



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:40 PM UTC

PDB ID : 6X6P / pdb_00006x6p
EMDB ID : EMD-22078
Title : Characterization of the SARS-CoV-2 S Protein: Biophysical, Biochemical, Structural, and Antigenic Analysis
Authors : Herrera, N.G.; Morano, N.C.; Celikgil, A.; Georgiev, G.I.; Malonis, R.; Lee, J.H.; Tong, K.; Vergnolle, O.; Massimi, A.; Yen, L.Y.; Noble, A.J.; Kopylov, M.; Bonanno, J.B.; Garrett-Thompson, S.C.; Hayes, D.B.; Brenowitz, M.; Garforth, S.J.; Eng, E.T.; Lai, J.R.; Almo, S.C.
Deposited on : 2020-05-28
Resolution : 3.22 Å(reported)
Based on initial model : 6VXX

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)

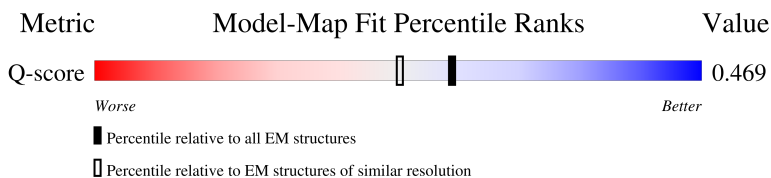
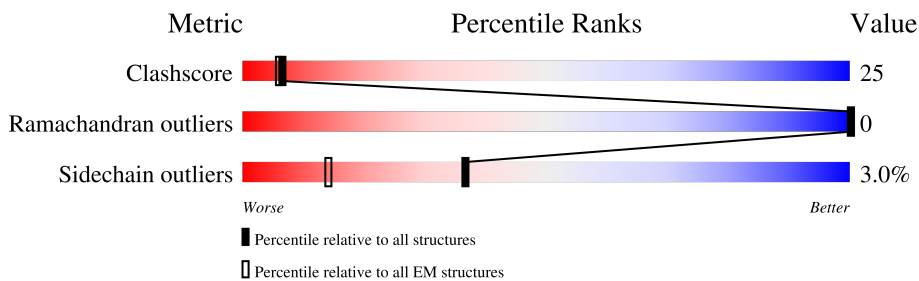
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 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	14612 (2.72 - 3.72)

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

Mol	Chain	Length	Quality of chain
1	A	1274	
1	B	1274	
1	C	1274	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	2	 100%
2	E	2	 50%50%
2	F	2	 50%50%
2	G	2	 50%50%
2	H	2	 100%
2	I	2	 50%50%
2	J	2	 50%50%
2	K	2	 50%50%
2	L	2	 100%
2	M	2	 50%50%
2	N	2	 50%50%
2	O	2	 50%50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0
			7939	5069	1319	1516	35		
1	B	1017	Total	C	N	O	S	0	0
			7939	5069	1319	1516	35		
1	C	1017	Total	C	N	O	S	0	0
			7939	5069	1319	1516	35		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

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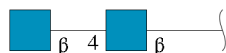
Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression 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	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

