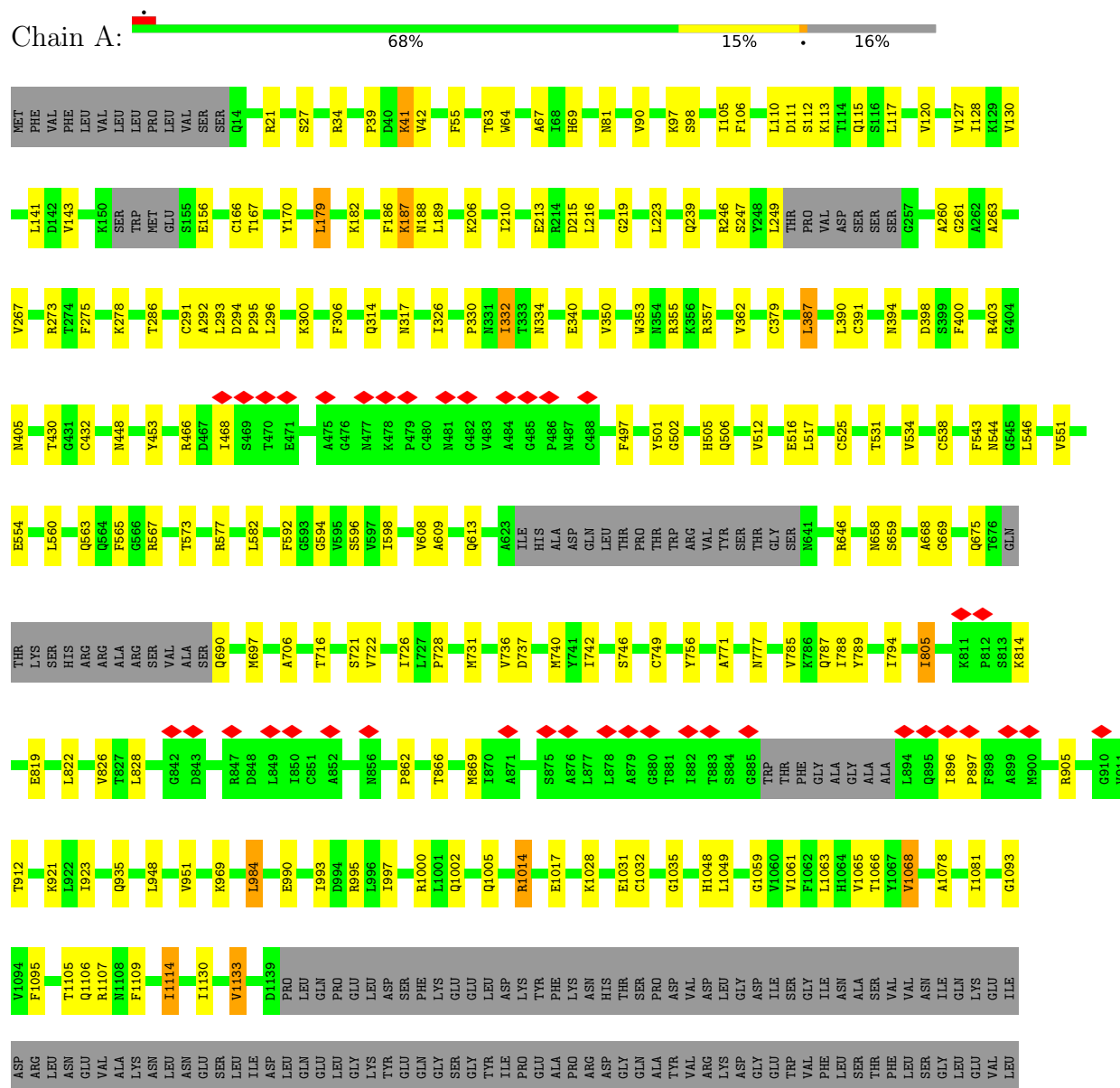
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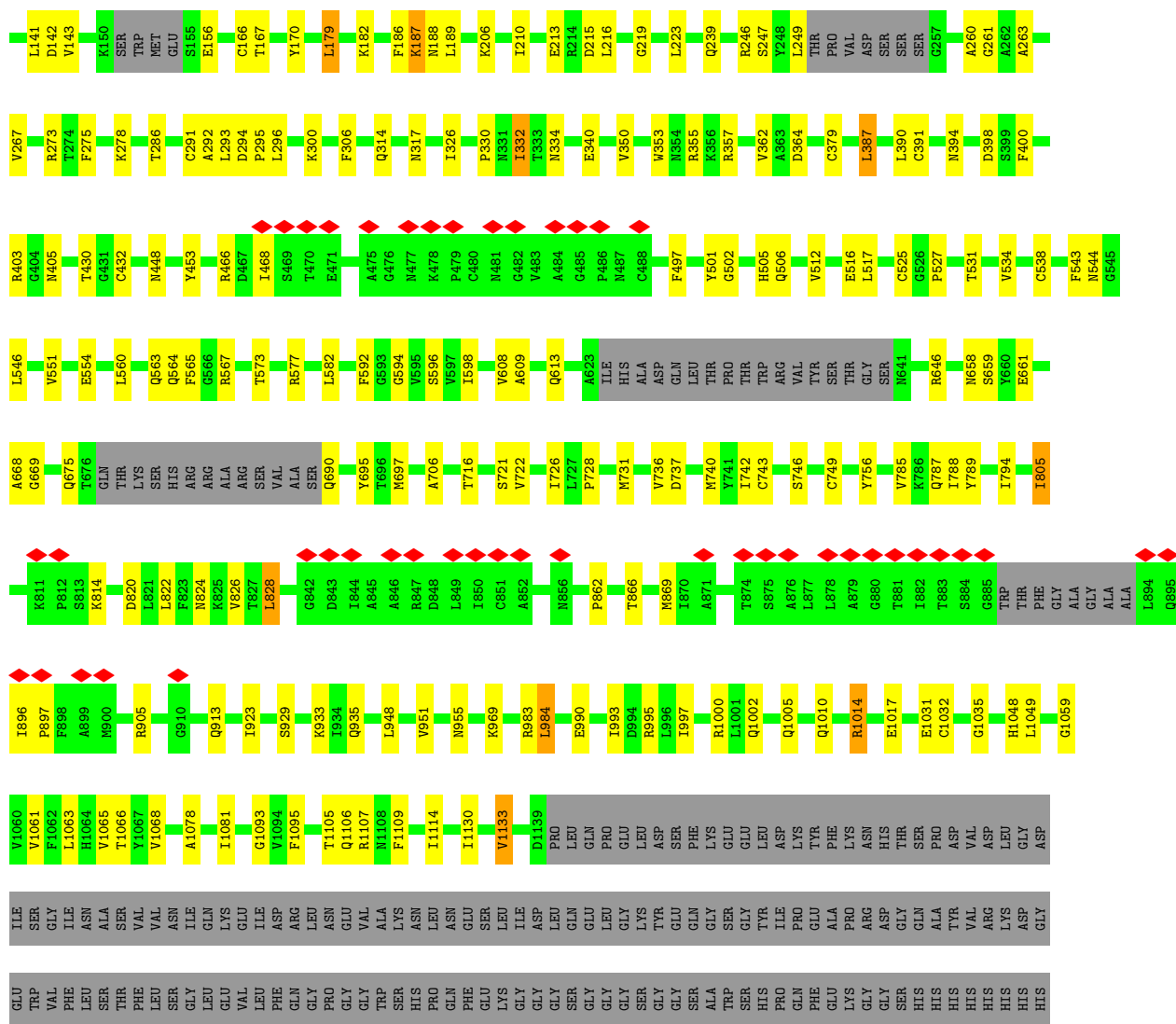
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6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

3 Residue-property plots [i](#)

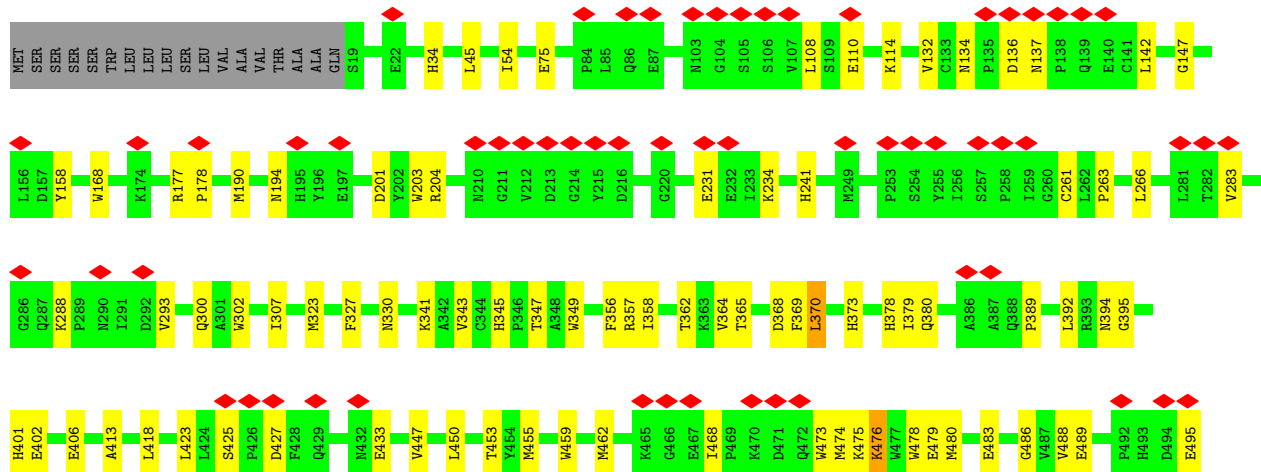
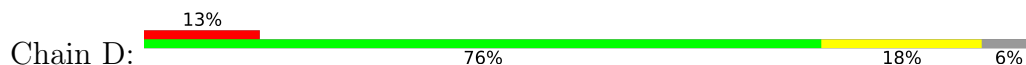
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

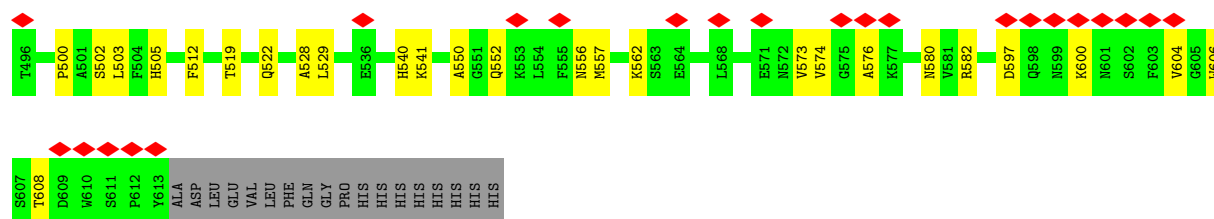
• Molecule 1: Spike glycoprotein



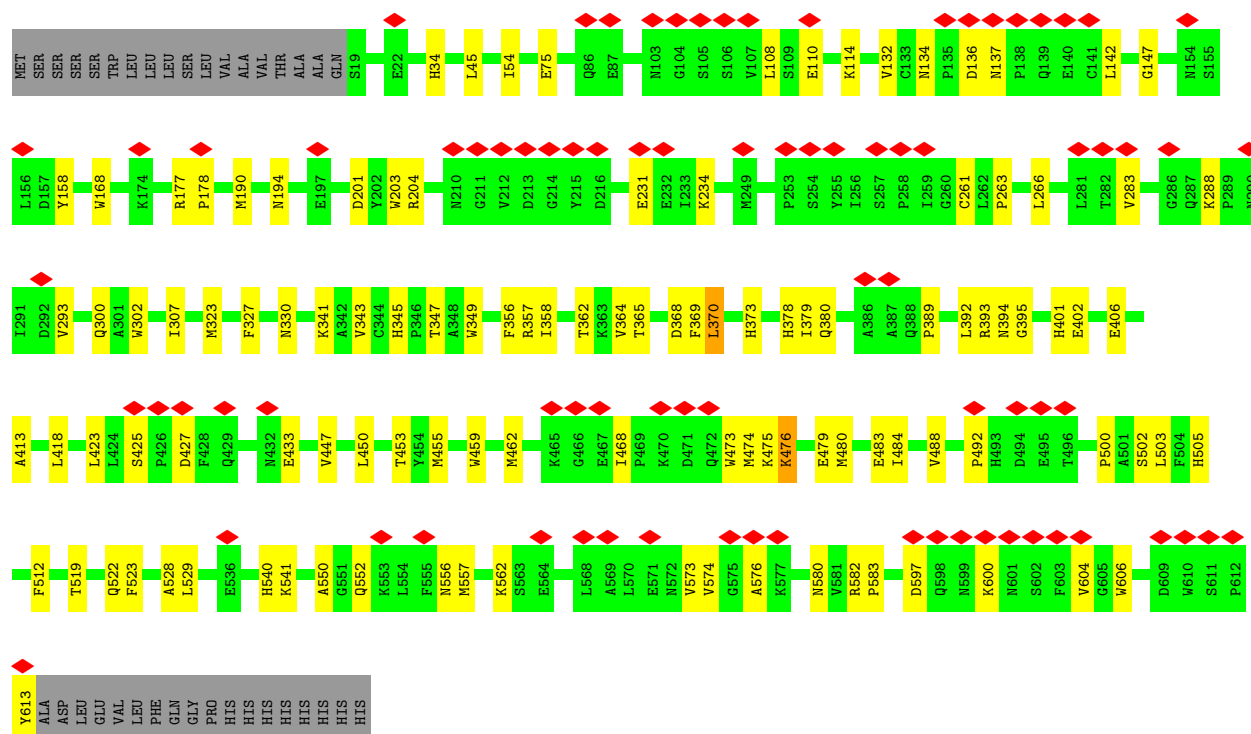
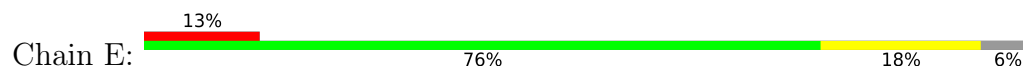


• Molecule 2: Angiotensin-converting enzyme 2

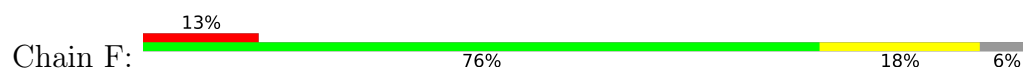


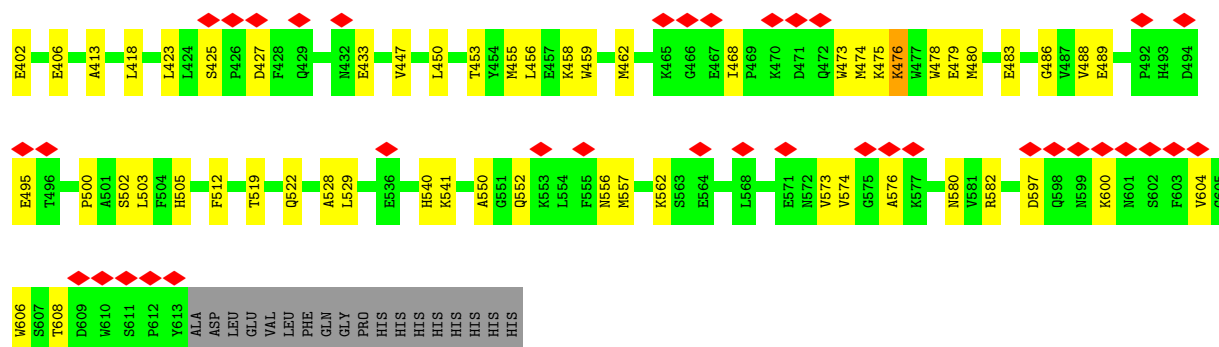


• Molecule 2: Angiotensin-converting enzyme 2

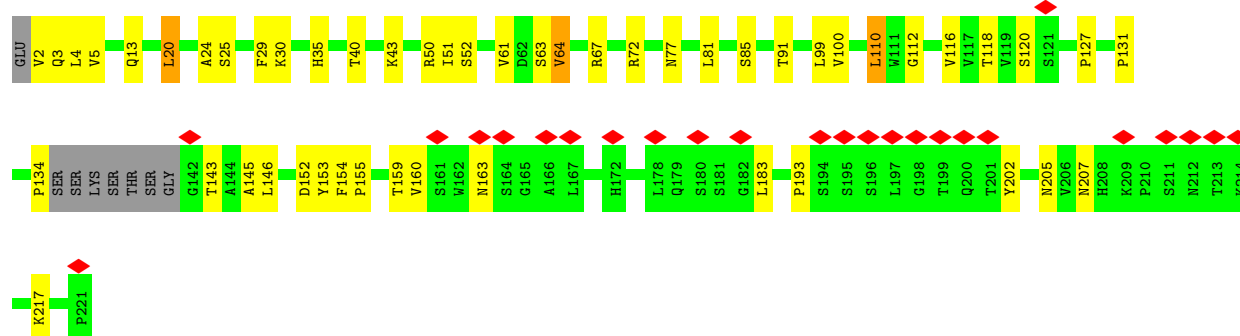


• Molecule 2: Angiotensin-converting enzyme 2

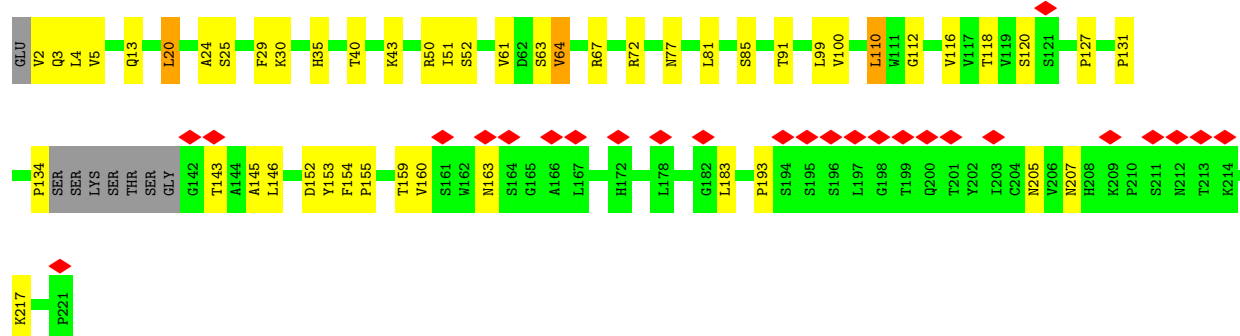




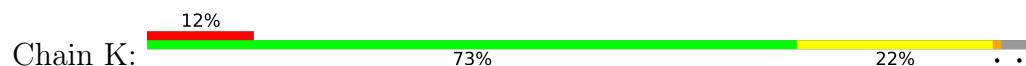
• Molecule 3: heavy chain of 76E1 Fab

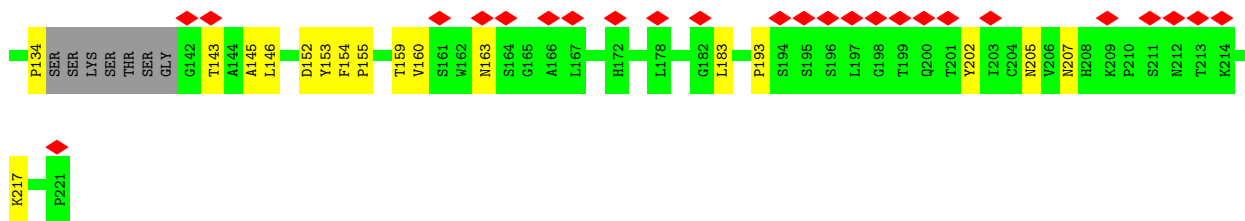


• Molecule 3: heavy chain of 76E1 Fab



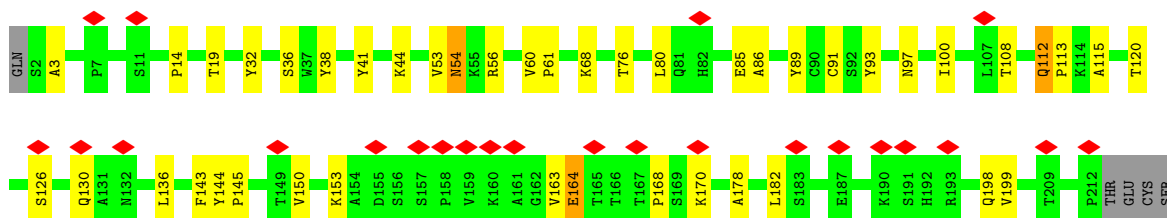
• Molecule 3: heavy chain of 76E1 Fab





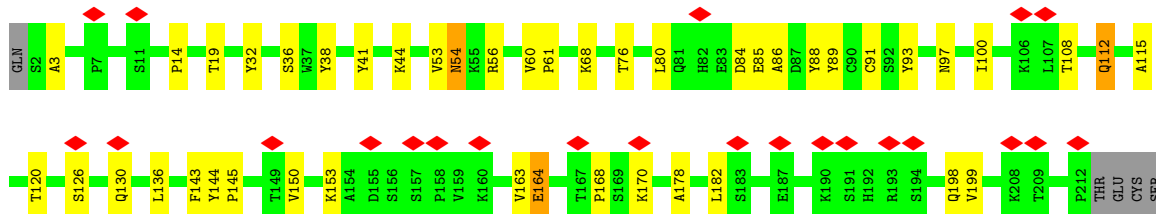
- Molecule 4: light chain of 76E1 Fab

Chain H: 11% 77% 19% ..



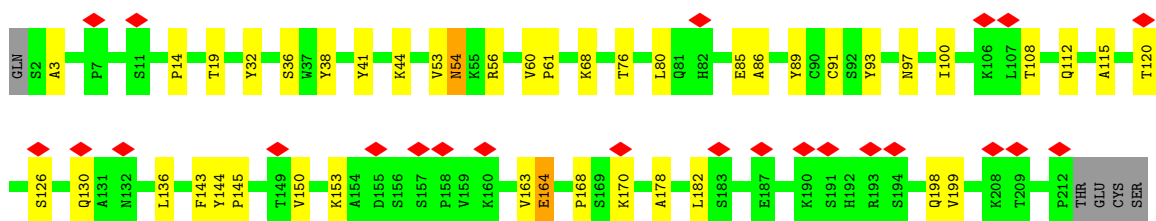
- Molecule 4: light chain of 76E1 Fab

Chain J: 11% 77% 19% ..



- Molecule 4: light chain of 76E1 Fab

Chain L: 11% 78% 19% ..



