



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:10 PM UTC

PDB ID : 8K46 / pdb_00008k46
EMDB ID : EMD-36878
Title : A potent and broad-spectrum neutralizing nanobody for SARS-CoV-2 viruses including all major Omicron strains
Authors : Lu, Y.; Gao, Y.; Yao, H.; Xu, W.; Yang, H.
Deposited on : 2023-07-17
Resolution : 3.37 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:

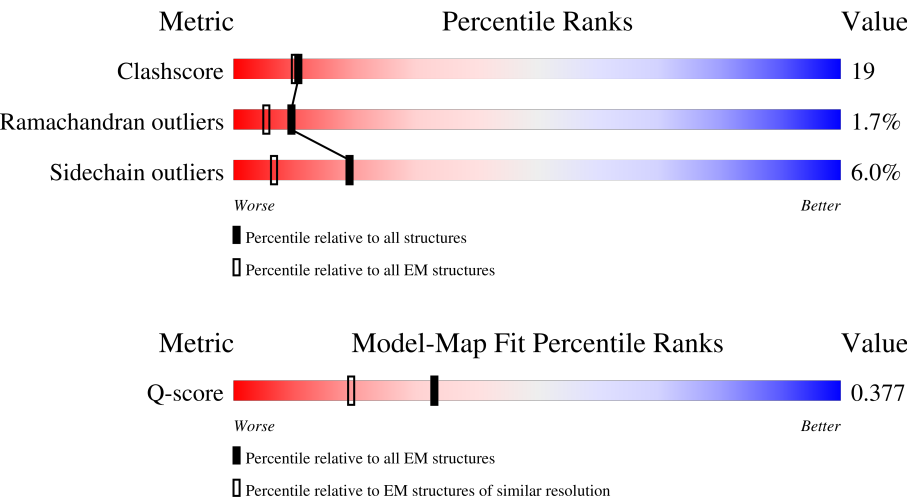
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.37 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14287 (2.87 - 3.87)

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	E	124	85% 63%37%
1	G	124	82% 61%38%
1	I	124	21% 48%50%
2	A	1288	6% 53%29%16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	1288	
2	C	1288	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 28908 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 nanobody Nb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	124	Total	C	N	O	S	1	0
			987	623	168	191	5		
1	G	124	Total	C	N	O	S	1	0
			977	617	164	191	5		
1	I	124	Total	C	N	O	S	1	0
			987	623	168	191	5		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1083	Total	C	N	O	S	0	0
			8410	5373	1397	1603	37		
2	B	1081	Total	C	N	O	S	0	0
			8413	5379	1392	1605	37		
2	C	1084	Total	C	N	O	S	0	0
			8448	5402	1401	1607	38		

There are 354 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	658	SER	ASN	conflict	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	conflict	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	655	TYR	HIS	variant	UNP P0DTC2
B	658	SER	ASN	conflict	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
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	conflict	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	658	SER	ASN	conflict	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	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
C	1241	GLU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
C	1283	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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 3 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
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

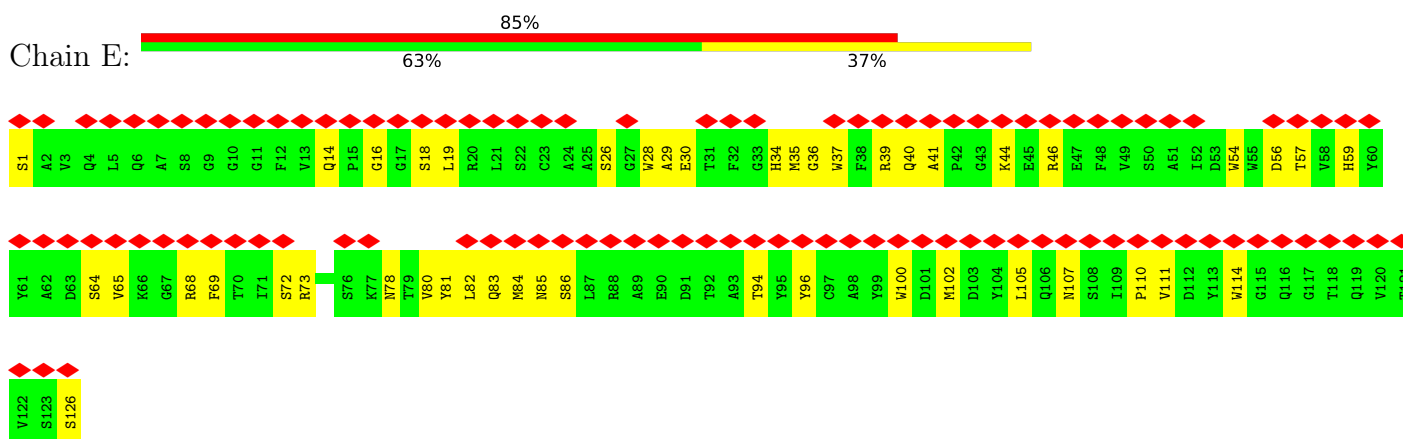
Continued from previous page...

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

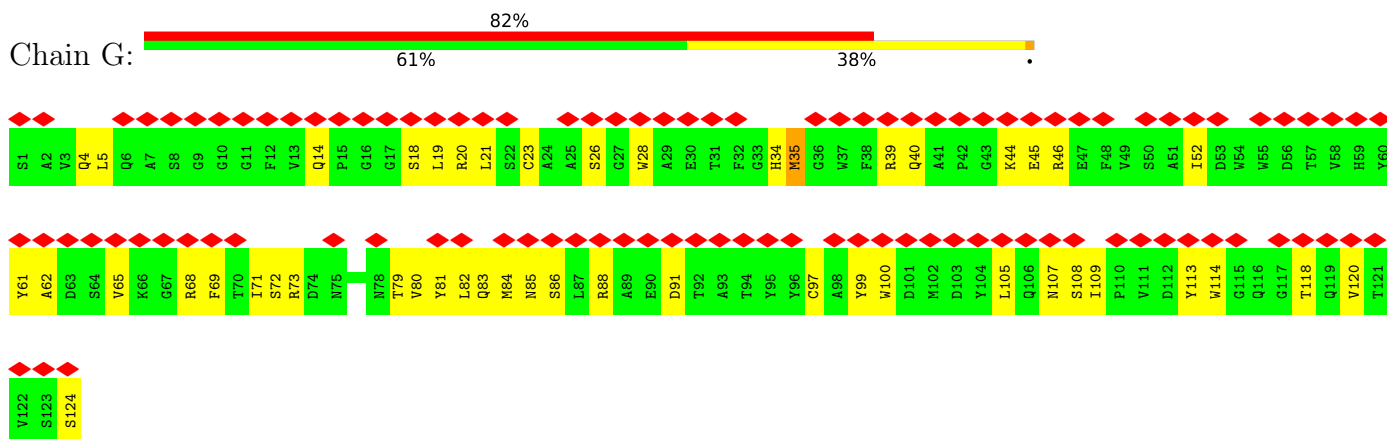
3 Residue-property plots

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

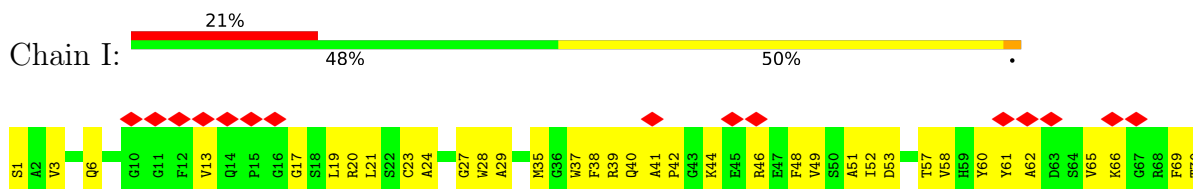
- Molecule 1: nanobody Nb4

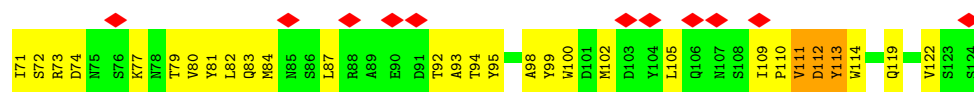


- Molecule 1: nanobody Nb4

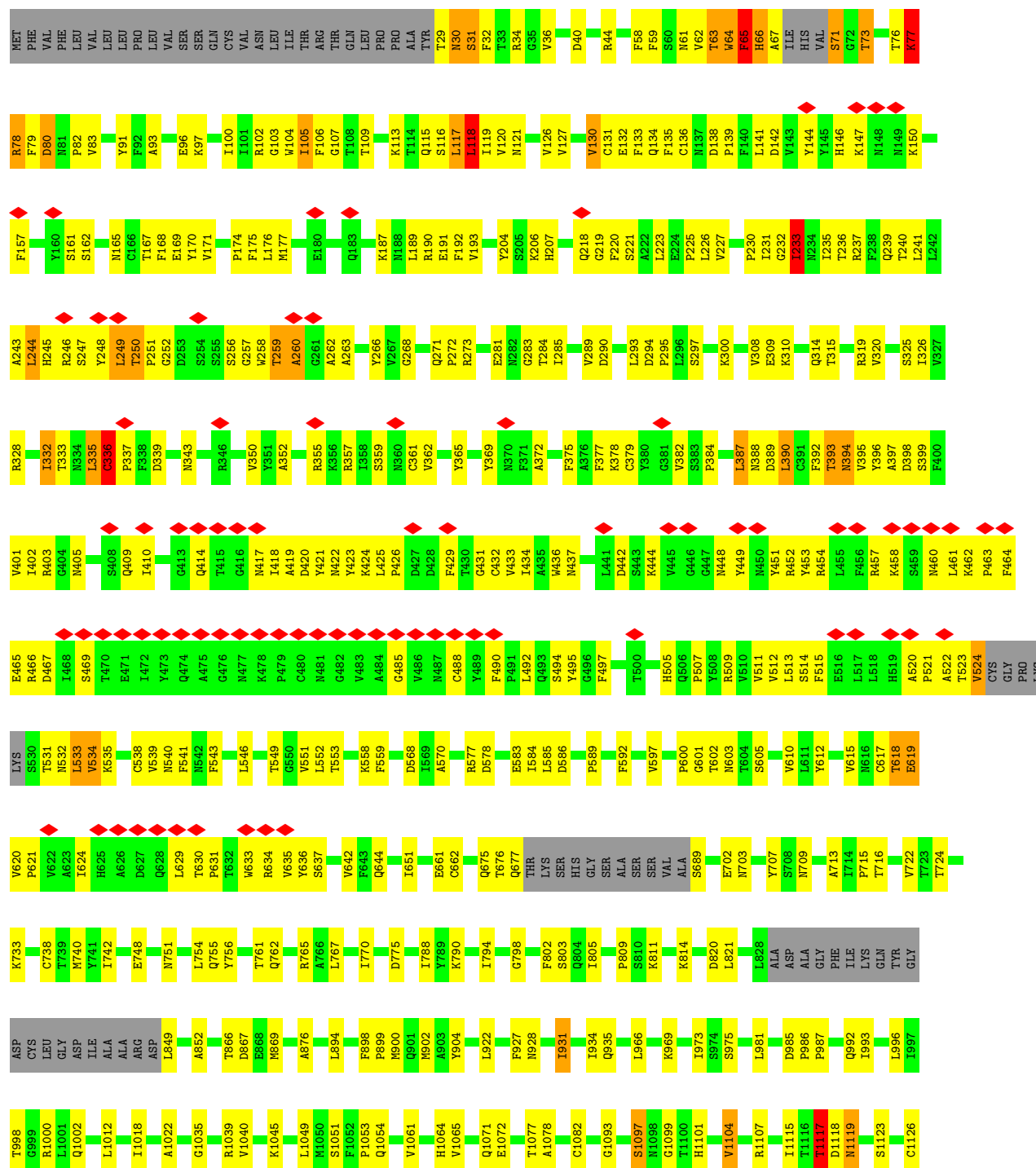


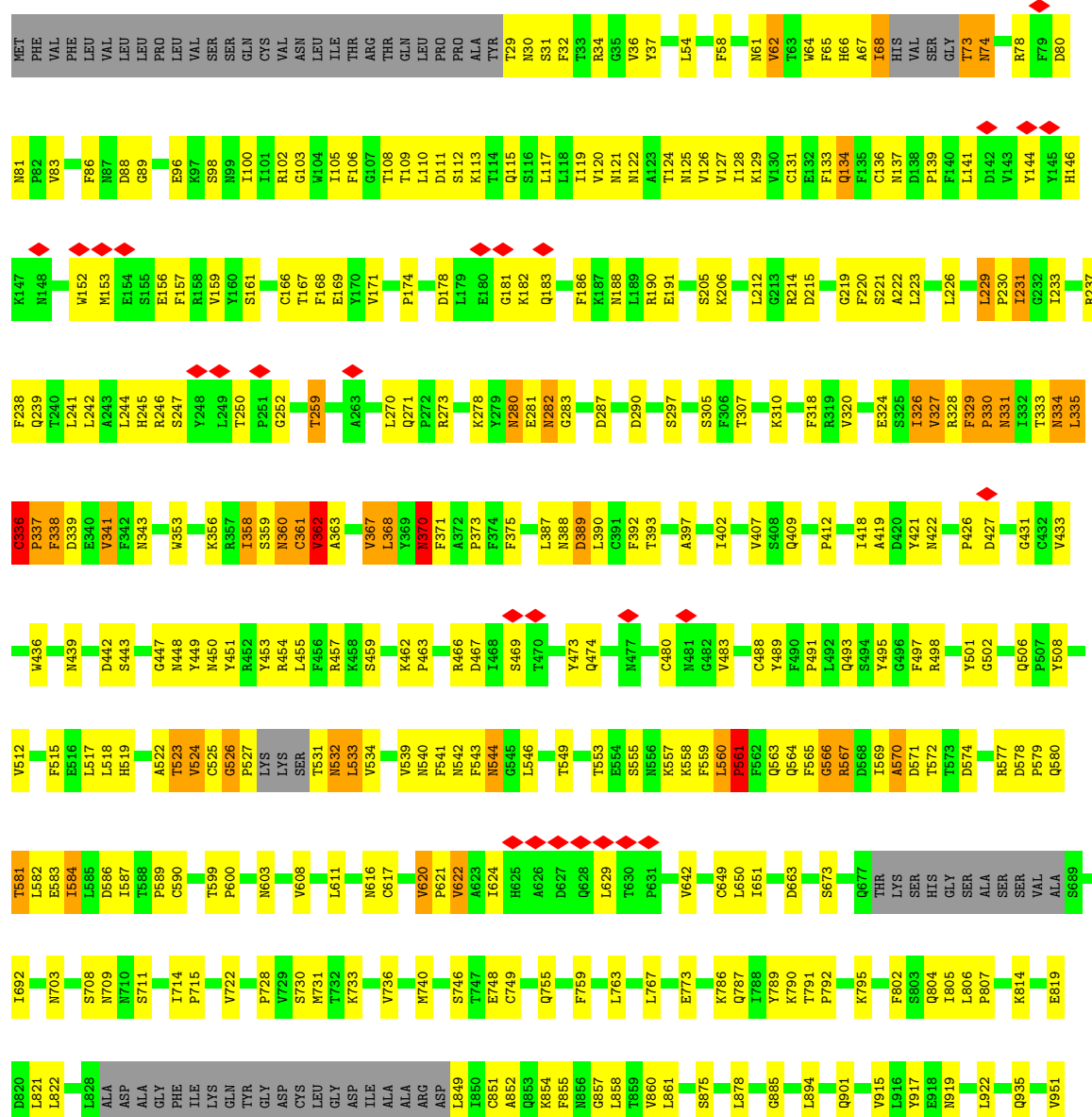
- Molecule 1: nanobody Nb4

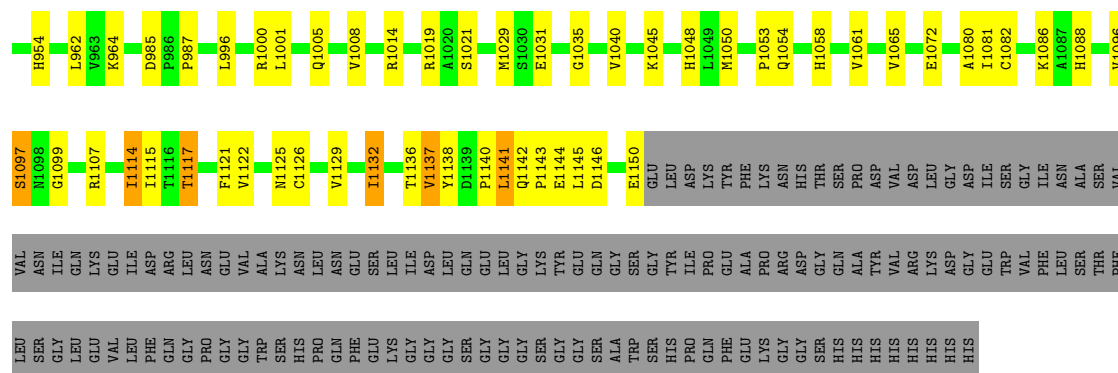




• Molecule 2: Spike glycoprotein







- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG2
MAG1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.778	Depositor
Minimum map value	-0.640	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.229	Depositor
Map size (Å)	417.792, 417.792, 417.792	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.816, 0.816, 0.816	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.11	0/1016	0.31	0/1382
1	G	0.37	0/1006	0.54	0/1371
1	I	0.28	0/1016	0.44	0/1382
2	A	0.38	0/8612	0.59	7/11736 (0.1%)
2	B	0.47	0/8616	0.68	6/11737 (0.1%)
2	C	0.38	0/8652	0.60	4/11785 (0.0%)
All	All	0.40	0/28918	0.61	17/39393 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	367	VAL	N-CA-C	-7.68	105.20	111.81
2	B	77	LYS	N-CA-C	-6.68	107.01	114.62
2	C	1121	PHE	CA-CB-CG	6.32	120.12	113.80
2	A	521	PRO	CB-CA-C	-6.24	103.91	111.46
2	C	622	VAL	N-CA-C	-5.93	104.85	110.42
2	A	107	GLY	CA-C-O	-5.67	118.04	122.52
2	B	242	LEU	N-CA-C	-5.52	105.17	113.89
2	B	282	ASN	N-CA-C	-5.46	107.18	112.97
2	C	337	PRO	N-CA-C	-5.28	101.60	112.47
2	B	1083	HIS	CB-CA-C	-5.20	102.62	110.83
2	A	1118	ASP	N-CA-C	-5.17	106.66	113.17
2	A	1119	ASN	N-CA-C	-5.17	107.65	114.31
2	A	1117	THR	N-CA-C	-5.12	105.93	113.61
2	B	561	PRO	N-CA-CB	-5.06	97.94	103.25
2	A	65	PHE	CA-C-N	-5.04	111.92	121.54
2	A	65	PHE	C-N-CA	-5.04	111.92	121.54
2	B	1117	THR	N-CA-C	-5.02	106.57	113.30

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	E	987	0	906	32	0
1	G	977	0	884	36	0
1	I	987	0	906	52	0
2	A	8410	0	8146	338	0
2	B	8413	0	8147	345	0
2	C	8448	0	8203	305	0
3	K	28	0	25	1	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	X	28	0	25	1	0
3	Y	28	0	25	0	0
3	Z	28	0	25	1	0
3	a	28	0	25	0	0
4	A	112	0	104	4	0
4	B	140	0	130	2	0
4	C	98	0	91	0	0
All	All	28908	0	27817	1062	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 19.