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



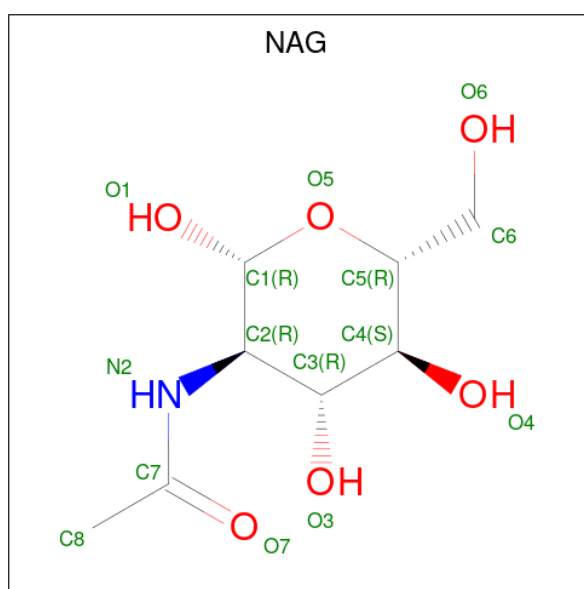
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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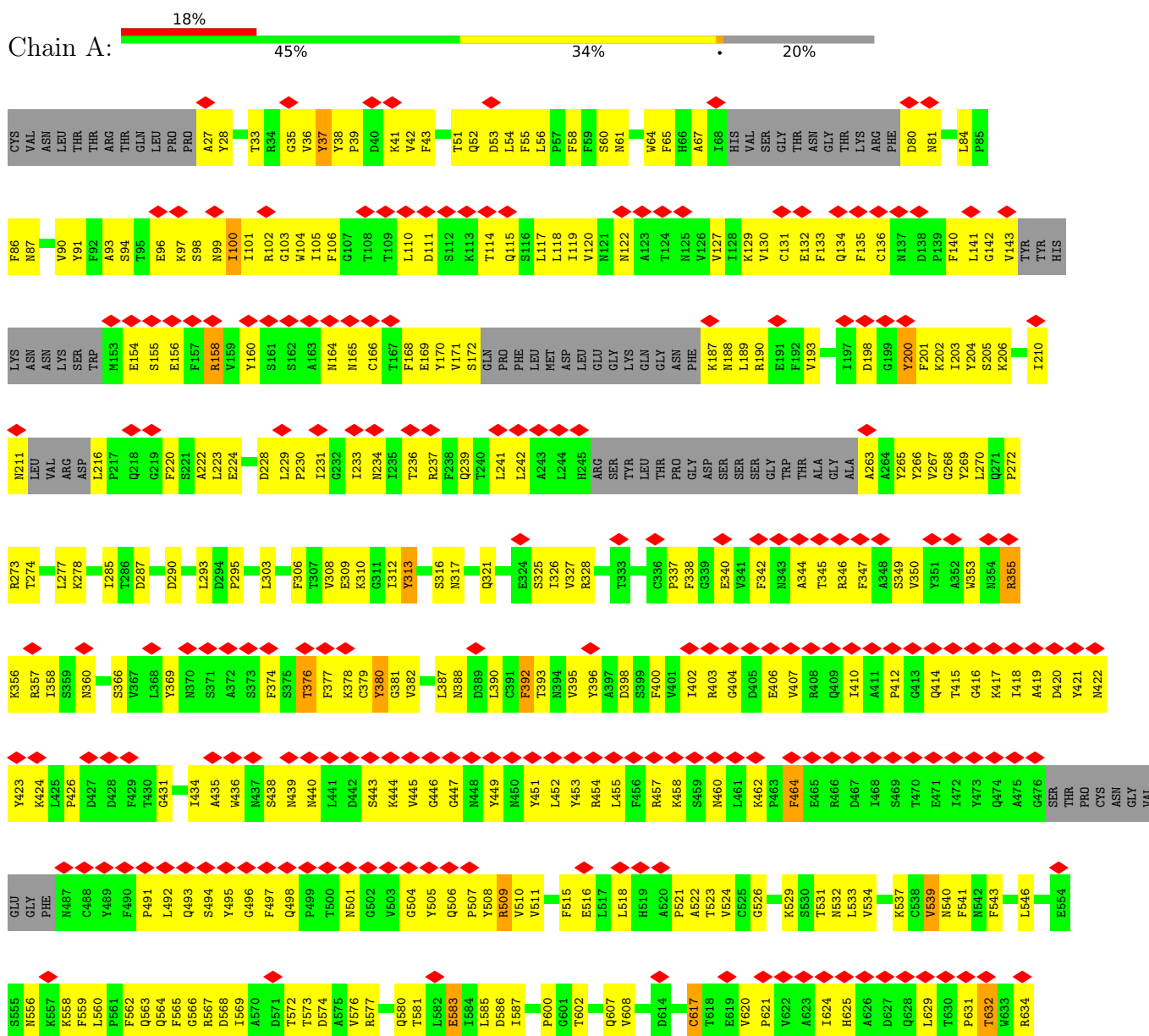
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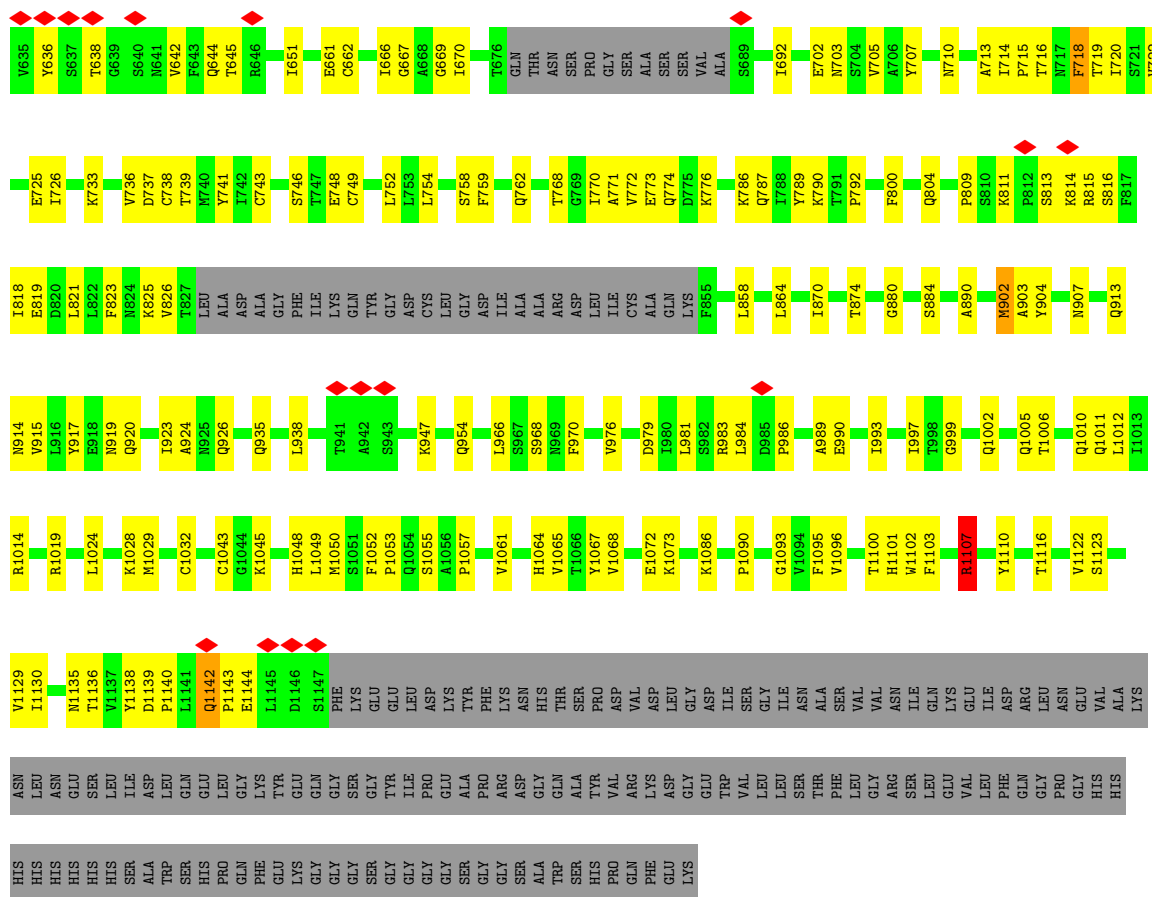
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