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

Chain M: 50% 50%



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

Chain N:  100%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  50% 50%



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

Chain T:  100%



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

Chain U:  50% 50%



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

Chain V:  100%



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

Chain W:  50% 50%



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

Chain X:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	93565	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)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.432	Depositor
Minimum map value	-0.722	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	372.8, 372.8, 372.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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	0.08	0/8583	0.24	0/11669
1	B	0.08	0/8583	0.24	0/11669
1	C	0.08	0/8583	0.24	0/11669
2	D	0.07	0/4994	0.20	0/6785
2	E	0.07	0/4994	0.20	0/6785
2	F	0.07	0/4994	0.20	0/6785
3	G	0.09	0/1625	0.26	0/2211
3	I	0.09	0/1625	0.25	0/2211
3	K	0.09	0/1625	0.25	0/2211
4	H	0.08	0/1613	0.25	0/2198
4	J	0.08	0/1613	0.25	0/2198
4	L	0.08	0/1613	0.25	0/2198
All	All	0.08	0/50445	0.23	0/68589

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	8393	0	8210	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8393	0	8210	118	0
1	C	8393	0	8210	124	0
2	D	4857	0	4631	63	0
2	E	4857	0	4631	63	0
2	F	4857	0	4631	64	0
3	G	1590	0	1561	26	0
3	I	1590	0	1561	24	0
3	K	1590	0	1561	25	0
4	H	1574	0	1530	25	0
4	J	1574	0	1530	26	0
4	L	1574	0	1530	22	0
5	M	28	0	25	1	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	1	0
5	R	28	0	25	0	0
5	S	28	0	25	1	0
5	T	28	0	25	0	0
5	U	28	0	25	1	0
5	V	28	0	25	0	0
5	W	28	0	25	1	0
5	X	28	0	25	0	0
6	A	126	0	117	0	0
6	B	126	0	117	2	0
6	C	126	0	117	1	0
6	D	28	0	26	1	0
6	E	28	0	26	1	0
6	F	28	0	26	1	0
All	All	50040	0	48525	658	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 7.