All (1062) 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)
2:B:379:CYS:HA	2:B:432:CYS:HA	1.42	1.02
2:A:71:SER:HA	2:A:79:PHE:HA	1.42	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:617:CYS:HA	2:A:621:PRO:HD2	1.46	0.95
2:A:617:CYS:C	2:A:619:GLU:H	1.74	0.95
2:B:44:ARG:HH21	2:B:49:HIS:CG	1.86	0.93
2:C:393:THR:HA	2:C:522:ALA:HA	1.50	0.92
2:A:620:VAL:HG13	2:A:621:PRO:HD3	1.52	0.92
2:C:337:PRO:HA	2:C:358:ILE:HD12	1.51	0.90
1:G:73:ARG:HA	1:G:80:VAL:HA	1.52	0.88
2:B:44:ARG:NH2	2:B:49:HIS:CE1	2.43	0.87
2:C:139:PRO:HA	2:C:157:PHE:HA	1.56	0.86
2:C:331:ASN:HA	2:C:580:GLN:HG3	1.57	0.85
2:C:519:HIS:CD2	2:C:567:ARG:HH21	1.95	0.84
2:B:337:PRO:HG2	2:B:358:ILE:HG23	1.60	0.83
1:E:1:SER:HB3	1:E:30:GLU:HB2	1.59	0.83
2:A:621:PRO:HA	2:A:624:ILE:HG23	1.59	0.82
2:B:79:PHE:HD1	2:B:242:LEU:HD12	1.42	0.81
2:A:617:CYS:HB2	2:A:621:PRO:HB2	1.63	0.81
2:B:426:PRO:HG2	2:B:429:PHE:HB2	1.62	0.81
2:B:44:ARG:NH2	2:B:49:HIS:ND1	2.32	0.77
2:B:624:ILE:HD11	2:B:637:SER:HA	1.66	0.77
2:A:61:ASN:HB3	2:A:258:TRP:HA	1.65	0.77
2:A:96:GLU:HB2	2:A:100:ILE:HB	1.67	0.76
2:B:102:ARG:HD3	2:B:244:LEU:HD13	1.67	0.76
2:C:336:CYS:HB3	2:C:362:VAL:H	1.49	0.76
2:B:107:GLY:H	2:B:235:ILE:HG23	1.49	0.76
2:A:403:ARG:HD2	2:A:505:HIS:HA	1.67	0.75
2:C:83:VAL:HG23	2:C:239:GLN:HB2	1.69	0.75
2:B:44:ARG:NH2	2:B:49:HIS:CG	2.55	0.74
2:B:40:ASP:CG	2:B:44:ARG:HH12	1.96	0.74
2:B:129:LYS:HE3	2:B:166:CYS:HB3	1.70	0.74
1:I:73:ARG:HA	1:I:80:VAL:HA	1.69	0.74
2:A:617:CYS:O	2:A:619:GLU:N	2.20	0.74
2:B:44:ARG:HH22	2:B:49:HIS:CE1	2.04	0.74
2:B:362:VAL:HA	2:B:524:VAL:HG11	1.69	0.74
2:B:336:CYS:HA	2:B:361:CYS:HA	1.69	0.73
2:A:126:VAL:HG13	2:A:174:PRO:HA	1.71	0.73
2:A:335:LEU:HB3	2:A:361:CYS:HB3	1.68	0.73
1:E:40:GLN:HB2	1:E:46:ARG:HG3	1.70	0.73
2:A:106:PHE:HB3	2:A:235:ILE:HD12	1.70	0.73
2:B:405:ASN:N	2:B:504:GLY:O	2.22	0.73
1:E:65:VAL:HB	1:E:69:PHE:HB2	1.69	0.72
2:A:335:LEU:HB3	2:A:361:CYS:CB	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:858:LEU:HD11	2:C:962:LEU:HD22	1.72	0.71
2:B:105:ILE:HD11	2:B:241:LEU:HD21	1.73	0.71
2:C:454:ARG:NH2	2:C:469:SER:O	2.24	0.71
2:B:42:VAL:CG2	2:B:44:ARG:HH11	2.03	0.71
2:B:112:SER:HB3	2:B:134:GLN:HA	1.72	0.71
2:B:303:LEU:HD22	2:B:308:VAL:HG12	1.73	0.71
2:A:193:VAL:HB	2:A:204:TYR:HB2	1.73	0.71
2:A:102:ARG:NH2	2:A:121:ASN:O	2.24	0.70
2:A:395:VAL:HG22	2:A:515:PHE:HB3	1.74	0.70
2:B:64:TRP:HE1	2:B:260:ALA:HA	1.55	0.70
2:A:263:ALA:HB3	2:A:266:TYR:CZ	2.27	0.70
2:A:740:MET:HG2	2:B:319:ARG:HE	1.57	0.69
2:B:905:ARG:NH1	2:B:1049:LEU:O	2.24	0.69
2:A:770:ILE:HD12	2:A:1012:LEU:HD22	1.75	0.69
1:G:61:TYR:HE1	1:G:71:ILE:H	1.38	0.69
2:B:422:ASN:ND2	2:B:454:ARG:O	2.26	0.68
2:A:437:ASN:ND2	2:A:507:PRO:O	2.27	0.68
2:A:401:VAL:HG22	2:A:509:ARG:HG2	1.74	0.68
2:B:773:GLU:OE1	2:B:774:GLN:NE2	2.26	0.68
2:C:519:HIS:HD2	2:C:567:ARG:HH21	1.41	0.68
2:C:624:ILE:HG21	2:C:629:LEU:HD13	1.76	0.68
2:B:451:TYR:HB3	2:B:495:TYR:HD2	1.57	0.68
2:A:378:LYS:HG3	2:A:433:VAL:HB	1.75	0.68
2:B:139:PRO:HB3	2:B:243:ALA:HB2	1.76	0.68
2:C:83:VAL:HG21	2:C:237:ARG:HH21	1.56	0.68
2:C:1053:PRO:O	2:C:1054:GLN:NE2	2.26	0.68
2:C:491:PRO:O	2:C:493:GLN:NE2	2.27	0.67
1:I:39:ARG:HG3	1:I:95:TYR:HD1	1.60	0.67
2:A:105:ILE:HG12	2:A:241:LEU:HD21	1.77	0.67
2:B:335:LEU:HG	2:B:360:ASN:HB2	1.77	0.67
2:B:100:ILE:O	2:B:242:LEU:HA	1.95	0.67
2:C:1138:TYR:HE1	2:C:1143:PRO:HG2	1.59	0.67
2:B:44:ARG:HG2	2:B:47:VAL:HG11	1.77	0.67
2:C:455:LEU:H	2:C:493:GLN:HE22	1.43	0.67
2:B:43:PHE:O	2:B:44:ARG:C	2.37	0.66
2:C:328:ARG:HH11	2:C:533:LEU:HB3	1.59	0.66
2:B:458:LYS:HG3	2:B:473:TYR:HD1	1.61	0.66
2:A:1053:PRO:O	2:A:1054:GLN:NE2	2.29	0.66
2:B:64:TRP:HE1	2:B:260:ALA:CA	2.09	0.66
2:B:336:CYS:CA	2:B:361:CYS:HA	2.25	0.66
2:B:821:LEU:HD22	2:B:935:GLN:HG3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:328:ARG:HH21	2:A:533:LEU:HA	1.61	0.66
2:C:81:ASN:O	2:C:239:GLN:NE2	2.28	0.66
1:G:20:ARG:HE	1:G:81:TYR:HB3	1.61	0.65
2:A:319:ARG:HH11	2:C:740:MET:HE2	1.61	0.65
2:A:393:THR:HB	2:A:520:ALA:HB3	1.78	0.65
2:A:444:LYS:H	2:A:448:ASN:HB2	1.62	0.65
2:C:98:SER:O	2:C:102:ARG:NH2	2.29	0.65
2:A:350:VAL:HG11	2:A:418:ILE:HD11	1.78	0.65
2:C:73:THR:HB	2:C:141:LEU:HD13	1.78	0.65
2:C:951:VAL:HA	2:C:954:HIS:CE1	2.32	0.65
2:B:454:ARG:HD3	2:B:457:ARG:HG3	1.79	0.65
1:E:36:GLY:HA3	1:E:100:TRP:HE1	1.62	0.65
2:C:326:ILE:HD11	2:C:534:VAL:HG13	1.79	0.65
2:A:100:ILE:HG23	2:A:244:LEU:HD23	1.77	0.65
2:A:434:ILE:HB	2:A:511:VAL:HB	1.79	0.65
2:B:401:VAL:HG13	2:B:509:ARG:HG2	1.79	0.65
2:B:426:PRO:HB3	2:B:463:PRO:HB3	1.77	0.65
2:A:64:TRP:CD2	2:A:259:THR:HB	2.32	0.65
2:A:91:TYR:N	2:A:268:GLY:O	2.26	0.65
2:B:176:LEU:HA	2:B:190:ARG:HH12	1.62	0.65
2:B:295:PRO:HG2	2:B:636:TYR:CE2	2.32	0.65
2:A:398:ASP:O	2:A:512:VAL:N	2.30	0.64
2:B:964:LYS:NZ	2:C:570:ALA:HA	2.11	0.64
2:A:147:LYS:HA	2:A:246:ARG:HA	1.79	0.64
2:C:985:ASP:HB2	2:C:987:PRO:HD2	1.79	0.64
2:C:74:ASN:HB2	2:C:78:ARG:HH21	1.63	0.64
2:A:175:PHE:O	2:A:207:HIS:NE2	2.27	0.64
2:A:615:VAL:HG21	2:A:621:PRO:HG2	1.80	0.64
2:B:271:GLN:HG2	2:B:272:PRO:HD2	1.78	0.64
2:B:144:TYR:O	2:B:145:TYR:C	2.41	0.64
2:A:620:VAL:CG1	2:A:621:PRO:HD3	2.26	0.64
2:C:553:THR:HG23	2:C:586:ASP:HB3	1.79	0.64
2:B:392:PHE:CB	2:B:515:PHE:HB3	2.28	0.64
2:A:738:CYS:HB3	2:A:742:ILE:HD12	1.80	0.64
2:B:379:CYS:HA	2:B:432:CYS:CA	2.25	0.64
2:A:485:GLY:H	2:A:488:CYS:HB2	1.62	0.64
2:B:133:PHE:CG	2:B:160:TYR:HA	2.32	0.63
2:C:339:ASP:C	2:C:341:VAL:H	2.05	0.63
2:C:418:ILE:HA	2:C:422:ASN:HB2	1.80	0.63
2:C:559:PHE:HB3	2:C:577:ARG:NH1	2.11	0.63
2:A:538:CYS:HB3	2:A:551:VAL:HG22	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:VAL:HA	2:B:410:ILE:HD12	1.78	0.63
2:C:68:ILE:HG12	2:C:252:GLY:HA2	1.80	0.63
1:E:68:ARG:NH1	1:E:86:SER:O	2.32	0.63
2:B:624:ILE:HG22	2:B:628:GLN:HB3	1.79	0.63
2:A:134:GLN:HB3	2:A:161:SER:HA	1.80	0.63
2:B:922:LEU:HD11	3:R:1:NAG:H5	1.81	0.63
2:B:452:ARG:HA	2:B:494:SER:HA	1.79	0.63
2:C:337:PRO:C	2:C:339:ASP:H	2.07	0.63
2:A:293:LEU:HD23	2:A:294:ASP:HB2	1.80	0.63
2:C:1138:TYR:CE1	2:C:1143:PRO:HG2	2.34	0.63
2:C:280:ASN:HD21	2:C:282:ASN:HD22	1.47	0.63
2:A:118:LEU:HB2	2:A:120:VAL:HG23	1.80	0.62
1:I:38:PHE:HE2	1:I:100:TRP:HE1	1.47	0.62
1:E:56:ASP:OD1	1:E:59:HIS:NE2	2.32	0.62
2:C:108:THR:HG22	2:C:109:THR:HG23	1.80	0.62
2:A:432:CYS:HB2	2:A:513:LEU:HG	1.81	0.62
2:B:42:VAL:HG21	2:B:44:ARG:HH11	1.63	0.62
2:B:79:PHE:CD1	2:B:242:LEU:HD12	2.32	0.62
2:B:886:TRP:HE1	2:C:1107:ARG:HH12	1.45	0.62
2:A:66:HIS:HA	2:A:263:ALA:HB1	1.81	0.62
2:A:387:LEU:HA	2:A:390:LEU:HB2	1.82	0.62
2:B:29:THR:OG1	2:B:30:ASN:N	2.26	0.62
2:C:244:LEU:O	2:C:246:ARG:N	2.30	0.62
2:C:111:ASP:OD2	2:C:113:LYS:NZ	2.28	0.62
2:C:792:PRO:O	2:C:795:LYS:NZ	2.32	0.62
2:A:403:ARG:HG3	2:A:495:TYR:HE1	1.64	0.61
2:B:456:PHE:H	2:B:491:PRO:HA	1.65	0.61
2:B:806:LEU:HD13	2:B:807:PRO:HD2	1.82	0.61
2:C:102:ARG:NH1	2:C:121:ASN:OD1	2.33	0.61
2:C:356:LYS:HB2	2:C:397:ALA:HB3	1.82	0.61
2:B:44:ARG:HH21	2:B:49:HIS:CD2	2.17	0.61
2:B:1142:GLN:HB3	2:B:1143:PRO:HD3	1.82	0.61
2:A:65:PHE:O	2:A:67:ALA:N	2.34	0.61
2:B:418:ILE:HD12	2:B:422:ASN:HD22	1.65	0.61
2:A:365:TYR:HD2	2:A:388:ASN:HA	1.66	0.61
2:B:600:PRO:HD3	2:B:692:ILE:HD11	1.83	0.61
2:A:821:LEU:HD13	2:A:935:GLN:HG3	1.83	0.61
2:A:34:ARG:HH22	2:A:221:SER:H	1.48	0.60
2:A:76:THR:O	2:A:77:LYS:C	2.44	0.60
2:A:263:ALA:HB3	2:A:266:TYR:CE1	2.36	0.60
2:A:534:VAL:HG22	2:A:535:LYS:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:ILE:H	2:C:80:ASP:HB3	1.66	0.60
2:C:310:LYS:HG3	2:C:600:PRO:HA	1.82	0.60
1:G:107:ASN:HB2	1:G:109:ILE:HG12	1.83	0.60
2:B:1143:PRO:HA	2:B:1146:ASP:HB2	1.82	0.60
2:C:64:TRP:O	2:C:65:PHE:C	2.44	0.60
2:A:106:PHE:HD2	2:A:235:ILE:HG21	1.64	0.60
2:C:359:SER:HA	2:C:523:THR:HB	1.82	0.60
2:C:915:VAL:O	2:C:919:ASN:ND2	2.34	0.60
2:A:248:TYR:O	2:A:249:LEU:C	2.44	0.60
2:B:196:ASN:HD21	2:B:233:ILE:HG23	1.67	0.60
2:B:850:ILE:O	2:B:854:LYS:NZ	2.35	0.60
2:C:791:THR:HG21	2:C:806:LEU:HD11	1.83	0.60
2:A:135:PHE:N	2:A:161:SER:OG	2.33	0.60
1:I:74:ASP:OD2	1:I:77:LYS:N	2.25	0.60
2:A:244:LEU:O	2:A:246:ARG:N	2.34	0.60
2:A:902:MET:HE2	2:A:1049:LEU:HD13	1.83	0.60
2:A:578:ASP:N	2:A:583:GLU:O	2.25	0.60
1:G:65:VAL:HB	1:G:69:PHE:HB2	1.83	0.60
1:E:68:ARG:O	1:E:85:ASN:ND2	2.34	0.60
2:B:567:ARG:NE	2:B:570:ALA:O	2.35	0.60
2:B:95:THR:HG21	2:B:212:LEU:HD22	1.83	0.59
2:B:915:VAL:O	2:B:919:ASN:ND2	2.34	0.59
2:C:804:GLN:NE2	2:C:935:GLN:OE1	2.29	0.59
2:A:403:ARG:HG3	2:A:495:TYR:CE1	2.36	0.59
2:C:338:PHE:HD2	2:C:356:LYS:HE3	1.67	0.59
1:E:34:HIS:HB2	1:E:100:TRP:HB2	1.85	0.59
2:B:1139:ASP:OD2	2:B:1142:GLN:N	2.33	0.59
2:A:66:HIS:HA	2:A:263:ALA:CB	2.32	0.59
2:A:71:SER:HA	2:A:79:PHE:CA	2.26	0.59
2:C:34:ARG:HH12	2:C:219:GLY:H	1.50	0.59
2:C:167:THR:HG22	2:C:168:PHE:H	1.67	0.59
2:C:442:ASP:O	2:C:448:ASN:ND2	2.35	0.59
2:A:34:ARG:NH1	2:A:219:GLY:O	2.36	0.59
2:A:142:ASP:HB2	2:A:146:HIS:HB3	1.84	0.59
2:B:393:THR:HG21	2:B:518:LEU:HB2	1.84	0.59
2:A:177:MET:O	2:A:190:ARG:NH2	2.34	0.59
2:A:365:TYR:CD2	2:A:388:ASN:HA	2.38	0.59
2:B:204:TYR:HA	2:B:225:PRO:HA	1.85	0.59
2:B:597:VAL:HG22	2:B:610:VAL:HG12	1.83	0.59
2:B:353:TRP:HB3	2:B:400:PHE:HD2	1.68	0.59
2:C:205:SER:HB3	2:C:226:LEU:HG	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:GLN:HG3	2:C:1143:PRO:HD3	1.85	0.59
2:A:401:VAL:HA	2:A:509:ARG:HA	1.83	0.59
2:A:617:CYS:C	2:A:619:GLU:N	2.42	0.59
1:I:83:GLN:NE2	1:I:84:MET:O	2.36	0.59
2:B:328:ARG:O	2:B:329:PHE:C	2.45	0.59
2:B:894:LEU:HD13	2:C:715:PRO:HD3	1.85	0.59
2:C:122:ASN:HD21	2:C:153:MET:HG3	1.67	0.59
1:I:41:ALA:HB3	1:I:44:LYS:HG3	1.84	0.58
1:I:92:THR:HG22	1:I:122:VAL:H	1.68	0.58
2:B:353:TRP:NE1	2:B:465:GLU:O	2.32	0.58
1:I:17:GLY:O	1:I:87:LEU:N	2.34	0.58
2:C:624:ILE:HB	2:C:629:LEU:HD22	1.85	0.58
2:B:128:ILE:H	2:B:128:ILE:HD12	1.68	0.58
1:I:98:ALA:HA	1:I:114:TRP:HA	1.86	0.58
2:C:330:PRO:O	2:C:331:ASN:C	2.46	0.58
2:A:295:PRO:HG3	2:A:633:TRP:CE2	2.38	0.58
2:B:273:ARG:NH1	2:B:290:ASP:OD2	2.37	0.58
2:B:336:CYS:N	2:B:361:CYS:HA	2.18	0.58
2:B:353:TRP:HB3	2:B:400:PHE:CD2	2.38	0.58
2:C:157:PHE:HD2	2:C:159:VAL:HG13	1.69	0.58
2:A:83:VAL:HA	2:A:239:GLN:HG2	1.86	0.58
2:A:83:VAL:HG11	2:A:237:ARG:HH21	1.67	0.58
2:A:414:GLN:O	2:A:424:LYS:NZ	2.37	0.58
2:A:973:ILE:HG22	2:A:992:GLN:HE21	1.69	0.58
2:A:187:LYS:O	2:A:189:LEU:N	2.37	0.57
2:A:63:THR:O	2:A:64:TRP:C	2.46	0.57
2:C:335:LEU:HD12	2:C:525:CYS:H	1.69	0.57
1:I:65:VAL:HB	1:I:69:PHE:HB2	1.86	0.57
2:A:1126:CYS:HB2	2:A:1132:ILE:HD13	1.85	0.57
2:B:64:TRP:CD1	2:B:259:THR:HG1	2.22	0.57
2:C:106:PHE:HB2	2:C:117:LEU:HB2	1.85	0.57
2:C:327:VAL:O	2:C:328:ARG:C	2.47	0.57
2:A:64:TRP:HE1	2:A:262:ALA:N	2.02	0.57
2:B:448:ASN:HB3	2:B:497:PHE:HB2	1.85	0.57
2:B:118:LEU:HD11	2:B:131:CYS:O	2.04	0.57
2:B:289:VAL:HG21	2:B:300:LYS:HD2	1.87	0.57
2:B:295:PRO:HD3	2:B:633:TRP:CD1	2.39	0.57
2:C:580:GLN:C	2:C:582:LEU:H	2.13	0.57
2:A:429:PHE:HE1	2:A:514:SER:HB3	1.70	0.57
1:I:6:GLN:HB2	1:I:24:ALA:HB3	1.87	0.57
2:A:738:CYS:O	2:A:742:ILE:N	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:HD12	2:B:276:LEU:HD21	1.87	0.57
2:C:103:GLY:HA3	2:C:120:VAL:HA	1.86	0.57
2:C:736:VAL:HG12	2:C:858:LEU:HD22	1.84	0.57
2:A:139:PRO:HA	2:A:157:PHE:HA	1.87	0.57
2:C:86:PHE:HB2	2:C:238:PHE:HB3	1.86	0.57
2:C:422:ASN:ND2	2:C:454:ARG:O	2.34	0.57
2:C:622:VAL:HG22	2:C:642:VAL:HG11	1.87	0.57
1:E:37:TRP:CD1	1:E:82:LEU:HD22	2.40	0.56
2:A:271:GLN:HG3	2:A:272:PRO:HD2	1.87	0.56
2:B:904:TYR:CE2	2:C:1107:ARG:HD3	2.40	0.56
2:C:581:THR:O	2:C:582:LEU:C	2.48	0.56
1:E:16:GLY:HA2	1:E:86:SER:H	1.69	0.56
2:A:396:TYR:N	2:A:514:SER:O	2.37	0.56
2:A:1051:SER:OG	2:A:1064:HIS:ND1	2.33	0.56
1:I:3:VAL:HG21	1:I:99:TYR:HE2	1.71	0.56
2:A:397:ALA:HA	2:A:513:LEU:HA	1.87	0.56
2:A:534:VAL:HG21	2:A:539:VAL:HG21	1.87	0.56
2:B:133:PHE:HA	2:B:163:ALA:HB2	1.85	0.56
2:C:1142:GLN:O	2:C:1146:ASP:N	2.31	0.56
2:A:62:VAL:O	2:A:64:TRP:N	2.37	0.56
2:C:96:GLU:HB2	2:C:100:ILE:HB	1.88	0.56
2:C:580:GLN:O	2:C:582:LEU:N	2.38	0.56
2:B:115:GLN:HA	2:B:132:GLU:HB3	1.86	0.56
1:I:46:ARG:HD2	1:I:114:TRP:CH2	2.40	0.56
2:B:110:LEU:HB3	2:B:136:CYS:SG	2.46	0.56
2:C:146:HIS:HB2	2:C:246:ARG:HA	1.86	0.56
2:B:215:ASP:O	2:B:216:LEU:C	2.49	0.56
2:B:351:TYR:HB2	2:B:467:ASP:HB2	1.88	0.56
2:C:985:ASP:OD1	2:C:985:ASP:N	2.39	0.56
2:A:65:PHE:O	2:A:66:HIS:C	2.46	0.55
2:A:592:PHE:HZ	2:C:857:GLY:H	1.54	0.55
2:B:34:ARG:NH1	2:B:219:GLY:O	2.39	0.55
2:C:338:PHE:CD2	2:C:356:LYS:HE3	2.41	0.55
2:A:226:LEU:HD23	2:A:227:VAL:HG23	1.88	0.55
2:A:369:TYR:OH	2:A:384:PRO:O	2.23	0.55
2:B:784:GLN:OE1	2:B:1030:SER:OG	2.23	0.55
2:C:392:PHE:HB3	2:C:515:PHE:HB3	1.87	0.55
2:C:620:VAL:HB	2:C:621:PRO:HD3	1.87	0.55
2:B:104:TRP:HB2	2:B:106:PHE:CE1	2.41	0.55
2:C:773:GLU:OE1	2:C:1019:ARG:NH1	2.38	0.55
2:C:922:LEU:HD11	3:K:1:NAG:H5	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1048:HIS:NE2	2:C:1050:MET:O	2.39	0.55
2:C:439:ASN:O	2:C:443:SER:OG	2.20	0.55
2:C:599:THR:HB	2:C:608:VAL:HG12	1.89	0.55
2:C:1086:LYS:HD2	2:C:1122:VAL:HG11	1.87	0.55
1:E:73:ARG:HA	1:E:80:VAL:HA	1.87	0.55
2:C:954:HIS:CD2	2:C:1014:ARG:HH11	2.24	0.55
1:I:51:ALA:HB3	1:I:60:TYR:HD2	1.71	0.55
2:B:356:LYS:HG3	2:B:358:ILE:HG13	1.88	0.55
2:C:543:PHE:O	2:C:544:ASN:C	2.50	0.55
1:E:28:TRP:HB3	2:A:375:PHE:HE1	1.70	0.55
1:I:62:ALA:O	1:I:66:LYS:N	2.39	0.55
2:A:1101:HIS:ND1	3:Z:1:NAG:H5	2.22	0.55
2:B:36:VAL:HG11	2:B:220:PHE:CE2	2.42	0.55
2:B:102:ARG:NH1	2:B:243:ALA:O	2.40	0.55
2:A:102:ARG:HG3	2:A:243:ALA:HB3	1.88	0.55
2:B:277:LEU:HD23	2:B:285:ILE:HD13	1.89	0.55
2:B:362:VAL:O	2:B:364:ASP:N	2.40	0.55
2:A:453:TYR:HB3	2:A:495:TYR:CZ	2.41	0.55
2:B:318:PHE:HE2	2:B:615:VAL:HG11	1.73	0.55
2:B:318:PHE:CD1	2:B:629:LEU:HA	2.42	0.55
2:C:29:THR:HA	2:C:61:ASN:HA	1.87	0.55
2:C:115:GLN:HG3	2:C:233:ILE:HG12	1.89	0.55
2:A:629:LEU:HD21	2:A:634:ARG:HA	1.89	0.54
2:B:72:GLY:O	2:B:73:THR:C	2.50	0.54
2:B:621:PRO:HA	2:B:624:ILE:HG23	1.88	0.54
2:C:29:THR:HA	2:C:62:VAL:N	2.22	0.54
1:E:19:LEU:HB3	1:E:84:MET:HE3	1.89	0.54
2:A:65:PHE:CZ	2:A:82:PRO:HD2	2.42	0.54
2:B:736:VAL:HG23	2:B:858:LEU:HD23	1.88	0.54
1:G:99:TYR:HB3	1:G:113:TYR:HB2	1.89	0.54
1:G:18:SER:OG	1:G:83:GLN:OE1	2.25	0.54
2:A:93:ALA:O	2:A:266:TYR:HD2	1.91	0.54
2:A:174:PRO:HG2	2:A:177:MET:HG3	1.89	0.54
2:A:326:ILE:HG23	2:A:541:PHE:HA	1.90	0.54
2:B:173:GLN:HB3	2:B:177:MET:HE1	1.89	0.54
1:G:4:GLN:HB3	2:C:489:TYR:HE1	1.72	0.54
2:A:29:THR:O	2:A:61:ASN:HA	2.08	0.54
2:A:1040:VAL:HG21	2:C:1035:GLY:HA3	1.88	0.54
2:B:157:PHE:HD1	2:B:158:ARG:N	2.05	0.54
2:B:566:GLY:HA3	2:B:575:ALA:HB3	1.88	0.54
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:77:LYS:O	2:A:78:ARG:C	2.50	0.54
2:A:900:MET:HE1	2:B:1094:VAL:HG23	1.89	0.54
2:C:178:ASP:N	2:C:178:ASP:OD1	2.39	0.54
1:I:61:TYR:HE1	1:I:70:THR:HA	1.72	0.54
2:B:418:ILE:HA	2:B:422:ASN:HB3	1.88	0.54
2:B:676:THR:HB	2:B:690:GLN:HG2	1.89	0.54
2:C:519:HIS:HB3	2:C:565:PHE:CD2	2.43	0.54
2:A:93:ALA:HB1	2:A:189:LEU:HG	1.90	0.54
2:A:811:LYS:NZ	2:A:820:ASP:OD2	2.33	0.54
2:B:617:CYS:O	2:B:621:PRO:HD2	2.08	0.54
2:C:1097:SER:C	2:C:1099:GLY:H	2.15	0.54
2:A:31:SER:O	2:A:32:PHE:C	2.51	0.54
2:B:106:PHE:HB3	2:B:235:ILE:CG2	2.38	0.54
2:B:555:SER:HB3	2:B:584:ILE:O	2.08	0.54
2:C:281:GLU:C	2:C:283:GLY:H	2.16	0.54
2:C:457:ARG:NE	2:C:459:SER:O	2.41	0.53
2:C:748:GLU:OE1	2:C:748:GLU:N	2.38	0.53
2:A:642:VAL:HG22	2:A:651:ILE:HG12	1.90	0.53
2:B:140:PHE:CE1	2:B:158:ARG:HB2	2.44	0.53
2:C:64:TRP:HB2	2:C:66:HIS:NE2	2.23	0.53
2:C:336:CYS:O	2:C:336:CYS:SG	2.66	0.53
2:A:724:THR:HB	2:A:934:ILE:HD11	1.89	0.53
2:B:339:ASP:O	2:B:340:GLU:C	2.51	0.53
2:C:206:LYS:HD2	2:C:221:SER:HB3	1.90	0.53
2:C:731:MET:O	2:C:733:LYS:NZ	2.42	0.53
2:A:337:PRO:C	2:A:339:ASP:H	2.15	0.53
2:A:904:TYR:OH	2:B:1094:VAL:HB	2.07	0.53
2:B:763:LEU:HD11	2:B:1005:GLN:HE22	1.74	0.53
1:E:57:THR:HG21	2:A:405:ASN:HD21	1.74	0.53
2:B:106:PHE:HB2	2:B:117:LEU:HB2	1.90	0.53
2:B:320:VAL:HG13	2:B:628:GLN:HE22	1.72	0.53
2:B:523:THR:OG1	2:B:524:VAL:N	2.38	0.53
2:B:617:CYS:O	2:B:619:GLU:N	2.38	0.53
2:C:110:LEU:HD13	2:C:136:CYS:SG	2.49	0.53
2:C:112:SER:HA	2:C:134:GLN:HA	1.91	0.53
1:G:34:HIS:HB2	1:G:100:TRP:HB2	1.91	0.53
2:A:36:VAL:HG11	2:A:220:PHE:CZ	2.44	0.53
2:A:120:VAL:HG13	2:A:157:PHE:HZ	1.74	0.53
2:B:42:VAL:O	2:C:563:GLN:NE2	2.40	0.53
2:B:339:ASP:HA	2:B:343:ASN:H	1.73	0.53
2:B:538:CYS:SG	2:B:590:CYS:HB3	2.48	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:454:ARG:NH1	2:A:469:SER:O	2.42	0.53
2:A:966:LEU:O	2:A:975:SER:OG	2.26	0.53
2:B:42:VAL:HG22	2:B:44:ARG:HH11	1.72	0.53
2:C:821:LEU:HD22	2:C:935:GLN:HG3	1.91	0.53
2:A:788:ILE:HG23	2:A:876:ALA:HB2	1.91	0.53
2:B:158:ARG:NH1	2:B:160:TYR:OH	2.42	0.53
2:B:294:ASP:H	2:B:297:SER:HB2	1.74	0.53
2:B:473:TYR:HB3	2:B:491:PRO:HD3	1.90	0.53
2:C:278:LYS:HG2	2:C:287:ASP:H	1.72	0.53
2:C:337:PRO:HD3	2:C:363:ALA:O	2.09	0.53
2:C:802:PHE:HD1	2:C:805:ILE:HD11	1.74	0.53
2:C:806:LEU:HG	2:C:807:PRO:HD2	1.91	0.53
2:B:73:THR:O	2:B:144:TYR:N	2.41	0.52
2:C:182:LYS:O	2:C:183:GLN:HG3	2.09	0.52
2:A:375:PHE:HB3	2:A:436:TRP:HB3	1.90	0.52
2:A:624:ILE:HG13	2:A:637:SER:HA	1.91	0.52
2:B:244:LEU:O	2:B:246:ARG:N	2.41	0.52
2:B:393:THR:HB	2:B:516:GLU:O	2.09	0.52
2:C:426:PRO:HD3	2:C:463:PRO:HB3	1.90	0.52
2:A:258:TRP:CE3	4:A:1302:NAG:H5	2.45	0.52
2:A:434:ILE:N	2:A:511:VAL:O	2.27	0.52
2:B:44:ARG:NH2	2:B:49:HIS:CD2	2.76	0.52
2:B:106:PHE:HB3	2:B:235:ILE:HG23	1.92	0.52
2:C:336:CYS:HB3	2:C:362:VAL:N	2.23	0.52
2:A:120:VAL:HB	2:A:127:VAL:HB	1.91	0.52
2:B:175:PHE:O	2:B:190:ARG:NH1	2.42	0.52
2:B:560:LEU:O	2:B:561:PRO:C	2.53	0.52
2:A:754:LEU:HD12	2:A:755:GLN:HG3	1.91	0.52
2:B:318:PHE:HD1	2:B:629:LEU:HA	1.74	0.52
2:B:448:ASN:HD21	2:B:451:TYR:HD2	1.58	0.52
2:B:777:ASN:OD1	2:B:1019:ARG:NH1	2.40	0.52
2:C:502:GLY:O	2:C:506:GLN:N	2.43	0.52
2:A:444:LYS:HE2	2:A:448:ASN:HA	1.92	0.52
1:I:27:GLY:N	2:C:373:PRO:O	2.43	0.52
2:A:629:LEU:HD23	2:A:629:LEU:H	1.75	0.52
2:B:91:TYR:HB3	2:B:268:GLY:HA3	1.92	0.52
2:B:445:VAL:HA	2:B:499:PRO:HG3	1.91	0.52
2:B:727:LEU:HD11	2:B:1028:LYS:HD3	1.92	0.52
2:A:29:THR:HA	2:A:259:THR:C	2.34	0.51
2:B:295:PRO:HD3	2:B:633:TRP:HD1	1.75	0.51
1:G:4:GLN:O	1:G:26[A]:SER:OG	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1077:THR:OG1	2:A:1078:ALA:N	2.41	0.51
2:B:133:PHE:CD2	2:B:160:TYR:HA	2.45	0.51
2:C:115:GLN:HB2	2:C:233:ILE:HG12	1.91	0.51
2:A:762:GLN:OE1	2:A:765:ARG:NH1	2.33	0.51
2:C:64:TRP:HD1	2:C:66:HIS:CD2	2.29	0.51
2:C:708:SER:HB3	2:C:711:SER:HB3	1.92	0.51
2:C:318:PHE:HZ	2:C:620:VAL:HG12	1.76	0.51
2:C:759:PHE:CD2	2:C:1001:LEU:HD21	2.46	0.51
2:B:187:LYS:CB	2:B:212:LEU:HB2	2.40	0.51
1:G:39:ARG:NH1	1:G:91:ASP:OD1	2.42	0.51
1:G:72:SER:O	1:G:81:TYR:N	2.44	0.51
2:A:244:LEU:HB2	2:A:247:SER:HB3	1.93	0.51
2:B:434:ILE:HG22	2:B:511:VAL:HB	1.92	0.51
2:B:480:CYS:HB3	2:B:483:VAL:O	2.11	0.51
2:A:91:TYR:OH	2:A:191:GLU:HG2	2.11	0.51
2:A:849:LEU:HD21	2:A:852:ALA:HB3	1.93	0.51
2:B:409:GLN:HB3	2:B:419:ALA:HB2	1.91	0.51
2:A:258:TRP:HE3	4:A:1302:NAG:HN2	1.58	0.51
2:A:326:ILE:HD11	2:A:328:ARG:HB2	1.93	0.51
2:A:661:GLU:OE2	2:A:662:CYS:N	2.42	0.51
1:E:37:TRP:HH2	1:E:80:VAL:HG13	1.76	0.51
2:A:436:TRP:O	2:A:509:ARG:N	2.44	0.51
2:A:457:ARG:NH1	2:A:467:ASP:HB3	2.26	0.51
2:B:855:PHE:HB3	2:C:589:PRO:HG2	1.92	0.51
2:C:29:THR:CA	2:C:61:ASN:HA	2.40	0.51
1:G:21:LEU:HD12	1:G:82:LEU:HD23	1.93	0.51
1:I:42:PRO:HD3	1:I:93:ALA:HB2	1.93	0.51
2:A:91:TYR:HE1	2:A:191:GLU:HB3	1.76	0.51
2:A:134:GLN:N	2:A:161:SER:OG	2.44	0.51
2:A:894:LEU:HD13	2:B:715:PRO:HD3	1.93	0.51
2:B:822:LEU:HD22	2:B:945:LEU:HD21	1.92	0.51
2:C:453:TYR:HB3	2:C:495:TYR:CE2	2.45	0.51
2:C:565:PHE:CB	2:C:567:ARG:HH22	2.24	0.50
2:A:1035:GLY:HA3	2:B:1040:VAL:HG21	1.92	0.50
2:B:42:VAL:CG2	2:B:44:ARG:NH1	2.73	0.50
2:B:450:ASN:O	2:B:452:ARG:NH1	2.45	0.50
2:C:335:LEU:HB3	2:C:524:VAL:HG12	1.93	0.50
2:A:63:THR:O	2:A:65:PHE:HB2	2.12	0.50
2:A:452:ARG:HG2	2:A:494:SER:HA	1.94	0.50
2:B:93:ALA:O	2:B:265:TYR:HA	2.10	0.50
2:B:359:SER:HB3	2:B:522:ALA:HB1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:964:LYS:HZ3	2:C:570:ALA:HA	1.76	0.50
2:B:1126:CYS:HB2	2:B:1132:ILE:HD13	1.93	0.50
1:I:100:TRP:CD1	1:I:105:LEU:HD11	2.46	0.50
2:A:426:PRO:HB3	2:A:463:PRO:HB3	1.93	0.50
2:A:624:ILE:HD12	2:A:629:LEU:HD22	1.94	0.50
2:B:392:PHE:HB2	2:B:515:PHE:HB3	1.92	0.50
2:C:389:ASP:OD1	2:C:527:PRO:HD2	2.12	0.50
2:A:541:PHE:HB3	2:A:552:LEU:HD11	1.94	0.50
2:B:387:LEU:HA	2:B:390:LEU:HB2	1.93	0.50
2:B:752:LEU:HD23	2:B:993:ILE:HG22	1.94	0.50
2:C:134:GLN:HG2	2:C:161:SER:HB3	1.93	0.50
1:G:14:GLN:HG3	1:G:124:SER:HA	1.94	0.50
2:B:29:THR:N	2:B:260:ALA:HA	2.27	0.50
2:B:115:GLN:NE2	2:B:130:VAL:O	2.45	0.50
2:B:602:THR:O	2:B:603:ASN:C	2.54	0.50
2:C:1082:CYS:HB2	2:C:1132:ILE:HG12	1.93	0.50
2:B:798:GLY:HA3	2:B:899:PRO:HG3	1.94	0.50
2:C:29:THR:CB	2:C:259:THR:HA	2.41	0.50
2:C:37:TYR:HA	2:C:223:LEU:H	1.76	0.50
2:C:714:ILE:HD12	2:C:1096:VAL:HG11	1.93	0.50
1:I:40:GLN:NE2	1:I:94:THR:O	2.45	0.50
2:A:190:ARG:HB3	2:A:192:PHE:CE2	2.47	0.50
2:A:206:LYS:HB3	2:A:223:LEU:HD22	1.94	0.50
2:A:762:GLN:HE22	2:A:765:ARG:HH22	1.58	0.50
2:B:43:PHE:H	2:C:566:GLY:HA2	1.76	0.50
2:B:79:PHE:CE2	2:B:139:PRO:HB2	2.47	0.50
2:B:119:ILE:HG12	2:B:128:ILE:HG23	1.93	0.50
2:B:387:LEU:O	2:B:388:ASN:C	2.54	0.50
2:B:448:ASN:O	2:B:498:ARG:NH1	2.45	0.50
2:A:748:GLU:HG3	2:A:981:LEU:HD11	1.93	0.49
2:B:40:ASP:CG	2:B:44:ARG:NH1	2.68	0.49
2:B:62:VAL:HG22	2:B:266:TYR:HB3	1.94	0.49
2:C:454:ARG:HE	2:C:491:PRO:HB2	1.77	0.49
2:A:328:ARG:NH1	2:A:578:ASP:OD2	2.45	0.49
2:A:393:THR:OG1	2:A:394:ASN:N	2.46	0.49
2:B:126:VAL:HG22	2:B:174:PRO:HA	1.93	0.49
2:B:802:PHE:HB3	2:B:806:LEU:HD23	1.93	0.49
2:C:334:ASN:HB2	2:C:361:CYS:C	2.37	0.49
2:C:1125:ASN:OD1	2:C:1126:CYS:N	2.45	0.49
2:A:802:PHE:O	2:A:803:SER:C	2.55	0.49
2:B:967:SER:O	2:B:975:SER:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:THR:HA	2:B:1138:TYR:O	2.12	0.49
1:E:28:TRP:HB3	2:A:375:PHE:CE1	2.48	0.49
2:B:616:ASN:O	2:B:617:CYS:C	2.55	0.49
1:G:40:GLN:HB2	1:G:46:ARG:HG3	1.94	0.49
2:A:392:PHE:H	2:A:524:VAL:HG23	1.77	0.49
2:B:131:CYS:HB3	2:B:133:PHE:CE2	2.47	0.49
2:B:595:VAL:HG21	2:B:631:PRO:HG2	1.94	0.49
2:C:431:GLY:HA2	2:C:515:PHE:CD2	2.47	0.49
2:C:443:SER:HB2	2:C:498:ARG:C	2.38	0.49
2:C:337:PRO:C	2:C:339:ASP:N	2.71	0.49
2:C:409:GLN:HB3	2:C:419:ALA:HB2	1.95	0.49
2:A:40:ASP:OD1	2:A:40:ASP:N	2.46	0.49
2:A:77:LYS:O	2:A:79:PHE:N	2.45	0.49
2:A:157:PHE:HB3	2:A:243:ALA:HB2	1.94	0.49
2:C:359:SER:HA	2:C:523:THR:CB	2.42	0.49
2:A:78:ARG:CB	2:A:251:PRO:HA	2.42	0.49
2:A:399:SER:HA	2:A:511:VAL:HA	1.95	0.49
2:B:133:PHE:O	2:B:134:GLN:C	2.55	0.49
2:B:789:TYR:HA	2:C:703:ASN:O	2.12	0.49
2:B:964:LYS:HZ2	2:C:570:ALA:HA	1.77	0.49
2:C:339:ASP:C	2:C:341:VAL:N	2.71	0.49
2:C:393:THR:HG21	2:C:519:HIS:O	2.12	0.49
1:E:41:ALA:HB3	1:E:44:LYS:HB2	1.95	0.49
2:B:543:PHE:O	2:B:544:ASN:C	2.55	0.49
2:C:807:PRO:HG3	2:C:875:SER:HB2	1.95	0.49
1:E:41:ALA:HA	1:E:94:THR:H	1.78	0.48
2:A:365:TYR:CE2	2:A:524:VAL:HG11	2.48	0.48
2:C:328:ARG:HH12	2:C:533:LEU:CD2	2.26	0.48
2:C:565:PHE:HB2	2:C:567:ARG:HH22	1.78	0.48
2:C:616:ASN:OD1	2:C:616:ASN:N	2.42	0.48
1:G:68:ARG:NH1	1:G:85:ASN:O	2.46	0.48
2:A:677:GLN:O	2:A:689:SER:OG	2.31	0.48
2:B:42:VAL:HG22	2:B:44:ARG:NH1	2.27	0.48
2:C:519:HIS:HD2	2:C:567:ARG:NH2	2.09	0.48
2:A:121:ASN:CG	2:A:176:LEU:HB2	2.38	0.48
2:B:392:PHE:HB3	2:B:515:PHE:HB3	1.94	0.48
2:C:480:CYS:HB3	2:C:483:VAL:O	2.14	0.48
2:C:600:PRO:HD3	2:C:692:ILE:HD11	1.94	0.48
2:A:553:THR:HG23	2:A:586:ASP:HB3	1.95	0.48
2:B:395:VAL:HA	2:B:514:SER:O	2.13	0.48
2:B:503:VAL:HA	2:B:506:GLN:HE21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:560:LEU:O	2:C:561:PRO:C	2.56	0.48