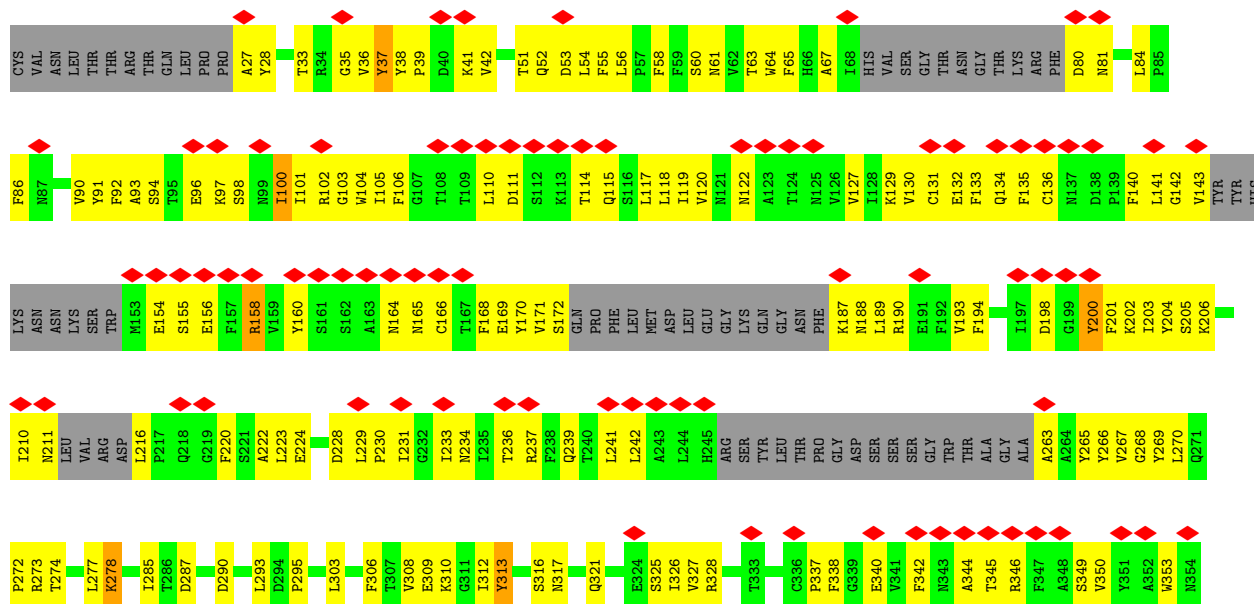
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein





• Molecule 1: Spike glycoprotein



V1129	V1130	N1135	T1136	V1137	Y1138	D1139	P1140	L1141	Q1142	P1143	E1144	L1145	D1146	S1147	PHE	LYS	GLU	GLU	GLU	LEU	ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	GLY	ILE	F1089	P1090	G1093	F1095	V1096	T1100	H1101	W1102	F1103	R1107	Y1110	T1116	V1122	S1123	ALA							
N907	Q913	N914	V915	L916	E917	E918	N919	Q920	I923	A924	N925	Q926	Q935	L938	A942	S943	K947	Q954	L956	S967	N968	N969	F970	V976	D979	I980	L981	S982	R983	L984	D985	A989	I993	I997	T998	G999	Q1002	Q1005	T1006	Q1010	Q1011	L1012															
I1013	R1014	R1019	L1024	K1028	M1029	P1109	L1141	Q1142	P1143	E1144	L1145	D1146	S1147	PHE	LYS	GLU	GLU	GLU	LEU	ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	GLY	ILE	F1089	P1090	G1093	F1095	V1096	T1100	H1101	W1102	F1103	R1107	Y1110	T1116	V1122	S1123	ALA								
P85	F86	N87	V90	F92	A93	S94	T95	E96	K97	S98	N99	I100	I101	R102	G103	W104	I105	F106	G107	T108	T109	L110	D111	S112	K113	T114	Q115	L117	L118	I119	V120	N121	N122	A123	T124	N125	V126	I127	I128	K129	V130	C131	E132	F133	Q134	F135	C136	N137	D138	I203	F139	F140	L141	G142	V143	TYR	TYR
HIS	LYS	ASN	LYS	ASP	TRP	M153	E154	S155	E156	F157	A158	V159	Y160	S161	S162	A163	N164	N165	C166	T167	F168	E169	Y170	V171	S172	GLN	PRO	PHE	LEU	MET	ASP	LEU	GLY	LYS	GLN	GLY	ASN	PHE	K187	N188	L189	R190	E191	F192	V193	I197	D198	G199	Y200	F201	K202	G268	Y269	L270	N354	R355	Q271
I210	N211	LEU	VAL	ARG	ASP	L216	P217	Q218	Q219	F220	S221	L223	E224	D228	L229	P230	T231	G232	T233	N234	T235	T236	R237	F238	Q239	T240	L241	L242	A243	L244	H245	ARG	SER	TYR	THR	PRO	GLY	ASP	SER	SER	SER	GLY	THR	ALA	ALA	A263	A264	Y265	Y266	V267	G268	Y269	L270	N354	R355	Q271	
P272	R273	T274	L277	K278	E281	L285	T286	D287	D290	P295	L303	F306	V308	E309	K310	G311	Y313	S316	N317	Q321	S325	L326	V327	R328	T333	C336	F337	G339	E340	F342	N343	A344	T345	R346	F347	A348	S349	V350	G413	Q414	A352	W353	N354	R355	Q271												
K356	R357	I358	S359	N360	C361	S366	L368	N370	S371	A372	S373	F374	S375	T376	F377	K378	C379	K380	G381	V382	L387	N388	D389	L390	C391	F392	T393	N394	V395	V396	A397	D398	S399	F400	V401	I402	R403	G404	D405	E406	V407	R408	Q409	I410	A411	P412	G413	Q414	A352	W353	N354	R355	Q271				
N422	Y423	K424	L425	P426	D427	D428	F429	T430	G431	C432	V433	I434	A435	H436	N437	S438	N439	N440	L441	D442	S443	K444	V445	G446	G447	N448	Y449	N450	Y451	L452	Y453	R454	L455	F456	R457	K458	S459	N460	L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	G475	A476	D476	SER	THR	PRO	CYS	ASN
GLY	VAL	GLU	GLY	PHE	N487	C488	Y489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	G504	Y505	Q506	P507	Y508	R509	V510	V511	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	K529	S530	T531	N532	L533	V534	K537	C538	V539	N540	F541	N542	F543	L546		
E554	S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565	G566	R567	D568	L569	A570	T572	T573	D574	A575	Y576	B577	Q580	T581	L582	E583	F584	D586	L587	S596	P600	G601	T602	Q607	V608	L611	P614	C617	V620	P621	V622	A623	T624	H625	A626	D627	Q628	L629									
T630	P631	T632	W633	R634	W635	W636	S637	T638	W639	C640	R641	W642	F643	Q644	T645	R646	T651	E661	C662	T666	G669	L670	T676	GLN	THR	ASN	SER	PRO	GLY	SER	ALA	ALA	SER	VAL	S689	I692	E702	N703	S704	W705	A706	Y707	N710	A713	T714	P715	T716	N717	F718								
T719	I720	S721	V722	E725	I726	K733	V736	D737	Q738	C739	T739	K740	V741	I742	C743	S746	T747	E748	C749	L752	L753	L754	S758	F759	Q762	T768	G769	I770	A771	V772	Q774	D775	K776	K786	Q787	I788	K789	T791	P792	D796	F800	Q804	P809	S810	K811												
F812	S813	K814	R815	S816	F817	R818	E819	R820	L821	L822	F823	R824	K825	V826	R827	LEU	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	GLY	ASP	ILE	ALA	ARG	ASP	ILE	ALA	VAL	L858	L864	I870	T874	A890	N900	Q901	R902	A903	Y904										
N907	Q913	N914	V915	L916	E917	E918	N919	Q920	I923	A924	N925	Q926	Q935	L938	A942	S943	K947	Q954	L956	S967	N968	N969	F970	V976	D979	I980	L981	S982	R983	L984	D985	A989	I993	I997	T998	G999	Q1002	Q1005	T1006	Q1010	Q1011	L1012															