All (658) 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)
4:L:36:SER:HG	4:L:91:CYS:HG	1.24	0.86
4:J:36:SER:HG	4:J:91:CYS:HG	1.32	0.77
4:H:36:SER:HG	4:H:91:CYS:HG	1.32	0.75
1:B:110:LEU:HD23	1:B:113:LYS:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:HD23	1:C:113:LYS:HB2	1.71	0.72
1:A:110:LEU:HD23	1:A:113:LYS:HB2	1.71	0.71
2:D:573:VAL:HG13	2:D:574:VAL:HG13	1.73	0.70
2:E:573:VAL:HG13	2:E:574:VAL:HG13	1.73	0.70
2:F:573:VAL:HG13	2:F:574:VAL:HG13	1.73	0.70
1:C:742:ILE:HA	1:C:1000:ARG:HG2	1.75	0.68
1:B:742:ILE:HA	1:B:1000:ARG:HG2	1.76	0.68
1:C:105:ILE:HB	1:C:239:GLN:HB2	1.76	0.68
3:G:163:ASN:H	3:G:205:ASN:HB2	1.59	0.68
1:B:105:ILE:HB	1:B:239:GLN:HB2	1.76	0.68
1:A:105:ILE:HB	1:A:239:GLN:HB2	1.75	0.67
1:A:27:SER:HB2	1:A:64:TRP:HB3	1.75	0.67
1:A:120:VAL:HB	1:A:127:VAL:HB	1.77	0.67
1:A:742:ILE:HA	1:A:1000:ARG:HG2	1.77	0.67
1:A:189:LEU:HB2	1:A:210:ILE:HB	1.77	0.66
1:B:189:LEU:HB2	1:B:210:ILE:HB	1.77	0.66
1:B:27:SER:HB2	1:B:64:TRP:HB3	1.76	0.66
1:C:120:VAL:HB	1:C:127:VAL:HB	1.78	0.66
1:B:120:VAL:HB	1:B:127:VAL:HB	1.77	0.66
1:C:27:SER:HB2	1:C:64:TRP:HB3	1.76	0.66
1:C:189:LEU:HB2	1:C:210:ILE:HB	1.77	0.66
3:K:163:ASN:H	3:K:205:ASN:HB2	1.59	0.66
3:I:163:ASN:H	3:I:205:ASN:HB2	1.60	0.66
1:C:326:ILE:HG13	1:C:531:THR:HB	1.78	0.65
3:G:29:PHE:O	3:G:72:ARG:NH1	2.30	0.65
1:B:326:ILE:HG13	1:B:531:THR:HB	1.79	0.64
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.80	0.64
3:K:29:PHE:O	3:K:72:ARG:NH1	2.31	0.64
4:H:85:GLU:OE2	4:H:170:LYS:NZ	2.31	0.64
3:I:29:PHE:O	3:I:72:ARG:NH1	2.31	0.64
1:A:326:ILE:HG13	1:A:531:THR:HB	1.78	0.63
4:H:53:VAL:O	4:H:54:ASN:ND2	2.29	0.63
2:E:356:PHE:HB3	2:E:379:ILE:HD12	1.80	0.63
4:L:85:GLU:OE2	4:L:170:LYS:NZ	2.31	0.63
1:B:394:ASN:HB2	1:B:516:GLU:HB3	1.79	0.63
4:H:126:SER:O	4:H:130:GLN:NE2	2.32	0.63
4:J:85:GLU:OE2	4:J:170:LYS:NZ	2.31	0.63
4:J:126:SER:O	4:J:130:GLN:NE2	2.32	0.63
1:A:394:ASN:HB2	1:A:516:GLU:HB3	1.81	0.62
4:J:168:PRO:HG3	4:J:178:ALA:HB2	1.81	0.62
2:F:356:PHE:HB3	2:F:379:ILE:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:168:PRO:HG3	4:H:178:ALA:HB2	1.82	0.62
4:J:53:VAL:O	4:J:54:ASN:ND2	2.29	0.62
4:L:168:PRO:HG3	4:L:178:ALA:HB2	1.81	0.62
4:L:126:SER:O	4:L:130:GLN:NE2	2.32	0.62
2:E:201:ASP:OD1	2:E:204:ARG:NH1	2.33	0.62
4:L:53:VAL:O	4:L:54:ASN:ND2	2.29	0.62
3:K:4:LEU:HB2	3:K:112:GLY:HA2	1.82	0.61
1:C:1078:ALA:HB3	1:C:1095:PHE:HB2	1.81	0.61
1:B:543:PHE:H	1:B:546:LEU:HB2	1.64	0.61
1:C:394:ASN:HB2	1:C:516:GLU:HB3	1.81	0.61
2:D:201:ASP:OD1	2:D:204:ARG:NH1	2.33	0.61
1:C:543:PHE:H	1:C:546:LEU:HB2	1.66	0.61
2:F:201:ASP:OD1	2:F:204:ARG:NH1	2.33	0.61
2:E:552:GLN:O	2:E:556:ASN:ND2	2.32	0.61
1:A:543:PHE:H	1:A:546:LEU:HB2	1.66	0.61
1:A:1078:ALA:HB3	1:A:1095:PHE:HB2	1.81	0.61
3:G:4:LEU:HB2	3:G:112:GLY:HA2	1.83	0.61
3:I:4:LEU:HB2	3:I:112:GLY:HA2	1.83	0.61
2:F:453:THR:HG23	2:F:512:PHE:HB3	1.83	0.60
1:B:869:MET:SD	1:B:905:ARG:NH1	2.74	0.60
1:A:869:MET:SD	1:A:905:ARG:NH1	2.74	0.60
1:B:1078:ALA:HB3	1:B:1095:PHE:HB2	1.82	0.60
1:A:826:VAL:HG11	1:A:923:ILE:HG12	1.84	0.60
2:D:453:THR:HG23	2:D:512:PHE:HB3	1.83	0.60
2:F:447:VAL:HG13	2:F:450:LEU:HD12	1.84	0.60
2:E:261:CYS:HB2	2:E:488:VAL:HB	1.84	0.60
1:C:805:ILE:HG23	1:C:951:VAL:HG11	1.84	0.59
4:L:38:TYR:HB2	4:L:89:TYR:HB2	1.83	0.59
2:D:552:GLN:O	2:D:556:ASN:ND2	2.32	0.59
4:H:38:TYR:HB2	4:H:89:TYR:HB2	1.85	0.59
2:E:453:THR:HG23	2:E:512:PHE:HB3	1.83	0.59
2:E:447:VAL:HG13	2:E:450:LEU:HD12	1.84	0.59
2:F:474:MET:SD	2:F:474:MET:N	2.76	0.59
4:H:136:LEU:HD12	4:H:182:LEU:HD23	1.85	0.59
4:J:38:TYR:HB2	4:J:89:TYR:HB2	1.85	0.59
2:D:447:VAL:HG13	2:D:450:LEU:HD12	1.85	0.59
3:I:13:GLN:NE2	3:I:120:SER:O	2.36	0.59
1:A:314:GLN:HE21	1:A:594:GLY:HA3	1.67	0.59
2:E:474:MET:SD	2:E:474:MET:N	2.76	0.58
1:C:826:VAL:HG11	1:C:923:ILE:HG12	1.83	0.58
4:L:136:LEU:HD12	4:L:182:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:HH22	1:C:292:ALA:HB3	1.68	0.58
2:F:261:CYS:HB2	2:F:488:VAL:HB	1.84	0.58
2:D:474:MET:SD	2:D:474:MET:N	2.76	0.58
1:C:278:LYS:NZ	1:C:286:THR:OG1	2.36	0.58
3:K:13:GLN:NE2	3:K:120:SER:O	2.36	0.58
1:A:805:ILE:HG23	1:A:951:VAL:HG11	1.86	0.58
1:B:826:VAL:HG11	1:B:923:ILE:HG12	1.85	0.58
4:J:163:VAL:HG12	4:J:164:GLU:HG3	1.85	0.58
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.84	0.58
4:L:163:VAL:HG12	4:L:164:GLU:HG3	1.85	0.58
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.85	0.58
1:B:314:GLN:HE21	1:B:594:GLY:HA3	1.67	0.58
1:C:314:GLN:HE21	1:C:594:GLY:HA3	1.67	0.58
1:B:273:ARG:HH22	1:B:292:ALA:HB3	1.67	0.58
1:C:97:LYS:HD2	1:C:179:LEU:HB3	1.86	0.58
2:F:552:GLN:O	2:F:556:ASN:ND2	2.32	0.58
1:A:1107:ARG:NH2	1:C:1035:GLY:O	2.37	0.58
2:F:455:MET:HG2	2:F:480:MET:HE2	1.85	0.58
3:G:13:GLN:NE2	3:G:120:SER:O	2.36	0.58
1:A:273:ARG:HH22	1:A:292:ALA:HB3	1.68	0.58
2:D:261:CYS:HB2	2:D:488:VAL:HB	1.84	0.58
4:J:136:LEU:HD12	4:J:182:LEU:HD23	1.85	0.58
1:A:97:LYS:HD2	1:A:179:LEU:HB3	1.86	0.57
2:D:455:MET:HG2	2:D:480:MET:HE2	1.86	0.57
1:B:805:ILE:HG12	1:B:951:VAL:HG11	1.85	0.57
4:J:32:TYR:O	4:J:68:LYS:NZ	2.37	0.57
4:H:32:TYR:O	4:H:68:LYS:NZ	2.37	0.57
1:B:1035:GLY:O	1:C:1107:ARG:NH2	2.37	0.57
2:E:455:MET:HG2	2:E:480:MET:HE2	1.86	0.57
1:A:822:LEU:HB2	1:B:935:GLN:HE22	1.69	0.57
1:A:278:LYS:NZ	1:A:286:THR:OG1	2.36	0.57
1:A:1035:GLY:O	1:B:1107:ARG:NH2	2.37	0.57
1:C:314:GLN:NE2	1:C:317:ASN:OD1	2.38	0.57
4:L:32:TYR:O	4:L:68:LYS:NZ	2.37	0.57
4:H:86:ALA:HB2	4:H:108:THR:HG22	1.86	0.57
1:B:314:GLN:NE2	1:B:317:ASN:OD1	2.38	0.57
1:C:869:MET:SD	1:C:905:ARG:NH1	2.78	0.57
4:L:56:ARG:NH1	4:L:61:PRO:O	2.38	0.57
1:B:39:PRO:HB3	1:B:55:PHE:HZ	1.70	0.57
3:K:91:THR:HG23	3:K:118:THR:HA	1.87	0.57
4:J:86:ALA:HB2	4:J:108:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:CYS:HA	1:B:525:CYS:HA	1.87	0.56
1:B:822:LEU:HB2	1:C:935:GLN:HE22	1.69	0.56
3:K:61:VAL:HG12	3:K:64:VAL:HG23	1.87	0.56
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.85	0.56
4:H:56:ARG:NH1	4:H:61:PRO:O	2.38	0.56
1:B:330:PRO:HD3	1:B:544:ASN:HD21	1.70	0.56
3:I:91:THR:HG23	3:I:118:THR:HA	1.87	0.56
1:A:330:PRO:HD3	1:A:544:ASN:HD21	1.70	0.56
4:H:163:VAL:HG12	4:H:164:GLU:HG3	1.85	0.56
1:A:97:LYS:HB2	1:A:187:LYS:HD3	1.88	0.56
3:G:91:THR:HG23	3:G:118:THR:HA	1.87	0.56
1:B:560:LEU:O	1:B:577:ARG:NH1	2.38	0.56
1:A:21:ARG:NH2	1:A:81:ASN:OD1	2.39	0.56
4:J:56:ARG:NH1	4:J:61:PRO:O	2.38	0.56
1:C:560:LEU:O	1:C:577:ARG:NH1	2.39	0.56
1:B:115:GLN:NE2	1:B:130:VAL:O	2.39	0.56
1:A:115:GLN:NE2	1:A:130:VAL:O	2.39	0.56
6:F:702:NAG:H3	6:F:702:NAG:H83	1.88	0.56
2:D:528:ALA:HB2	2:D:574:VAL:HG12	1.88	0.55
3:G:4:LEU:HD11	3:G:110:LEU:HD13	1.88	0.55
2:E:406:GLU:OE1	2:E:522:GLN:NE2	2.40	0.55
1:C:330:PRO:HD3	1:C:544:ASN:HD21	1.71	0.55
2:F:177:ARG:NH2	2:F:474:MET:SD	2.79	0.55
1:A:314:GLN:NE2	1:A:317:ASN:OD1	2.37	0.55
2:D:330:ASN:O	2:D:357:ARG:NH1	2.39	0.55
1:C:391:CYS:HA	1:C:525:CYS:HA	1.88	0.55
2:F:528:ALA:HB2	2:F:574:VAL:HG12	1.88	0.55
1:B:97:LYS:HD2	1:B:179:LEU:HB3	1.87	0.55
1:C:21:ARG:NH2	1:C:81:ASN:OD1	2.39	0.55
1:C:97:LYS:HB2	1:C:187:LYS:HD3	1.88	0.55
1:A:39:PRO:HB3	1:A:55:PHE:HZ	1.71	0.55
4:L:86:ALA:HB2	4:L:108:THR:HG22	1.87	0.55
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.89	0.55
6:D:702:NAG:H3	6:D:702:NAG:H83	1.88	0.55
2:E:330:ASN:O	2:E:357:ARG:NH1	2.39	0.55
3:I:4:LEU:HD11	3:I:110:LEU:HD13	1.88	0.55
4:J:36:SER:OG	4:J:91:CYS:SG	2.54	0.55
1:A:391:CYS:HA	1:A:525:CYS:HA	1.87	0.55
2:D:177:ARG:NH2	2:D:474:MET:SD	2.79	0.55
1:B:97:LYS:HB2	1:B:187:LYS:HD3	1.88	0.55
2:E:528:ALA:HB2	2:E:574:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:O	1:A:577:ARG:NH1	2.39	0.55
2:E:110:GLU:OE2	2:E:114:LYS:NZ	2.40	0.54
2:F:136:ASP:OD2	2:F:137:ASN:ND2	2.40	0.54
2:D:136:ASP:OD2	2:D:137:ASN:ND2	2.40	0.54
2:D:406:GLU:OE1	2:D:522:GLN:NE2	2.40	0.54
2:D:110:GLU:OE2	2:D:114:LYS:NZ	2.40	0.54
2:F:450:LEU:HD11	2:F:519:THR:HG21	1.90	0.54
3:K:4:LEU:HD11	3:K:110:LEU:HD13	1.88	0.54
1:B:21:ARG:NH2	1:B:81:ASN:OD1	2.39	0.54
1:B:278:LYS:NZ	1:B:286:THR:OG1	2.36	0.54
1:C:115:GLN:NE2	1:C:130:VAL:O	2.39	0.54
3:I:61:VAL:HG12	3:I:64:VAL:HG23	1.88	0.54
1:C:213:GLU:HG2	1:C:215:ASP:H	1.73	0.54
6:E:702:NAG:H83	6:E:702:NAG:H3	1.88	0.54
2:D:450:LEU:HD11	2:D:519:THR:HG21	1.90	0.54
2:E:450:LEU:HD11	2:E:519:THR:HG21	1.90	0.54
2:F:54:ILE:HD12	2:F:341:LYS:HG2	1.90	0.54
2:F:110:GLU:OE2	2:F:114:LYS:NZ	2.40	0.54
2:F:395:GLY:H	2:F:401:HIS:HE1	1.56	0.54
2:F:330:ASN:O	2:F:357:ARG:NH1	2.39	0.54
2:D:190:MET:SD	2:D:194:ASN:ND2	2.81	0.54
1:C:721:SER:HB3	1:C:1068:VAL:HG22	1.90	0.54
2:E:136:ASP:OD2	2:E:137:ASN:ND2	2.41	0.54
2:E:190:MET:SD	2:E:194:ASN:ND2	2.81	0.54
1:B:213:GLU:HG2	1:B:215:ASP:H	1.73	0.53
2:E:394:ASN:HB3	2:E:562:LYS:HD2	1.91	0.53
2:F:190:MET:SD	2:F:194:ASN:ND2	2.81	0.53
2:D:394:ASN:HB3	2:D:562:LYS:HD2	1.91	0.53
2:F:263:PRO:HG2	2:F:266:LEU:HB2	1.90	0.53
1:A:213:GLU:HG2	1:A:215:ASP:H	1.73	0.53
3:G:61:VAL:HG12	3:G:64:VAL:HG23	1.89	0.53
4:H:14:PRO:HA	4:H:80:LEU:HB2	1.91	0.53
2:E:177:ARG:NH2	2:E:474:MET:SD	2.79	0.53
2:E:263:PRO:HG2	2:E:266:LEU:HB2	1.91	0.53
1:C:39:PRO:HB3	1:C:55:PHE:HZ	1.72	0.53
2:D:54:ILE:HD12	2:D:341:LYS:HG2	1.89	0.53
2:D:395:GLY:H	2:D:401:HIS:HE1	1.56	0.53
2:E:54:ILE:HD12	2:E:341:LYS:HG2	1.90	0.53
1:A:387:LEU:HA	1:A:390:LEU:HD12	1.91	0.53
1:B:387:LEU:HA	1:B:390:LEU:HD12	1.90	0.53
2:F:406:GLU:OE1	2:F:522:GLN:NE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:395:GLY:H	2:E:401:HIS:HE1	1.56	0.53
2:D:362:THR:HG23	2:D:368:ASP:HB3	1.91	0.53
2:F:394:ASN:HB3	2:F:562:LYS:HD2	1.91	0.53
1:B:721:SER:HB3	1:B:1068:VAL:HG22	1.91	0.53
1:C:387:LEU:HA	1:C:390:LEU:HD12	1.91	0.53
2:D:483:GLU:HA	2:D:606:TRP:HE1	1.74	0.52
1:C:951:VAL:O	1:C:955:ASN:ND2	2.35	0.52
1:B:166:CYS:O	1:C:357:ARG:NH2	2.41	0.52
3:K:24:ALA:HB3	3:K:77:ASN:HB3	1.91	0.52
2:F:483:GLU:HA	2:F:606:TRP:HE1	1.74	0.52
3:G:52:SER:O	3:G:72:ARG:NH2	2.40	0.52
1:B:1105:THR:OG1	1:B:1109:PHE:O	2.27	0.52
2:E:362:THR:HG23	2:E:368:ASP:HB3	1.92	0.52
2:F:362:THR:HG23	2:F:368:ASP:HB3	1.91	0.52
1:C:794:ILE:O	1:C:969:LYS:NZ	2.38	0.52
1:A:721:SER:HB3	1:A:1068:VAL:HG22	1.91	0.52
2:D:263:PRO:HG2	2:D:266:LEU:HB2	1.91	0.52
3:G:24:ALA:HB3	3:G:77:ASN:HB3	1.91	0.51
2:E:483:GLU:HA	2:E:606:TRP:HE1	1.74	0.51
1:A:819:GLU:HG2	3:G:50:ARG:HH12	1.75	0.51
1:B:295:PRO:HD2	1:B:608:VAL:HG21	1.93	0.51
3:I:24:ALA:HB3	3:I:77:ASN:HB3	1.91	0.51
3:I:145:ALA:HB3	4:J:120:THR:HG21	1.93	0.51
1:A:166:CYS:O	1:B:357:ARG:NH2	2.41	0.51
1:B:862:PRO:O	1:B:905:ARG:NH2	2.43	0.51
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.93	0.51
1:A:295:PRO:HD2	1:A:608:VAL:HG21	1.92	0.51
1:C:706:ALA:HB1	1:C:1130:ILE:HD13	1.93	0.51
3:K:52:SER:O	3:K:72:ARG:NH2	2.41	0.51
4:L:14:PRO:HA	4:L:80:LEU:HB2	1.93	0.51
2:D:134:ASN:ND2	2:D:136:ASP:O	2.44	0.51
1:B:1032:CYS:O	1:B:1048:HIS:NE2	2.42	0.51
2:E:327:PHE:HE1	2:E:358:ILE:HD12	1.76	0.51
4:L:93:TYR:OH	4:L:97:ASN:OD1	2.26	0.51
1:B:1005:GLN:OE1	1:C:1002:GLN:NE2	2.44	0.50
1:A:187:LYS:O	1:A:188:ASN:ND2	2.44	0.50
1:B:187:LYS:O	1:B:188:ASN:ND2	2.44	0.50
3:I:61:VAL:HG13	3:I:63:SER:H	1.76	0.50
1:A:706:ALA:HB1	1:A:1130:ILE:HD13	1.93	0.50
2:D:327:PHE:HE1	2:D:358:ILE:HD12	1.76	0.50
2:E:529:LEU:HD22	2:E:550:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:14:PRO:HA	4:J:80:LEU:HB2	1.94	0.50
1:C:187:LYS:O	1:C:188:ASN:ND2	2.44	0.50
2:D:529:LEU:HD22	2:D:550:ALA:HB1	1.93	0.50
1:C:862:PRO:O	1:C:905:ARG:NH2	2.44	0.50
1:A:1105:THR:OG1	1:A:1109:PHE:O	2.27	0.50
3:G:159:THR:OG1	3:G:207:ASN:O	2.29	0.50
4:H:93:TYR:OH	4:H:97:ASN:OD1	2.25	0.50
1:C:1032:CYS:O	1:C:1048:HIS:NE2	2.44	0.50
3:K:145:ALA:HB3	4:L:120:THR:HG21	1.93	0.50
1:A:582:LEU:HD21	5:O:1:NAG:H83	1.94	0.50
1:C:295:PRO:HD2	1:C:608:VAL:HG21	1.93	0.50
1:A:862:PRO:O	1:A:905:ARG:NH2	2.44	0.50
1:B:69:HIS:HD2	1:B:260:ALA:HA	1.77	0.50
2:E:134:ASN:ND2	2:E:136:ASP:O	2.44	0.50
2:F:134:ASN:ND2	2:F:136:ASP:O	2.44	0.50
2:F:608:THR:HG1	3:K:202:TYR:HH	1.58	0.50
1:A:69:HIS:HD2	1:A:260:ALA:HA	1.77	0.49
1:A:794:ILE:O	1:A:969:LYS:NZ	2.36	0.49
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.94	0.49
1:B:706:ALA:HB1	1:B:1130:ILE:HD13	1.94	0.49
1:C:69:HIS:HD2	1:C:260:ALA:HA	1.77	0.49
2:F:327:PHE:HE1	2:F:358:ILE:HD12	1.76	0.49
2:F:529:LEU:HD22	2:F:550:ALA:HB1	1.93	0.49
3:K:67:ARG:HD2	3:K:85:SER:HB3	1.94	0.49
2:D:389:PRO:HD2	2:D:392:LEU:HD12	1.95	0.49
1:A:34:ARG:NH2	1:A:219:GLY:O	2.45	0.49
1:A:296:LEU:HG	1:A:300:LYS:HE2	1.95	0.49
1:A:1032:CYS:O	1:A:1048:HIS:NE2	2.42	0.49
1:C:34:ARG:NH2	1:C:219:GLY:O	2.45	0.49
3:I:67:ARG:HD2	3:I:85:SER:HB3	1.94	0.49
3:G:145:ALA:HB3	4:H:120:THR:HG21	1.93	0.49
1:B:658:ASN:OD1	1:B:659:SER:N	2.45	0.49
1:C:582:LEU:HD21	5:W:1:NAG:H83	1.94	0.49
1:A:41:LYS:HB2	1:B:563:GLN:HA	1.95	0.49
1:A:737:ASP:HB3	1:A:740:MET:HG2	1.95	0.49
1:A:453:TYR:OH	2:D:34:HIS:ND1	2.46	0.49
1:B:41:LYS:HB2	1:C:563:GLN:HA	1.94	0.49
1:B:582:LEU:HD21	5:S:1:NAG:H83	1.94	0.49
3:G:67:ARG:HD2	3:G:85:SER:HB3	1.94	0.48
1:A:771:ALA:HA	1:B:1010:GLN:HE22	1.78	0.48
1:B:34:ARG:NH2	1:B:219:GLY:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.94	0.48
1:A:90:VAL:HG13	1:A:267:VAL:HG13	1.94	0.48
1:A:563:GLN:HA	1:C:41:LYS:HB2	1.94	0.48
1:C:142:ASP:OD1	1:C:142:ASP:N	2.44	0.48
1:A:273:ARG:NH2	1:A:291:CYS:O	2.46	0.48
1:C:186:PHE:HB2	1:C:210:ILE:HG23	1.95	0.48
1:C:658:ASN:OD1	1:C:659:SER:N	2.46	0.48
1:B:186:PHE:HB2	1:B:210:ILE:HG23	1.95	0.48
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.95	0.48
4:H:3:ALA:HA	4:H:100:ILE:HG21	1.95	0.48
1:B:777:ASN:ND2	1:C:743:CYS:O	2.41	0.48
3:I:134:PRO:HD3	3:I:146:LEU:HB3	1.96	0.48
4:L:3:ALA:HA	4:L:100:ILE:HG21	1.95	0.48
2:F:389:PRO:HD2	2:F:392:LEU:HD12	1.95	0.48
3:K:40:THR:HG23	3:K:43:LYS:HB2	1.95	0.48
1:A:186:PHE:HB2	1:A:210:ILE:HG23	1.95	0.48
1:A:332:ILE:HB	1:A:362:VAL:HG11	1.96	0.48
2:E:142:LEU:H	2:E:142:LEU:HD23	1.79	0.48
3:I:159:THR:OG1	3:I:207:ASN:O	2.29	0.48
1:A:746:SER:HB2	1:A:749:CYS:SG	2.54	0.48
2:E:389:PRO:HD2	2:E:392:LEU:HD12	1.95	0.48
3:I:152:ASP:HA	3:I:183:LEU:HD13	1.96	0.48
1:C:273:ARG:NH2	1:C:291:CYS:O	2.47	0.48
1:A:1002:GLN:NE2	1:C:1005:GLN:OE1	2.47	0.48
2:D:142:LEU:HD23	2:D:142:LEU:H	1.79	0.48
2:D:608:THR:HG1	3:G:202:TYR:HH	1.58	0.48
1:B:273:ARG:NH2	1:B:291:CYS:O	2.47	0.48
4:J:3:ALA:HA	4:J:100:ILE:HG21	1.95	0.48
1:C:296:LEU:HG	1:C:300:LYS:HE2	1.95	0.48
1:C:453:TYR:OH	2:F:34:HIS:ND1	2.46	0.48
2:F:425:SER:OG	2:F:427:ASP:OD1	2.32	0.48
2:F:597:ASP:O	2:F:600:LYS:NZ	2.36	0.48
3:K:134:PRO:HD3	3:K:146:LEU:HB3	1.96	0.48
1:C:90:VAL:HG13	1:C:267:VAL:HG13	1.95	0.47
1:C:403:ARG:HB2	1:C:505:HIS:HA	1.96	0.47
2:F:142:LEU:HD23	2:F:142:LEU:H	1.79	0.47
2:D:323:MET:SD	2:D:380:GLN:NE2	2.87	0.47
2:E:418:LEU:HD22	2:E:423:LEU:HD12	1.96	0.47
2:E:468:ILE:HG23	2:E:476:LYS:HZ3	1.79	0.47
2:F:418:LEU:HD22	2:F:423:LEU:HD12	1.96	0.47
3:K:61:VAL:HG13	3:K:63:SER:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:159:THR:OG1	3:K:207:ASN:O	2.29	0.47
2:D:418:LEU:HD22	2:D:423:LEU:HD12	1.97	0.47
3:G:143:THR:HA	3:G:193:PRO:HA	1.95	0.47
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.78	0.47
1:B:453:TYR:OH	2:E:34:HIS:ND1	2.46	0.47
3:I:52:SER:O	3:I:72:ARG:NH2	2.41	0.47
3:I:127:PRO:HB3	3:I:153:TYR:HB3	1.97	0.47
3:I:143:THR:HA	3:I:193:PRO:HA	1.95	0.47
2:F:323:MET:SD	2:F:380:GLN:NE2	2.87	0.47
3:K:127:PRO:HB3	3:K:153:TYR:HB3	1.96	0.47
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.96	0.47
3:G:152:ASP:HA	3:G:183:LEU:HD13	1.95	0.47
1:B:90:VAL:HG13	1:B:267:VAL:HG13	1.96	0.47
1:B:332:ILE:HB	1:B:362:VAL:HG11	1.96	0.47
3:G:127:PRO:HB3	3:G:153:TYR:HB3	1.96	0.47
3:G:134:PRO:HD3	3:G:146:LEU:HB3	1.96	0.47
2:E:468:ILE:HD13	2:E:476:LYS:HG2	1.96	0.47
1:A:777:ASN:ND2	1:B:743:CYS:O	2.40	0.47
1:B:69:HIS:HB3	1:B:261:GLY:H	1.80	0.47
1:B:296:LEU:HG	1:B:300:LYS:HE2	1.95	0.47
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.96	0.47
2:D:370:LEU:HD11	2:D:413:ALA:HB2	1.97	0.47
4:H:115:ALA:HB3	4:H:143:PHE:HA	1.96	0.47
1:B:141:LEU:HD12	1:B:156:GLU:HG3	1.97	0.47
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.95	0.47
2:E:231:GLU:HA	2:E:234:LYS:HE2	1.97	0.47
2:E:370:LEU:HD11	2:E:413:ALA:HB2	1.96	0.47
3:I:40:THR:HG23	3:I:43:LYS:HB2	1.96	0.47
1:C:746:SER:HB2	1:C:749:CYS:SG	2.55	0.47
1:B:538:CYS:HB2	1:B:551:VAL:HG22	1.97	0.47
3:K:143:THR:HA	3:K:193:PRO:HA	1.96	0.47
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.96	0.47
1:B:746:SER:HB2	1:B:749:CYS:SG	2.54	0.47
1:A:247:SER:HB2	1:A:249:LEU:HD23	1.97	0.47
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.79	0.47
3:G:61:VAL:HG13	3:G:63:SER:H	1.79	0.47
1:B:247:SER:HB2	1:B:249:LEU:HD23	1.97	0.47
1:C:1105:THR:OG1	1:C:1109:PHE:O	2.27	0.47
2:F:462:MET:HE3	2:F:468:ILE:HD11	1.97	0.47
1:A:353:TRP:CE2	1:A:466:ARG:HB3	2.50	0.46
3:G:40:THR:HG23	3:G:43:LYS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:370:LEU:HD11	2:F:413:ALA:HB2	1.96	0.46
2:F:580:ASN:HD21	2:F:582:ARG:HB2	1.80	0.46
4:L:115:ALA:HB3	4:L:143:PHE:HA	1.96	0.46
1:A:69:HIS:HB3	1:A:261:GLY:H	1.80	0.46
1:A:756:TYR:CZ	1:B:995:ARG:HG3	2.50	0.46
1:C:141:LEU:HD12	1:C:156:GLU:HG3	1.97	0.46
2:F:300:GLN:HB3	2:F:302:TRP:CD1	2.51	0.46
1:A:141:LEU:HD12	1:A:156:GLU:HG3	1.97	0.46
4:J:153:LYS:HD2	4:J:198:GLN:HE22	1.81	0.46
1:C:332:ILE:HB	1:C:362:VAL:HG11	1.96	0.46
1:C:353:TRP:CE2	1:C:466:ARG:HB3	2.50	0.46
1:C:353:TRP:HZ3	1:C:355:ARG:HB2	1.79	0.46
2:E:323:MET:SD	2:E:380:GLN:NE2	2.87	0.46
2:E:425:SER:OG	2:E:427:ASP:OD1	2.32	0.46
4:J:115:ALA:HB3	4:J:143:PHE:HA	1.97	0.46
1:A:658:ASN:OD1	1:A:659:SER:N	2.45	0.46
2:D:231:GLU:HA	2:D:234:LYS:HE2	1.97	0.46
4:H:108:THR:O	4:H:144:TYR:OH	2.34	0.46
1:B:387:LEU:HD13	1:B:387:LEU:H	1.80	0.46
1:C:69:HIS:HB3	1:C:261:GLY:H	1.80	0.46
1:C:247:SER:HB2	1:C:249:LEU:HD23	1.97	0.46
1:C:538:CYS:HB2	1:C:551:VAL:HG22	1.98	0.46
3:K:152:ASP:HA	3:K:183:LEU:HD13	1.96	0.46
1:A:55:PHE:HB2	1:A:275:PHE:CZ	2.51	0.46
2:D:462:MET:HE3	2:D:468:ILE:HD11	1.97	0.46
1:B:353:TRP:CE2	1:B:466:ARG:HB3	2.50	0.46
1:B:669:GLY:HA2	1:B:697:MET:HE2	1.98	0.46
2:F:231:GLU:HA	2:F:234:LYS:HE2	1.97	0.46
4:L:153:LYS:HD2	4:L:198:GLN:HE22	1.81	0.46
1:A:246:ARG:H	1:A:246:ARG:HG3	1.62	0.46
1:A:921:LYS:HG2	1:C:828:LEU:HD21	1.96	0.46
2:D:300:GLN:HB3	2:D:302:TRP:CD1	2.50	0.46
4:H:150:VAL:HG22	4:H:199:VAL:HG22	1.98	0.46
2:D:557:MET:HG3	2:D:573:VAL:HB	1.98	0.46
1:C:55:PHE:HB2	1:C:275:PHE:CZ	2.51	0.46
4:H:153:LYS:HD2	4:H:198:GLN:HE22	1.81	0.45
2:F:158:TYR:HD2	2:F:266:LEU:HD11	1.81	0.45
2:D:468:ILE:HD13	2:D:476:LYS:HG2	1.98	0.45
2:E:300:GLN:HB3	2:E:302:TRP:CD1	2.50	0.45
4:J:93:TYR:OH	4:J:97:ASN:OD1	2.26	0.45
1:C:387:LEU:HD13	1:C:387:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:O	1:B:357:ARG:NH1	2.49	0.45
2:D:580:ASN:HD21	2:D:582:ARG:HB2	1.82	0.45
1:B:403:ARG:HB2	1:B:505:HIS:HA	1.98	0.45
2:E:557:MET:HG3	2:E:573:VAL:HB	1.99	0.45
1:C:737:ASP:HB3	1:C:740:MET:HG2	1.98	0.45
4:L:150:VAL:HG22	4:L:199:VAL:HG22	1.98	0.45
1:A:403:ARG:HB2	1:A:505:HIS:HA	1.99	0.45
1:A:794:ILE:HB	1:A:969:LYS:HD3	1.99	0.45
3:G:154:PHE:HB3	3:G:155:PRO:HD3	1.99	0.45
1:B:34:ARG:HD3	1:B:216:LEU:HD13	1.98	0.45
1:B:756:TYR:CZ	1:C:995:ARG:HG3	2.51	0.45
1:B:983:ARG:HH11	1:C:984:LEU:HD12	1.80	0.45
1:C:67:ALA:N	1:C:263:ALA:O	2.50	0.45
1:A:387:LEU:HD13	1:A:387:LEU:H	1.81	0.45
1:B:820:ASP:O	1:B:824:ASN:HB2	2.16	0.45
2:E:580:ASN:HD21	2:E:582:ARG:HB2	1.82	0.45
1:A:984:LEU:HD12	1:C:983:ARG:HH11	1.80	0.45
2:D:468:ILE:HG23	2:D:476:LYS:HZ3	1.81	0.45
2:F:168:TRP:HE1	2:F:502:SER:HB2	1.82	0.45
3:K:154:PHE:HB3	3:K:155:PRO:HD3	1.99	0.45
1:A:538:CYS:HB2	1:A:551:VAL:HG22	1.98	0.45
1:B:55:PHE:HB2	1:B:275:PHE:CZ	2.51	0.45
1:B:737:ASP:HB3	1:B:740:MET:HG2	1.98	0.45
2:E:503:LEU:HG	2:E:505:HIS:H	1.82	0.45
3:I:154:PHE:HB3	3:I:155:PRO:HD3	1.99	0.45
1:C:246:ARG:H	1:C:246:ARG:HG3	1.63	0.45
1:A:34:ARG:HD3	1:A:216:LEU:HD13	1.98	0.45
1:B:1093:GLY:HA2	1:B:1106:GLN:HA	1.99	0.45
1:C:1093:GLY:HA2	1:C:1106:GLN:HA	1.98	0.45
2:E:392:LEU:HA	2:E:562:LYS:HD3	1.99	0.45
4:J:150:VAL:HG22	4:J:199:VAL:HG22	1.98	0.45
1:A:669:GLY:HA2	1:A:697:MET:HE2	1.99	0.44
2:E:462:MET:HE3	2:E:468:ILE:HD11	1.99	0.44
1:C:646:ARG:HD2	1:C:668:ALA:HB1	1.99	0.44
1:A:67:ALA:N	1:A:263:ALA:O	2.50	0.44
1:B:67:ALA:N	1:B:263:ALA:O	2.50	0.44
1:C:97:LYS:HG2	1:C:98:SER:H	1.83	0.44
2:D:108:LEU:HD11	2:D:190:MET:HB2	1.99	0.44
2:D:392:LEU:HA	2:D:562:LYS:HD3	1.99	0.44
3:G:35:HIS:CE1	3:G:50:ARG:HH21	2.35	0.44
1:A:357:ARG:NH2	1:C:166:CYS:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:ILE:HG12	1:B:789:TYR:HD2	1.83	0.44
2:E:108:LEU:HD11	2:E:190:MET:HB2	1.99	0.44
1:C:34:ARG:HD3	1:C:216:LEU:HD13	1.98	0.44
1:C:661:GLU:O	1:C:695:TYR:OH	2.33	0.44
2:F:142:LEU:HD12	2:F:147:GLY:HA3	2.00	0.44
1:C:820:ASP:O	1:C:824:ASN:HB2	2.17	0.44
2:F:468:ILE:HG23	2:F:476:LYS:HZ3	1.83	0.44
2:F:557:MET:HG3	2:F:573:VAL:HB	1.99	0.44
2:D:142:LEU:HD12	2:D:147:GLY:HA3	2.00	0.44
2:D:503:LEU:HG	2:D:505:HIS:H	1.82	0.44
2:D:574:VAL:HG23	2:D:576:ALA:H	1.82	0.44
2:D:597:ASP:O	2:D:600:LYS:NZ	2.36	0.44
1:B:771:ALA:HA	1:C:1010:GLN:HE22	1.82	0.44
2:E:142:LEU:HD12	2:E:147:GLY:HA3	2.00	0.44
1:C:669:GLY:HA2	1:C:697:MET:HE2	1.99	0.44
2:F:468:ILE:HD13	2:F:476:LYS:HG2	1.98	0.44
2:F:574:VAL:HG23	2:F:576:ALA:H	1.82	0.44
1:A:97:LYS:HG2	1:A:98:SER:H	1.83	0.44
1:A:596:SER:OG	1:A:613:GLN:OE1	2.36	0.44
1:A:995:ARG:HG3	1:C:756:TYR:CZ	2.53	0.44
2:D:425:SER:OG	2:D:427:ASP:OD1	2.32	0.44
1:B:596:SER:OG	1:B:613:GLN:OE1	2.36	0.44
1:C:501:TYR:HB3	1:C:505:HIS:HB2	2.00	0.44
1:A:206:LYS:HB2	1:A:223:LEU:HA	1.99	0.44
1:A:646:ARG:HD2	1:A:668:ALA:HB1	1.99	0.44
1:C:1081:ILE:HA	1:C:1133:VAL:HG23	2.00	0.44
2:F:108:LEU:HD11	2:F:190:MET:HB2	1.99	0.44
1:A:726:ILE:HG13	1:A:1061:VAL:HG12	2.00	0.44
1:B:726:ILE:HG13	1:B:1061:VAL:HG12	2.00	0.44
1:B:794:ILE:HB	1:B:969:LYS:HD3	2.00	0.44
2:E:574:VAL:HG23	2:E:576:ALA:H	1.82	0.44
2:F:540:HIS:ND1	2:F:541:LYS:HG3	2.33	0.44
1:A:379:CYS:HA	1:A:432:CYS:HA	2.00	0.43
2:D:158:TYR:HD2	2:D:266:LEU:HD11	1.82	0.43
2:D:347:THR:OG1	2:D:349:TRP:NE1	2.51	0.43
1:B:111:ASP:OD1	1:B:112:SER:N	2.49	0.43
2:E:158:TYR:HD2	2:E:266:LEU:HD11	1.82	0.43
4:J:84:ASP:O	4:J:88:TYR:OH	2.33	0.43
1:C:788:ILE:HG12	1:C:789:TYR:HD2	1.84	0.43
1:B:822:LEU:HB2	1:C:935:GLN:NE2	2.32	0.43
2:E:459:TRP:HZ2	2:E:473:TRP:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:597:ASP:O	2:E:600:LYS:NZ	2.36	0.43
2:F:503:LEU:HD21	2:F:512:PHE:HE1	1.84	0.43
1:A:403:ARG:NE	1:A:405:ASN:OD1	2.52	0.43
1:A:788:ILE:HG12	1:A:789:TYR:HD2	1.83	0.43
2:D:168:TRP:HE1	2:D:502:SER:HB2	1.84	0.43
2:F:347:THR:OG1	2:F:349:TRP:NE1	2.51	0.43
1:A:332:ILE:HA	1:A:362:VAL:HG21	2.01	0.43
1:A:935:GLN:HE22	1:C:822:LEU:HB2	1.82	0.43
1:A:1093:GLY:HA2	1:A:1106:GLN:HA	1.99	0.43
2:D:540:HIS:ND1	2:D:541:LYS:HG3	2.33	0.43
1:B:332:ILE:HA	1:B:362:VAL:HG21	2.00	0.43
1:B:379:CYS:HA	1:B:432:CYS:HA	2.01	0.43
1:B:501:TYR:HB3	1:B:505:HIS:HB2	2.00	0.43
1:C:379:CYS:HA	1:C:432:CYS:HA	2.01	0.43
1:C:403:ARG:NE	1:C:405:ASN:OD1	2.51	0.43
2:F:392:LEU:HA	2:F:562:LYS:HD3	1.99	0.43
2:D:459:TRP:HZ2	2:D:473:TRP:HB3	1.83	0.43
1:C:787:GLN:NE2	1:C:789:TYR:O	2.34	0.43
2:F:459:TRP:HZ2	2:F:473:TRP:HB3	1.84	0.43
1:A:787:GLN:NE2	1:A:789:TYR:O	2.33	0.43
1:B:646:ARG:HD2	1:B:668:ALA:HB1	1.99	0.43
2:E:347:THR:OG1	2:E:349:TRP:NE1	2.51	0.43
1:A:111:ASP:OD1	1:A:112:SER:N	2.49	0.43
1:A:1028:LYS:HE2	1:A:1028:LYS:HB2	1.89	0.43
1:C:127:VAL:HG22	5:U:1:NAG:H61	2.01	0.43
1:A:42:VAL:HA	1:B:565:PHE:HB2	2.00	0.43
1:A:675:GLN:O	1:A:690:GLN:N	2.52	0.43
3:I:35:HIS:CE1	3:I:50:ARG:HH21	2.37	0.43
1:A:398:ASP:HB2	1:A:512:VAL:HB	2.01	0.43
1:A:565:PHE:HB2	1:C:42:VAL:HA	2.01	0.43
1:B:97:LYS:HG2	1:B:98:SER:H	1.83	0.43
1:C:596:SER:OG	1:C:613:GLN:OE1	2.36	0.43
1:A:935:GLN:NE2	1:C:822:LEU:HB2	2.33	0.42
1:B:127:VAL:HG22	5:Q:1:NAG:H61	2.01	0.42
4:J:108:THR:O	4:J:144:TYR:OH	2.33	0.42
1:A:728:PRO:HA	1:A:1059:GLY:HA2	2.02	0.42
1:A:1081:ILE:HA	1:A:1133:VAL:HG23	2.01	0.42
2:D:503:LEU:HD21	2:D:512:PHE:HE1	1.84	0.42
3:G:2:VAL:HG13	3:G:25:SER:HB3	2.01	0.42
3:G:20:LEU:HB3	3:G:81:LEU:HB3	2.01	0.42
1:B:108:THR:OG1	1:B:234:ASN:O	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:NE	1:B:405:ASN:OD1	2.52	0.42
2:E:540:HIS:ND1	2:E:541:LYS:HG3	2.33	0.42
1:C:564:GLN:HG2	1:C:577:ARG:HD2	2.01	0.42
1:C:726:ILE:HG13	1:C:1061:VAL:HG12	2.00	0.42
3:K:20:LEU:HB3	3:K:81:LEU:HB3	2.00	0.42
3:K:35:HIS:CE1	3:K:50:ARG:HH21	2.36	0.42
2:D:343:VAL:HG12	2:D:345:HIS:H	1.85	0.42
1:B:115:GLN:OE1	6:B:1306:NAG:O6	2.38	0.42
1:B:1081:ILE:HA	1:B:1133:VAL:HG23	2.01	0.42
1:C:567:ARG:HG2	1:C:573:THR:HA	2.02	0.42
2:D:293:VAL:HG11	2:D:418:LEU:HD13	2.01	0.42
2:E:378:HIS:HE1	2:E:402:GLU:HA	1.85	0.42
3:I:2:VAL:HG13	3:I:25:SER:HB3	2.02	0.42
4:J:41:TYR:HB2	4:J:44:LYS:HB2	2.02	0.42
1:C:206:LYS:HB2	1:C:223:LEU:HA	2.01	0.42
2:F:293:VAL:HG11	2:F:418:LEU:HD13	2.02	0.42
2:F:378:HIS:HE1	2:F:402:GLU:HA	1.85	0.42
3:K:2:VAL:HG13	3:K:25:SER:HB3	2.01	0.42
1:A:357:ARG:NH1	1:C:167:THR:O	2.52	0.42
1:B:929:SER:O	1:B:933:LYS:HG2	2.20	0.42
2:E:343:VAL:HG12	2:E:345:HIS:H	1.85	0.42
3:I:20:LEU:HB3	3:I:81:LEU:HB3	2.00	0.42
3:I:99:LEU:HD22	3:I:99:LEU:H	1.85	0.42
1:A:896:ILE:HB	1:A:897:PRO:HD3	2.02	0.42
3:G:131:PRO:HD3	3:G:217:LYS:HG2	2.02	0.42
1:B:675:GLN:O	1:B:690:GLN:N	2.53	0.42
2:F:343:VAL:HG12	2:F:345:HIS:H	1.85	0.42
1:B:41:LYS:HE2	1:B:41:LYS:HB3	1.93	0.42
1:B:206:LYS:HB2	1:B:223:LEU:HA	2.02	0.42
1:C:334:ASN:O	1:C:362:VAL:N	2.50	0.42
4:L:108:THR:O	4:L:144:TYR:OH	2.33	0.42
1:A:41:LYS:HE2	1:A:41:LYS:HB3	1.93	0.42
1:A:501:TYR:HB3	1:A:505:HIS:HB2	2.01	0.42
2:E:293:VAL:HG11	2:E:418:LEU:HD13	2.02	0.42
2:F:307:ILE:HG23	2:F:369:PHE:HD1	1.85	0.42
2:F:459:TRP:CH2	2:F:500:PRO:HG2	2.55	0.42
1:A:567:ARG:HG2	1:A:573:THR:HA	2.01	0.41
1:A:1005:GLN:OE1	1:B:1002:GLN:NE2	2.53	0.41
4:H:19:THR:HG22	4:H:76:THR:HA	2.02	0.41
1:B:293:LEU:HG	1:B:294:ASP:H	1.85	0.41
2:E:168:TRP:HE1	2:E:502:SER:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:503:LEU:HD21	2:E:512:PHE:HE1	1.85	0.41
1:A:334:ASN:O	1:A:362:VAL:N	2.50	0.41
4:H:144:TYR:CG	4:H:145:PRO:HD2	2.56	0.41
1:C:111:ASP:OD1	1:C:112:SER:N	2.49	0.41
3:K:131:PRO:HD3	3:K:217:LYS:HG2	2.01	0.41
1:A:293:LEU:HG	1:A:294:ASP:H	1.85	0.41
1:A:350:VAL:HA	1:A:400:PHE:HB2	2.03	0.41
1:A:1014:ARG:HH11	1:A:1017:GLU:HG2	1.86	0.41
1:B:896:ILE:HB	1:B:897:PRO:HD3	2.02	0.41
1:C:293:LEU:HG	1:C:294:ASP:H	1.86	0.41
1:A:127:VAL:HG22	5:M:1:NAG:H61	2.01	0.41
2:D:241:HIS:NE2	2:D:486:GLY:O	2.53	0.41
1:B:42:VAL:HA	1:C:565:PHE:HB2	2.01	0.41
1:B:912:THR:HG21	1:C:913:GLN:NE2	2.35	0.41
1:C:1014:ARG:HH11	1:C:1017:GLU:HG2	1.85	0.41
4:L:144:TYR:CG	4:L:145:PRO:HD2	2.56	0.41
1:A:912:THR:HG21	1:B:913:GLN:NE2	2.36	0.41
2:D:177:ARG:HB3	2:D:178:PRO:HD3	2.03	0.41
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.85	0.41
4:H:41:TYR:HB2	4:H:44:LYS:HB2	2.02	0.41
1:C:896:ILE:HB	1:C:897:PRO:HD3	2.03	0.41
1:C:929:SER:O	1:C:933:LYS:HG2	2.20	0.41
2:D:307:ILE:HG23	2:D:369:PHE:HD1	1.85	0.41
2:D:474:MET:HE3	2:D:495:GLU:HA	2.02	0.41
1:B:233:ILE:HA	6:B:1307:NAG:H82	2.03	0.41
1:C:398:ASP:HB2	1:C:512:VAL:HB	2.02	0.41
1:C:675:GLN:O	1:C:690:GLN:N	2.53	0.41
2:F:288:LYS:HD2	2:F:433:GLU:HB2	2.03	0.41
2:F:458:LYS:HB3	2:F:480:MET:HE1	2.02	0.41
1:B:728:PRO:HA	1:B:1059:GLY:HA2	2.01	0.41
1:B:1014:ARG:HH11	1:B:1017:GLU:HG2	1.85	0.41
2:E:480:MET:O	2:E:484:ILE:HB	2.21	0.41
2:D:459:TRP:CH2	2:D:500:PRO:HG2	2.55	0.41
1:B:350:VAL:HA	1:B:400:PHE:HB2	2.03	0.41
1:C:332:ILE:HA	1:C:362:VAL:HG21	2.01	0.41
1:A:822:LEU:O	4:H:93:TYR:OH	2.39	0.41
1:A:990:GLU:O	1:A:993:ILE:HG13	2.21	0.41
2:D:478:TRP:CE3	2:D:489:GLU:HB3	2.56	0.41
4:H:36:SER:OG	4:H:91:CYS:SG	2.54	0.41
2:E:288:LYS:HD2	2:E:433:GLU:HB2	2.03	0.41
2:E:459:TRP:CH2	2:E:500:PRO:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:131:PRO:HD3	3:I:217:LYS:HG2	2.02	0.41
4:J:112:GLN:HE21	4:J:112:GLN:HB2	1.71	0.41
4:J:144:TYR:CG	4:J:145:PRO:HD2	2.55	0.41
1:C:990:GLU:O	1:C:993:ILE:HG13	2.21	0.41
2:F:478:TRP:CE3	2:F:489:GLU:HB3	2.56	0.41
1:A:300:LYS:NZ	1:A:306:PHE:O	2.54	0.41
4:J:19:THR:HG22	4:J:76:THR:HA	2.03	0.41
1:C:350:VAL:HA	1:C:400:PHE:HB2	2.02	0.41
2:F:503:LEU:HG	2:F:505:HIS:H	1.85	0.41
1:B:398:ASP:HB2	1:B:512:VAL:HB	2.02	0.40
1:B:567:ARG:HG2	1:B:573:THR:HA	2.02	0.40
1:B:794:ILE:O	1:B:969:LYS:NZ	2.38	0.40
1:C:300:LYS:NZ	1:C:306:PHE:O	2.54	0.40
1:C:794:ILE:HB	1:C:969:LYS:HD3	2.04	0.40
2:F:474:MET:HE3	2:F:495:GLU:HA	2.02	0.40
4:L:19:THR:HG22	4:L:76:THR:HA	2.03	0.40
1:A:502:GLY:O	1:A:506:GLN:HG3	2.21	0.40
1:B:142:ASP:OD1	1:B:142:ASP:N	2.44	0.40
1:B:990:GLU:O	1:B:993:ILE:HG13	2.21	0.40
1:C:502:GLY:O	1:C:506:GLN:HG3	2.21	0.40
1:C:824:ASN:ND2	1:C:824:ASN:O	2.55	0.40
2:F:241:HIS:NE2	2:F:486:GLY:O	2.54	0.40
2:F:456:LEU:HD11	2:F:503:LEU:HD22	2.03	0.40
3:K:99:LEU:H	3:K:99:LEU:HD22	1.86	0.40
4:L:41:TYR:HB2	4:L:44:LYS:HB2	2.02	0.40
3:G:99:LEU:HD22	3:G:99:LEU:H	1.85	0.40
4:H:112:GLN:NE2	4:H:113:PRO:O	2.55	0.40
2:E:389:PRO:O	2:E:393:ARG:HG3	2.22	0.40
2:E:492:PRO:HG3	2:E:613:TYR:CZ	2.56	0.40
1:C:115:GLN:OE1	6:C:1306:NAG:O6	2.38	0.40
1:C:728:PRO:HA	1:C:1059:GLY:HA2	2.02	0.40
1:B:787:GLN:NE2	1:B:789:TYR:O	2.34	0.40
2:E:307:ILE:HG23	2:E:369:PHE:HD1	1.85	0.40
1:A:1114:ILE:H	1:A:1114:ILE:HG13	1.59	0.40
2:D:288:LYS:HD2	2:D:433:GLU:HB2	2.03	0.40
2:E:177:ARG:HB3	2:E:178:PRO:HD3	2.03	0.40
2:E:523:PHE:HB3	2:E:583:PRO:HB2	2.04	0.40
4:J:85:GLU:H	4:J:85:GLU:CD	2.30	0.40
1:C:364:ASP:HA	1:C:527:PRO:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1061/1284 (83%)	1003 (94%)	58 (6%)	0	100	100
1	B	1061/1284 (83%)	1006 (95%)	55 (5%)	0	100	100
1	C	1061/1284 (83%)	1005 (95%)	56 (5%)	0	100	100
2	D	593/631 (94%)	585 (99%)	8 (1%)	0	100	100
2	E	593/631 (94%)	585 (99%)	8 (1%)	0	100	100
2	F	593/631 (94%)	584 (98%)	9 (2%)	0	100	100
3	G	209/221 (95%)	198 (95%)	11 (5%)	0	100	100
3	I	209/221 (95%)	199 (95%)	10 (5%)	0	100	100
3	K	209/221 (95%)	199 (95%)	10 (5%)	0	100	100
4	H	209/216 (97%)	186 (89%)	23 (11%)	0	100	100
4	J	209/216 (97%)	189 (90%)	20 (10%)	0	100	100
4	L	209/216 (97%)	188 (90%)	21 (10%)	0	100	100
All	All	6216/7056 (88%)	5927 (95%)	289 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	934/1110 (84%)	898 (96%)	36 (4%)	27	48
1	B	934/1110 (84%)	898 (96%)	36 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	934/1110 (84%)	899 (96%)	35 (4%)	29	49
2	D	526/557 (94%)	513 (98%)	13 (2%)	42	61
2	E	526/557 (94%)	513 (98%)	13 (2%)	42	61
2	F	526/557 (94%)	513 (98%)	13 (2%)	42	61
3	G	179/186 (96%)	169 (94%)	10 (6%)	17	38
3	I	179/186 (96%)	169 (94%)	10 (6%)	17	38
3	K	179/186 (96%)	169 (94%)	10 (6%)	17	38
4	H	178/183 (97%)	174 (98%)	4 (2%)	47	65
4	J	178/183 (97%)	174 (98%)	4 (2%)	47	65
4	L	178/183 (97%)	174 (98%)	4 (2%)	47	65
All	All	5451/6108 (89%)	5263 (97%)	188 (3%)	34	51