2:A:273:ARG:HA	2:A:273:ARG:HD3	1.52	0.48
2:A:452:ARG:HA	2:A:495:TYR:H	1.78	0.48
2:A:927:PHE:O	2:A:928:ASN:C	2.56	0.48
2:B:983:ARG:HG2	2:C:517:LEU:HD22	1.94	0.48
2:B:1145:LEU:HA	2:B:1148:PHE:HB3	1.95	0.48
2:A:457:ARG:HG2	2:A:458:LYS:H	1.79	0.48
2:C:457:ARG:NH1	2:C:467:ASP:OD2	2.46	0.48
2:A:809:PRO:O	2:A:814:LYS:NZ	2.40	0.48
2:C:328:ARG:HH12	2:C:533:LEU:HD23	1.79	0.48
2:A:61:ASN:HB3	2:A:258:TRP:CA	2.37	0.48
2:A:109:THR:HG21	2:A:113:LYS:HB2	1.96	0.48
2:A:635:VAL:HG23	2:A:636:TYR:HD1	1.79	0.48
2:A:1097:SER:C	2:A:1099:GLY:H	2.20	0.48
2:B:75:GLY:O	2:B:76:THR:C	2.56	0.48
2:B:599:THR:HB	2:B:608:VAL:HG12	1.96	0.48
1:E:46:ARG:HD3	1:E:114:TRP:CZ2	2.49	0.48
1:I:109:ILE:HG13	1:I:110:PRO:HD3	1.94	0.48
2:A:379:CYS:HA	2:A:432:CYS:HA	1.96	0.48
2:B:121:ASN:ND2	2:B:176:LEU:HB2	2.29	0.48
2:B:435:ALA:HA	2:B:509:ARG:O	2.14	0.48
2:C:328:ARG:NH1	2:C:533:LEU:HB3	2.27	0.48
2:C:329:PHE:CG	2:C:330:PRO:HD2	2.49	0.48
2:C:525:CYS:O	2:C:526:GLY:C	2.56	0.48
2:A:702:GLU:HG3	2:C:790:LYS:HE2	1.96	0.47
2:C:767:LEU:HD13	2:C:1008:VAL:HG22	1.96	0.47
1:G:68:ARG:NH1	1:G:86:SER:O	2.47	0.47
1:I:28:TRP:HB3	2:C:375:PHE:CZ	2.49	0.47
1:I:98:ALA:HB1	1:I:111:VAL:HG11	1.97	0.47
2:A:131:CYS:SG	2:A:165:ASN:O	2.72	0.47
2:A:336:CYS:N	2:A:361:CYS:HB2	2.29	0.47
2:B:77:LYS:O	2:B:78:ARG:C	2.57	0.47
2:B:379:CYS:CA	2:B:432:CYS:HA	2.28	0.47
2:B:452:ARG:HG3	2:B:494:SER:HA	1.96	0.47
1:E:111:VAL:HG21	1:E:114:TRP:CZ2	2.49	0.47
2:A:176:LEU:HD23	2:A:190:ARG:HG2	1.96	0.47
2:A:335:LEU:HB3	2:A:361:CYS:HB2	1.97	0.47
2:A:402:ILE:HG21	2:A:410:ILE:HG13	1.94	0.47
2:B:164:ASN:O	2:B:166:CYS:SG	2.72	0.47
1:I:1:SER:HB2	1:I:29:ALA:HA	1.96	0.47
2:A:568:ASP:OD1	2:A:570:ALA:N	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:715:PRO:HA	2:B:1072:GLU:HA	1.96	0.47
2:A:328:ARG:HD3	2:A:531:THR:OG1	2.14	0.47
2:A:355:ARG:HH12	2:A:464:PHE:HB3	1.80	0.47
2:A:761:THR:OG1	2:A:762:GLN:NE2	2.47	0.47
2:A:767:LEU:O	2:A:770:ILE:HG22	2.14	0.47
2:C:498:ARG:HG3	2:C:501:TYR:HE2	1.80	0.47
1:I:23:CYS:HB2	1:I:37:TRP:CH2	2.49	0.47
2:A:44:ARG:O	2:A:283:GLY:HA2	2.14	0.47
2:B:325:SER:HB2	2:B:539:VAL:HG12	1.94	0.47
2:C:102:ARG:O	2:C:121:ASN:HB3	2.15	0.47
1:E:14:GLN:HG3	1:E:126:SER:HA	1.97	0.47
1:I:20:ARG:HG3	1:I:83:GLN:HB2	1.96	0.47
2:A:392:PHE:C	2:A:522:ALA:HA	2.40	0.47
2:A:448:ASN:HB3	2:A:497:PHE:HB2	1.96	0.47
2:A:534:VAL:HG11	2:A:552:LEU:HD22	1.96	0.47
2:A:922:LEU:HD11	3:X:1:NAG:H5	1.95	0.47
2:B:451:TYR:HB3	2:B:495:TYR:CD2	2.45	0.47
2:B:453:TYR:CE1	2:B:455:LEU:HB2	2.49	0.47
2:C:106:PHE:CE1	2:C:119:ILE:HD12	2.49	0.47
2:C:819:GLU:HA	2:C:822:LEU:HD12	1.96	0.47
1:I:40:GLN:H	1:I:40:GLN:CD	2.21	0.47
2:A:80:ASP:OD1	2:A:252:GLY:HA2	2.13	0.47
2:A:117:LEU:O	2:A:119:ILE:N	2.48	0.47
2:A:372:ALA:N	2:A:375:PHE:HE2	2.13	0.47
2:A:589:PRO:HB3	2:C:855:PHE:HD1	1.80	0.47
2:A:748:GLU:H	2:A:748:GLU:CD	2.22	0.47
2:C:36:VAL:HG13	2:C:222:ALA:HA	1.97	0.47
1:G:69:PHE:HB3	1:G:82:LEU:HD11	1.97	0.47
1:I:13:VAL:HG23	1:I:122:VAL:HG13	1.96	0.47
2:A:65:PHE:HZ	2:A:82:PRO:HD2	1.79	0.47
2:A:339:ASP:HA	2:A:343:ASN:HB2	1.97	0.47
2:C:449:TYR:OH	2:C:498:ARG:NH2	2.47	0.47
2:C:474:GLN:HA	2:C:488:CYS:SG	2.55	0.47
2:C:555:SER:HB2	2:C:586:ASP:HB2	1.97	0.47
2:A:866:THR:HG23	2:A:869:MET:HE2	1.97	0.47
2:A:103:GLY:O	2:A:241:LEU:N	2.48	0.46
2:A:157:PHE:HD1	2:A:157:PHE:H	1.62	0.46
2:A:283:GLY:HA3	2:B:560:LEU:HD11	1.97	0.46
2:A:1117:THR:HG22	2:A:1140:PRO:HD2	1.97	0.46
2:B:121:ASN:CG	2:B:176:LEU:HB2	2.40	0.46
2:B:131:CYS:HB2	2:B:166:CYS:HB3	1.75	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:421:TYR:HB3	2:C:457:ARG:HB3	1.97	0.46
1:I:112:ASP:OD1	1:I:112:ASP:N	2.46	0.46
2:B:299:THR:OG1	2:B:308:VAL:HG11	2.15	0.46
2:B:454:ARG:NH2	2:B:469:SER:O	2.48	0.46
2:C:181:GLY:HA3	2:C:186:PHE:CE2	2.51	0.46
2:C:247:SER:OG	2:C:247:SER:O	2.31	0.46
2:A:34:ARG:NH2	2:A:221:SER:OG	2.48	0.46
2:A:71:SER:N	2:A:80:ASP:OD1	2.48	0.46
2:B:758:SER:O	2:B:762:GLN:NE2	2.38	0.46
1:G:19:LEU:HD12	1:G:19:LEU:HA	1.79	0.46
2:B:986:PRO:N	2:B:987:PRO:HD2	2.30	0.46
2:B:1107:ARG:H	2:B:1107:ARG:HD2	1.80	0.46
1:I:19:LEU:H	1:I:84:MET:HG2	1.79	0.46
1:I:94:THR:OG1	1:I:119:GLN:OE1	2.29	0.46
2:B:75:GLY:O	2:B:77:LYS:N	2.49	0.46
2:C:212:LEU:HD13	2:C:215:ASP:HA	1.97	0.46
2:C:290:ASP:O	2:C:297:SER:HB3	2.15	0.46
1:I:35:MET:N	1:I:35:MET:SD	2.89	0.46
2:A:104:TRP:CD1	2:A:240:THR:HG23	2.50	0.46
2:A:713:ALA:HB3	2:C:894:LEU:HB3	1.96	0.46
2:A:1082:CYS:HB2	2:A:1126:CYS:HB2	1.90	0.46
2:C:242:LEU:HD12	2:C:242:LEU:HA	1.79	0.46
1:G:68:ARG:HD3	1:G:88:ARG:HH21	1.80	0.46
2:A:372:ALA:H	2:A:375:PHE:HE2	1.62	0.46
2:C:36:VAL:HG11	2:C:220:PHE:CE2	2.50	0.46
2:C:387:LEU:HD23	2:C:392:PHE:CZ	2.50	0.46
2:C:746:SER:HB2	2:C:749:CYS:HB3	1.98	0.46
1:G:35:MET:HE3	1:G:35:MET:HB2	1.79	0.46
1:I:72:SER:O	1:I:81:TYR:N	2.42	0.46
2:A:337:PRO:O	2:A:339:ASP:N	2.46	0.46
2:B:983:ARG:HA	2:C:390:LEU:HD11	1.98	0.46
2:C:433:VAL:HG12	2:C:512:VAL:HG13	1.98	0.46
2:B:190:ARG:HB3	2:B:192:PHE:CZ	2.50	0.46
2:B:290:ASP:O	2:B:297:SER:HB3	2.16	0.46
2:B:404:GLY:HA2	2:B:407:VAL:HG23	1.97	0.46
2:B:559:PHE:O	2:B:560:LEU:C	2.59	0.46
2:B:1035:GLY:HA3	2:C:1040:VAL:HG21	1.97	0.46
2:B:1102:TRP:CZ2	2:B:1133:VAL:HG11	2.51	0.46
2:C:339:ASP:O	2:C:341:VAL:N	2.45	0.46
1:I:48:PHE:HZ	1:I:60:TYR:HB3	1.81	0.46
2:A:136:CYS:SG	2:A:138:ASP:HB2	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:167:THR:HG22	2:A:168:PHE:H	1.79	0.46
2:A:715:PRO:HA	2:A:1072:GLU:HA	1.98	0.46
2:B:97:LYS:HA	2:B:97:LYS:HD2	1.75	0.46
2:B:176:LEU:O	2:B:178:ASP:N	2.49	0.46
2:B:246:ARG:O	2:B:247:SER:C	2.59	0.46
2:B:1077:THR:OG1	2:B:1078:ALA:N	2.49	0.46
2:C:153:MET:SD	2:C:156:GLU:HG3	2.56	0.46
2:C:559:PHE:HB2	2:C:584:ILE:HD12	1.98	0.46
2:C:878:LEU:HD12	2:C:878:LEU:HA	1.76	0.46
1:I:71:ILE:HG13	1:I:81:TYR:O	2.16	0.45
2:A:147:LYS:HE3	2:A:248:TYR:HB2	1.98	0.45
2:A:382:VAL:HG21	2:A:390:LEU:HD12	1.97	0.45
2:A:675:GLN:O	2:A:677:GLN:NE2	2.46	0.45
2:A:756:TYR:OH	2:A:998:THR:HG22	2.16	0.45
2:B:242:LEU:O	2:B:243:ALA:C	2.59	0.45
2:B:406:GLU:O	2:B:410:ILE:N	2.50	0.45
2:C:519:HIS:HB3	2:C:565:PHE:HD2	1.81	0.45
1:G:34:HIS:HB3	1:G:100:TRP:HE3	1.82	0.45
2:A:462:LYS:HB2	2:A:465:GLU:HB2	1.98	0.45
2:A:894:LEU:HB3	2:B:713:ALA:HB3	1.98	0.45
2:B:118:LEU:HD12	2:B:118:LEU:H	1.80	0.45
2:B:352:ALA:O	2:B:466:ARG:NH2	2.49	0.45
2:B:555:SER:HB3	2:B:584:ILE:C	2.42	0.45
2:B:629:LEU:HG	2:B:632:THR:H	1.80	0.45
2:C:131:CYS:HB3	2:C:133:PHE:CE1	2.52	0.45
2:C:402:ILE:O	2:C:508:TYR:N	2.39	0.45
1:G:118:THR:HG22	1:G:120:VAL:HG23	1.98	0.45
2:A:996:LEU:HD21	2:A:1000:ARG:CZ	2.46	0.45
2:A:1104:VAL:HG11	2:A:1119:ASN:OD1	2.17	0.45
2:A:1123:SER:O	2:A:1123:SER:OG	2.33	0.45
2:C:650:LEU:HD12	2:C:650:LEU:HA	1.79	0.45
2:C:1029:MET:HE2	2:C:1029:MET:HB2	1.69	0.45
2:A:119:ILE:HG22	2:A:175:PHE:CZ	2.52	0.45
2:A:543:PHE:O	2:A:546:LEU:HB2	2.16	0.45
2:A:798:GLY:HA3	2:A:899:PRO:HG3	1.96	0.45
2:B:236:THR:HG21	4:B:1302:NAG:H5	1.99	0.45
2:B:320:VAL:HB	2:B:590:CYS:HB2	1.98	0.45
2:C:457:ARG:NH2	2:C:459:SER:OG	2.49	0.45
2:C:786:LYS:HG3	2:C:787:GLN:HG3	1.98	0.45
2:A:32:PHE:HD2	2:A:218:GLN:HG2	1.82	0.45
2:A:190:ARG:HE	2:A:207:HIS:CG	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:191:GLU:O	2:A:223:LEU:HD13	2.16	0.45
2:A:589:PRO:HG3	2:C:855:PHE:HB2	1.99	0.45
2:A:931:ILE:O	2:A:934:ILE:HG22	2.17	0.45
2:B:33:THR:OG1	2:B:219:GLY:O	2.23	0.45
2:B:853:GLN:HB2	2:B:854:LYS:HZ2	1.81	0.45
2:C:137:ASN:H	2:C:159:VAL:HA	1.81	0.45
1:E:107:ASN:HB2	1:E:110:PRO:HD3	1.98	0.45
2:A:289:VAL:HG21	2:A:300:LYS:HD2	1.99	0.45
2:A:451:TYR:HD2	2:A:495:TYR:CD2	2.35	0.45
2:A:794:ILE:HG21	4:B:1308:NAG:H61	1.99	0.45
2:B:147:LYS:HA	2:B:147:LYS:HD3	1.78	0.45
2:C:128:ILE:HG13	2:C:229:LEU:HD11	1.99	0.45
2:C:1088:HIS:CE1	2:C:1137:VAL:HG11	2.52	0.45
1:G:45:GLU:OE2	2:C:450:ASN:ND2	2.50	0.45
2:A:294:ASP:HB3	2:A:297:SER:H	1.82	0.45
2:B:139:PRO:HA	2:B:157:PHE:HA	1.97	0.45
2:B:516:GLU:H	2:B:516:GLU:HG3	1.44	0.45
2:B:612:TYR:OH	2:B:629:LEU:HD13	2.16	0.45
2:C:29:THR:C	2:C:61:ASN:HA	2.42	0.45
2:C:30:ASN:HB3	2:C:32:PHE:CE1	2.52	0.45
1:G:28:TRP:CD1	1:G:28:TRP:H	2.35	0.45
1:I:39:ARG:HG3	1:I:95:TYR:CD1	2.47	0.45
2:A:118:LEU:H	2:A:118:LEU:HG	1.40	0.45
2:A:451:TYR:HD2	2:A:495:TYR:HD2	1.64	0.45
2:B:1138:TYR:HE1	2:B:1143:PRO:HG2	1.81	0.45
2:C:320:VAL:HG23	2:C:590:CYS:HB2	1.98	0.45
2:C:802:PHE:CD1	2:C:805:ILE:HD11	2.52	0.45
2:B:43:PHE:HA	2:C:563:GLN:OE1	2.17	0.45
2:B:64:TRP:HD1	2:B:259:THR:HG23	1.82	0.45
2:B:449:TYR:O	2:B:494:SER:OG	2.35	0.45
2:C:964:LYS:HB2	2:C:964:LYS:HE2	1.82	0.45
1:E:73:ARG:HG3	1:E:80:VAL:HB	1.98	0.45
2:B:64:TRP:CZ3	2:B:262:ALA:HA	2.52	0.45
2:B:130:VAL:HG11	2:B:231:ILE:HG12	1.98	0.45
2:B:339:ASP:O	2:B:341:VAL:N	2.50	0.45
2:B:558:LYS:HE3	2:B:558:LYS:HB3	1.33	0.45
2:B:620:VAL:HB	2:B:621:PRO:HD3	1.98	0.45
2:B:917:TYR:HB3	2:C:1129:VAL:HG13	1.99	0.45
2:C:524:VAL:O	2:C:525:CYS:SG	2.74	0.45
1:G:68:ARG:HB3	1:G:85:ASN:O	2.17	0.44
2:A:490:PHE:CE2	2:A:492:LEU:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:HIS:CE1	2:B:51:THR:HB	2.52	0.44
2:B:502:GLY:O	2:B:506:GLN:N	2.50	0.44
2:B:673:SER:HB3	2:B:695:TYR:HE2	1.80	0.44
2:A:431:GLY:HA3	2:A:514:SER:HA	1.98	0.44
2:B:553:THR:HG23	2:B:586:ASP:HB3	1.99	0.44
2:B:1125:ASN:OD1	2:B:1125:ASN:N	2.50	0.44
2:C:86:PHE:CZ	2:C:89:GLY:HA2	2.52	0.44
1:G:69:PHE:CE2	1:G:84:MET:HG2	2.52	0.44
2:A:150:LYS:HD2	2:A:150:LYS:HA	1.68	0.44
2:B:411:ALA:O	2:B:414:GLN:HG2	2.18	0.44
2:B:537:LYS:HG3	2:B:539:VAL:HG13	1.99	0.44
2:B:1050:MET:HE3	2:B:1052:PHE:CE1	2.52	0.44
2:A:204:TYR:HA	2:A:225:PRO:HA	1.99	0.44
2:B:339:ASP:C	2:B:341:VAL:N	2.76	0.44
2:B:955:ASN:OD1	2:B:956:ALA:N	2.50	0.44
1:G:44:LYS:HD2	1:G:44:LYS:HA	1.77	0.44
1:I:99:TYR:HB3	1:I:113:TYR:HB3	1.99	0.44
2:B:106:PHE:HD2	2:B:235:ILE:HG21	1.82	0.44
2:B:206:LYS:HB3	2:B:223:LEU:HD22	2.00	0.44
2:B:178:ASP:N	2:B:178:ASP:OD1	2.42	0.44
1:E:35:MET:HE3	1:E:54:TRP:CH2	2.53	0.44
2:A:676:THR:HG1	2:A:689:SER:HG	1.59	0.44
2:A:709:ASN:ND2	4:A:1307:NAG:O5	2.49	0.44
2:B:157:PHE:CD1	2:B:158:ARG:N	2.85	0.44
2:B:318:PHE:CE2	2:B:615:VAL:HG11	2.52	0.44
1:G:61:TYR:CE1	1:G:71:ILE:HG22	2.53	0.44
1:G:109:ILE:HD12	2:C:501:TYR:HA	2.00	0.44
2:A:105:ILE:HD12	2:A:116:SER:HB2	1.98	0.44
2:A:357:ARG:HD2	2:A:359:SER:HB2	1.99	0.44
2:B:722:VAL:HG22	2:B:1065:VAL:HG22	2.00	0.44
2:B:1097:SER:C	2:B:1099:GLY:H	2.25	0.44
2:C:29:THR:HA	2:C:61:ASN:CA	2.48	0.44
2:C:329:PHE:O	2:C:331:ASN:N	2.50	0.44
2:A:59:PHE:HB2	2:A:293:LEU:HD11	1.99	0.44
2:C:125:ASN:OD1	2:C:171:VAL:HG23	2.17	0.44
1:I:53:ASP:OD2	1:I:57:THR:OG1	2.33	0.43
1:I:111:VAL:O	1:I:112:ASP:C	2.60	0.43
2:B:78:ARG:HD2	2:B:78:ARG:HA	1.36	0.43
2:B:613:GLN:HE21	2:B:613:GLN:HB2	1.57	0.43
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.77	0.43
2:B:1050:MET:HB2	2:B:1065:VAL:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:ILE:HG21	2:C:229:LEU:HD11	1.99	0.43
2:C:555:SER:HB3	2:C:584:ILE:O	2.18	0.43
1:E:29:ALA:O	2:A:377:PHE:N	2.51	0.43
1:G:105:LEU:HD11	1:G:108:SER:HA	2.00	0.43
2:A:325:SER:HB2	2:A:540:ASN:HD22	1.83	0.43
2:A:715:PRO:HD3	2:C:894:LEU:HD13	1.99	0.43
2:B:281:GLU:OE1	2:B:281:GLU:C	2.61	0.43
2:B:858:LEU:HD13	2:B:959:LEU:HD22	1.99	0.43
2:C:168:PHE:CZ	2:C:230:PRO:HG2	2.53	0.43
2:C:733:LYS:HB2	2:C:861:LEU:HB2	1.99	0.43
2:C:854:LYS:HZ1	2:C:860:VAL:HB	1.83	0.43
1:I:38:PHE:HE2	1:I:100:TRP:NE1	2.16	0.43
2:A:44:ARG:HH11	2:B:567:ARG:HH11	1.65	0.43
2:A:58:PHE:HB2	2:A:290:ASP:HB2	2.00	0.43
2:A:147:LYS:HA	2:A:147:LYS:HD3	1.86	0.43
2:A:603:ASN:N	2:A:603:ASN:OD1	2.51	0.43
2:A:1129:VAL:HG13	2:C:917:TYR:HB3	2.01	0.43
2:B:1145:LEU:O	2:B:1149:LYS:N	2.41	0.43
2:C:335:LEU:HD23	2:C:363:ALA:HA	2.00	0.43
2:C:763:LEU:HD21	2:C:1005:GLN:CD	2.44	0.43
2:A:597:VAL:HG22	2:A:610:VAL:HG12	2.00	0.43
2:A:601:GLY:O	2:A:602:THR:C	2.61	0.43
2:B:1123:SER:O	2:B:1123:SER:OG	2.31	0.43
2:C:54:LEU:HB3	2:C:270:LEU:HB3	2.01	0.43
2:C:146:HIS:CG	2:C:247:SER:H	2.37	0.43
2:C:230:PRO:O	2:C:231:ILE:C	2.61	0.43
2:C:328:ARG:HA	2:C:328:ARG:HD2	1.76	0.43
2:C:885:GLY:HA2	2:C:901:GLN:NE2	2.33	0.43
2:C:1097:SER:C	2:C:1099:GLY:N	2.77	0.43
2:C:1117:THR:HG22	2:C:1140:PRO:HD2	2.01	0.43
2:A:540:ASN:HA	2:A:549:THR:HA	2.00	0.43
2:A:612:TYR:HE1	2:A:651:ILE:HD12	1.83	0.43
2:A:703:ASN:O	2:C:789:TYR:HA	2.18	0.43
2:A:1148:PHE:CE2	2:B:1145:LEU:HD13	2.53	0.43
2:B:621:PRO:C	2:B:624:ILE:HG23	2.43	0.43
1:E:68:ARG:HD2	1:E:86:SER:HB3	2.00	0.43
1:I:49:VAL:HG13	1:I:65:VAL:HG11	1.99	0.43
1:I:53:ASP:HB3	1:I:58:VAL:H	1.83	0.43
2:A:531:THR:OG1	2:A:532:ASN:N	2.52	0.43
2:A:644:GLN:HG2	4:A:1305:NAG:H82	2.00	0.43
2:B:191:GLU:O	2:B:223:LEU:HD13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:GLN:H	2:B:563:GLN:HG2	1.68	0.43
2:B:212:LEU:O	2:B:213:GLY:C	2.62	0.43
2:B:224:GLU:OE1	2:B:224:GLU:N	2.49	0.43
2:B:501:TYR:HB3	2:B:505:HIS:HB2	2.01	0.43
2:B:853:GLN:OE1	2:B:854:LYS:NZ	2.44	0.43
2:B:1073:LYS:HD3	2:B:1075:PHE:CZ	2.54	0.43
2:A:97:LYS:HD3	2:A:97:LYS:HA	1.78	0.43
2:A:434:ILE:O	2:A:511:VAL:N	2.35	0.43
2:A:733:LYS:NZ	2:A:775:ASP:OD1	2.51	0.43
2:A:900:MET:HE2	2:A:900:MET:HB3	1.66	0.43
2:A:1104:VAL:HG11	2:A:1119:ASN:CG	2.44	0.43
2:B:320:VAL:HA	2:B:628:GLN:OE1	2.19	0.43
2:B:756:TYR:OH	2:B:994:ASP:OD1	2.35	0.43
2:C:519:HIS:CD2	2:C:567:ARG:NH2	2.75	0.43
2:A:30:ASN:O	2:A:32:PHE:N	2.51	0.43
2:A:490:PHE:HE2	2:A:492:LEU:HB2	1.84	0.43
2:A:1039:ARG:NE	2:C:1031:GLU:OE2	2.49	0.43
2:B:197:ILE:HG13	2:B:202:LYS:HZ3	1.83	0.43
2:B:366:SER:O	2:B:369:TYR:HB2	2.19	0.43
2:C:125:ASN:OD1	2:C:127:VAL:N	2.52	0.43
2:C:281:GLU:C	2:C:283:GLY:N	2.77	0.43
2:C:454:ARG:HD3	2:C:457:ARG:HB2	2.00	0.43
1:I:74:ASP:HB2	1:I:81:TYR:CZ	2.53	0.43
2:A:29:THR:C	2:A:61:ASN:HA	2.44	0.43
2:A:421:TYR:O	2:A:457:ARG:NE	2.52	0.43
2:B:73:THR:OG1	2:B:247:SER:HB3	2.19	0.43
2:C:119:ILE:HG23	2:C:128:ILE:HD12	2.00	0.43
2:C:131:CYS:SG	2:C:166:CYS:N	2.91	0.43
2:C:191:GLU:H	2:C:191:GLU:HG2	1.61	0.43
2:C:572:THR:O	2:C:574:ASP:N	2.52	0.43
2:A:71:SER:O	2:A:250:THR:HB	2.19	0.42
2:A:559:PHE:HB3	2:A:577:ARG:HH21	1.84	0.42
2:A:1045:LYS:HE3	2:A:1045:LYS:HB2	1.80	0.42
2:B:1114:ILE:O	2:B:1119:ASN:ND2	2.52	0.42
1:I:19:LEU:HD13	1:I:87:LEU:HD13	2.01	0.42
2:A:117:LEU:O	2:A:119:ILE:HG12	2.19	0.42
2:A:314:GLN:OE1	2:A:315:THR:N	2.52	0.42
2:A:442:ASP:O	2:A:448:ASN:ND2	2.52	0.42
2:A:969:LYS:HD2	2:C:755:GLN:HE22	1.84	0.42
2:B:416:GLY:O	2:B:420:ASP:N	2.50	0.42
2:B:421:TYR:HB3	2:B:457:ARG:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:VAL:HG21	2:B:539:VAL:HG21	2.01	0.42
2:B:657:ASN:O	2:B:658:SER:C	2.61	0.42
2:C:30:ASN:O	2:C:32:PHE:N	2.53	0.42
2:C:88:ASP:O	2:C:270:LEU:HB2	2.19	0.42
2:C:447:GLY:HA2	2:C:498:ARG:HG2	2.01	0.42
1:E:102:MET:HE3	1:E:105:LEU:HA	1.99	0.42
1:G:62:ALA:HB3	1:G:65:VAL:HG22	2.00	0.42
2:A:248:TYR:O	2:A:250:THR:N	2.51	0.42
2:A:546:LEU:HD23	2:A:546:LEU:HA	1.77	0.42
2:A:1018:ILE:O	2:A:1022:ALA:N	2.41	0.42
2:B:318:PHE:HA	2:B:630:THR:OG1	2.19	0.42
2:B:359:SER:O	2:B:360:ASN:C	2.62	0.42
2:B:416:GLY:O	2:B:420:ASP:HB2	2.19	0.42
2:B:624:ILE:H	2:B:624:ILE:HG12	1.40	0.42
2:B:650:LEU:HD12	2:B:650:LEU:HA	1.89	0.42
2:C:567:ARG:HH11	2:C:567:ARG:H	1.65	0.42
1:I:52:ILE:HB	1:I:71:ILE:HG23	2.01	0.42
2:A:790:LYS:HD3	2:A:790:LYS:HA	1.84	0.42
2:B:37:TYR:OH	2:B:53:ASP:OD1	2.37	0.42
2:C:188:ASN:O	2:C:190:ARG:HG3	2.19	0.42
2:A:36:VAL:HG11	2:A:220:PHE:CE2	2.55	0.42
2:A:985:ASP:HB2	2:A:987:PRO:HD2	2.00	0.42
2:B:37:TYR:OH	2:B:195:LYS:NZ	2.52	0.42
2:B:37:TYR:HA	2:B:223:LEU:H	1.83	0.42
2:C:152:TRP:CD1	2:C:153:MET:H	2.37	0.42
2:C:533:LEU:O	2:C:533:LEU:HG	2.18	0.42
1:G:23:CYS:HB2	1:G:97:CYS:HB2	1.81	0.42
2:A:64:TRP:HB2	2:A:259:THR:H	1.84	0.42
2:A:309:GLU:OE1	2:A:310:LYS:N	2.52	0.42
2:A:422:ASN:OD1	2:A:454:ARG:HB3	2.20	0.42
2:A:751:ASN:O	2:A:755:GLN:NE2	2.38	0.42
2:B:977:LEU:HD23	2:B:977:LEU:H	1.85	0.42
2:B:1047:TYR:O	2:B:1067:TYR:N	2.46	0.42
2:C:68:ILE:HA	2:C:250:THR:HB	2.01	0.42
2:C:462:LYS:HA	2:C:462:LYS:HD2	1.65	0.42
1:E:18:SER:HB3	1:E:83:GLN:HE21	1.84	0.42
1:I:40:GLN:HE22	1:I:94:THR:HB	1.85	0.42
2:A:78:ARG:HA	2:A:252:GLY:N	2.35	0.42
2:A:126:VAL:O	2:A:171:VAL:HA	2.19	0.42
2:A:350:VAL:HG22	2:A:422:ASN:HB3	2.02	0.42
2:C:214:ARG:NH1	2:C:215:ASP:OD1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1114:ILE:HD13	2:C:1114:ILE:HA	1.80	0.42
2:C:1144:GLU:OE1	2:C:1144:GLU:N	2.51	0.42
2:A:133:PHE:CD2	2:A:136:CYS:HA	2.54	0.42
2:A:146:HIS:CD2	2:A:147:LYS:H	2.38	0.42
2:A:716:THR:OG1	2:A:1071:GLN:O	2.36	0.42
2:A:998:THR:O	2:A:1002:GLN:HB2	2.20	0.42
2:B:36:VAL:O	2:B:223:LEU:HG	2.20	0.42
2:B:376:ALA:N	2:B:435:ALA:O	2.50	0.42
2:B:993:ILE:HD13	2:B:993:ILE:HA	1.91	0.42
2:C:137:ASN:HB2	2:C:159:VAL:HA	2.00	0.42
2:C:451:TYR:HD2	2:C:497:PHE:HD2	1.68	0.42
1:G:65:VAL:HB	1:G:69:PHE:CG	2.54	0.42
2:A:993:ILE:HD13	2:A:993:ILE:HA	1.87	0.42
2:B:1125:ASN:ND2	2:B:1127:ASP:OD1	2.53	0.42
2:C:157:PHE:CD2	2:C:159:VAL:HG13	2.52	0.42
2:C:518:LEU:HD12	2:C:518:LEU:HA	1.84	0.42
2:C:523:THR:HG23	2:C:524:VAL:HG22	2.02	0.42
1:I:37:TRP:CD2	1:I:82:LEU:HD22	2.54	0.42
2:A:117:LEU:HD13	2:A:130:VAL:HG13	2.01	0.42
2:A:170:TYR:CE1	2:A:231:ILE:HD11	2.54	0.42
2:A:390:LEU:HB3	2:A:392:PHE:CZ	2.54	0.42
2:B:190:ARG:O	2:B:192:PHE:N	2.52	0.42
2:B:201:PHE:HB3	2:B:229:LEU:HB3	2.02	0.42
2:B:234:ASN:OD1	2:B:234:ASN:N	2.52	0.42
2:B:362:VAL:C	2:B:524:VAL:HG21	2.45	0.42
2:C:100:ILE:H	2:C:100:ILE:HG13	1.63	0.42
1:I:100:TRP:CD1	1:I:111:VAL:HG13	2.54	0.41
2:A:115:GLN:HE22	2:A:165:ASN:C	2.28	0.41
2:A:190:ARG:O	2:A:192:PHE:N	2.49	0.41
2:A:352:ALA:C	2:A:466:ARG:HH21	2.28	0.41
2:A:802:PHE:HZ	2:A:898:PHE:CZ	2.38	0.41
2:B:64:TRP:CD1	2:B:259:THR:HG23	2.55	0.41
2:B:143:VAL:HG13	2:B:245:HIS:CE1	2.54	0.41
2:B:559:PHE:HE2	2:B:564:GLN:O	2.03	0.41
2:B:1004:LEU:HD23	2:B:1004:LEU:HA	1.89	0.41
2:C:278:LYS:HE3	2:C:278:LYS:HB2	1.93	0.41
2:C:353:TRP:O	2:C:466:ARG:NE	2.39	0.41
2:C:1141:LEU:O	2:C:1142:GLN:C	2.62	0.41
2:A:169:GLU:OE2	2:A:171:VAL:HB	2.20	0.41
2:A:248:TYR:HD2	2:A:249:LEU:HG	1.84	0.41
2:A:707:TYR:HB3	2:C:792:PRO:HG2	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:PHE:HD1	2:B:158:ARG:H	1.66	0.41
2:C:67:ALA:O	2:C:250:THR:HB	2.19	0.41
2:C:129:LYS:HE3	2:C:129:LYS:HB2	1.83	0.41
2:C:329:PHE:O	2:C:330:PRO:C	2.63	0.41
2:C:728:PRO:HB3	2:C:951:VAL:HG21	2.01	0.41
1:E:39:ARG:NH2	1:E:64:SER:OG	2.52	0.41
1:G:71:ILE:HA	1:G:82:LEU:HA	2.03	0.41
2:A:138:ASP:OD1	2:A:139:PRO:HD2	2.21	0.41
2:B:131:CYS:HB3	2:B:133:PHE:CZ	2.55	0.41
2:C:305:SER:OG	2:C:307:THR:O	2.38	0.41
2:C:371:PHE:HZ	2:C:436:TRP:CE3	2.38	0.41
2:C:524:VAL:C	2:C:525:CYS:SG	3.03	0.41
2:C:1045:LYS:HB2	2:C:1045:LYS:HE2	1.72	0.41
1:E:73:ARG:HH12	1:E:78:ASN:HA	1.85	0.41
1:I:24:ALA:HB2	1:I:79:THR:HG22	2.01	0.41
2:A:58:PHE:O	2:A:59:PHE:C	2.63	0.41
2:B:176:LEU:HA	2:B:190:ARG:HH22	1.85	0.41
2:B:335:LEU:HD13	2:B:335:LEU:HA	1.85	0.41
2:B:461:LEU:HA	2:B:461:LEU:HD23	1.81	0.41
2:C:540:ASN:OD1	2:C:549:THR:OG1	2.38	0.41
2:C:849:LEU:HG	2:C:851:CYS:H	1.85	0.41
2:C:1054:GLN:N	2:C:1061:VAL:O	2.50	0.41
1:I:69:PHE:HA	1:I:84:MET:HB3	2.01	0.41
2:A:29:THR:HA	2:A:260:ALA:N	2.35	0.41
2:A:83:VAL:HG11	2:A:237:ARG:NH2	2.35	0.41
2:A:811:LYS:HE3	2:A:811:LYS:HB2	1.80	0.41
2:B:73:THR:HG23	2:B:79:PHE:CZ	2.55	0.41
2:B:189:LEU:O	2:B:191:GLU:HG3	2.21	0.41
2:B:375:PHE:HA	2:B:436:TRP:HB3	2.03	0.41
2:C:127:VAL:HG23	2:C:169:GLU:HB3	2.02	0.41
2:C:402:ILE:HD11	2:C:407:VAL:HA	2.01	0.41
1:I:100:TRP:HB3	1:I:102:MET:SD	2.60	0.41
2:A:34:ARG:HH22	2:A:221:SER:N	2.14	0.41
2:A:144:TYR:HA	2:A:146:HIS:CE1	2.56	0.41
2:A:423:TYR:HA	2:A:461:LEU:HD12	2.02	0.41
2:A:433:VAL:HG22	2:A:512:VAL:HG22	2.03	0.41
2:A:986:PRO:N	2:A:987:PRO:HD2	2.35	0.41
2:B:473:TYR:CZ	2:B:475:ALA:HB2	2.56	0.41
2:C:126:VAL:HG13	2:C:174:PRO:HA	2.03	0.41
2:C:715:PRO:HA	2:C:1072:GLU:HA	2.03	0.41
2:C:996:LEU:HD21	2:C:1000:ARG:CZ	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:232:GLY:C	2:A:233:ILE:HG13	2.45	0.41
2:B:99:ASN:CG	2:B:102:ARG:HD2	2.46	0.41
2:B:347:PHE:HE2	2:B:511:VAL:HG22	1.86	0.41
2:B:1114:ILE:HD12	2:B:1114:ILE:HA	1.75	0.41
2:C:280:ASN:O	2:C:281:GLU:C	2.63	0.41
2:C:412:PRO:HB3	2:C:427:ASP:HA	2.02	0.41
2:C:728:PRO:O	2:C:1021:SER:OG	2.31	0.41
1:I:21:LEU:HD23	1:I:21:LEU:HA	1.94	0.41
2:A:409:GLN:O	2:A:419:ALA:HB2	2.21	0.41
2:A:420:ASP:O	2:A:460:ASN:HA	2.20	0.41
2:A:1104:VAL:HG21	2:A:1119:ASN:OD1	2.21	0.41
2:B:45:SER:O	2:B:46:SER:C	2.63	0.41
2:B:122:ASN:HB3	2:B:153:MET:SD	2.61	0.41
2:B:222:ALA:HB2	2:B:285:ILE:HB	2.02	0.41
2:B:748:GLU:H	2:B:748:GLU:CD	2.29	0.41
2:C:141:LEU:HD12	2:C:144:TYR:HA	2.03	0.41
2:C:663:ASP:HB3	2:C:673:SER:HB3	2.03	0.41
1:E:40:GLN:HB3	1:E:96:TYR:CE1	2.56	0.41
1:G:5:LEU:HD13	1:G:114:TRP:O	2.21	0.41
2:A:141:LEU:HD23	2:A:141:LEU:HA	1.85	0.41
2:A:375:PHE:HB3	2:A:436:TRP:CB	2.50	0.41
2:A:417:ASN:HA	2:A:421:TYR:CD2	2.55	0.41
2:A:449:TYR:O	2:A:494:SER:OG	2.38	0.41
2:A:578:ASP:HB2	2:A:585:LEU:HD23	2.02	0.41
2:A:722:VAL:HG22	2:A:1065:VAL:HG22	2.03	0.41
2:A:1093:GLY:HA2	2:A:1107:ARG:HD2	2.02	0.41
2:B:117:LEU:CD2	2:B:233:ILE:HD13	2.50	0.41
2:B:273:ARG:HD3	2:B:273:ARG:HA	1.91	0.41
2:B:314:GLN:HA	2:B:596:SER:HA	2.02	0.41
2:B:369:TYR:HD1	2:B:369:TYR:HA	1.79	0.41
2:C:370:ASN:O	2:C:371:PHE:C	2.64	0.41
2:C:578:ASP:O	2:C:579:PRO:C	2.61	0.41
2:C:730:SER:O	2:C:1058:HIS:HB3	2.20	0.41
2:A:320:VAL:HG21	2:A:620:VAL:HG21	2.03	0.41
2:B:117:LEU:HD23	2:B:233:ILE:HD13	2.03	0.41
2:B:242:LEU:O	2:B:244:LEU:N	2.54	0.41
2:B:454:ARG:HG3	2:B:491:PRO:HB2	2.03	0.41
2:C:324:GLU:C	2:C:539:VAL:HG13	2.46	0.41
2:C:584:ILE:H	2:C:584:ILE:HG12	1.53	0.41
2:C:852:ALA:O	2:C:855:PHE:HB3	2.21	0.41
2:C:1080:ALA:HB3	2:C:1132:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:SER:O	1:E:81:TYR:N	2.28	0.40
2:A:63:THR:HA	2:A:257:GLY:HA2	2.04	0.40
2:A:170:TYR:OH	2:A:230:PRO:HD2	2.21	0.40
2:A:559:PHE:CD1	2:A:584:ILE:HD12	2.57	0.40
2:A:805:ILE:HD13	2:A:931:ILE:HD11	2.03	0.40
2:B:359:SER:HB3	2:B:522:ALA:CB	2.51	0.40
2:C:124:THR:O	2:C:124:THR:OG1	2.38	0.40
2:C:281:GLU:O	2:C:283:GLY:N	2.53	0.40
2:A:133:PHE:HA	2:A:162:SER:HA	2.02	0.40
2:A:631:PRO:O	2:A:633:TRP:NE1	2.54	0.40
2:B:164:ASN:HB3	2:B:165:ASN:H	1.59	0.40
2:B:350:VAL:CG1	2:B:422:ASN:HD21	2.34	0.40
2:B:985:ASP:N	2:B:985:ASP:OD1	2.52	0.40
2:C:64:TRP:CD1	2:C:66:HIS:CD2	3.08	0.40
2:C:541:PHE:CZ	2:C:587:ILE:HD13	2.57	0.40
2:C:1146:ASP:O	2:C:1150:GLU:N	2.42	0.40
2:A:167:THR:HG22	2:A:168:PHE:N	2.36	0.40
2:A:425:LEU:HD23	2:A:425:LEU:HA	1.93	0.40
2:A:867:ASP:OD1	2:A:867:ASP:N	2.52	0.40
2:A:1054:GLN:N	2:A:1061:VAL:O	2.53	0.40
2:C:542:ASN:O	2:C:543:PHE:C	2.65	0.40
2:B:195:LYS:HB3	2:B:195:LYS:HE2	1.84	0.40
2:B:386:LYS:O	2:B:387:LEU:C	2.64	0.40
2:B:453:TYR:HB3	2:B:495:TYR:CD1	2.56	0.40
2:C:271:GLN:O	2:C:273:ARG:N	2.55	0.40
2:C:473:TYR:H	2:C:491:PRO:HD3	1.85	0.40
2:C:814:LYS:HA	2:C:814:LYS:HD3	1.84	0.40
2:C:1141:LEU:O	2:C:1145:LEU:N	2.55	0.40
2:B:54:LEU:HB3	2:B:270:LEU:HD23	2.03	0.40
2:B:387:LEU:HA	2:B:387:LEU:HD22	1.90	0.40
2:B:453:TYR:OH	2:B:455:LEU:HD22	2.21	0.40
2:C:58:PHE:HD1	2:C:58:PHE:HA	1.75	0.40
2:C:105:ILE:HB	2:C:241:LEU:HD11	2.03	0.40
2:C:368:LEU:C	2:C:370:ASN:H	2.30	0.40
2:C:611:LEU:HD12	2:C:649:CYS:O	2.21	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	E	123/124 (99%)	112 (91%)	11 (9%)	0	100	100
1	G	123/124 (99%)	113 (92%)	10 (8%)	0	100	100
1	I	123/124 (99%)	115 (94%)	8 (6%)	0	100	100
2	A	1073/1288 (83%)	949 (88%)	104 (10%)	20 (2%)	6	25
2	B	1071/1288 (83%)	903 (84%)	147 (14%)	21 (2%)	6	24
2	C	1074/1288 (83%)	932 (87%)	121 (11%)	21 (2%)	6	24
All	All	3587/4236 (85%)	3124 (87%)	401 (11%)	62 (2%)	9	27