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

NAG1
NAG2

NAG1
NAG2

NAG1
NAG2

NAG1
NAG2

NAG1
NAG2



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



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



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



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



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



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	54395	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 ($e^-/\text{\AA}^2$)	66.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.126	Depositor
Minimum map value	-0.478	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	406.27197, 406.27197, 406.27197	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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	A	0.52	0/8118	0.61	3/11050 (0.0%)
1	B	0.52	0/8118	0.61	3/11050 (0.0%)
1	C	0.52	0/8118	0.61	3/11050 (0.0%)
All	All	0.52	0/24354	0.61	9/33150 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ILE	N-CA-C	-7.00	105.96	112.96
1	A	100	ILE	N-CA-C	-6.97	105.99	112.96
1	B	100	ILE	N-CA-C	-6.96	106.00	112.96
1	A	355	ARG	CG-CD-NE	-6.94	96.74	112.00
1	B	355	ARG	CG-CD-NE	-6.92	96.77	112.00
1	C	355	ARG	CG-CD-NE	-6.91	96.80	112.00
1	A	1107	ARG	CB-CG-CD	5.83	124.70	111.30
1	C	1107	ARG	CB-CG-CD	5.83	124.70	111.30
1	B	1107	ARG	CB-CG-CD	5.81	124.65	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	617	CYS	Peptide
1	B	617	CYS	Peptide
1	C	617	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7939	0	7732	441	0
1	B	7939	0	7732	421	0
1	C	7939	0	7732	440	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
3	A	154	0	143	3	0
3	B	154	0	143	3	0
3	C	154	0	143	3	0
All	All	24615	0	23925	1220	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 25.