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	63	THR
1	A	143	VAL
1	A	179	LEU
1	A	182	LYS
1	A	187	LYS
1	A	332	ILE
1	A	340	GLU
1	A	387	LEU
1	A	430	THR
1	A	468	ILE
1	A	517	LEU
1	A	534	VAL
1	A	554	GLU
1	A	592	PHE
1	A	716	THR
1	A	722	VAL
1	A	731	MET
1	A	736	VAL
1	A	785	VAL
1	A	805	ILE
1	A	814	LYS
1	A	828	LEU

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Mol	Chain	Res	Type
1	A	866	THR
1	A	948	LEU
1	A	984	LEU
1	A	997	ILE
1	A	1014	ARG
1	A	1031	GLU
1	A	1049	LEU
1	A	1063	LEU
1	A	1065	VAL
1	A	1066	THR
1	A	1068	VAL
1	A	1114	ILE
1	A	1133	VAL
2	D	45	LEU
2	D	75	GLU
2	D	132	VAL
2	D	203	TRP
2	D	283	VAL
2	D	364	VAL
2	D	365	THR
2	D	370	LEU
2	D	373	HIS
2	D	475	LYS
2	D	476	LYS
2	D	479	GLU
2	D	604	VAL
3	G	3	GLN
3	G	5	VAL
3	G	20	LEU
3	G	30	LYS
3	G	51	ILE
3	G	64	VAL
3	G	100	VAL
3	G	110	LEU
3	G	116	VAL
3	G	160	VAL
4	H	54	ASN
4	H	60	VAL
4	H	112	GLN
4	H	164	GLU
1	B	41	LYS
1	B	63	THR

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Mol	Chain	Res	Type
1	B	143	VAL
1	B	179	LEU
1	B	182	LYS
1	B	187	LYS
1	B	332	ILE
1	B	340	GLU
1	B	387	LEU
1	B	430	THR
1	B	468	ILE
1	B	517	LEU
1	B	534	VAL
1	B	554	GLU
1	B	592	PHE
1	B	716	THR
1	B	722	VAL
1	B	731	MET
1	B	736	VAL
1	B	785	VAL
1	B	805	ILE
1	B	814	LYS
1	B	828	LEU
1	B	866	THR
1	B	948	LEU
1	B	984	LEU
1	B	997	ILE
1	B	1014	ARG
1	B	1031	GLU
1	B	1049	LEU
1	B	1063	LEU
1	B	1065	VAL
1	B	1066	THR
1	B	1068	VAL
1	B	1114	ILE
1	B	1133	VAL
2	E	45	LEU
2	E	75	GLU
2	E	132	VAL
2	E	203	TRP
2	E	283	VAL
2	E	364	VAL
2	E	365	THR
2	E	370	LEU

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Mol	Chain	Res	Type
2	E	373	HIS
2	E	475	LYS
2	E	476	LYS
2	E	479	GLU
2	E	604	VAL
3	I	3	GLN
3	I	5	VAL
3	I	20	LEU
3	I	30	LYS
3	I	51	ILE
3	I	64	VAL
3	I	100	VAL
3	I	110	LEU
3	I	116	VAL
3	I	160	VAL
4	J	54	ASN
4	J	60	VAL
4	J	112	GLN
4	J	164	GLU
1	C	41	LYS
1	C	63	THR
1	C	143	VAL
1	C	179	LEU
1	C	182	LYS
1	C	187	LYS
1	C	332	ILE
1	C	340	GLU
1	C	387	LEU
1	C	430	THR
1	C	468	ILE
1	C	517	LEU
1	C	534	VAL
1	C	554	GLU
1	C	592	PHE
1	C	716	THR
1	C	722	VAL
1	C	731	MET
1	C	736	VAL
1	C	785	VAL
1	C	805	ILE
1	C	814	LYS
1	C	828	LEU

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Mol	Chain	Res	Type
1	C	866	THR
1	C	948	LEU
1	C	984	LEU
1	C	997	ILE
1	C	1014	ARG
1	C	1031	GLU
1	C	1049	LEU
1	C	1063	LEU
1	C	1065	VAL
1	C	1066	THR
1	C	1114	ILE
1	C	1133	VAL
2	F	45	LEU
2	F	75	GLU
2	F	132	VAL
2	F	203	TRP
2	F	283	VAL
2	F	364	VAL
2	F	365	THR
2	F	370	LEU
2	F	373	HIS
2	F	475	LYS
2	F	476	LYS
2	F	479	GLU
2	F	604	VAL
3	K	3	GLN
3	K	5	VAL
3	K	20	LEU
3	K	30	LYS
3	K	51	ILE
3	K	64	VAL
3	K	100	VAL
3	K	110	LEU
3	K	116	VAL
3	K	160	VAL
4	L	54	ASN
4	L	60	VAL
4	L	112	GLN
4	L	164	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	49	HIS
1	A	69	HIS
1	A	87	ASN
1	A	173	GLN
1	A	188	ASN
1	A	271	GLN
1	A	321	GLN
1	A	339	HIS
1	A	370	ASN
1	A	409	GLN
1	A	422	ASN
1	A	439	ASN
1	A	544	ASN
1	A	563	GLN
1	A	564	GLN
1	A	603	ASN
1	A	607	GLN
1	A	641	ASN
1	A	690	GLN
1	A	717	ASN
1	A	774	GLN
1	A	836	GLN
1	A	872	GLN
1	A	913	GLN
1	A	954	HIS
1	A	957	GLN
1	A	960	ASN
1	A	992	GLN
1	A	1002	GLN
1	A	1005	GLN
1	A	1010	GLN
1	A	1011	GLN
1	A	1071	GLN
1	A	1106	GLN
2	D	42	GLN
2	D	81	GLN
2	D	89	GLN
2	D	98	GLN
2	D	101	GLN
2	D	149	ASN
2	D	290	ASN
2	D	300	GLN

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Mol	Chain	Res	Type
2	D	442	GLN
2	D	552	GLN
3	G	3	GLN
3	G	13	GLN
3	G	35	HIS
3	G	113	GLN
3	G	179	GLN
3	G	205	ASN
4	H	40	GLN
4	H	54	ASN
4	H	98	ASN
4	H	112	GLN
4	H	130	GLN
4	H	171	GLN
1	B	14	GLN
1	B	49	HIS
1	B	69	HIS
1	B	87	ASN
1	B	173	GLN
1	B	188	ASN
1	B	271	GLN
1	B	321	GLN
1	B	339	HIS
1	B	370	ASN
1	B	409	GLN
1	B	422	ASN
1	B	439	ASN
1	B	544	ASN
1	B	563	GLN
1	B	564	GLN
1	B	607	GLN
1	B	641	ASN
1	B	644	GLN
1	B	690	GLN
1	B	774	GLN
1	B	836	GLN
1	B	872	GLN
1	B	907	ASN
1	B	913	GLN
1	B	954	HIS
1	B	957	GLN
1	B	960	ASN

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Mol	Chain	Res	Type
1	B	992	GLN
1	B	1002	GLN
1	B	1005	GLN
1	B	1010	GLN
1	B	1011	GLN
1	B	1106	GLN
2	E	42	GLN
2	E	89	GLN
2	E	98	GLN
2	E	101	GLN
2	E	290	ASN
2	E	300	GLN
2	E	442	GLN
2	E	552	GLN
3	I	3	GLN
3	I	13	GLN
3	I	35	HIS
3	I	113	GLN
3	I	172	HIS
3	I	179	GLN
3	I	205	ASN
4	J	40	GLN
4	J	54	ASN
4	J	98	ASN
4	J	112	GLN
4	J	130	GLN
4	J	171	GLN
1	C	14	GLN
1	C	49	HIS
1	C	69	HIS
1	C	87	ASN
1	C	173	GLN
1	C	271	GLN
1	C	321	GLN
1	C	339	HIS
1	C	370	ASN
1	C	409	GLN
1	C	422	ASN
1	C	439	ASN
1	C	544	ASN
1	C	563	GLN
1	C	564	GLN

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Mol	Chain	Res	Type
1	C	603	ASN
1	C	607	GLN
1	C	641	ASN
1	C	690	GLN
1	C	774	GLN
1	C	836	GLN
1	C	872	GLN
1	C	913	GLN
1	C	935	GLN
1	C	953	ASN
1	C	954	HIS
1	C	960	ASN
1	C	992	GLN
1	C	1002	GLN
1	C	1005	GLN
1	C	1010	GLN
1	C	1011	GLN
1	C	1106	GLN
2	F	42	GLN
2	F	81	GLN
2	F	89	GLN
2	F	98	GLN
2	F	101	GLN
2	F	290	ASN
2	F	300	GLN
2	F	442	GLN
2	F	552	GLN
3	K	3	GLN
3	K	13	GLN
3	K	35	HIS
3	K	113	GLN
3	K	179	GLN
3	K	205	ASN
4	L	40	GLN
4	L	54	ASN
4	L	98	ASN
4	L	112	GLN
4	L	130	GLN
4	L	171	GLN

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 ⓘ

24 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	5,1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	M	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	N	1	5,1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	N	2	5	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	O	1	5,1	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	O	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	P	1	5,2	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	P	2	5	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	Q	1	5,1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	Q	2	5	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	R	1	5,1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	R	2	5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	S	1	5,1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	S	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	T	1	5,2	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	T	2	5	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	U	1	5,1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	U	2	5	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	V	1	5,1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	W	1	5,1	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	W	2	5	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	X	1	5,2	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	X	2	5	14,14,15	0.25	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	5,1	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	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	5,2	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	NAG	T	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	NAG	X	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	X	2	5	-	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 (21) torsion outliers are listed below:

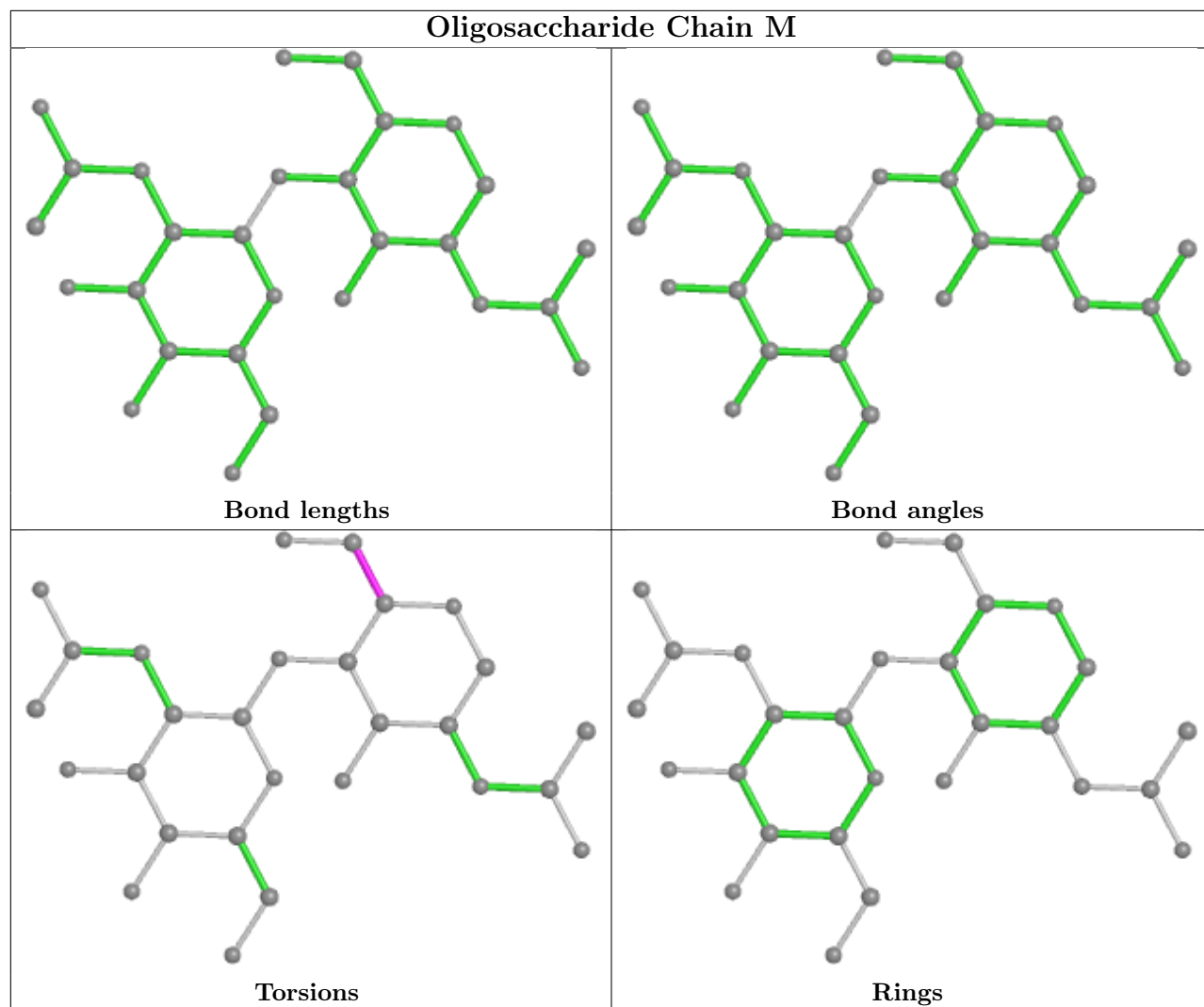
Mol	Chain	Res	Type	Atoms
5	O	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6

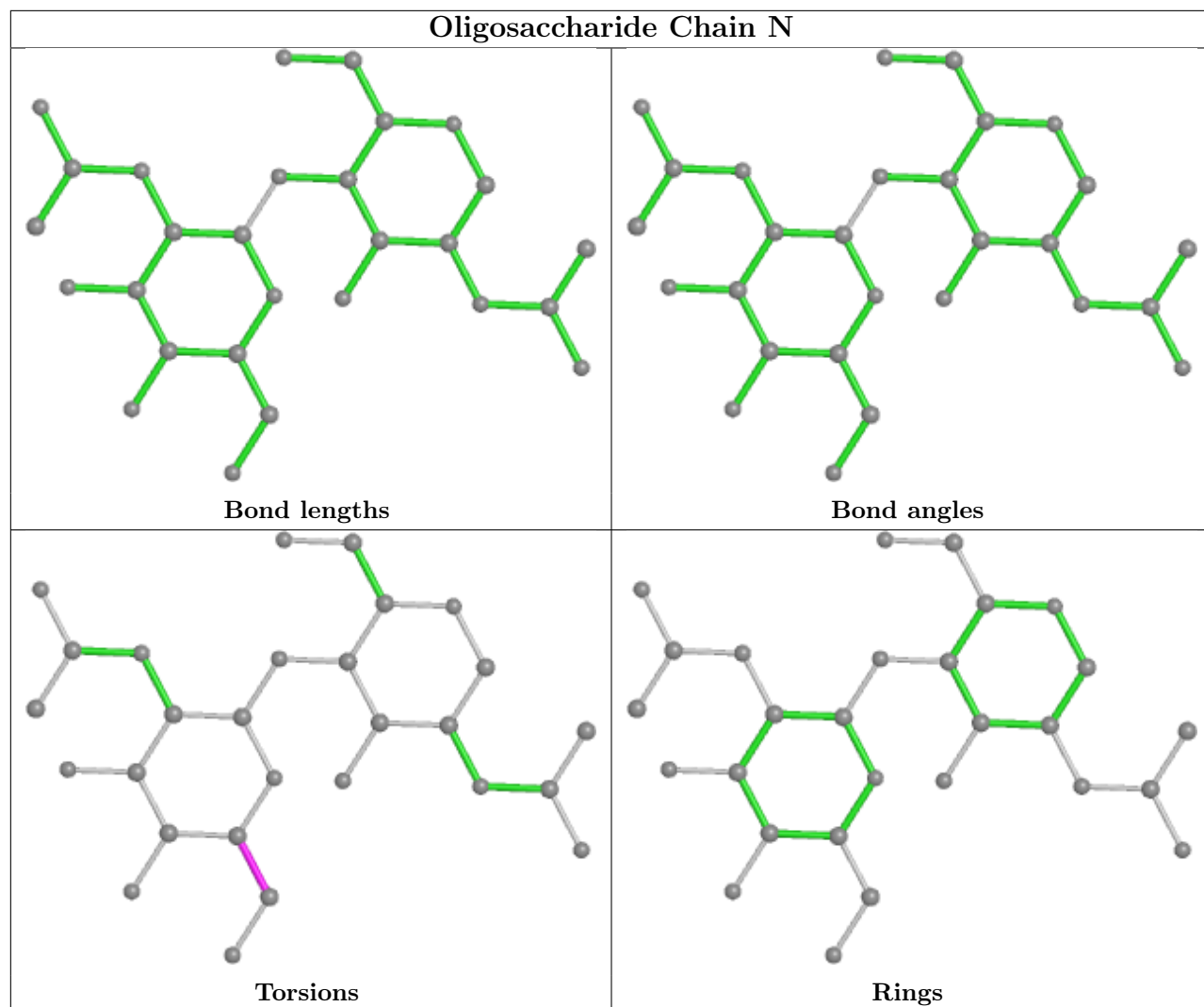
There are no ring outliers.

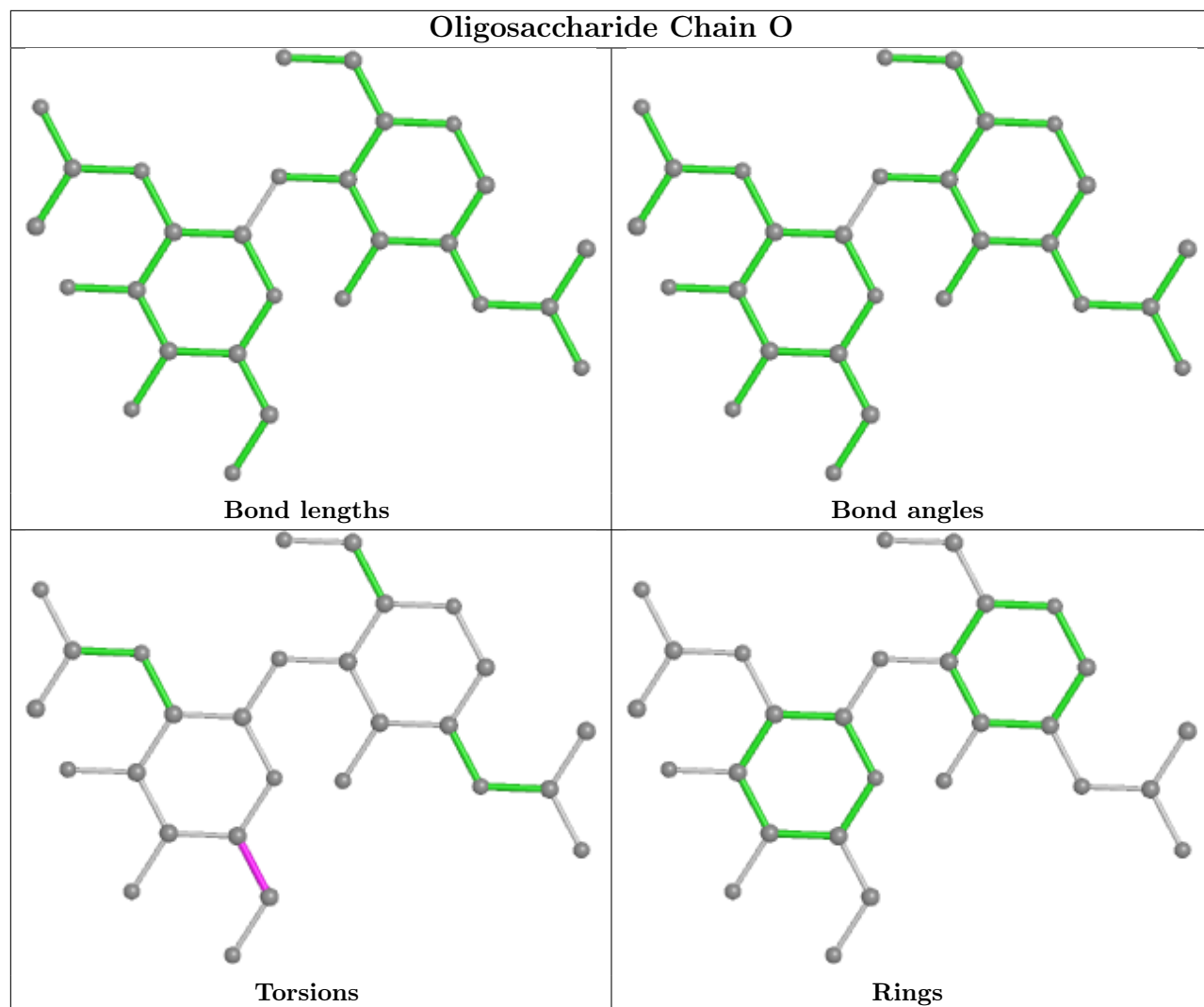
6 monomers are involved in 6 short contacts:

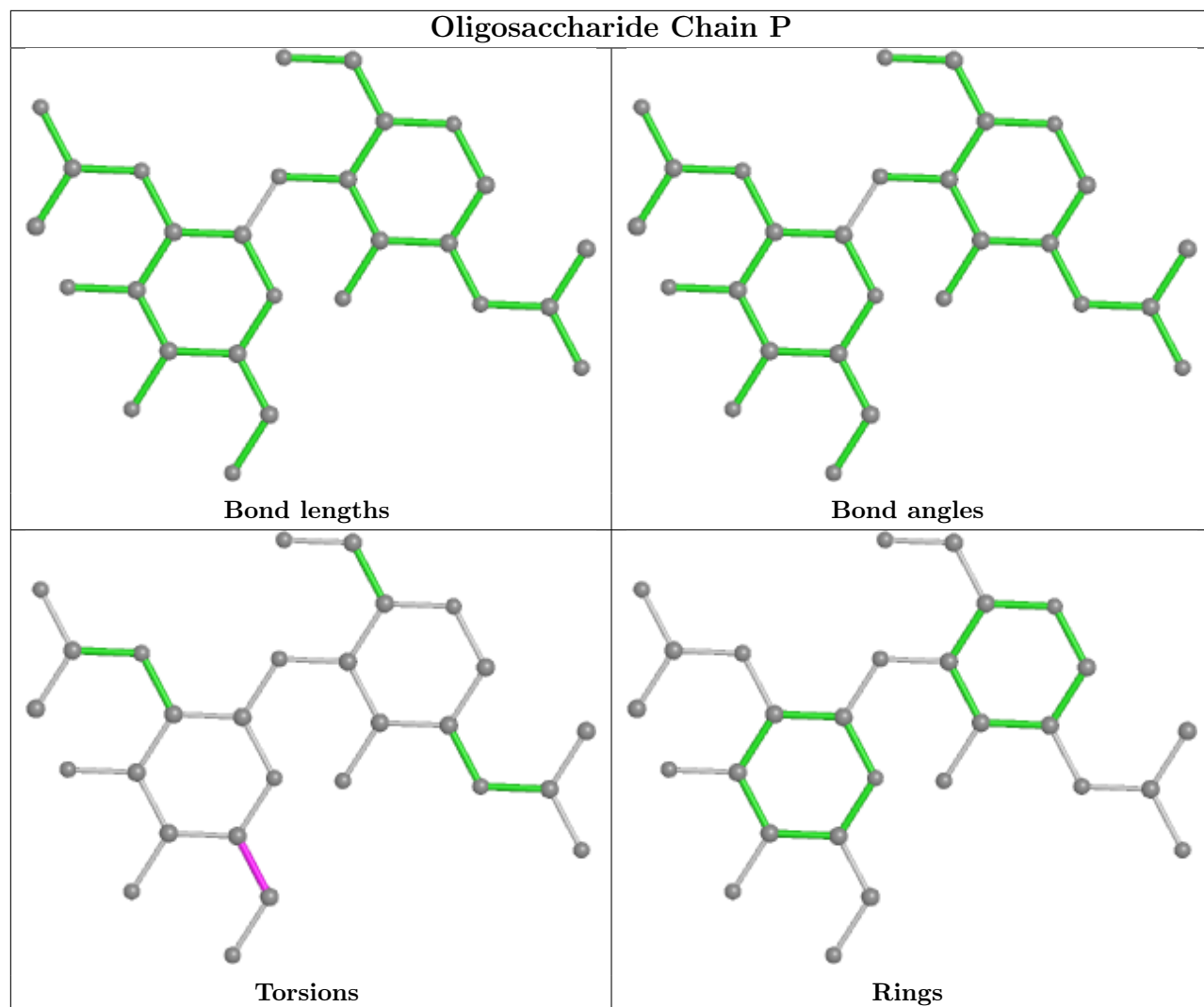
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	1	0
5	Q	1	NAG	1	0
5	M	1	NAG	1	0
5	U	1	NAG	1	0
5	W	1	NAG	1	0
5	S	1	NAG	1	0

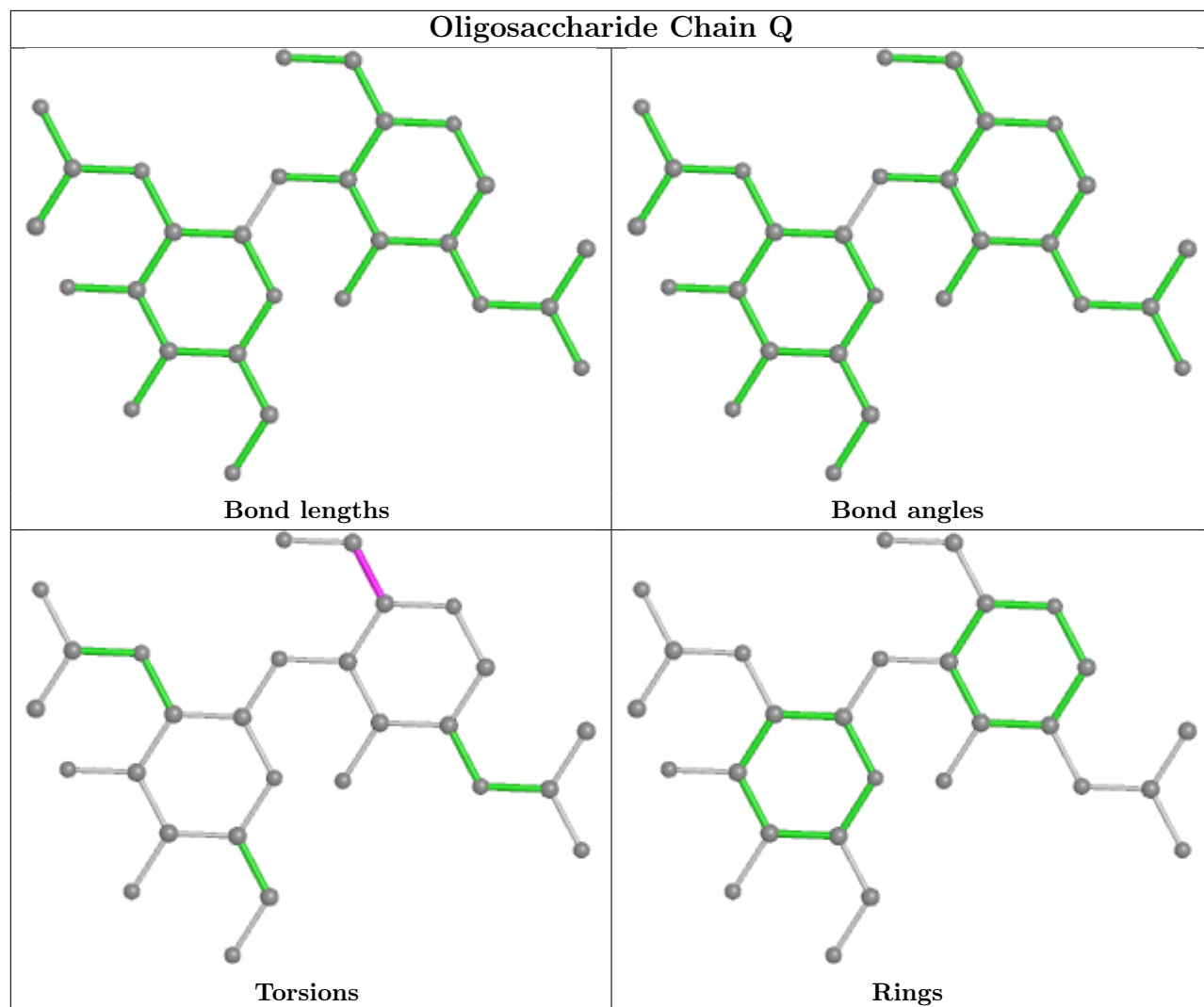
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