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	77	LYS
2	A	78	ARG
2	A	245	HIS
2	A	333	THR
2	A	618	THR
2	B	44	ARG
2	B	251	PRO
2	B	363	ALA
2	C	231	ILE
2	C	330	PRO
2	C	370	ASN
2	C	570	ALA
2	A	31	SER
2	A	64	TRP
2	A	73	THR
2	A	118	LEU
2	A	332	ILE
2	B	73	THR
2	B	76	THR
2	B	145	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	163	ALA
2	B	248	TYR
2	B	330	PRO
2	B	619	GLU
2	C	245	HIS
2	C	282	ASN
2	C	526	GLY
2	C	544	ASN
2	C	571	ASP
2	C	581	THR
2	A	30	ASN
2	A	63	THR
2	A	260	ALA
2	B	78	ARG
2	B	243	ALA
2	B	340	GLU
2	B	561	PRO
2	B	617	CYS
2	C	331	ASN
2	A	66	HIS
2	A	249	LEU
2	A	336	CYS
2	A	393	THR
2	B	329	PHE
2	B	360	ASN
2	B	618	THR
2	C	336	CYS
2	C	532	ASN
2	C	546	LEU
2	C	564	GLN
2	A	534	VAL
2	B	381	GLY
2	C	360	ASN
2	C	361	CYS
2	C	620	VAL
2	A	285	ILE
2	B	245	HIS
2	C	362	VAL
2	A	233	ILE
2	B	336	CYS
2	C	566	GLY
2	C	561	PRO