All (1220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HG3	1:B:158:ARG:HH11	1.20	1.05
1:A:158:ARG:HG3	1:A:158:ARG:HH11	1.20	1.04
1:C:158:ARG:HG3	1:C:158:ARG:HH11	1.20	1.03
1:C:328:ARG:HE	1:C:533:LEU:HB2	1.25	1.00
1:A:328:ARG:HE	1:A:533:LEU:HB2	1.25	0.98
1:B:328:ARG:HE	1:B:533:LEU:HB2	1.25	0.96
1:B:104:TRP:HB3	1:B:106:PHE:HE1	1.31	0.95
1:A:104:TRP:HB3	1:A:106:PHE:HE1	1.31	0.94
1:C:104:TRP:HB3	1:C:106:PHE:HE1	1.31	0.94
1:A:904:TYR:CZ	1:C:1107:ARG:HD2	2.06	0.90
1:C:342:PHE:HE2	1:C:511:VAL:HG11	1.37	0.89
1:B:342:PHE:HE2	1:B:511:VAL:HG11	1.37	0.88
1:C:53:ASP:HB3	1:C:55:PHE:HE2	1.39	0.88
1:A:53:ASP:HB3	1:A:55:PHE:HE2	1.39	0.87
1:B:1107:ARG:HD2	1:C:904:TYR:CZ	2.09	0.87
1:A:342:PHE:HE2	1:A:511:VAL:HG11	1.37	0.87
1:C:236:THR:HG23	1:C:237:ARG:HG3	1.57	0.87
1:B:53:ASP:HB3	1:B:55:PHE:HE2	1.40	0.86
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.57	0.86
1:B:236:THR:HG23	1:B:237:ARG:HG3	1.56	0.85
1:A:720:ILE:HG13	1:A:923:ILE:HG23	1.57	0.85
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.56	0.85
1:A:236:THR:HG23	1:A:237:ARG:HG3	1.57	0.84
1:A:1107:ARG:HD2	1:B:904:TYR:CZ	2.12	0.84
1:A:417:LYS:O	1:A:421:TYR:HB2	1.77	0.84
1:B:453:TYR:HD2	1:B:495:TYR:HE1	1.26	0.84
1:C:417:LYS:O	1:C:421:TYR:HB2	1.77	0.84
1:A:568:ASP:OD1	1:A:569:ILE:N	2.11	0.83
1:C:568:ASP:OD1	1:C:569:ILE:N	2.11	0.83
1:B:417:LYS:O	1:B:421:TYR:HB2	1.77	0.83
1:B:568:ASP:OD1	1:B:569:ILE:N	2.11	0.83
1:A:453:TYR:HD2	1:A:495:TYR:HE1	1.26	0.83
1:C:453:TYR:HD2	1:C:495:TYR:HE1	1.26	0.82
1:A:560:LEU:H	1:A:563:GLN:HE21	1.28	0.81
1:B:231:ILE:HG13	1:B:233:ILE:H	1.46	0.80
1:B:452:LEU:HD11	1:B:492:LEU:HB3	1.64	0.80
1:C:231:ILE:HG13	1:C:233:ILE:H	1.47	0.80
1:C:131:CYS:HB3	1:C:133:PHE:HE1	1.48	0.80
1:A:131:CYS:HB3	1:A:133:PHE:HE1	1.47	0.79
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.66	0.78
1:A:231:ILE:HG13	1:A:233:ILE:H	1.47	0.78
1:A:452:LEU:HD11	1:A:492:LEU:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:HH22	1:B:396:TYR:HB3	1.49	0.78
1:C:355:ARG:HH22	1:C:396:TYR:HB3	1.49	0.78
1:A:387:LEU:HA	1:A:390:LEU:HD12	1.66	0.78
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.66	0.78
1:C:387:LEU:HA	1:C:390:LEU:HD12	1.66	0.78
1:B:403:ARG:NH2	1:B:504:GLY:O	2.17	0.78
1:A:355:ARG:HH22	1:A:396:TYR:HB3	1.49	0.78
1:A:493:GLN:NE2	1:A:494:SER:O	2.17	0.78
1:C:452:LEU:HD11	1:C:492:LEU:HB3	1.64	0.77
1:B:493:GLN:NE2	1:B:494:SER:O	2.17	0.77
1:C:1028:LYS:O	1:C:1032:CYS:HB3	1.85	0.77
1:C:96:GLU:OE2	1:C:100:ILE:N	2.17	0.77
1:B:96:GLU:OE2	1:B:100:ILE:N	2.17	0.77
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.66	0.77
1:A:1028:LYS:O	1:A:1032:CYS:HB3	1.85	0.77
1:B:387:LEU:HA	1:B:390:LEU:HD12	1.66	0.77
1:B:719:THR:HA	1:B:926:GLN:HE22	1.50	0.77
1:B:131:CYS:HB3	1:B:133:PHE:HE1	1.47	0.77
1:B:1028:LYS:O	1:B:1032:CYS:HB3	1.85	0.76
1:C:403:ARG:NH2	1:C:504:GLY:O	2.17	0.76
1:A:403:ARG:NH2	1:A:504:GLY:O	2.17	0.76
1:A:96:GLU:OE2	1:A:100:ILE:N	2.17	0.76