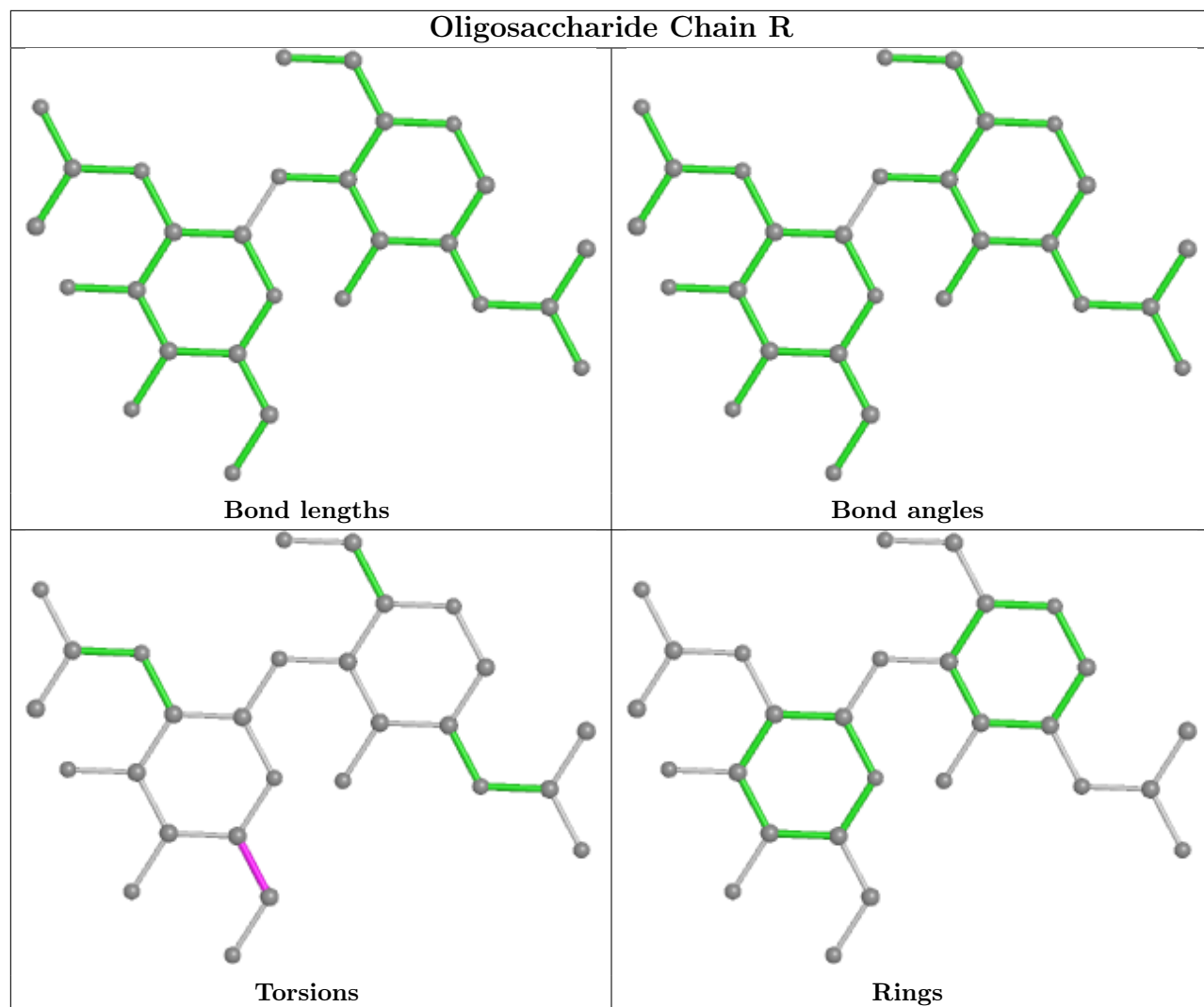


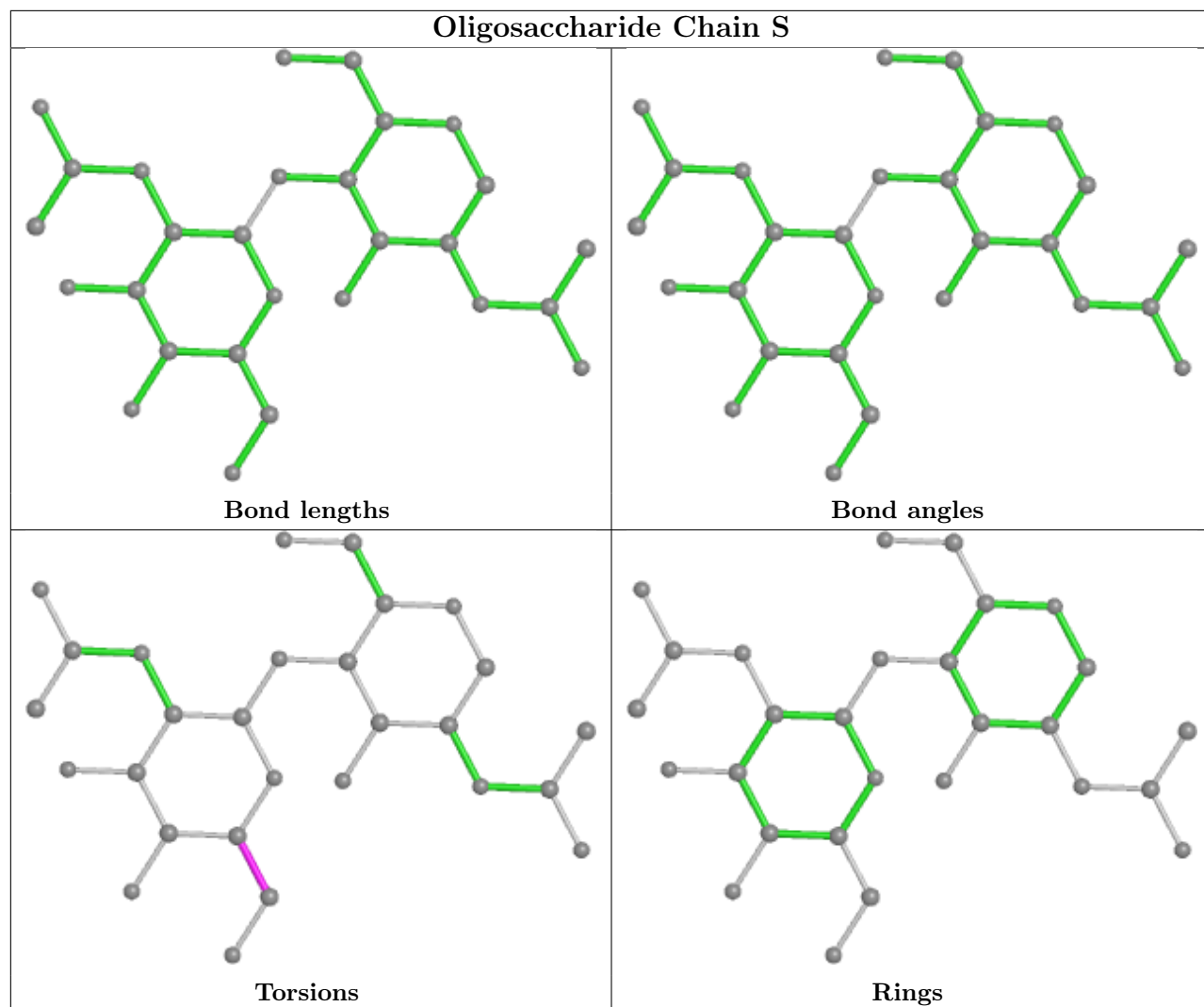


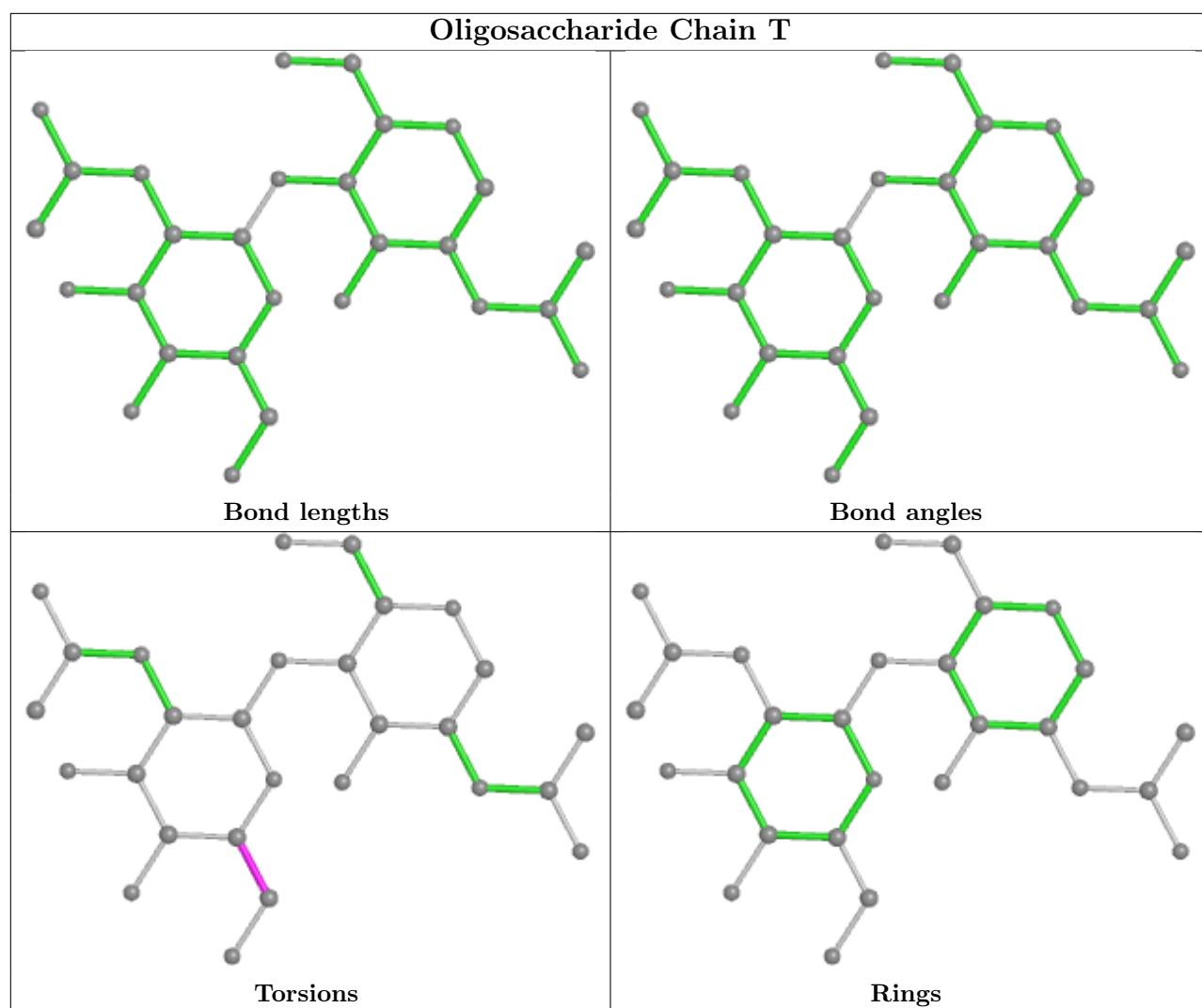


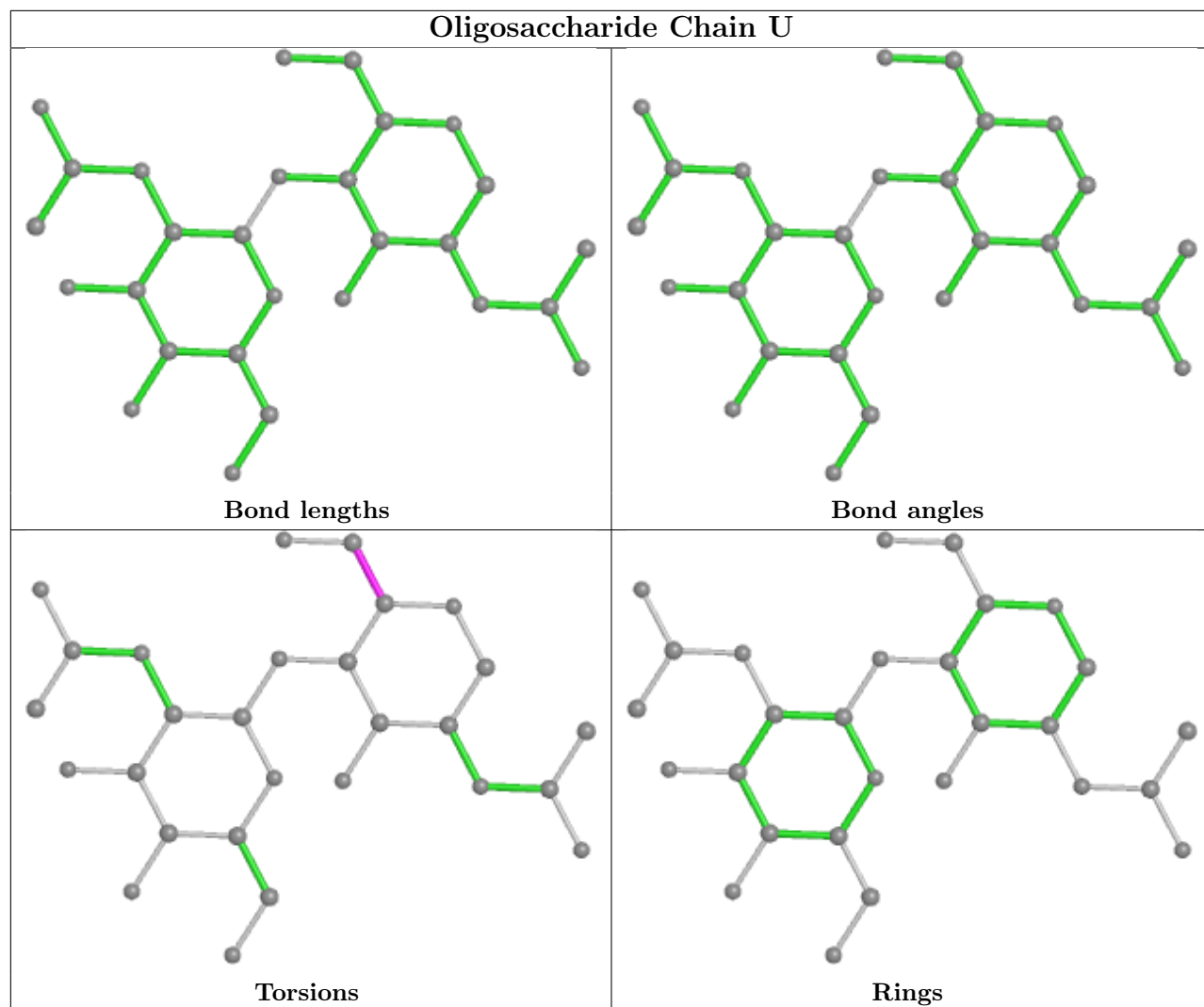


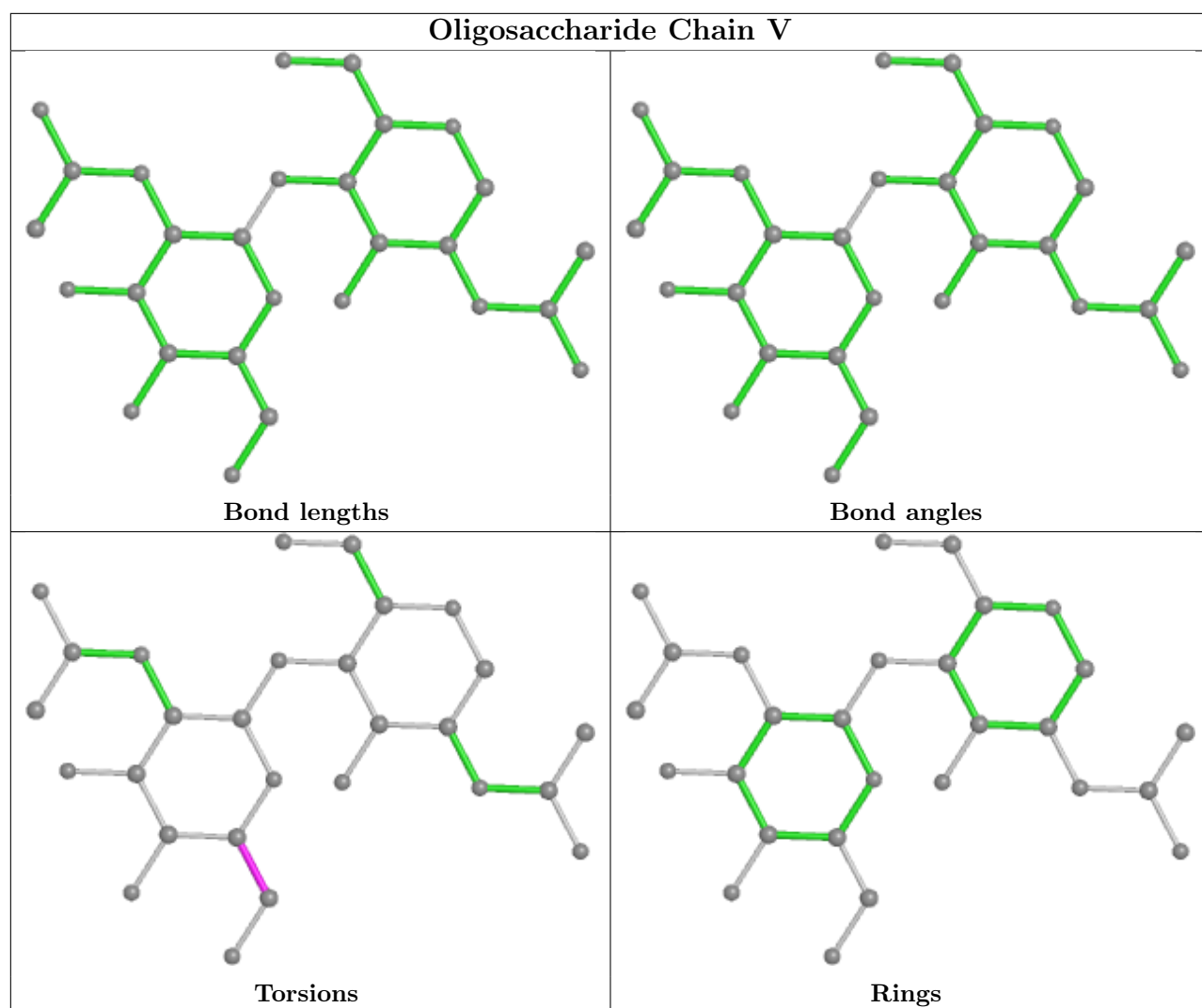


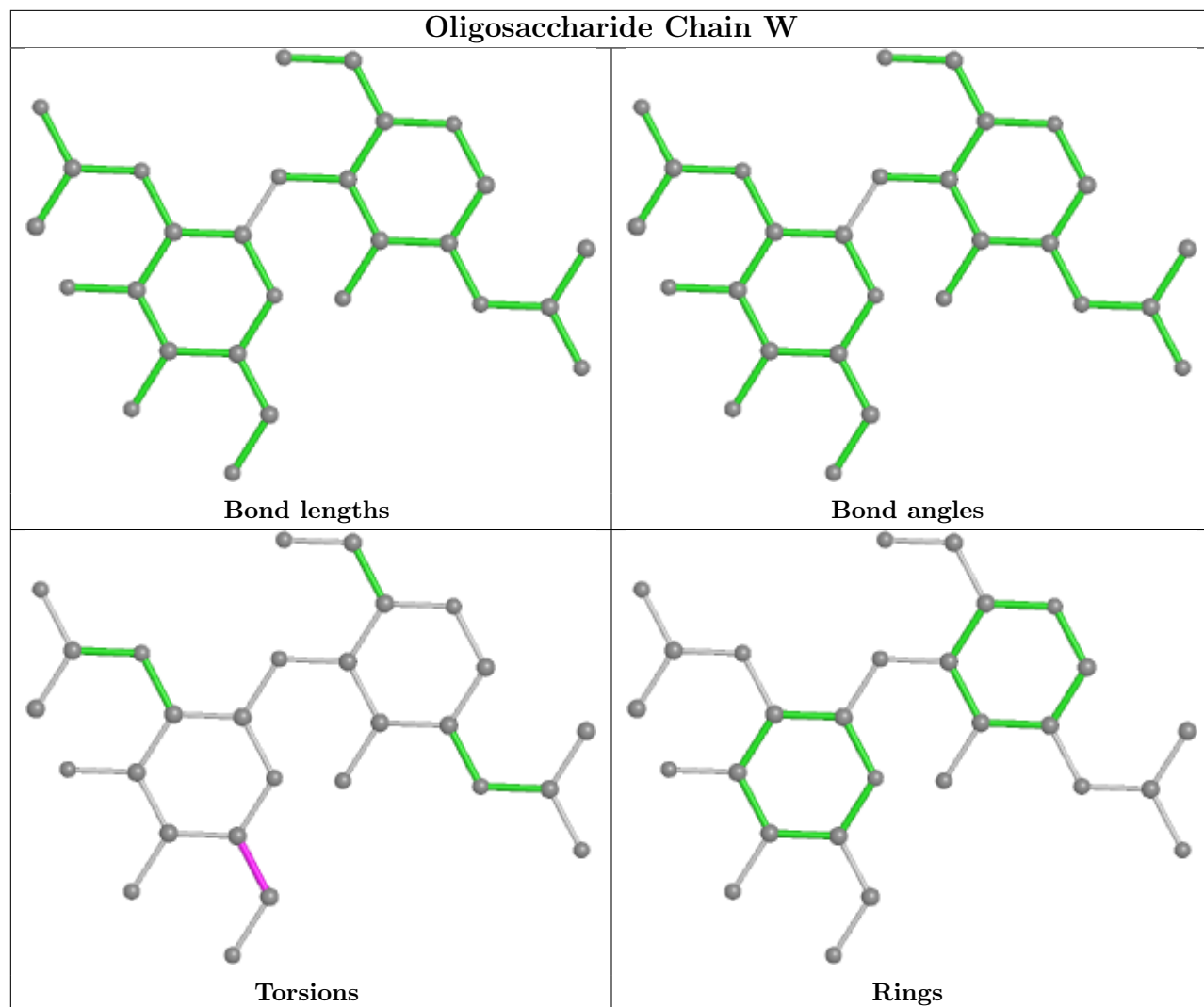


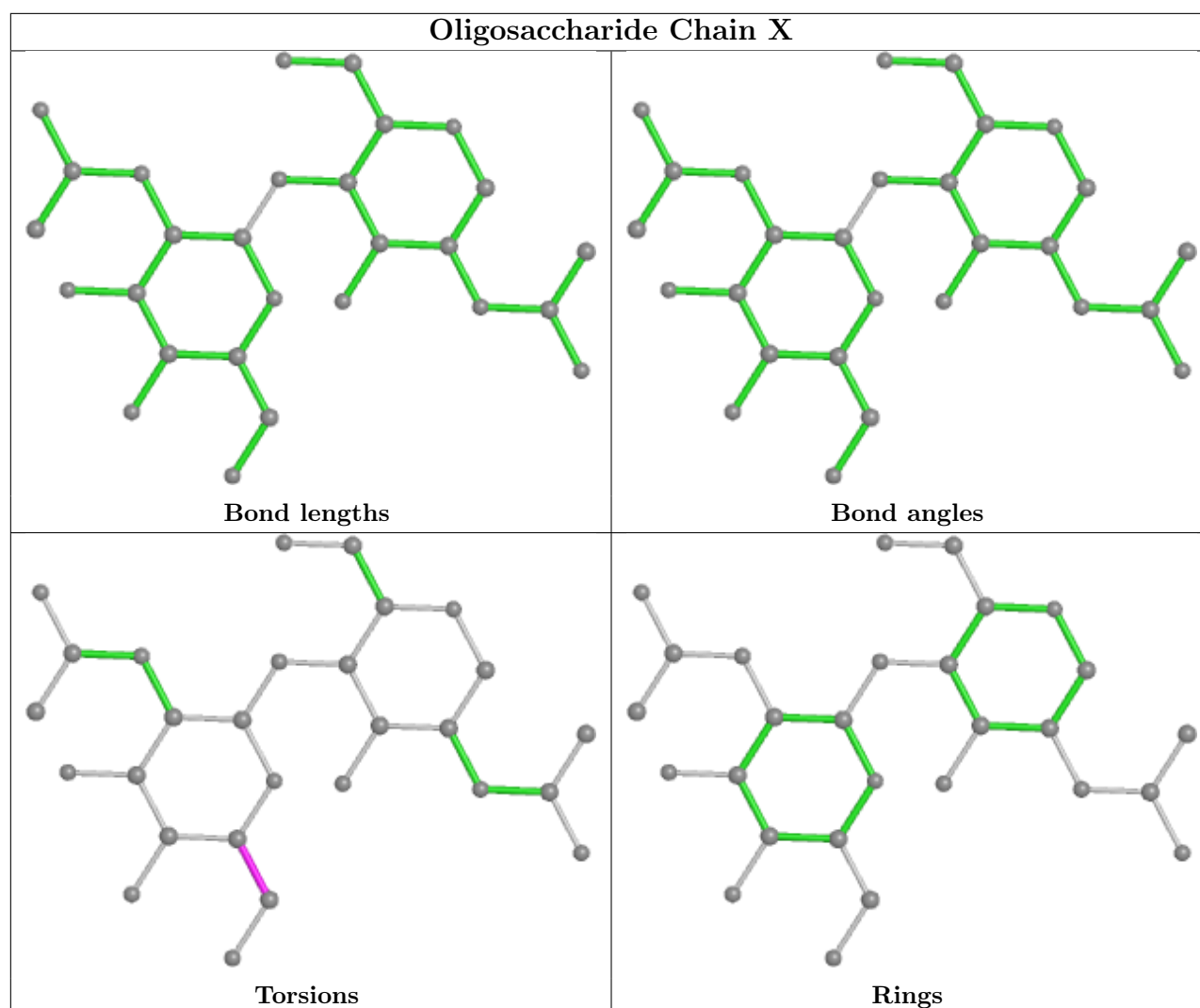












5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
6	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.42	0
6	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	C	1302	1	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	B	1307	1	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	D	702	2	14,14,15	0.45	0	17,19,21	1.26	1 (5%)
6	NAG	D	701	2	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	A	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	1302	1	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	F	701	2	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	E	702	2	14,14,15	0.44	0	17,19,21	1.27	1 (5%)
6	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	E	701	2	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	F	702	2	14,14,15	0.44	0	17,19,21	1.26	1 (5%)
6	NAG	B	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	C	1304	1	14,14,15	0.23	0	17,19,21	0.42	0
6	NAG	C	1307	1	14,14,15	0.22	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
6	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	D	702	2	-	5/6/23/26	0/1/1/1
6	NAG	D	701	2	-	4/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	F	701	2	-	4/6/23/26	0/1/1/1
6	NAG	E	702	2	-	5/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	E	701	2	-	4/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	F	702	2	-	5/6/23/26	0/1/1/1
6	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	NAG	C2-N2-C7	4.35	129.10	122.90
6	D	702	NAG	C2-N2-C7	4.33	129.07	122.90
6	F	702	NAG	C2-N2-C7	4.32	129.06	122.90

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1305	NAG	O5-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	D	702	NAG	O5-C5-C6-O6
6	E	702	NAG	O5-C5-C6-O6
6	F	702	NAG	O5-C5-C6-O6
6	A	1305	NAG	C4-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	D	701	NAG	C8-C7-N2-C2
6	D	701	NAG	O7-C7-N2-C2
6	D	702	NAG	C8-C7-N2-C2
6	D	702	NAG	O7-C7-N2-C2
6	E	701	NAG	C8-C7-N2-C2
6	E	701	NAG	O7-C7-N2-C2
6	E	702	NAG	C8-C7-N2-C2
6	E	702	NAG	O7-C7-N2-C2
6	F	701	NAG	C8-C7-N2-C2
6	F	701	NAG	O7-C7-N2-C2
6	F	702	NAG	C8-C7-N2-C2
6	F	702	NAG	O7-C7-N2-C2
6	F	702	NAG	C4-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	D	702	NAG	C4-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	E	702	NAG	C4-C5-C6-O6
6	C	1302	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	B	1306	NAG	C4-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	D	701	NAG	C4-C5-C6-O6

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Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	F	701	NAG	C4-C5-C6-O6
6	E	701	NAG	C4-C5-C6-O6
6	D	701	NAG	O5-C5-C6-O6
6	F	701	NAG	O5-C5-C6-O6
6	E	701	NAG	O5-C5-C6-O6
6	D	702	NAG	C3-C2-N2-C7
6	E	702	NAG	C3-C2-N2-C7
6	F	702	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1306	NAG	1	0
6	B	1307	NAG	1	0
6	D	702	NAG	1	0
6	E	702	NAG	1	0
6	B	1306	NAG	1	0
6	F	702	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.