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	E	102/101 (101%)	100 (98%)	2 (2%)	48	66
1	G	100/101 (99%)	97 (97%)	3 (3%)	36	60
1	I	102/101 (101%)	99 (97%)	3 (3%)	37	60
2	A	931/1113 (84%)	890 (96%)	41 (4%)	25	51
2	B	934/1113 (84%)	848 (91%)	86 (9%)	8	30
2	C	939/1113 (84%)	886 (94%)	53 (6%)	19	46
All	All	3108/3642 (85%)	2920 (94%)	188 (6%)	19	43

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

Mol	Chain	Res	Type
1	E	26[A]	SER
1	E	26[B]	SER
1	G	35	MET
1	G	52	ILE
1	G	79	THR
1	I	111	VAL
1	I	112	ASP
1	I	113	TYR
2	A	65	PHE
2	A	71	SER
2	A	73	THR
2	A	77	LYS
2	A	80	ASP
2	A	105	ILE
2	A	117	LEU
2	A	118	LEU
2	A	130	VAL
2	A	132	GLU
2	A	233	ILE
2	A	236	THR
2	A	244	LEU
2	A	250	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	256	SER
2	A	259	THR
2	A	281	GLU
2	A	284	THR
2	A	308	VAL
2	A	332	ILE
2	A	335	LEU
2	A	336	CYS
2	A	362	VAL
2	A	387	LEU
2	A	389	ASP
2	A	390	LEU
2	A	394	ASN
2	A	523	THR
2	A	524	VAL
2	A	533	LEU
2	A	558	LYS
2	A	600	PRO
2	A	605	SER
2	A	618	THR
2	A	619	GLU
2	A	630	THR
2	A	931	ILE
2	A	1097	SER
2	A	1104	VAL
2	A	1115	ILE
2	A	1117	THR
2	B	40	ASP
2	B	42	VAL
2	B	44	ARG
2	B	46	SER
2	B	61	ASN
2	B	66	HIS
2	B	73	THR
2	B	77	LYS
2	B	78	ARG
2	B	100	ILE
2	B	126	VAL
2	B	132	GLU
2	B	143	VAL
2	B	212	LEU
2	B	214	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	215	ASP
2	B	233	ILE
2	B	239	GLN
2	B	240	THR
2	B	242	LEU
2	B	248	TYR
2	B	249	LEU
2	B	255	SER
2	B	259	THR
2	B	281	GLU
2	B	307	THR
2	B	308	VAL
2	B	309	GLU
2	B	327	VAL
2	B	329	PHE
2	B	333	THR
2	B	334	ASN
2	B	335	LEU
2	B	336	CYS
2	B	338	PHE
2	B	347	PHE
2	B	359	SER
2	B	360	ASN
2	B	361	CYS
2	B	369	TYR
2	B	375	PHE
2	B	378	LYS
2	B	382	VAL
2	B	383	SER
2	B	386	LYS
2	B	387	LEU
2	B	389	ASP
2	B	390	LEU
2	B	391	CYS
2	B	395	VAL
2	B	400	PHE
2	B	402	ILE
2	B	428	ASP
2	B	433	VAL
2	B	434	ILE
2	B	438	SER
2	B	503	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	513	LEU
2	B	516	GLU
2	B	517	LEU
2	B	524	VAL
2	B	557	LYS
2	B	558	LYS
2	B	561	PRO
2	B	580	GLN
2	B	581	THR
2	B	582	LEU
2	B	584	ILE
2	B	602	THR
2	B	605	SER
2	B	617	CYS
2	B	618	THR
2	B	619	GLU
2	B	624	ILE
2	B	657	ASN
2	B	710	ASN
2	B	873	TYR
2	B	963	VAL
2	B	967	SER
2	B	1081	ILE
2	B	1096	VAL
2	B	1101	HIS
2	B	1104	VAL
2	B	1114	ILE
2	B	1115	ILE
2	B	1119	ASN
2	C	31	SER
2	C	62	VAL
2	C	68	ILE
2	C	73	THR
2	C	74	ASN
2	C	134	GLN
2	C	229	LEU
2	C	259	THR
2	C	280	ASN
2	C	326	ILE
2	C	327	VAL
2	C	329	PHE
2	C	333	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	334	ASN
2	C	335	LEU
2	C	336	CYS
2	C	338	PHE
2	C	341	VAL
2	C	343	ASN
2	C	358	ILE
2	C	360	ASN
2	C	362	VAL
2	C	367	VAL
2	C	368	LEU
2	C	370	ASN
2	C	388	ASN
2	C	389	ASP
2	C	523	THR
2	C	524	VAL
2	C	531	THR
2	C	532	ASN
2	C	533	LEU
2	C	557	LYS
2	C	558	LYS
2	C	560	LEU
2	C	561	PRO
2	C	567	ARG
2	C	569	ILE
2	C	583	GLU
2	C	584	ILE
2	C	603	ASN
2	C	617	CYS
2	C	651	ILE
2	C	709	ASN
2	C	1081	ILE
2	C	1097	SER
2	C	1114	ILE
2	C	1115	ILE
2	C	1117	THR
2	C	1132	ILE
2	C	1136	THR
2	C	1137	VAL
2	C	1141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	14	GLN
1	E	40	GLN
1	E	106	GLN
1	E	107	ASN
1	G	4	GLN
1	G	107	ASN
1	G	116	GLN
1	I	4	GLN
1	I	14	GLN
1	I	83	GLN
1	I	85	ASN
1	I	107	ASN
2	A	173	GLN
2	A	196	ASN
2	A	394	ASN
2	A	405	ASN
2	A	439	ASN
2	A	448	ASN
2	A	804	GLN
2	A	949	GLN
2	A	992	GLN
2	A	1142	GLN
2	B	30	ASN
2	B	49	HIS
2	B	74	ASN
2	B	196	ASN
2	B	245	HIS
2	B	331	ASN
2	B	354	ASN
2	B	388	ASN
2	B	417	ASN
2	B	422	ASN
2	B	460	ASN
2	B	481	ASN
2	B	506	GLN
2	B	580	GLN
2	B	644	GLN
2	B	675	GLN
2	B	1108	ASN
2	C	87	ASN
2	C	134	GLN
2	C	245	HIS
2	C	474	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	493	GLN
2	C	519	HIS
2	C	641	ASN
2	C	690	GLN
2	C	784	GLN
2	C	901	GLN
2	C	919	ASN
2	C	926	GLN
2	C	954	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
3	NAG	K	1	3,2	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.40	0
3	NAG	L	1	3,2	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	L	2	3	14,14,15	0.18	0	17,19,21	0.38	0
3	NAG	M	1	3,2	14,14,15	0.37	0	17,19,21	0.41	0
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	0.51	0
3	NAG	N	1	3,2	14,14,15	0.39	0	17,19,21	0.59	0
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	0.44	0
3	NAG	R	1	3,2	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	R	2	3	14,14,15	0.17	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	S	1	3,2	14,14,15	0.37	0	17,19,21	0.41	0
3	NAG	S	2	3	14,14,15	0.17	0	17,19,21	0.42	0
3	NAG	T	1	3,2	14,14,15	0.38	0	17,19,21	0.91	2 (11%)
3	NAG	T	2	3	14,14,15	0.39	0	17,19,21	0.34	0
3	NAG	U	1	3,2	14,14,15	0.39	0	17,19,21	0.57	0
3	NAG	U	2	3	14,14,15	0.39	0	17,19,21	0.70	0
3	NAG	X	1	3,2	14,14,15	0.36	0	17,19,21	0.42	0
3	NAG	X	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	Y	1	3,2	14,14,15	0.41	0	17,19,21	0.58	0
3	NAG	Y	2	3	14,14,15	0.41	0	17,19,21	0.40	0
3	NAG	Z	1	3,2	14,14,15	0.39	0	17,19,21	0.89	2 (11%)
3	NAG	Z	2	3	14,14,15	0.40	0	17,19,21	0.38	0
3	NAG	a	1	3,2	14,14,15	0.56	0	17,19,21	0.46	0
3	NAG	a	2	3	14,14,15	0.22	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	3,2	-	5/6/23/26	0/1/1/1
3	NAG	T	2	3	-	6/6/23/26	0/1/1/1
3	NAG	U	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C1-O5-C5	2.28	115.24	112.19
3	T	1	NAG	O5-C1-C2	2.25	114.78	111.29
3	Z	1	NAG	C2-N2-C7	-2.17	120.00	122.90
3	Z	1	NAG	O5-C1-C2	-2.10	108.04	111.29

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C8-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	M	2	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

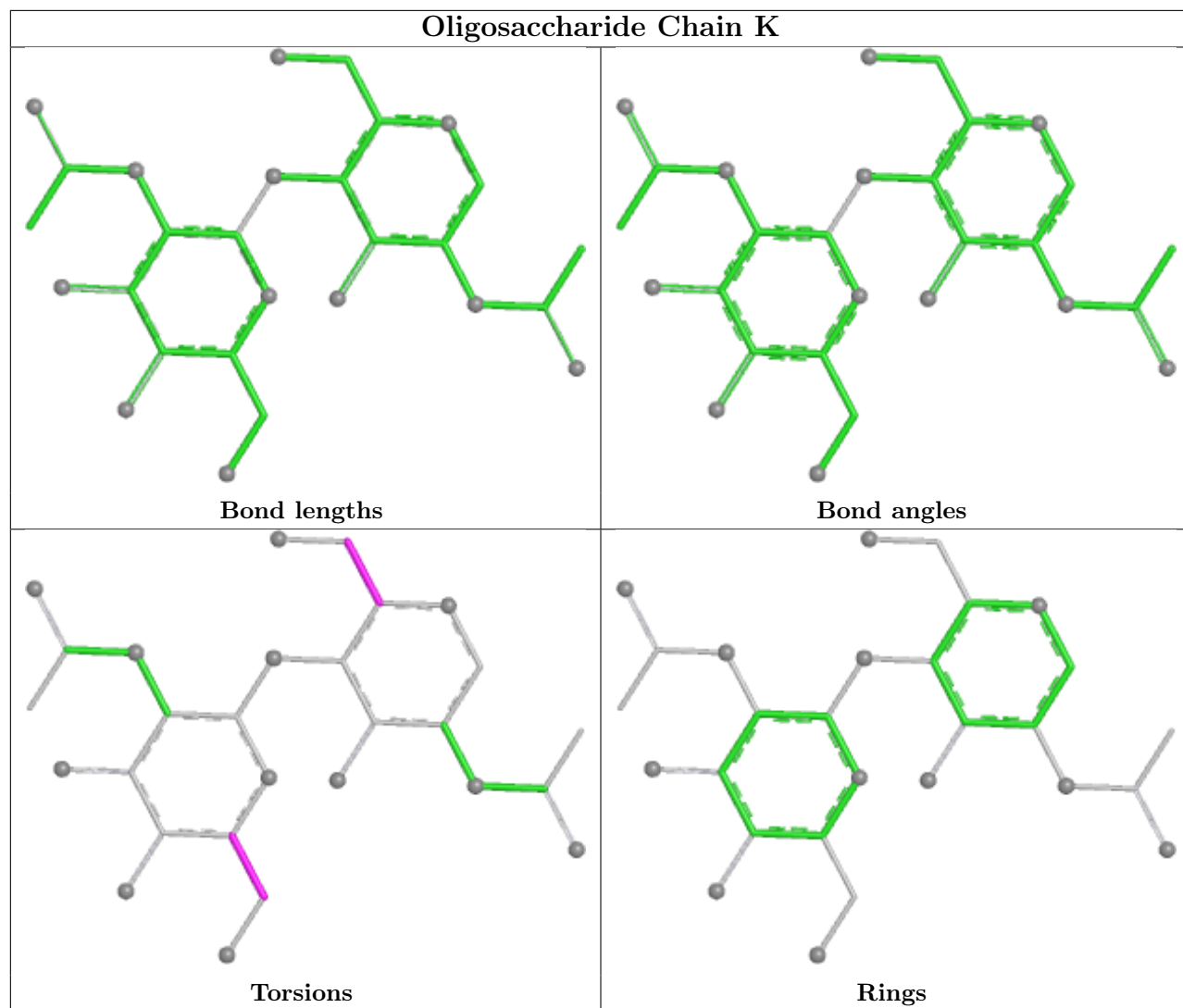
Mol	Chain	Res	Type	Atoms
3	U	1	NAG	O7-C7-N2-C2
3	N	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C1-C2-N2-C7
3	T	2	NAG	C1-C2-N2-C7
3	U	1	NAG	C1-C2-N2-C7
3	Y	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C3-C2-N2-C7
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2

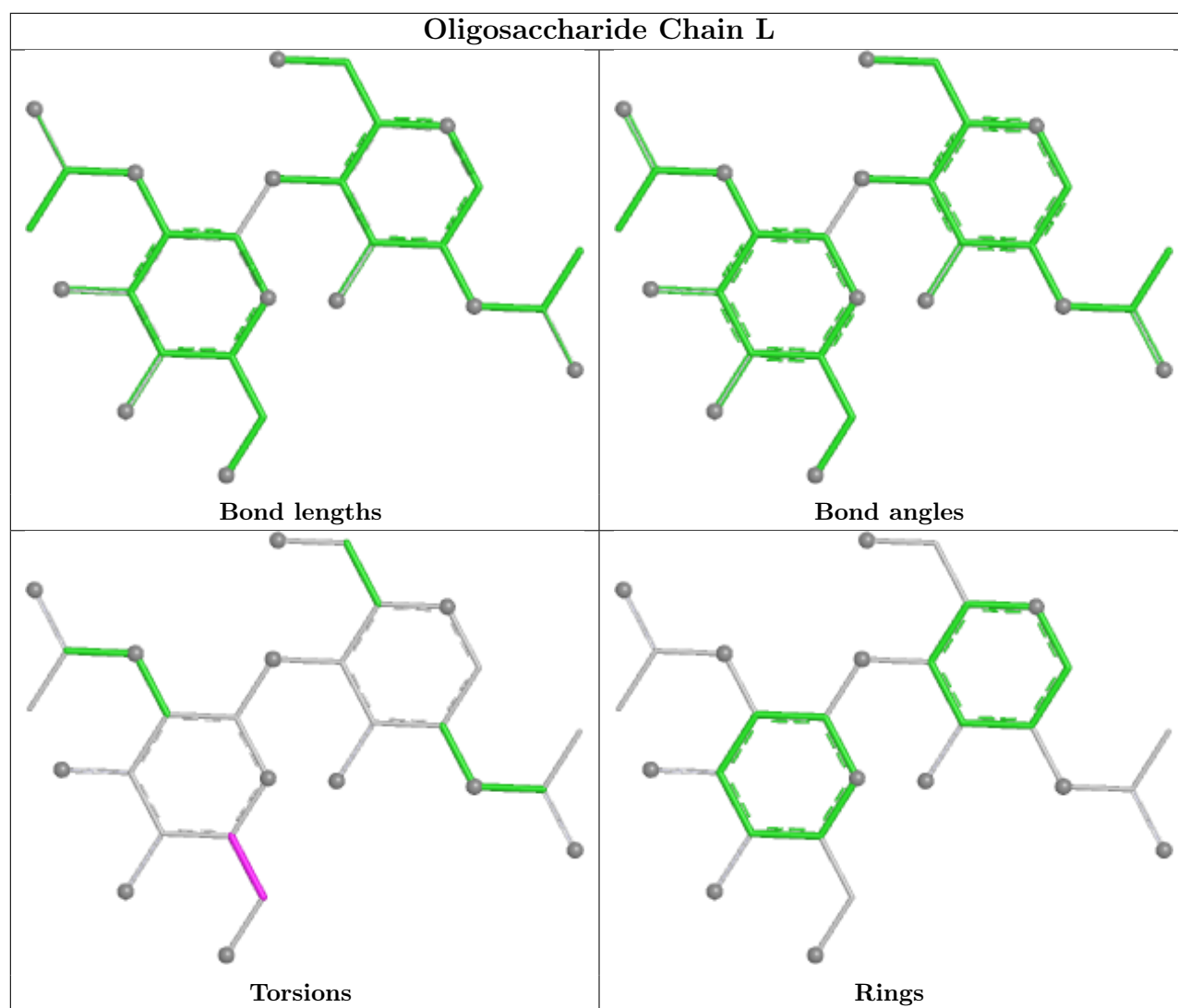
There are no ring outliers.