1:C:493:GLN:NE2	1:C:494:SER:O	2.17	0.76
1:C:719:THR:HA	1:C:926:GLN:HE22	1.50	0.75
1:A:392:PHE:HD2	1:A:515:PHE:HB3	1.51	0.75
1:B:392:PHE:HD2	1:B:515:PHE:HB3	1.51	0.75
1:A:455:LEU:HD21	1:A:493:GLN:HB3	1.69	0.74
1:A:719:THR:HA	1:A:926:GLN:HE22	1.50	0.74
1:C:392:PHE:HD2	1:C:515:PHE:HB3	1.51	0.74
1:B:455:LEU:HD21	1:B:493:GLN:HB3	1.69	0.73
1:C:455:LEU:HD21	1:C:493:GLN:HB3	1.69	0.73
1:C:1028:LYS:O	1:C:1032:CYS:CB	2.37	0.73
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.22	0.73
1:A:369:TYR:OH	1:C:415:THR:OG1	2.06	0.72
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.22	0.72
1:B:1028:LYS:O	1:B:1032:CYS:CB	2.37	0.72
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.22	0.72
1:B:422:ASN:HD21	1:B:454:ARG:H	1.38	0.72
1:C:355:ARG:HH22	1:C:396:TYR:CB	2.03	0.72
1:C:559:PHE:HB2	1:C:577:ARG:HH21	1.55	0.72
1:A:355:ARG:HH22	1:A:396:TYR:CB	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:HB2	1:B:577:ARG:HH21	1.55	0.71
1:A:1028:LYS:O	1:A:1032:CYS:CB	2.37	0.71
1:B:642:VAL:HG23	1:B:651:ILE:HG12	1.72	0.71
1:A:170:TYR:OH	1:A:172:SER:OG	2.08	0.71
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.72	0.71
1:A:559:PHE:HB2	1:A:577:ARG:HH21	1.55	0.71
1:C:642:VAL:HG23	1:C:651:ILE:HG12	1.72	0.71
1:A:560:LEU:H	1:A:563:GLN:NE2	1.88	0.71
1:B:355:ARG:HH22	1:B:396:TYR:CB	2.03	0.71
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.72	0.70
1:A:131:CYS:HB3	1:A:133:PHE:CE1	2.26	0.70
1:A:422:ASN:HD21	1:A:454:ARG:H	1.38	0.70
1:A:642:VAL:HG23	1:A:651:ILE:HG12	1.72	0.70
1:C:228:ASP:OD1	1:C:229:LEU:N	2.25	0.70
1:C:158:ARG:HG3	1:C:158:ARG:NH1	1.97	0.70
1:A:228:ASP:OD1	1:A:229:LEU:N	2.25	0.70
1:A:395:VAL:HG23	1:A:524:VAL:HG11	1.72	0.70
1:A:417:LYS:NZ	1:A:455:LEU:O	2.24	0.70
1:B:170:TYR:OH	1:B:172:SER:OG	2.08	0.70
1:C:170:TYR:OH	1:C:172:SER:OG	2.08	0.70
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.22	0.70
1:C:422:ASN:HD21	1:C:454:ARG:H	1.38	0.70
1:B:228:ASP:OD1	1:B:229:LEU:N	2.25	0.70
1:B:392:PHE:CD2	1:B:515:PHE:HB3	2.27	0.70
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.22	0.69
1:B:131:CYS:HB3	1:B:133:PHE:CE1	2.26	0.69
1:B:415:THR:OG1	1:C:369:TYR:OH	2.10	0.69
1:C:131:CYS:HB3	1:C:133:PHE:CE1	2.26	0.69
1:A:453:TYR:CD2	1:A:495:TYR:HE1	2.10	0.69
1:C:392:PHE:CD2	1:C:515:PHE:HB3	2.27	0.69
1:A:380:TYR:HE2	1:A:412:PRO:HD2	1.58	0.69
1:A:392:PHE:CD2	1:A:515:PHE:HB3	2.27	0.69
1:C:342:PHE:CE2	1:C:511:VAL:HG11	2.26	0.69
1:B:417:LYS:NZ	1:B:455:LEU:O	2.24	0.69
1:B:380:TYR:HE2	1:B:412:PRO:HD2	1.58	0.68
1:C:417:LYS:NZ	1:C:455:LEU:O	2.24	0.68
1:A:327:VAL:H	1:A:531:THR:HG22	1.58	0.68
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.22	0.68
1:C:380:TYR:HE2	1:C:412:PRO:HD2	1.58	0.68
1:B:327:VAL:H	1:B:531:THR:HG22	1.58	0.67
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HG3	1:A:158:ARG:NH1	1.97	0.67
1:B:496:GLY:O	1:B:505:TYR:OH	2.08	0.67
1:C:403:ARG:HD2	1:C:497:PHE:HZ	1.60	0.67
1:A:403:ARG:HD2	1:A:497:PHE:HZ	1.60	0.67
1:C:1024:LEU:HD21	1:C:1028:LYS:HE3	1.76	0.67