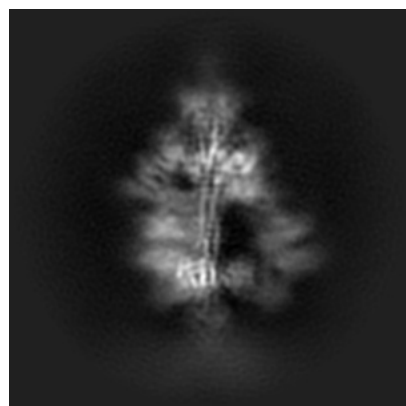
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65168. These allow visual inspection of the internal detail of the map and identification of artifacts.

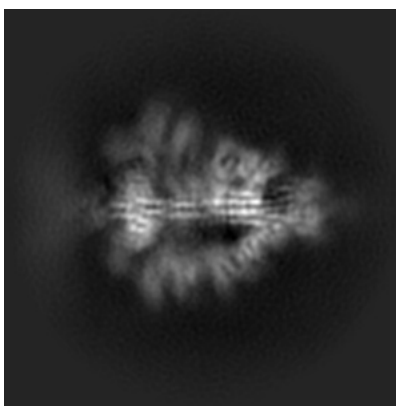
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

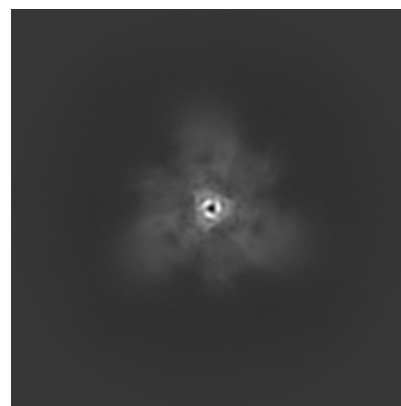
6.1.1 Primary map



X

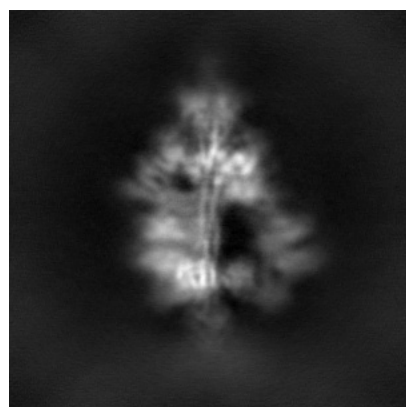


Y

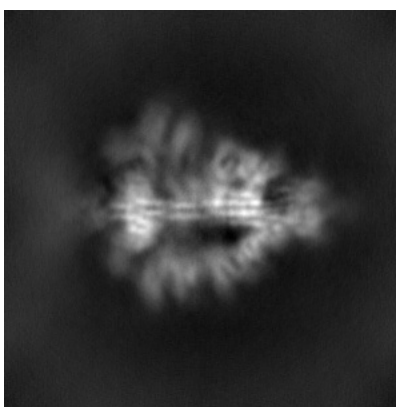


Z

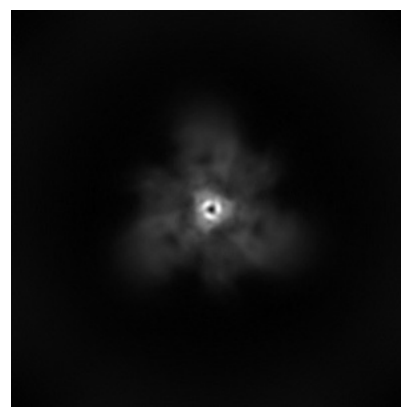
6.1.2 Raw map



X



Y

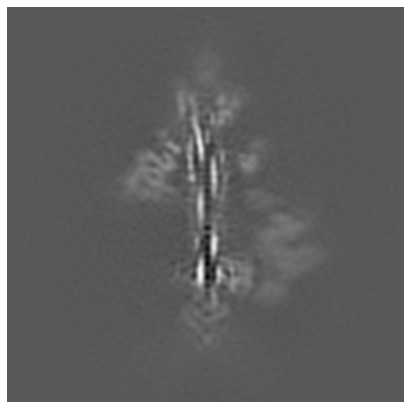


Z

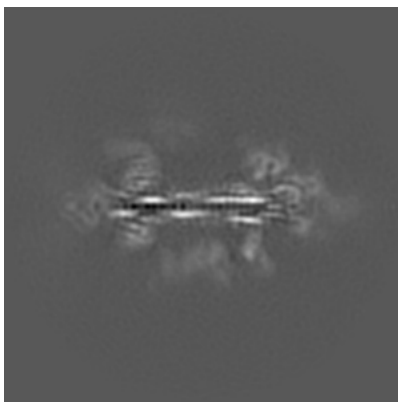
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

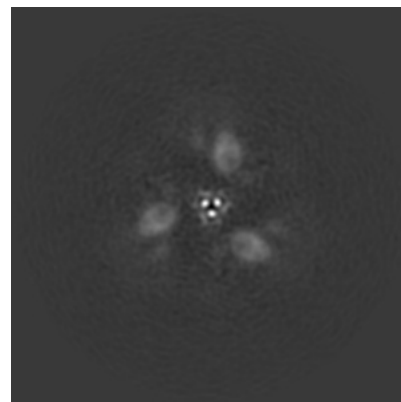
6.2.1 Primary map



X Index: 200

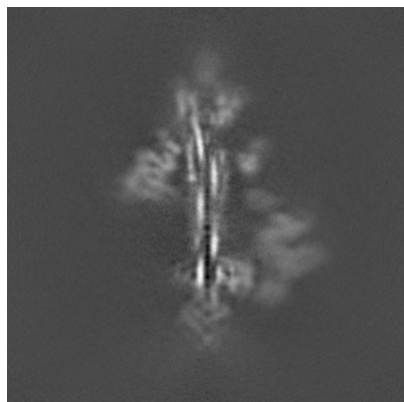


Y Index: 200

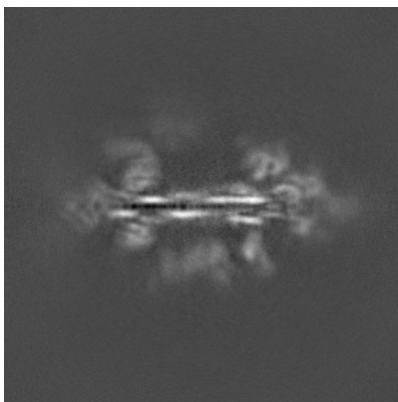


Z Index: 200

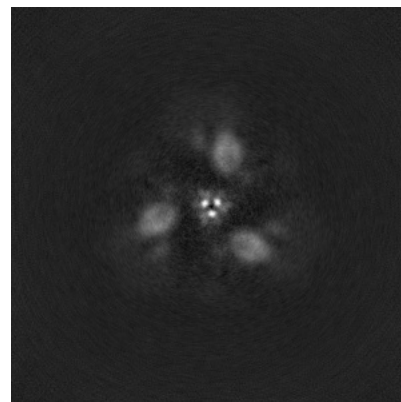
6.2.2 Raw map



X Index: 200



Y Index: 200

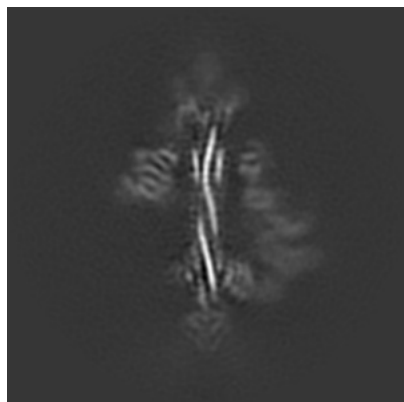


Z Index: 200

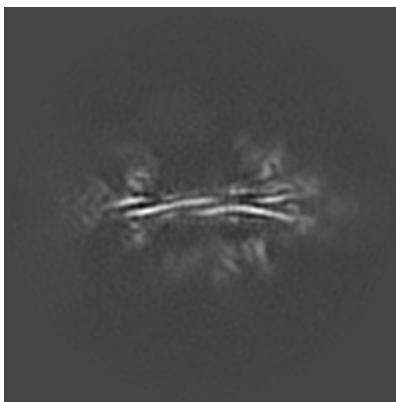
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

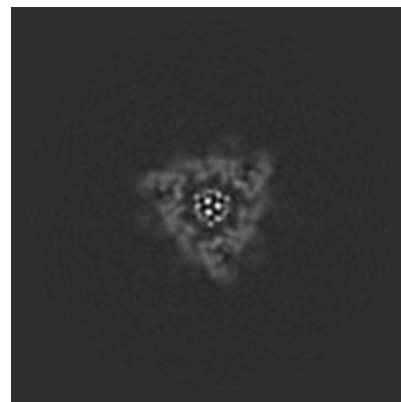
6.3.1 Primary map



X Index: 206

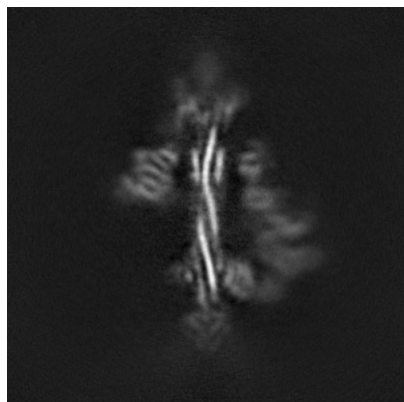


Y Index: 205

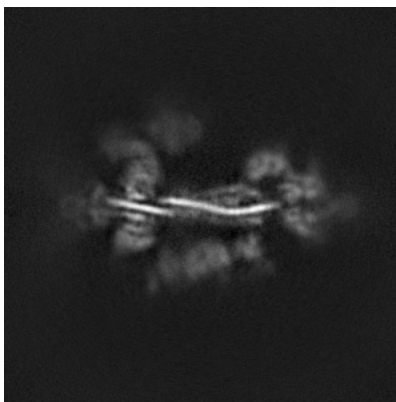


Z Index: 249

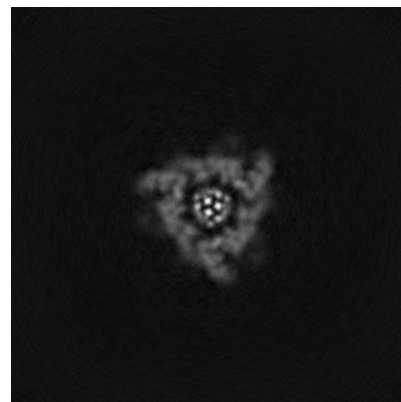
6.3.2 Raw map



X Index: 206



Y Index: 194

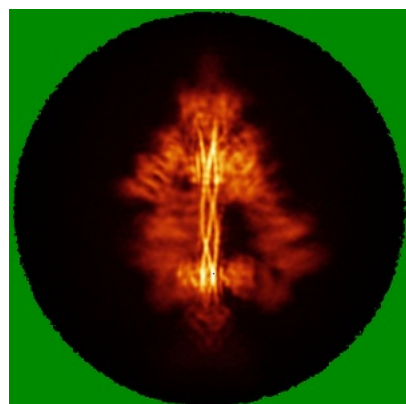


Z Index: 249

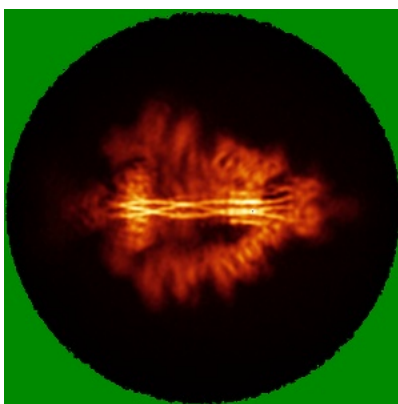
The images above show the largest variance slices of the map in three orthogonal directions.

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

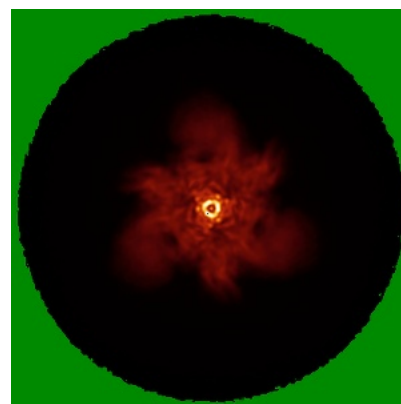
6.4.1 Primary map



X

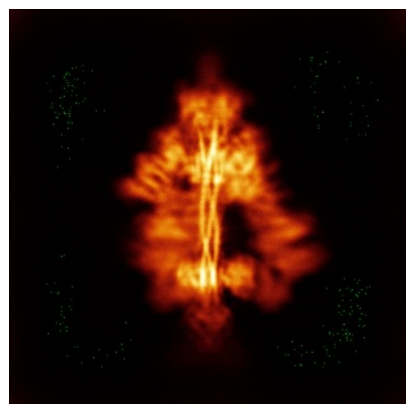


Y

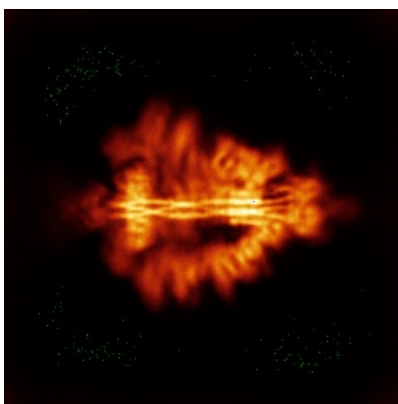


Z

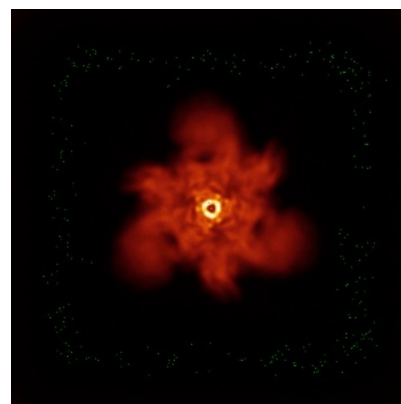
6.4.2 Raw map



X



Y

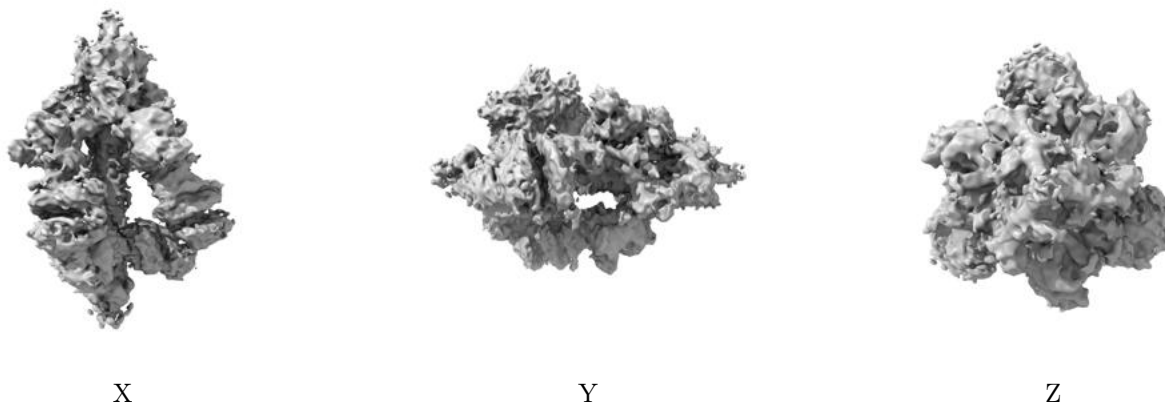


Z

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.

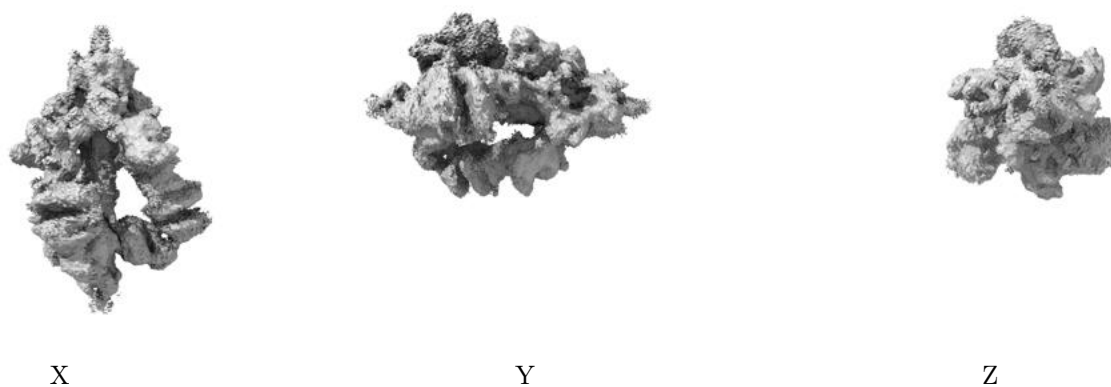
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

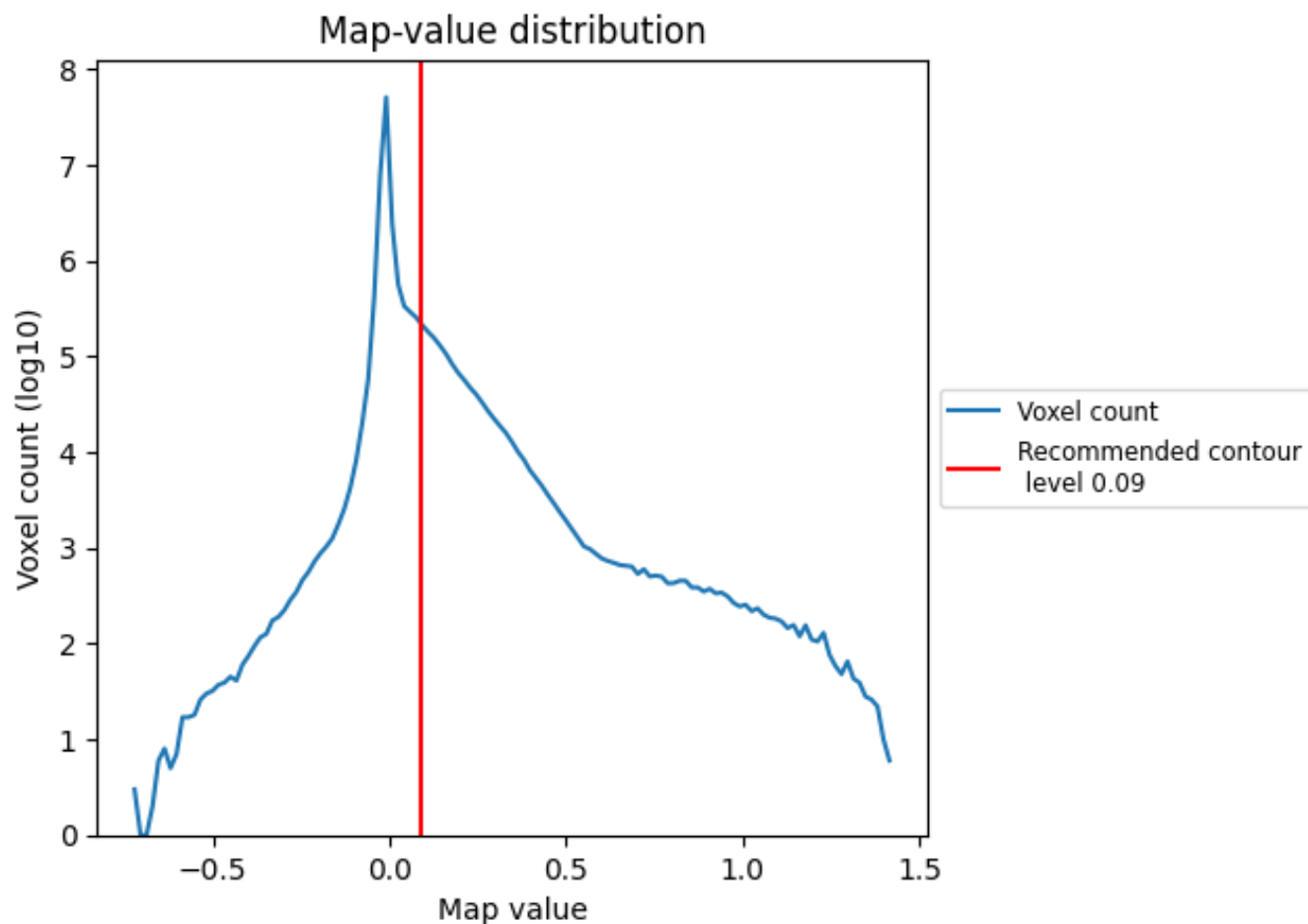
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