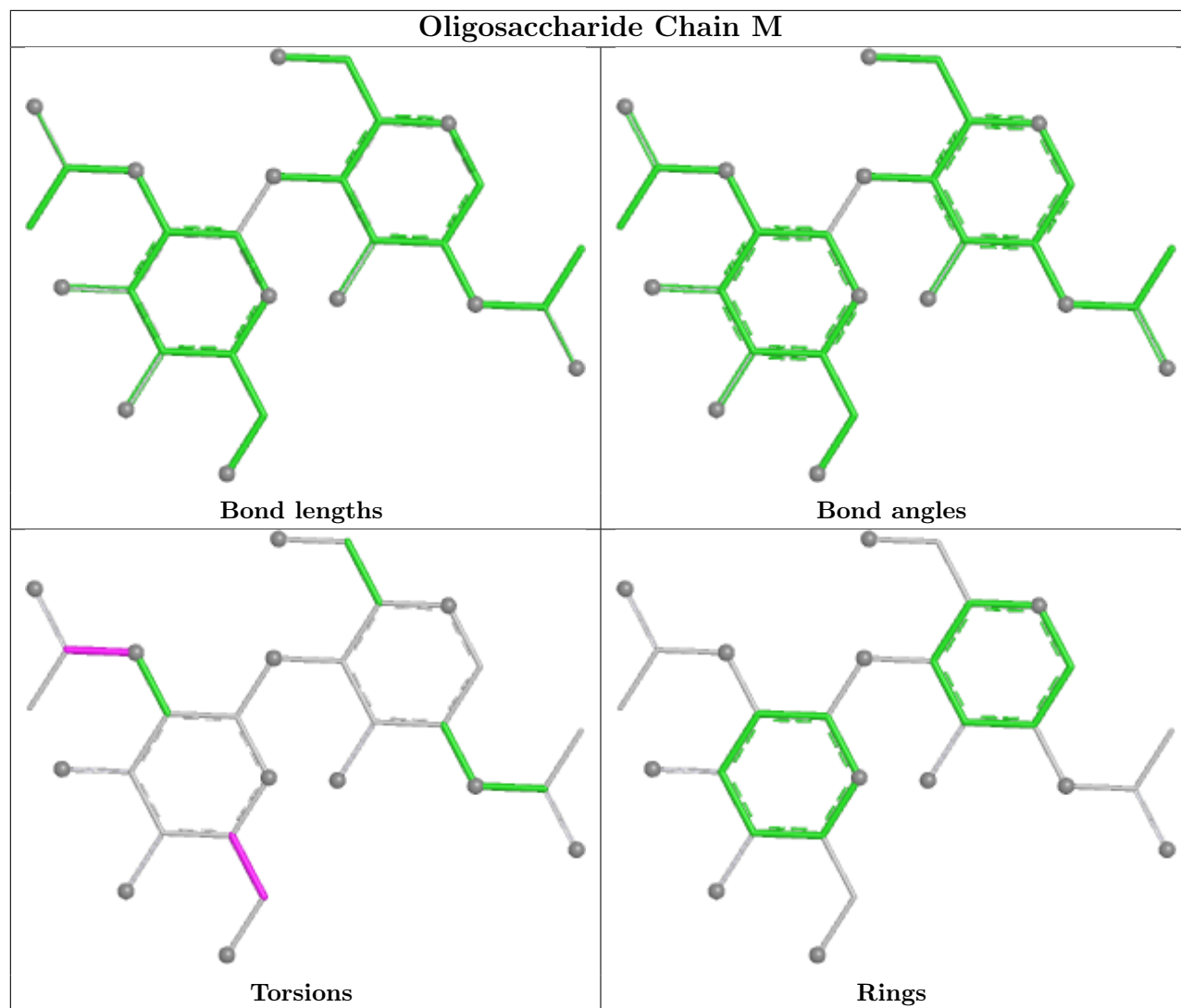
4 monomers are involved in 4 short contacts:

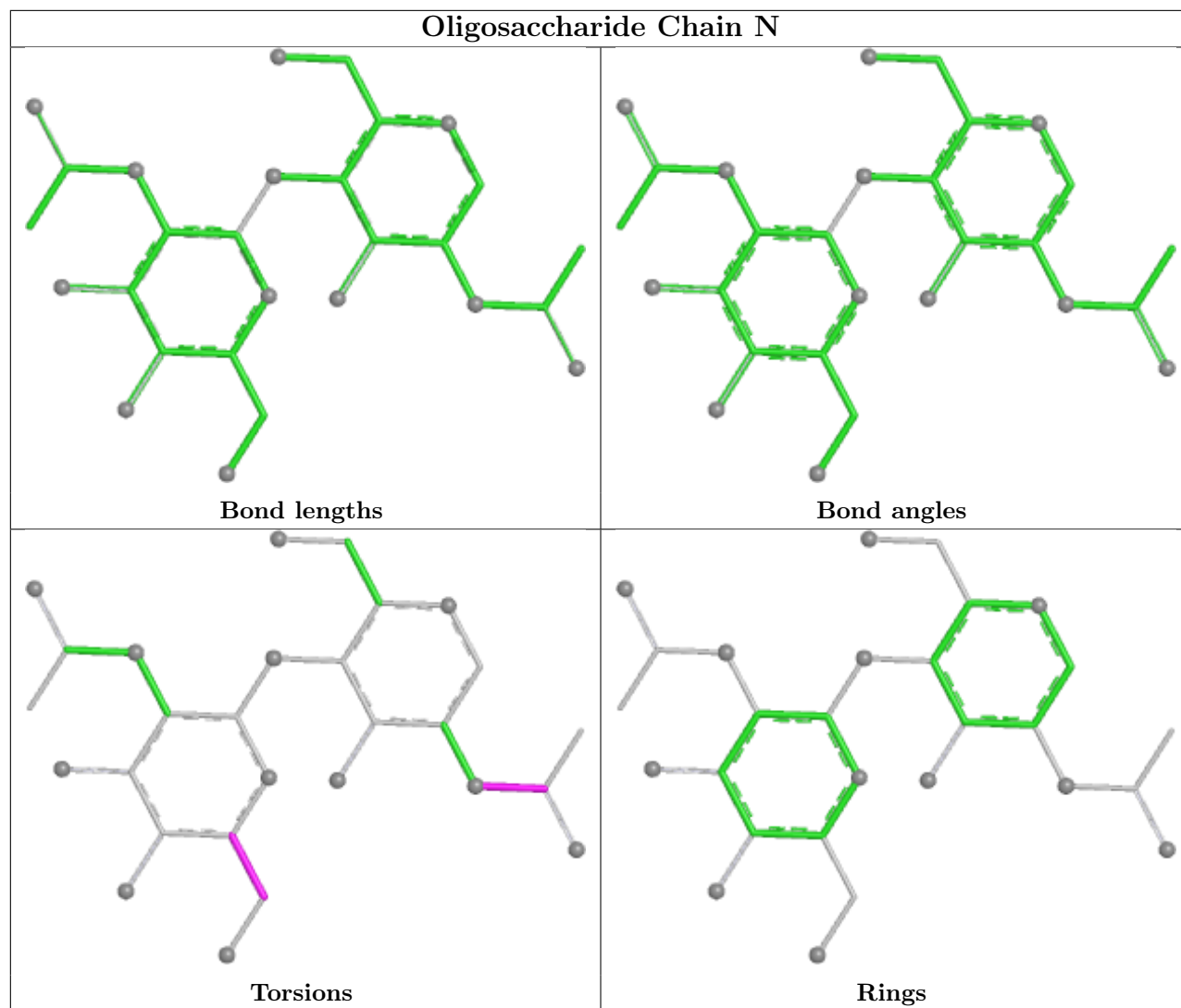
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	1	NAG	1	0
3	K	1	NAG	1	0
3	R	1	NAG	1	0
3	Z	1	NAG	1	0

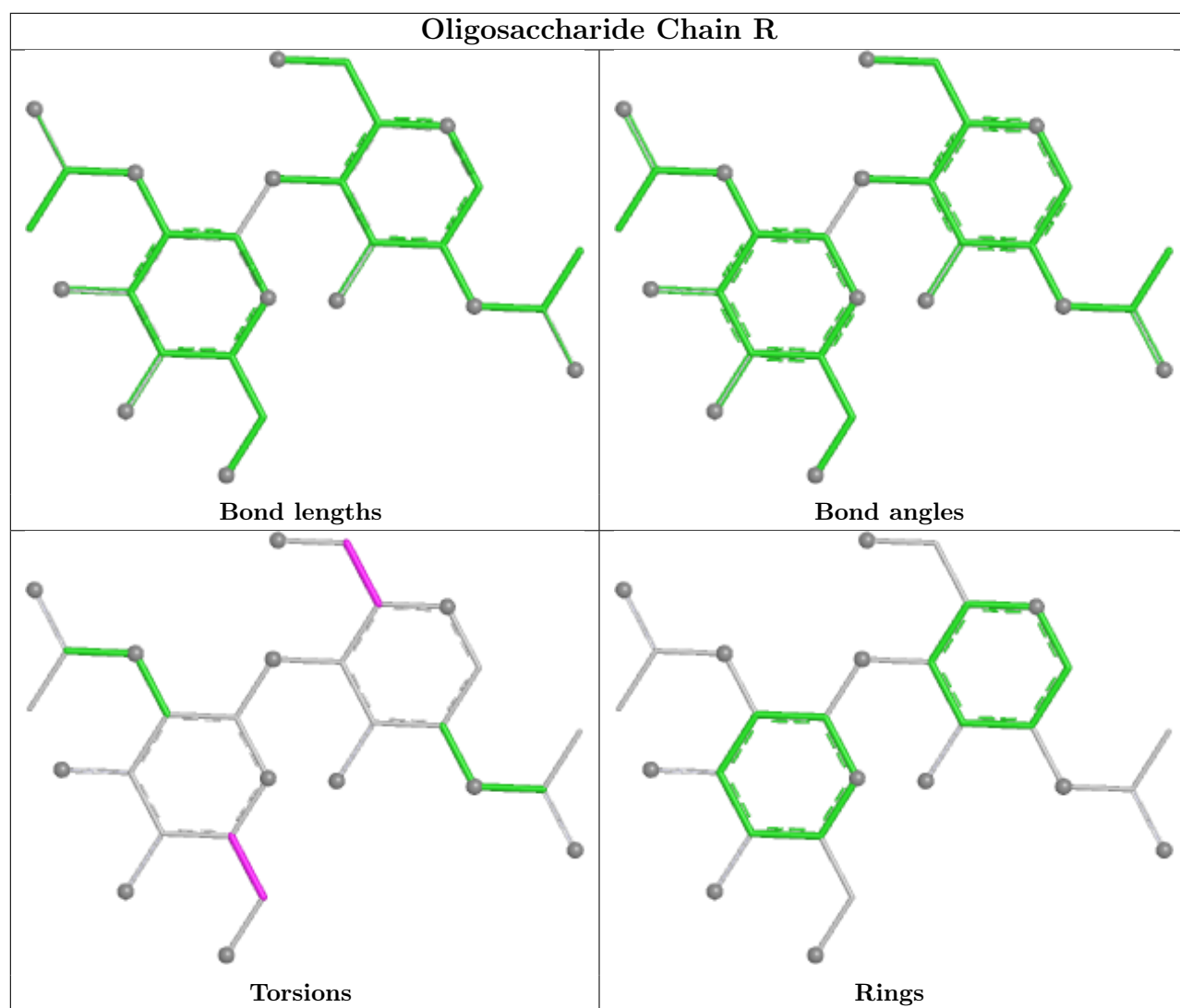
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

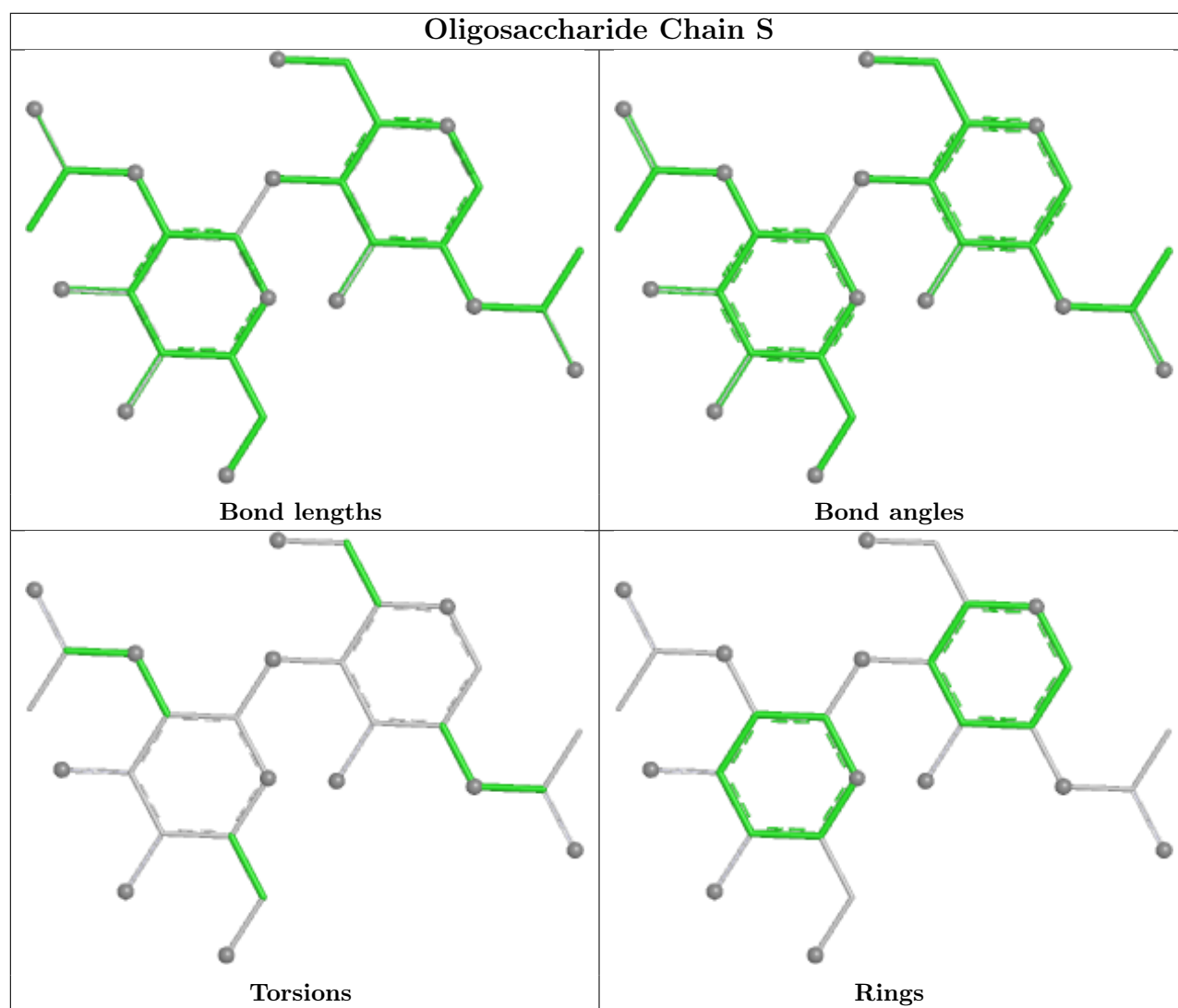


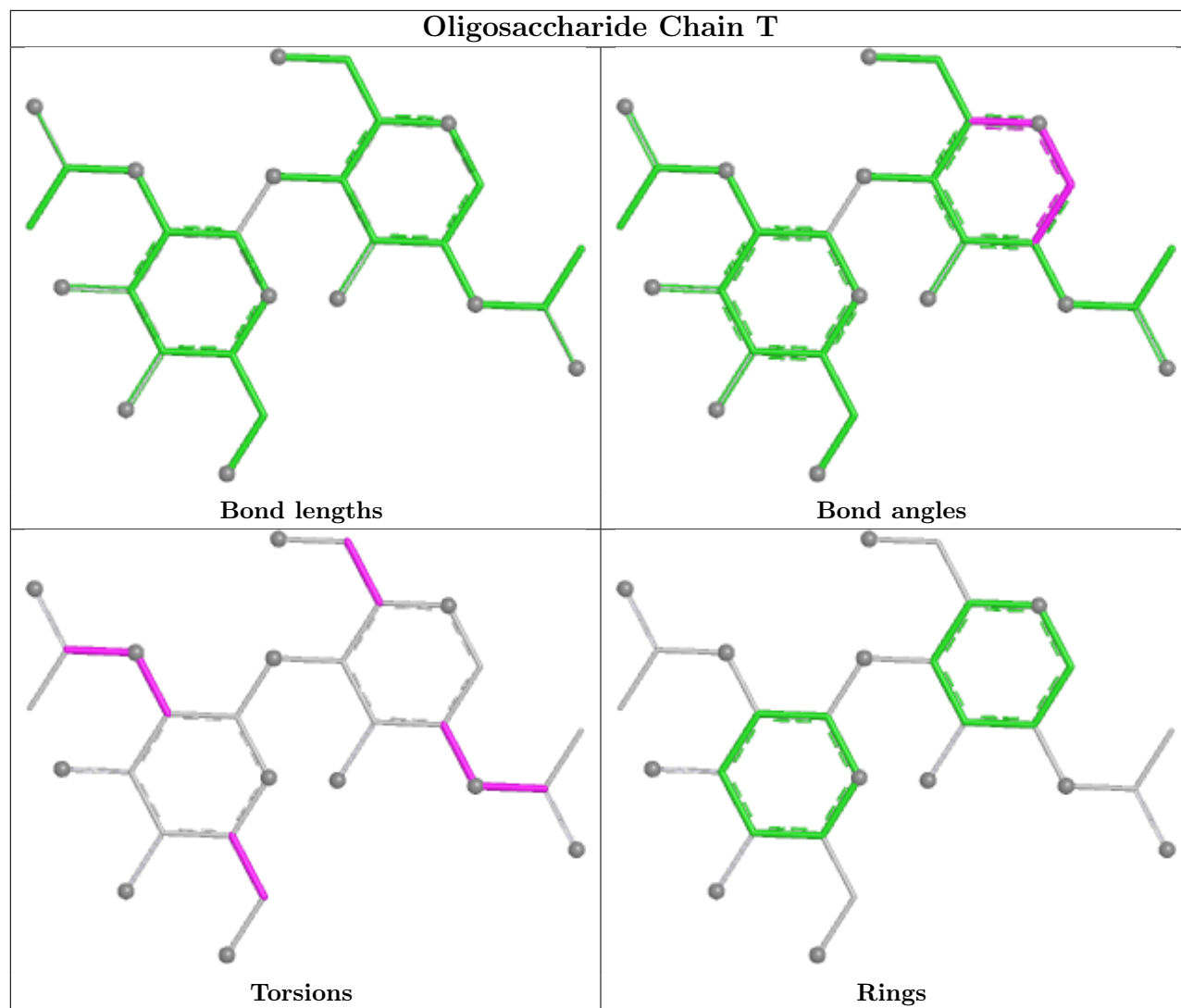


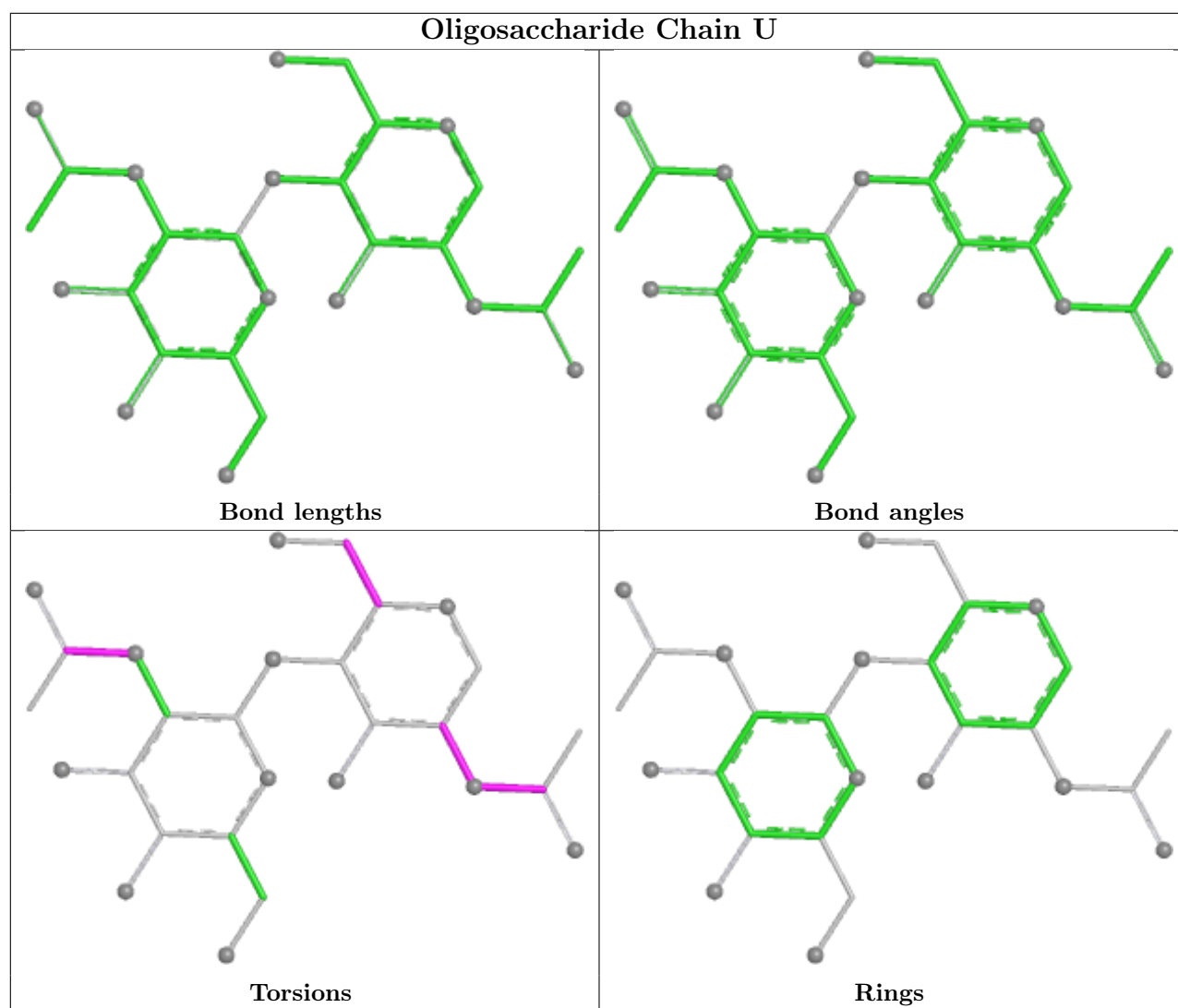


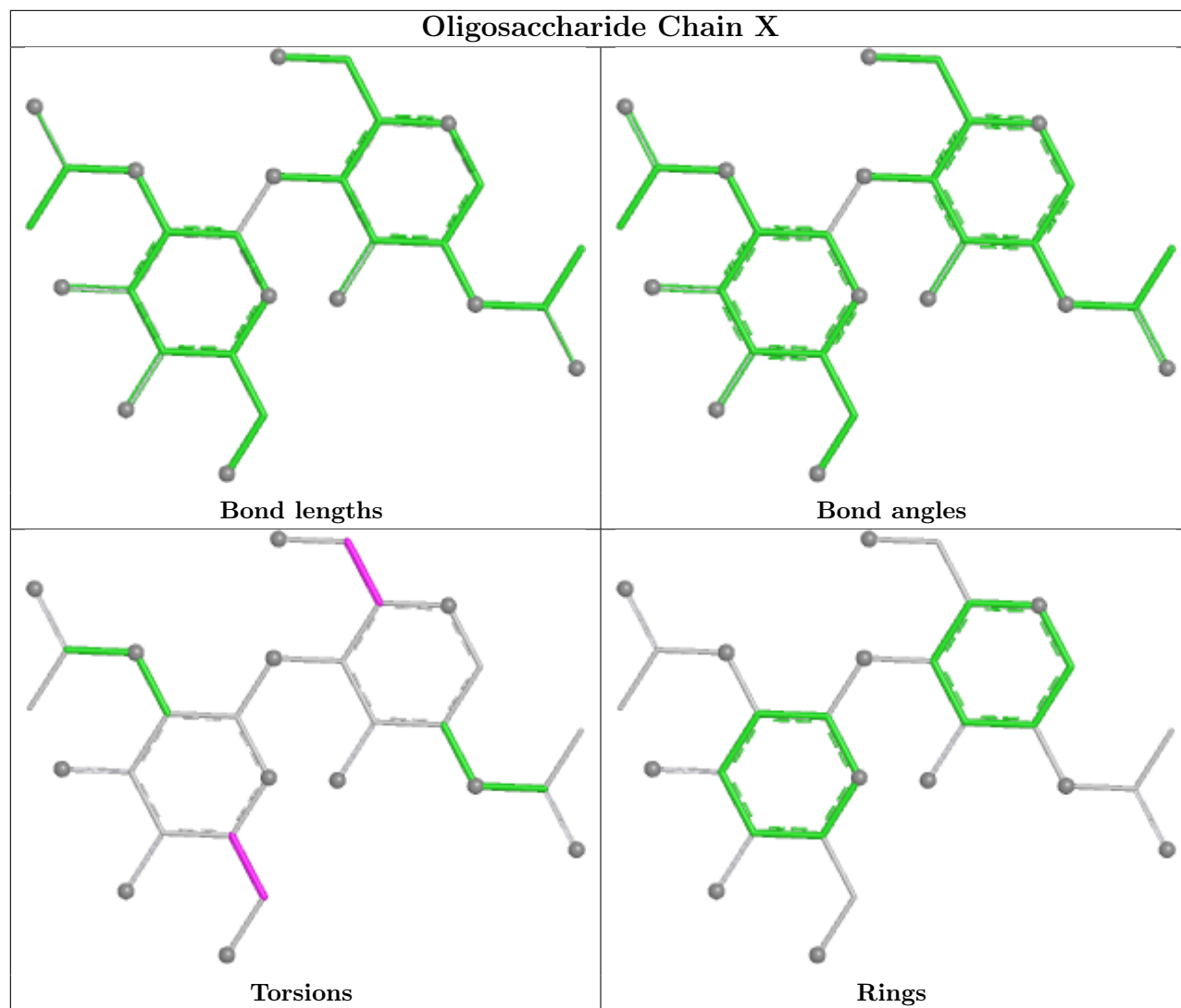


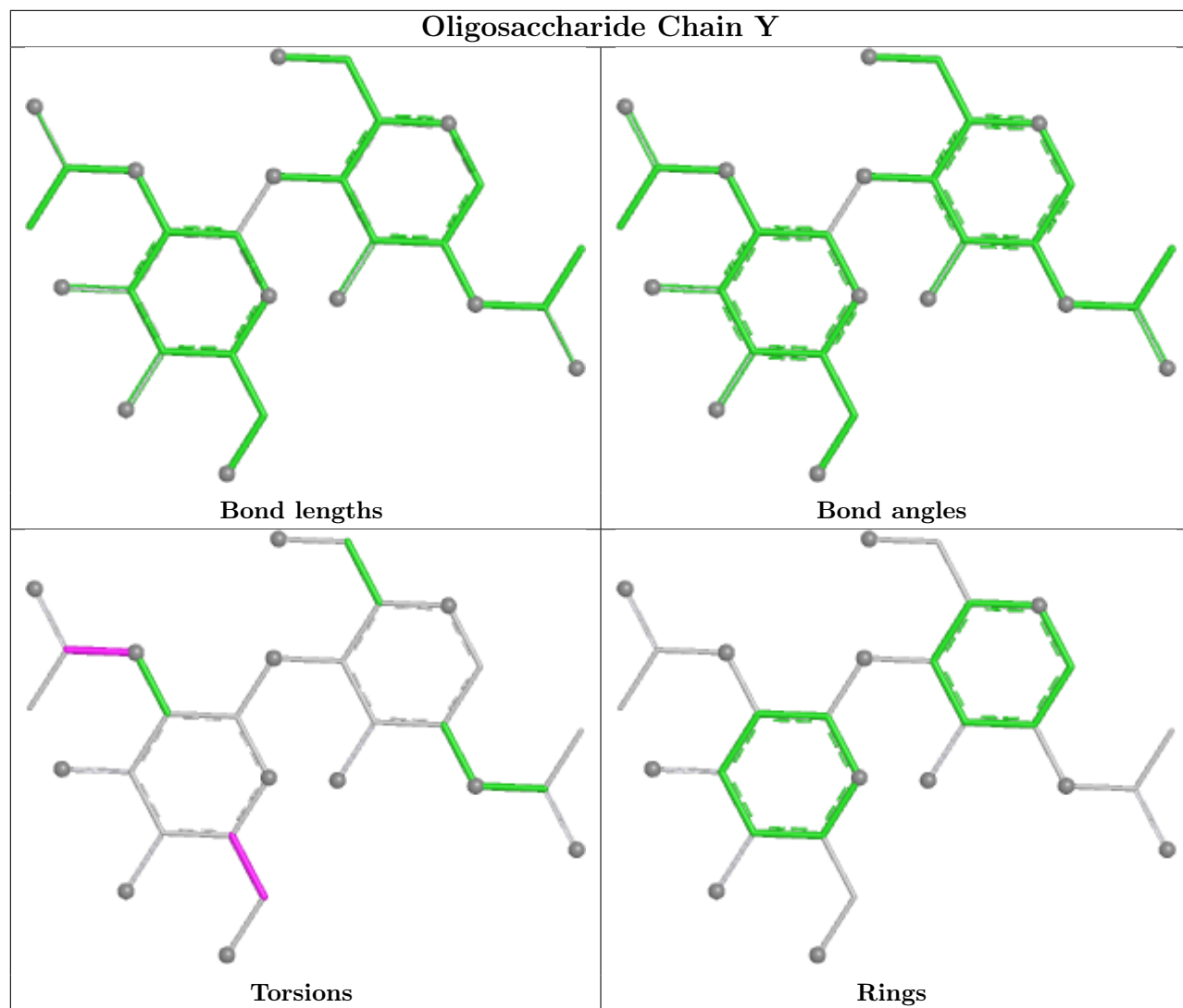


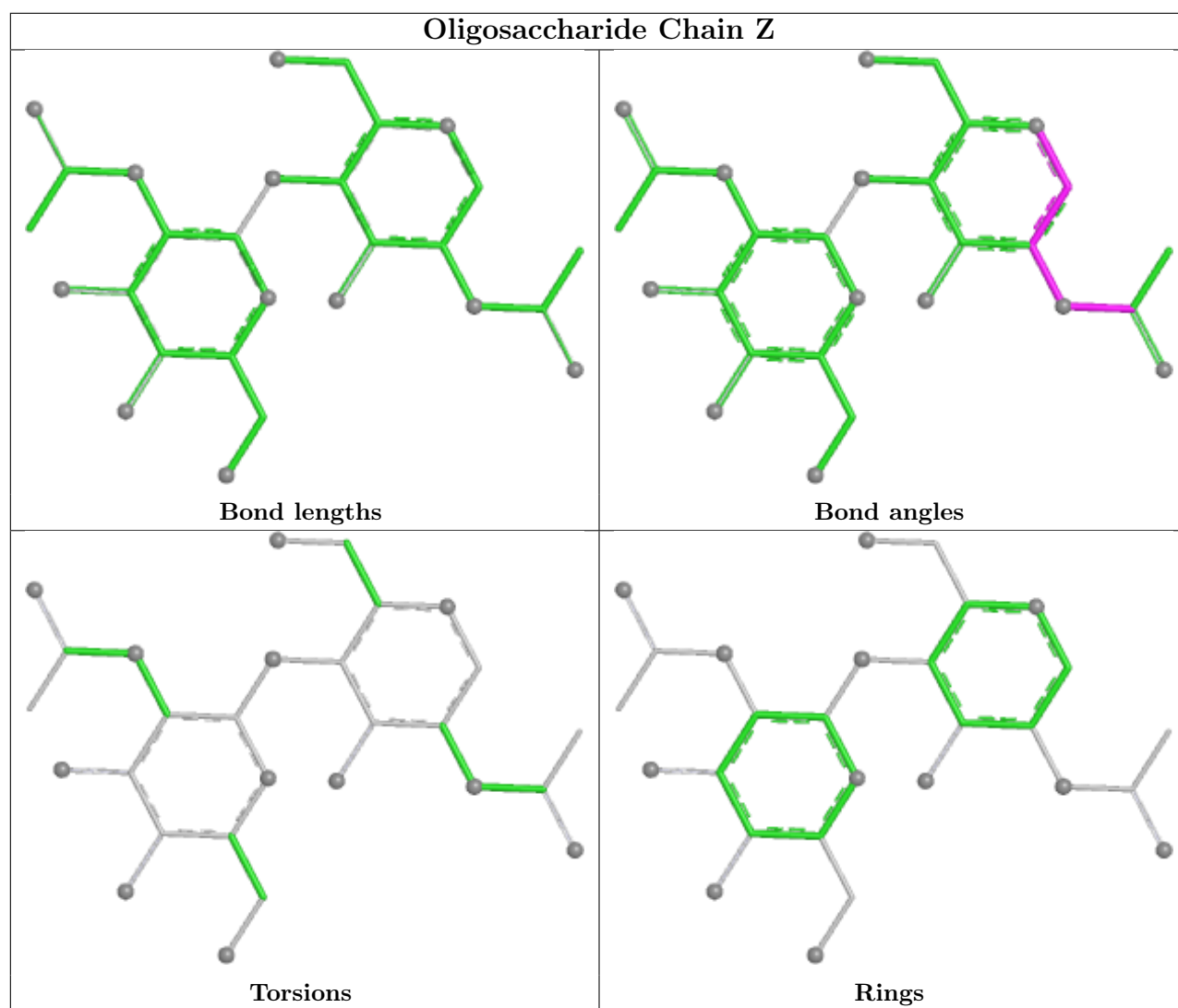


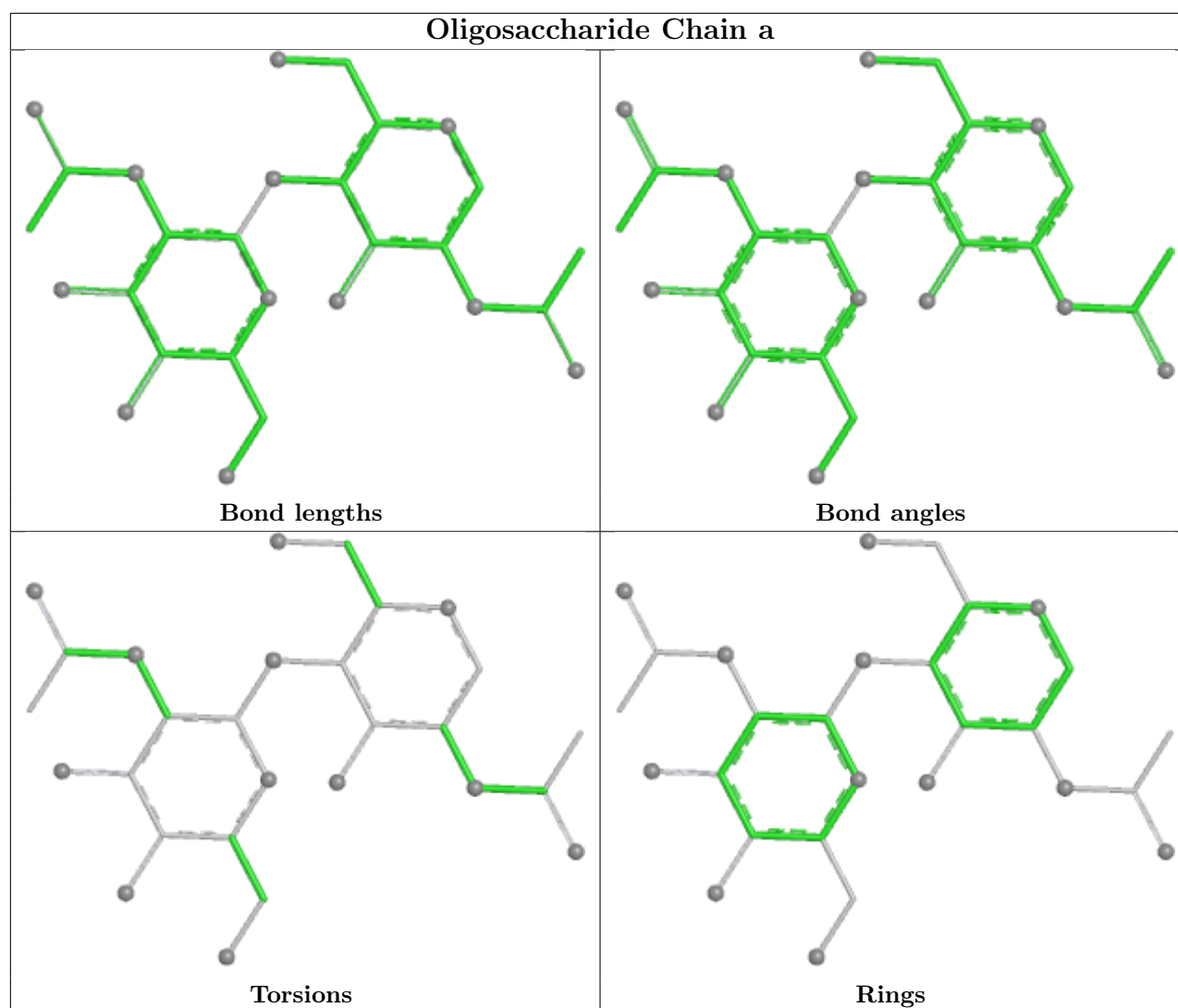












5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1302	2	14,14,15	0.41	0	17,19,21	0.59	0
4	NAG	C	1306	-	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	A	1304	2	14,14,15	0.39	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1307	2	14,14,15	0.38	0	17,19,21	0.67	1 (5%)
4	NAG	A	1307	-	14,14,15	0.24	0	17,19,21	0.64	1 (5%)
4	NAG	A	1305	2	14,14,15	0.39	0	17,19,21	0.75	1 (5%)
4	NAG	B	1304	2	14,14,15	0.39	0	17,19,21	0.42	0
4	NAG	A	1302	-	14,14,15	0.40	0	17,19,21	0.84	0
4	NAG	A	1308	2	14,14,15	0.25	0	17,19,21	0.58	0
4	NAG	C	1304	-	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	C	1303	2	14,14,15	0.41	0	17,19,21	0.53	0
4	NAG	B	1308	2	14,14,15	0.42	0	17,19,21	0.99	1 (5%)
4	NAG	B	1303	2	14,14,15	0.41	0	17,19,21	0.65	0
4	NAG	B	1310	-	14,14,15	0.20	0	17,19,21	0.38	0
4	NAG	C	1301	2	14,14,15	0.38	0	17,19,21	1.24	2 (11%)
4	NAG	B	1301	2	14,14,15	0.40	0	17,19,21	0.34	0
4	NAG	C	1302	2	14,14,15	0.41	0	17,19,21	0.72	0
4	NAG	C	1305	-	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	A	1301	2	14,14,15	0.40	0	17,19,21	0.42	0
4	NAG	A	1303	2	14,14,15	0.39	0	17,19,21	0.36	0
4	NAG	A	1306	-	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1307	2	14,14,15	0.40	0	17,19,21	0.43	0
4	NAG	B	1305	2	14,14,15	0.41	0	17,19,21	0.39	0
4	NAG	B	1306	2	14,14,15	0.42	0	17,19,21	1.63	1 (5%)
4	NAG	B	1309	2	14,14,15	0.22	0	17,19,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1306	NAG	O5-C1-C2	6.30	121.04	111.29
4	C	1301	NAG	O5-C1-C2	4.34	118.01	111.29
4	B	1308	NAG	O5-C1-C2	3.42	116.59	111.29
4	A	1304	NAG	O5-C1-C2	-2.79	106.97	111.29
4	B	1307	NAG	C1-O5-C5	2.36	115.35	112.19
4	A	1307	NAG	C1-O5-C5	2.19	115.12	112.19
4	C	1301	NAG	C1-O5-C5	2.16	115.08	112.19
4	A	1305	NAG	C1-O5-C5	2.14	115.05	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	O7-C7-N2-C2
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	B	1301	NAG	C8-C7-N2-C2
4	B	1301	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	C	1302	NAG	C8-C7-N2-C2
4	C	1302	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	C	1307	NAG	C1-C2-N2-C7
4	C	1307	NAG	C8-C7-N2-C2
4	C	1307	NAG	O7-C7-N2-C2
4	A	1308	NAG	C4-C5-C6-O6
4	A	1301	NAG	C8-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	C	1304	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	C	1304	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1304	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	A	1302	NAG	C8-C7-N2-C2
4	C	1307	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	A	1302	NAG	O7-C7-N2-C2
4	C	1301	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1305	NAG	C8-C7-N2-C2
4	C	1303	NAG	C4-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	A	1305	NAG	O7-C7-N2-C2
4	B	1308	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	NAG	1	0
4	A	1307	NAG	1	0
4	A	1305	NAG	1	0
4	A	1302	NAG	2	0
4	B	1308	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.

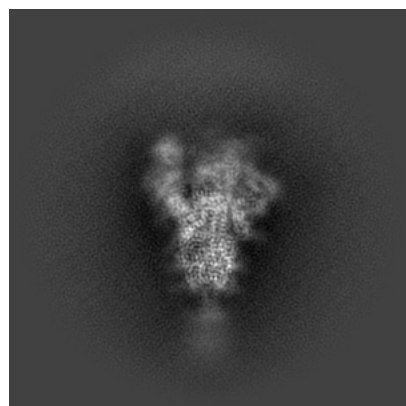
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36878. These allow visual inspection of the internal detail of the map and identification of artifacts.

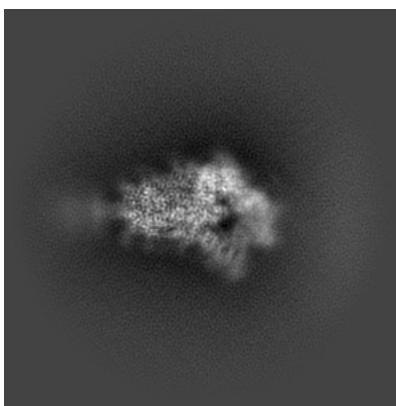
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

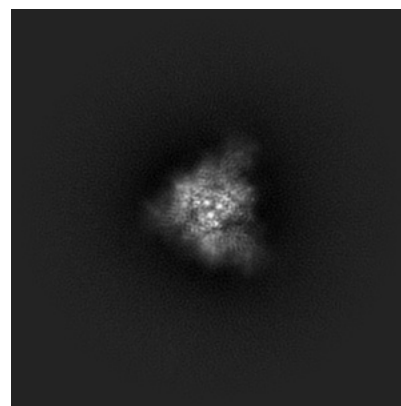
6.1.1 Primary map



X

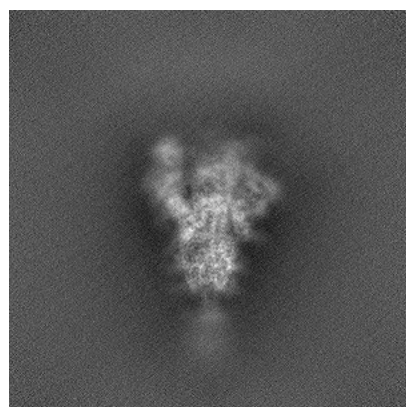


Y

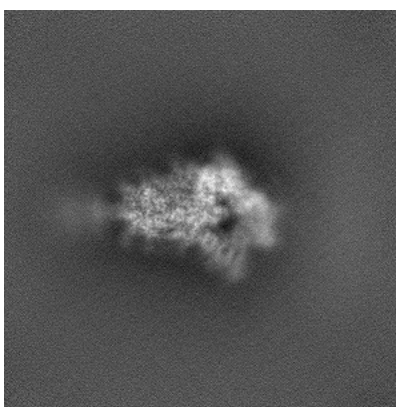


Z

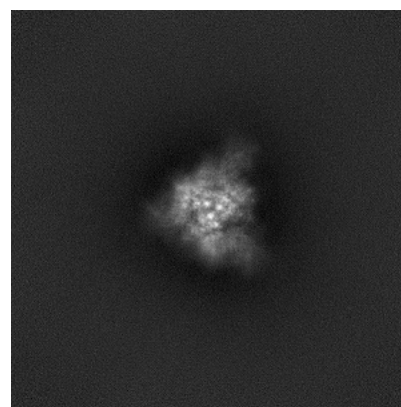
6.1.2 Raw map



X



Y

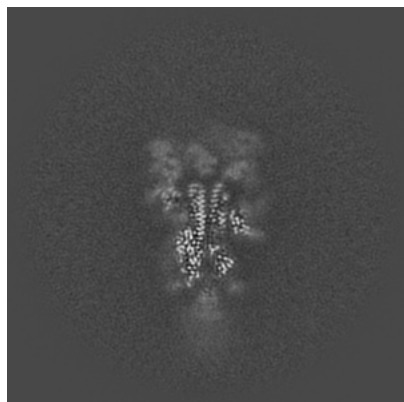


Z

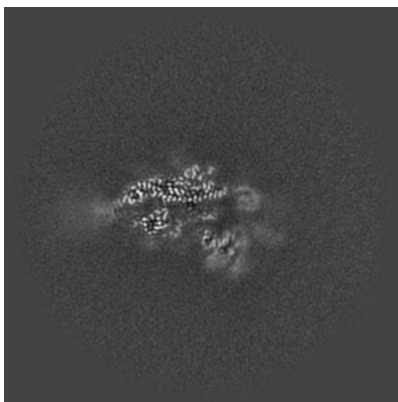
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

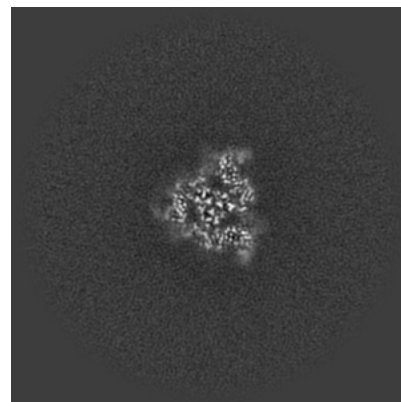
6.2.1 Primary map



X Index: 256

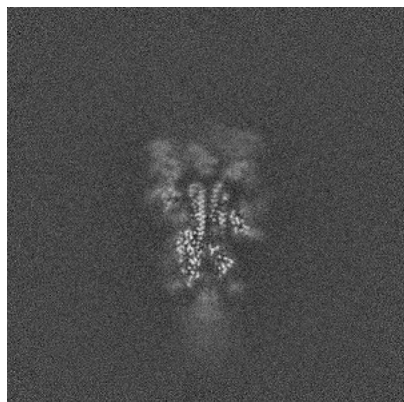


Y Index: 256

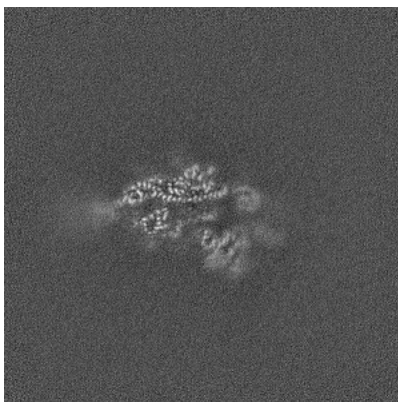


Z Index: 256

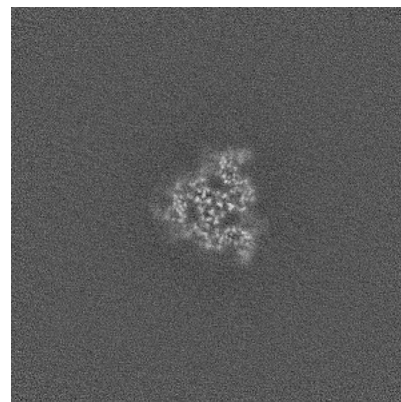
6.2.2 Raw map



X Index: 256



Y Index: 256

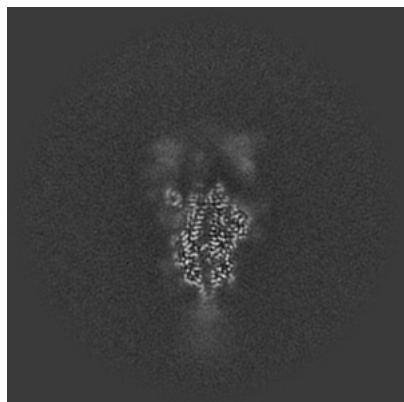


Z Index: 256

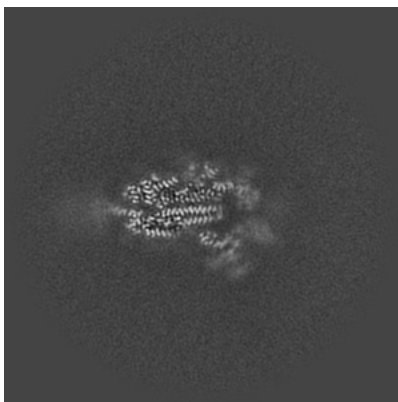
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

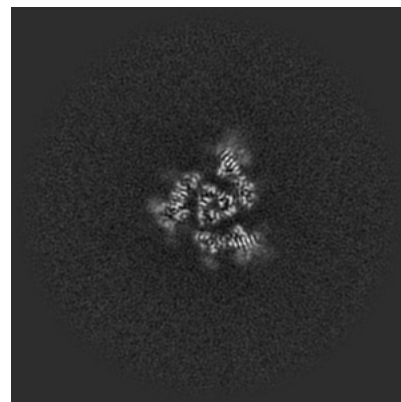
6.3.1 Primary map



X Index: 246

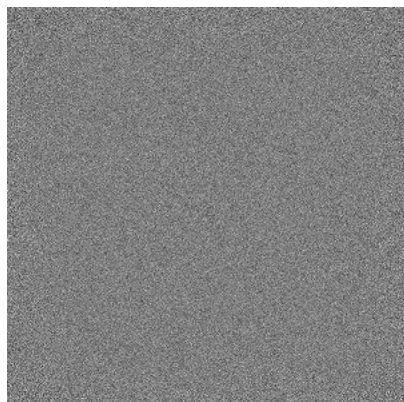


Y Index: 263

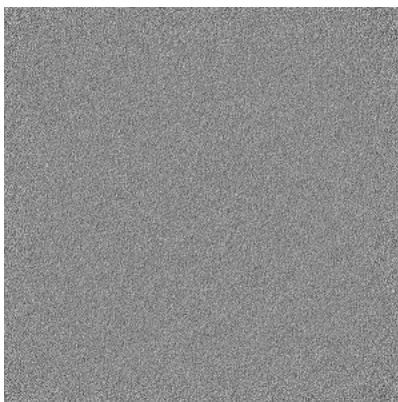


Z Index: 268

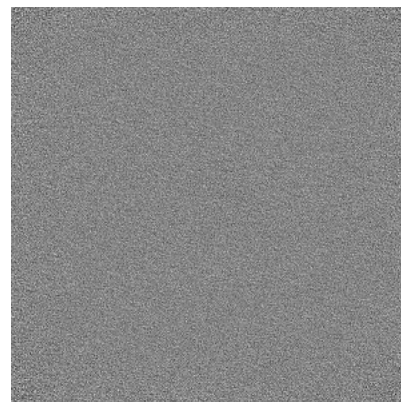
6.3.2 Raw map



X Index: 0



Y Index: 0

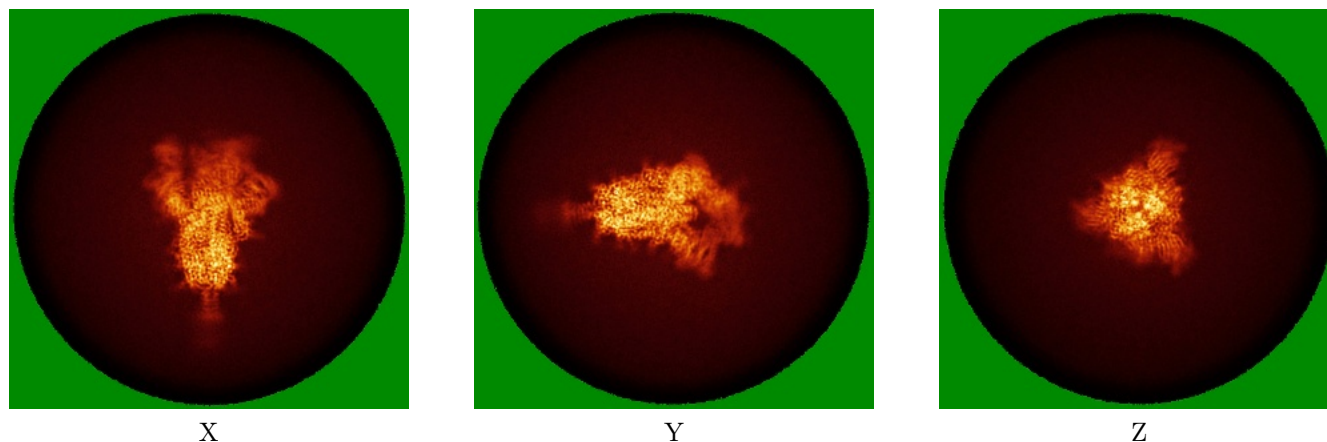


Z Index: 511

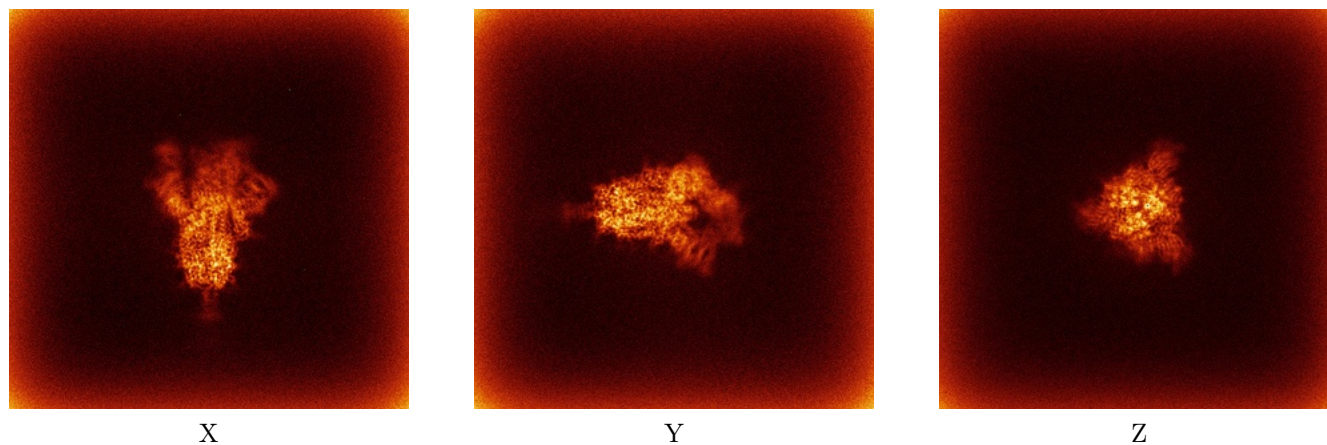
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

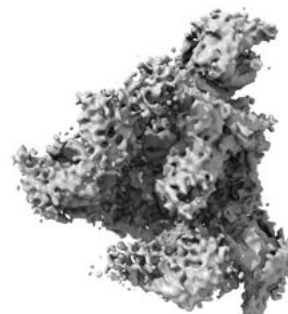
6.5.1 Primary map



X



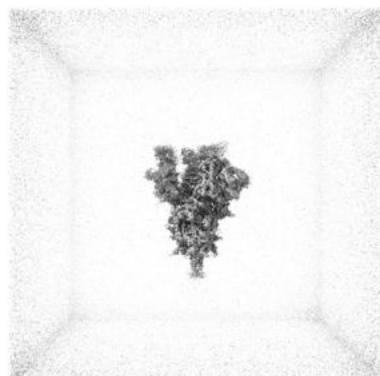
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.229. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

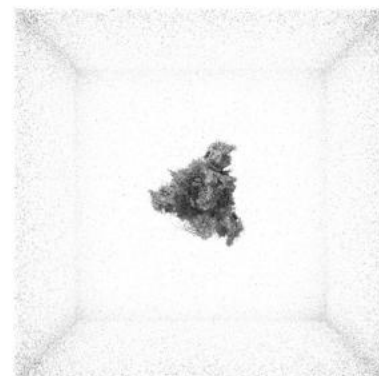
6.5.2 Raw map



X



Y



Z

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.