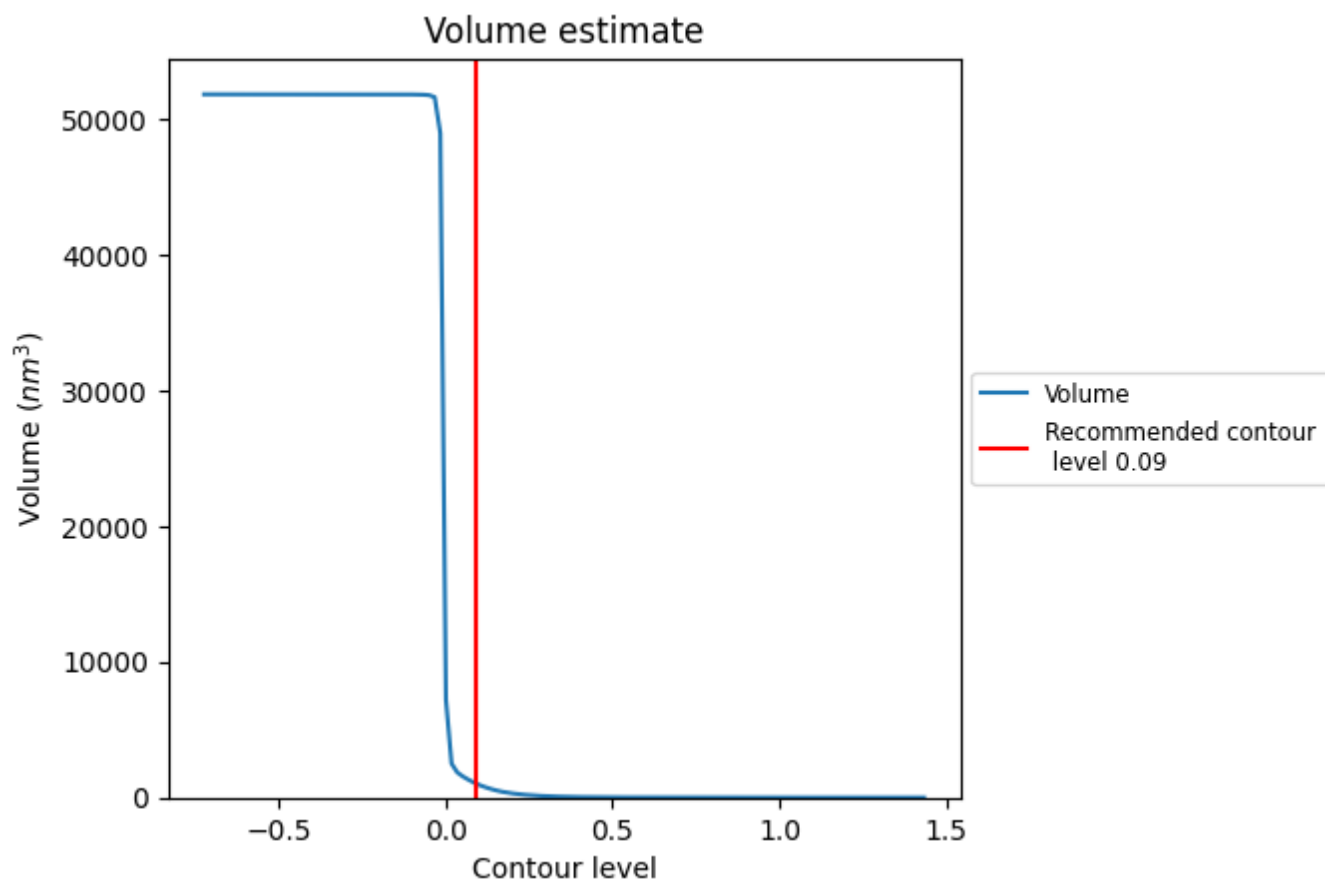
This section contains the results of statistical analysis of the map.

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.

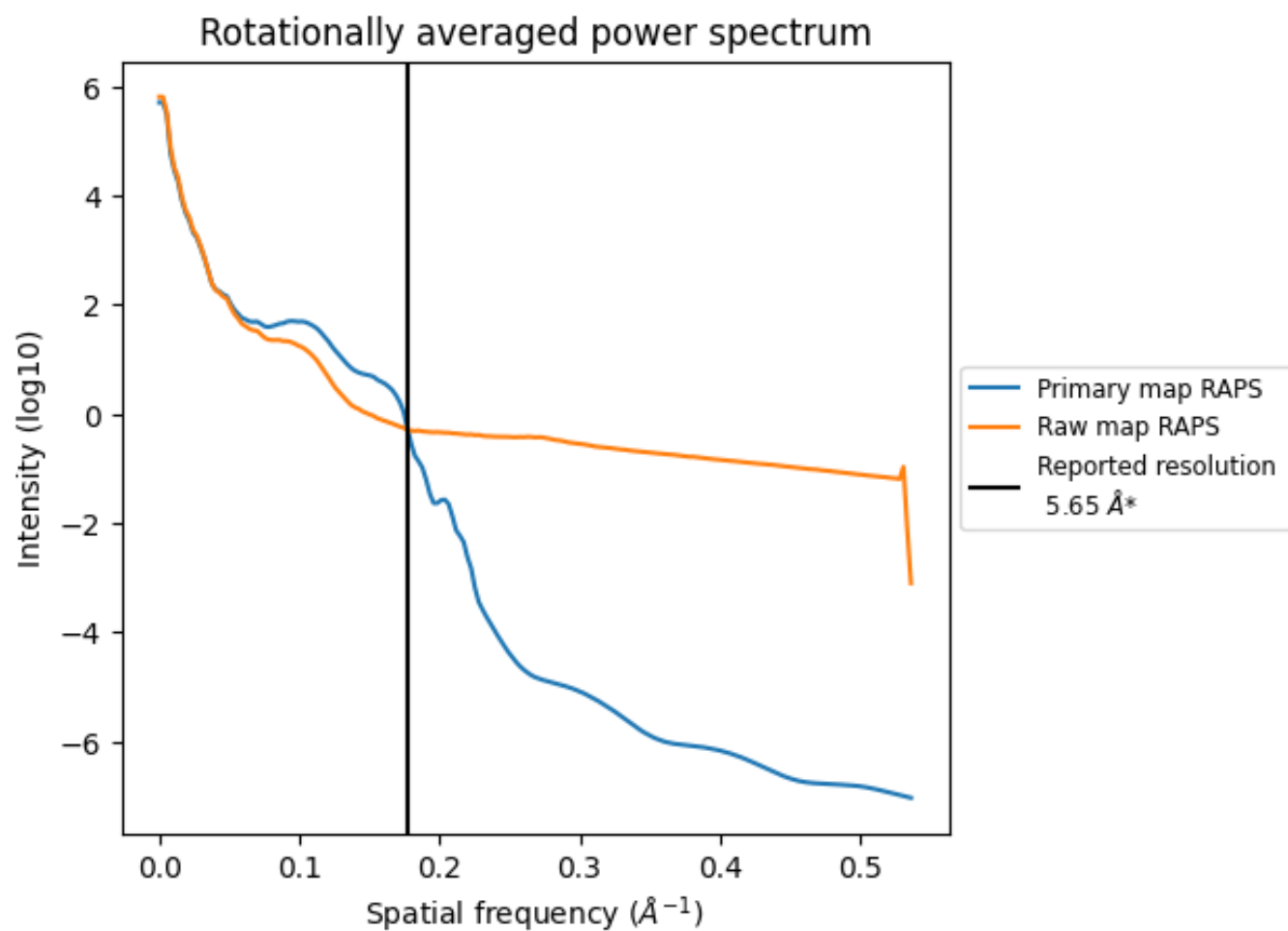
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1055 nm^3 ; this corresponds to an approximate mass of 953 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 ⓘ

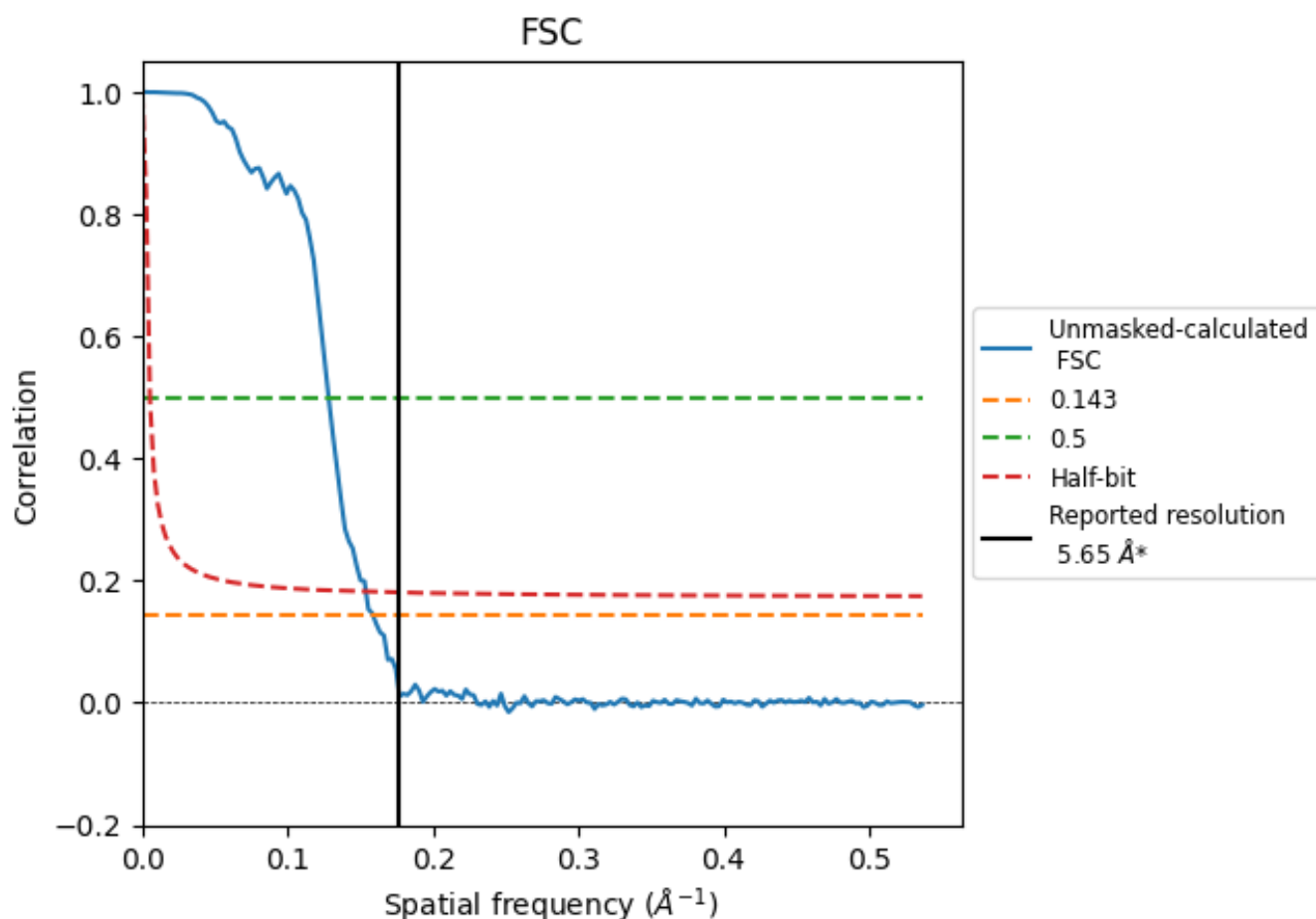


*Reported resolution corresponds to spatial frequency of 0.177 Å⁻¹

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 0.177 \AA^{-1}

8.2 Resolution estimates [i](#)

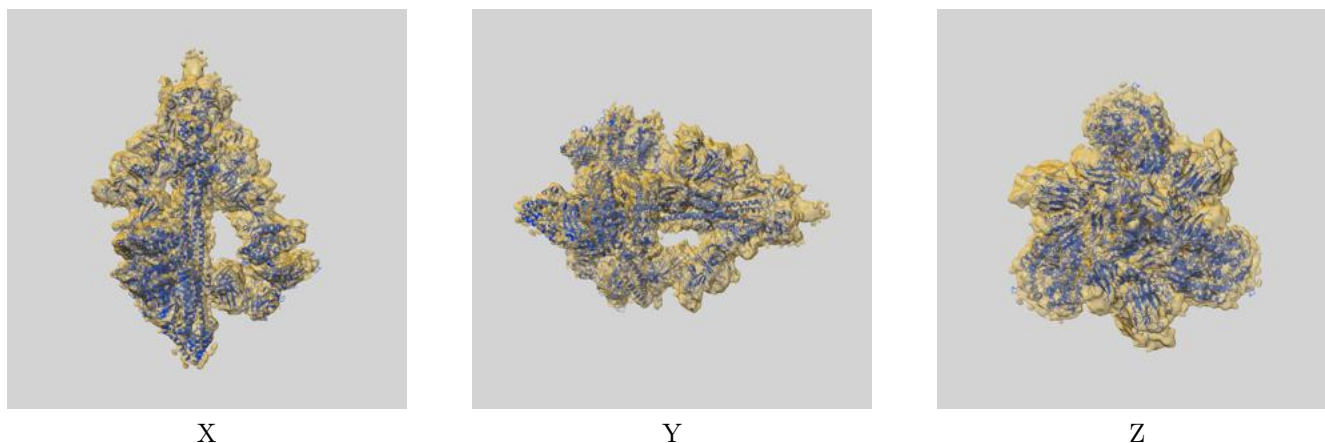
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.30	7.80	6.50

*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 6.30 differs from the reported value 5.65 by more than 10 %

9 Map-model fit [i](#)

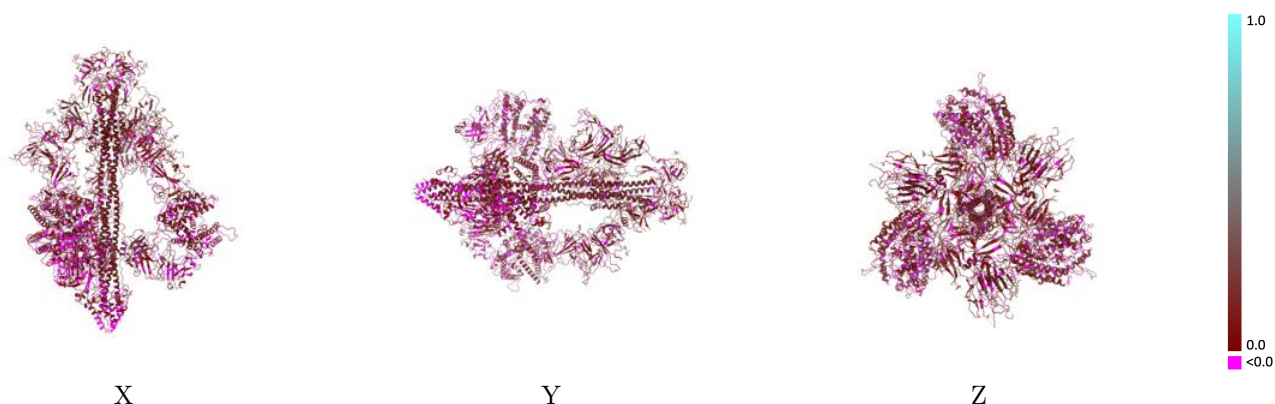
This section contains information regarding the fit between EMDB map EMD-65168 and PDB model 9VLT. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



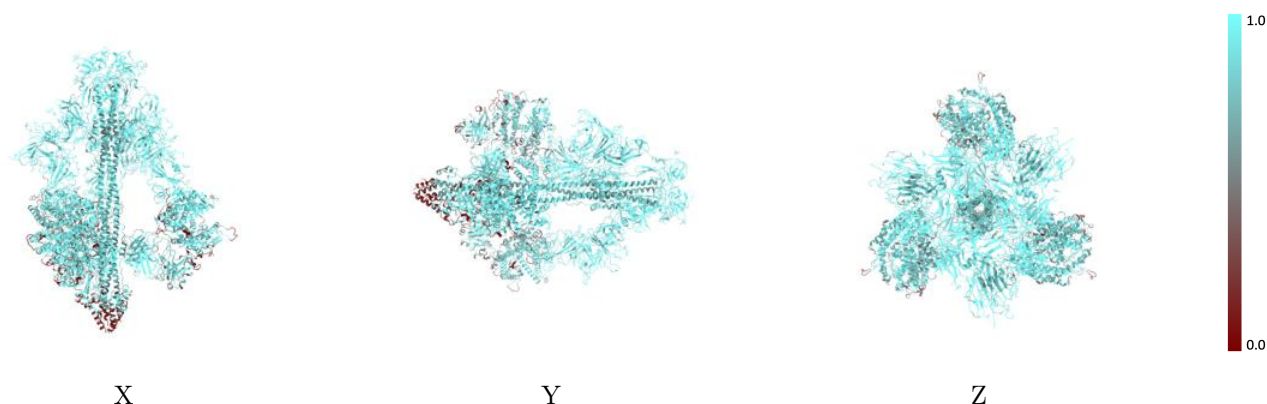
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



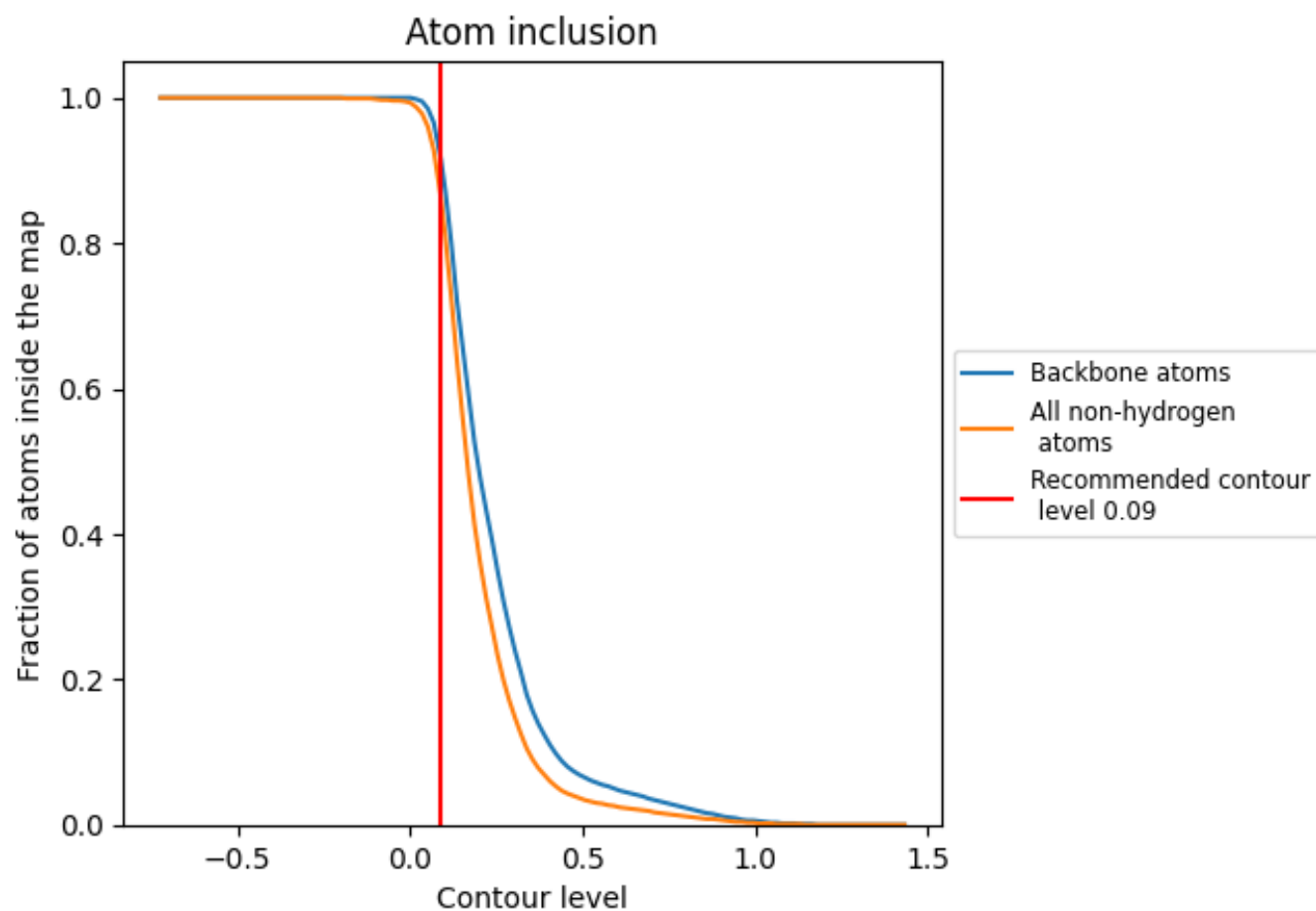
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.1080
A	 0.9030	 0.1340
B	 0.9000	 0.1350
C	 0.8990	 0.1350
D	 0.8090	 0.0720
E	 0.8090	 0.0730
F	 0.8070	 0.0730
G	 0.8430	 0.0860
H	 0.8260	 0.0860
I	 0.8420	 0.0880
J	 0.8250	 0.0900
K	 0.8460	 0.0900
L	 0.8230	 0.0900
M	 0.8930	 0.1350
N	 1.0000	 0.3010
O	 0.9640	 0.2890
P	 0.9640	 0.1950
Q	 0.9290	 0.1400
R	 1.0000	 0.3250
S	 0.9640	 0.2810
T	 0.9640	 0.2080
U	 0.9290	 0.1540
V	 1.0000	 0.3110
W	 0.9640	 0.2750
X	 0.9640	 0.1920