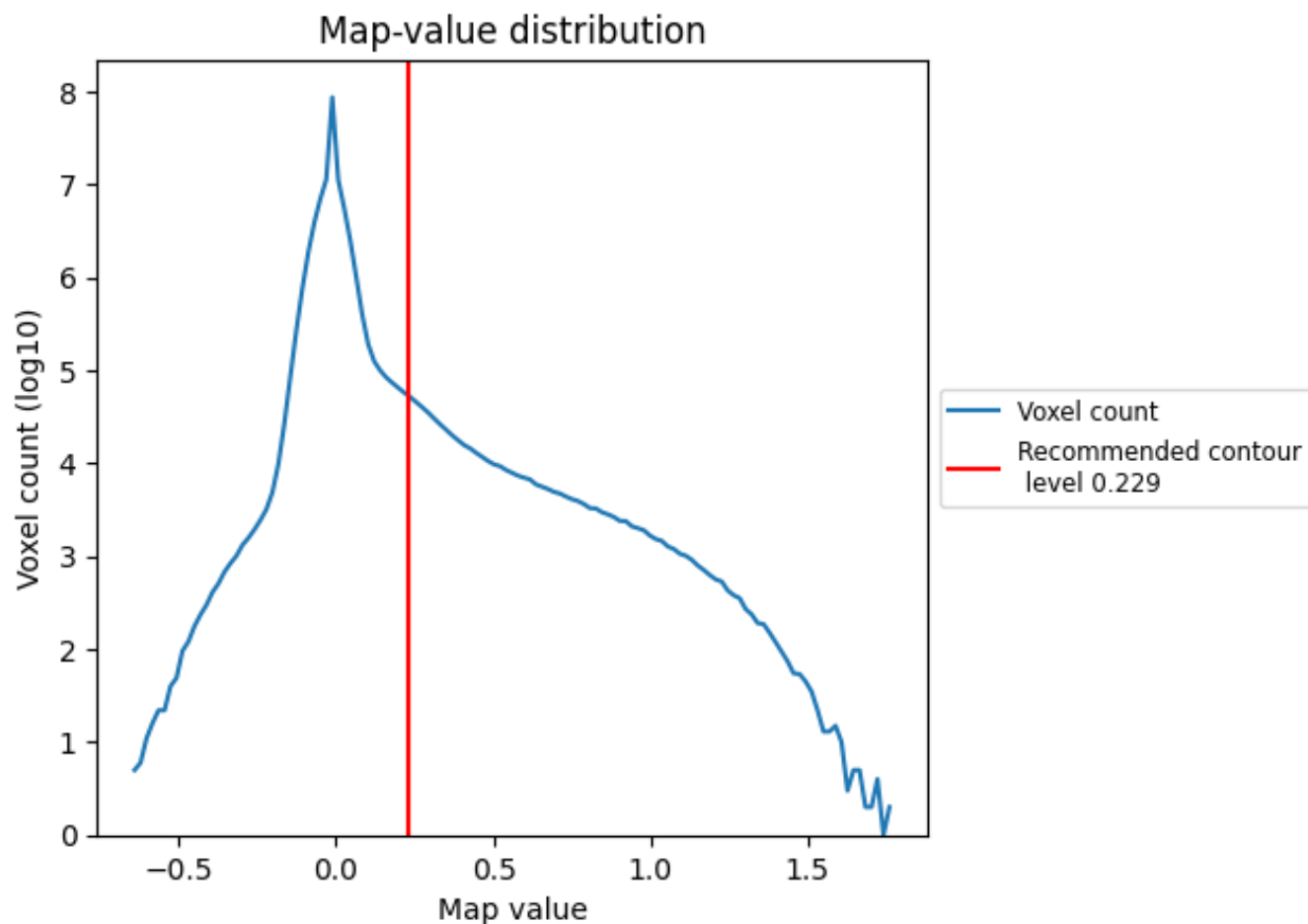
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

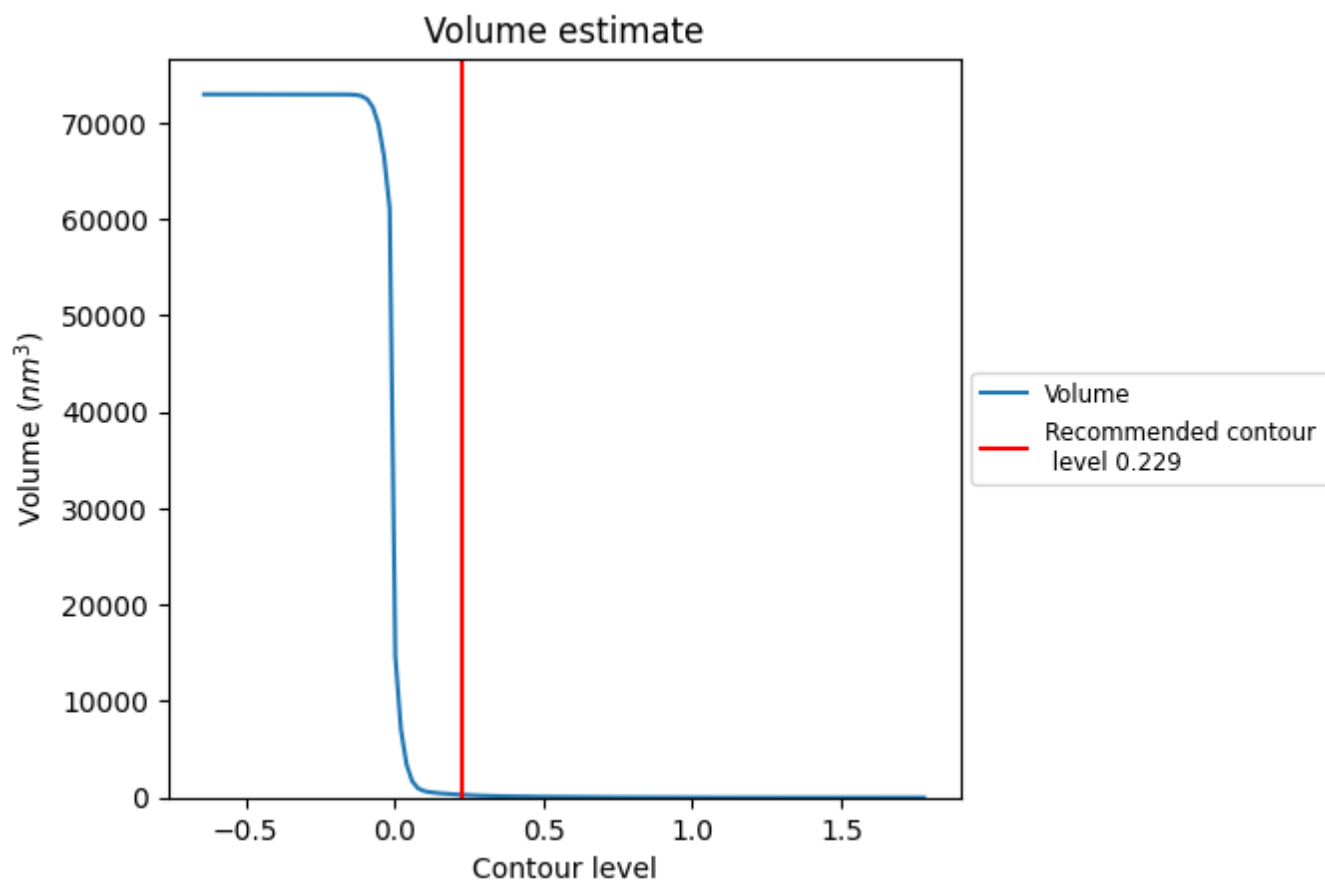
This section contains the results of statistical analysis of the map.

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.

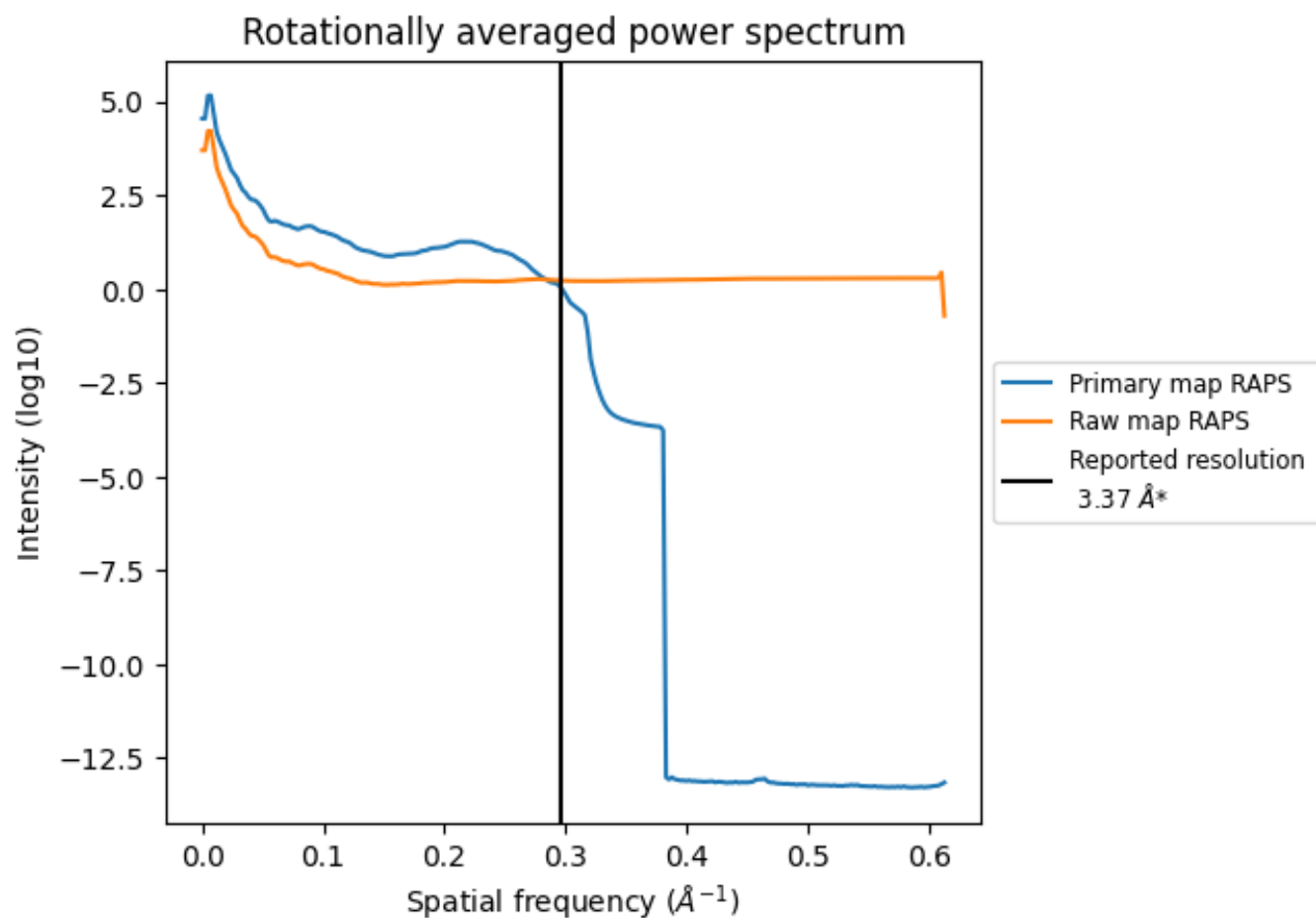
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm^3 ; this corresponds to an approximate mass of 254 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 ⓘ

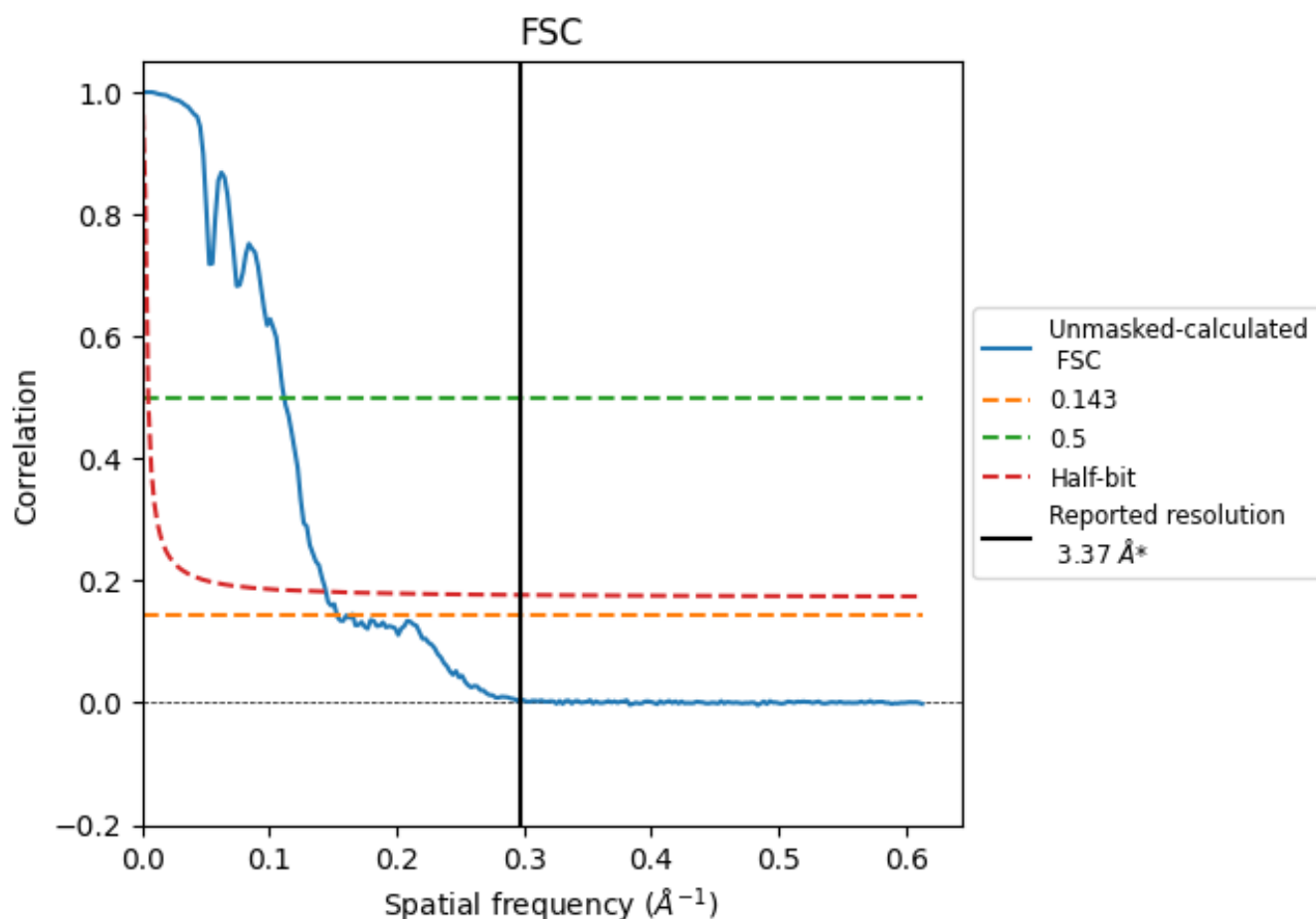


*Reported resolution corresponds to spatial frequency of 0.297 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.297 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.54	8.97	6.93

*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 6.54 differs from the reported value 3.37 by more than 10 %

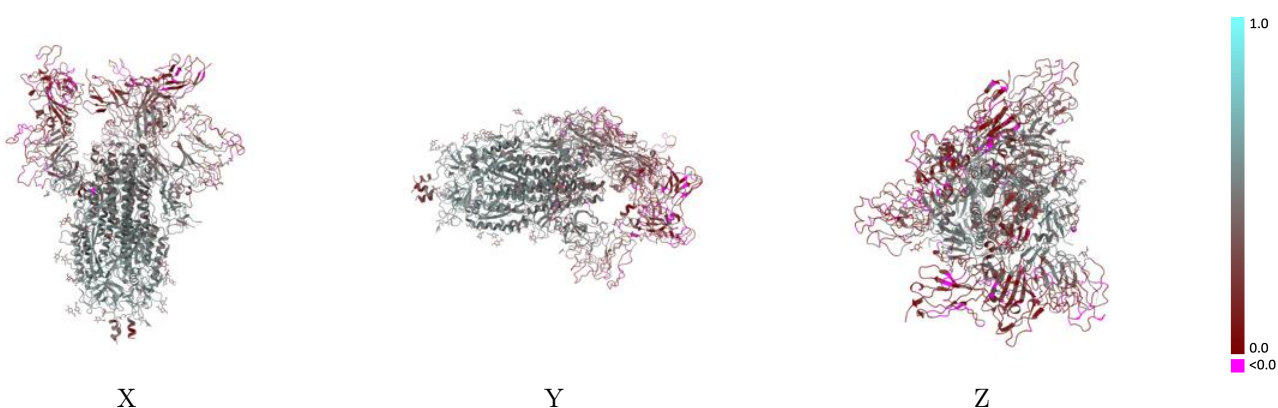
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36878 and PDB model 8K46. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

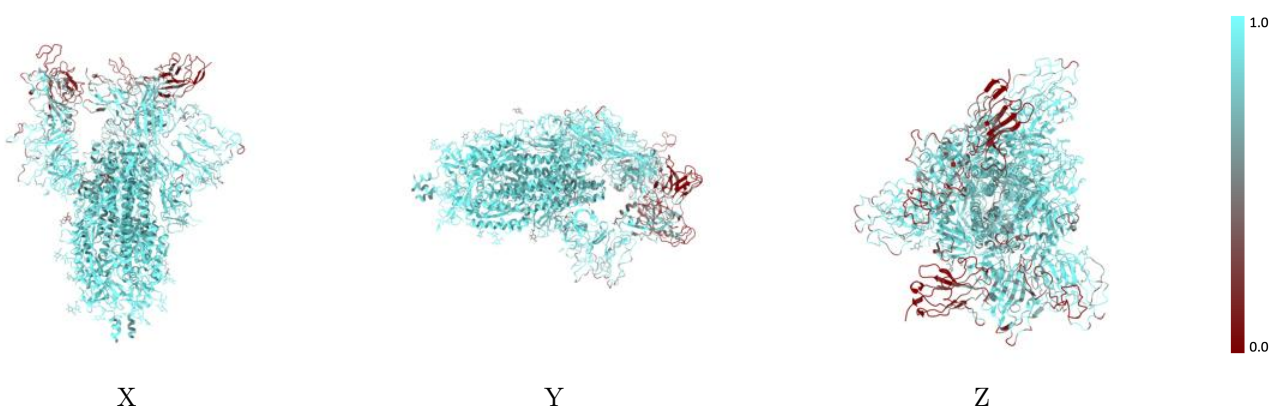
This section was not generated.

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



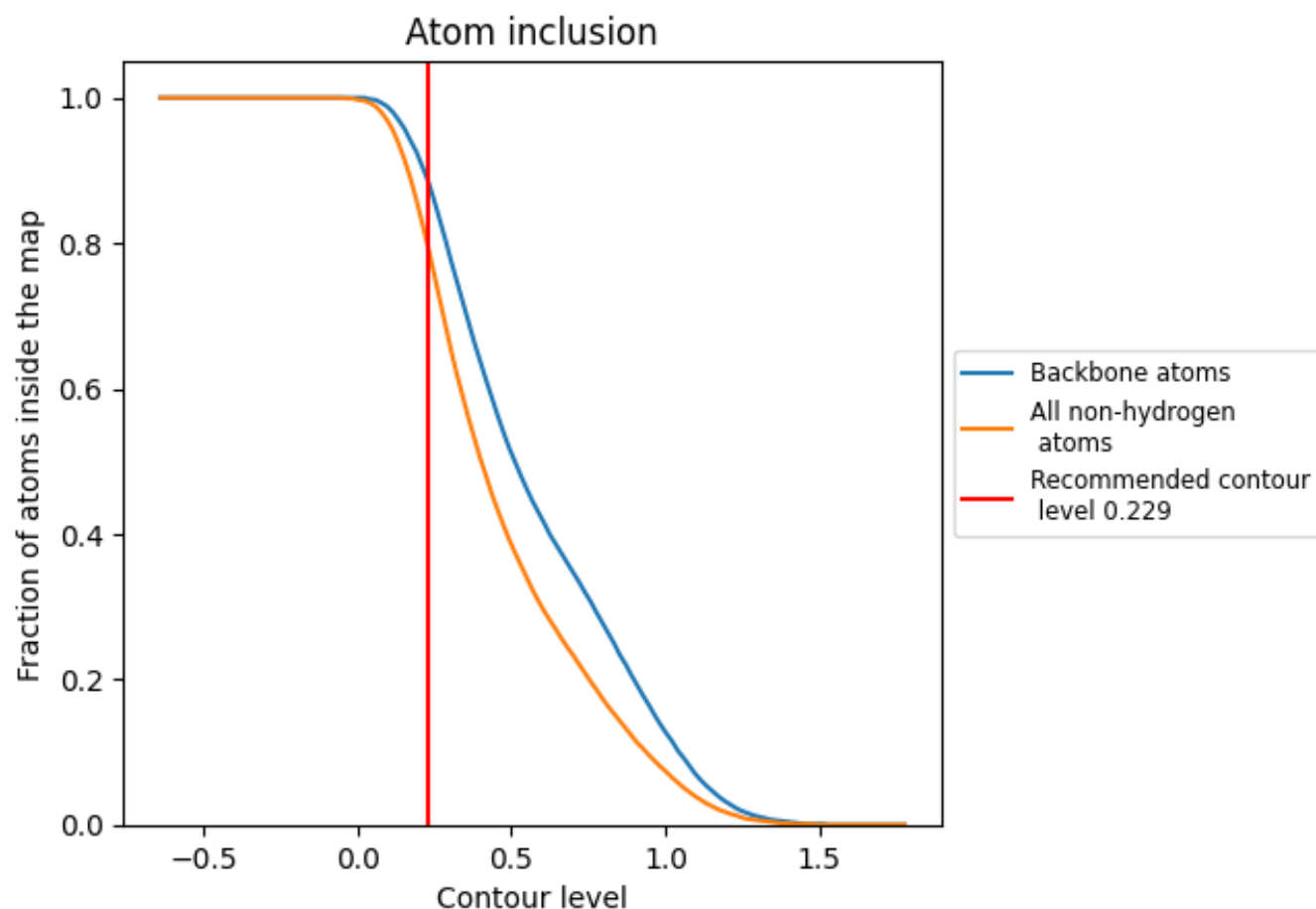
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.229).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.229) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.3770
A	 0.8260	 0.3840
B	 0.8260	 0.3940
C	 0.8820	 0.4190
E	 0.1850	 0.1510
G	 0.1930	 0.1410
I	 0.6700	 0.2330
K	 0.9290	 0.4730
L	 0.8570	 0.4000
M	 0.9640	 0.3980
N	 0.8930	 0.4380
R	 0.8930	 0.4630
S	 0.7860	 0.3180
T	 0.9640	 0.3870
U	 0.9640	 0.4660
X	 0.8930	 0.4480
Y	 0.8930	 0.4180
Z	 1.0000	 0.4880
a	 0.8210	 0.3840