1:A:496:GLY:O	1:A:505:TYR:OH	2.08	0.67
1:B:1024:LEU:HD21	1:B:1028:LYS:HE3	1.76	0.67
1:C:393:THR:OG1	1:C:516:GLU:O	2.13	0.67
1:A:624:ILE:HG12	1:A:629:LEU:HD21	1.77	0.67
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.76	0.67
1:B:403:ARG:HD2	1:B:497:PHE:HZ	1.60	0.67
1:C:327:VAL:H	1:C:531:THR:HG22	1.58	0.66
1:B:360:ASN:H	1:B:523:THR:HB	1.60	0.66
1:A:393:THR:OG1	1:A:516:GLU:O	2.12	0.66
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.76	0.66
1:C:353:TRP:HZ3	1:C:355:ARG:HG3	1.61	0.66
1:A:360:ASN:H	1:A:523:THR:HB	1.60	0.66
1:C:349:SER:OG	1:C:452:LEU:O	2.14	0.66
1:A:342:PHE:CE2	1:A:511:VAL:HG11	2.26	0.66
1:B:393:THR:OG1	1:B:516:GLU:O	2.13	0.66
1:B:624:ILE:HG12	1:B:629:LEU:HD21	1.77	0.66
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.28	0.66
1:A:158:ARG:HH11	1:A:158:ARG:CG	2.04	0.66
1:B:96:GLU:HG2	1:B:97:LYS:N	2.10	0.66
1:A:96:GLU:CD	1:A:100:ILE:H	2.04	0.66
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.28	0.66
1:B:96:GLU:CD	1:B:100:ILE:H	2.04	0.66
1:A:1024:LEU:HD21	1:A:1028:LYS:HE3	1.76	0.66
1:C:96:GLU:CD	1:C:100:ILE:H	2.04	0.66
1:A:80:ASP:O	1:A:265:TYR:OH	2.14	0.66
1:B:326:ILE:HD11	1:B:534:VAL:HG22	1.78	0.66
1:C:96:GLU:HG2	1:C:97:LYS:N	2.10	0.66
1:A:415:THR:OG1	1:B:369:TYR:OH	2.13	0.65
1:B:80:ASP:O	1:B:265:TYR:OH	2.14	0.65
1:B:349:SER:OG	1:B:452:LEU:O	2.14	0.65
1:A:96:GLU:HG2	1:A:97:LYS:N	2.10	0.65
1:B:342:PHE:CE2	1:B:511:VAL:HG11	2.26	0.65
1:C:360:ASN:H	1:C:523:THR:HB	1.60	0.65
1:A:349:SER:OG	1:A:452:LEU:O	2.14	0.65
1:B:725:GLU:OE1	1:B:1028:LYS:NZ	2.29	0.65
1:C:624:ILE:HG12	1:C:629:LEU:HD21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:TRP:HZ3	1:B:355:ARG:HG3	1.61	0.65
1:A:308:VAL:HB	1:A:602:THR:HG23	1.80	0.65
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.79	0.65
1:B:97:LYS:HZ3	1:B:188:ASN:H	1.45	0.64
1:A:353:TRP:HZ3	1:A:355:ARG:HG3	1.61	0.64
1:C:80:ASP:O	1:C:265:TYR:OH	2.14	0.64
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.30	0.64
1:A:326:ILE:HD11	1:A:534:VAL:HG22	1.78	0.64
1:B:118:LEU:HD11	1:B:135:PHE:HZ	1.63	0.64
1:B:308:VAL:HB	1:B:602:THR:HG23	1.79	0.64
1:B:453:TYR:CD2	1:B:495:TYR:HE1	2.10	0.64
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.30	0.64
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.79	0.64
1:A:105:ILE:HB	1:A:239:GLN:HB3	1.79	0.64
1:A:993:ILE:O	1:A:997:ILE:HD12	1.98	0.64
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.79	0.64
1:C:403:ARG:HH12	1:C:506:GLN:C	2.06	0.64
1:A:403:ARG:HH12	1:A:506:GLN:C	2.06	0.64
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.31	0.64
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.28	0.64
1:C:97:LYS:HZ3	1:C:188:ASN:H	1.46	0.63
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.30	0.63
1:B:317:ASN:ND2	1:C:737:ASP:OD1	2.32	0.63
1:A:737:ASP:OD1	1:C:317:ASN:ND2	2.30	0.63
1:C:105:ILE:HB	1:C:239:GLN:HB3	1.79	0.63
1:C:118:LEU:HD11	1:C:135:PHE:HZ	1.63	0.63
1:C:426:PRO:HD3	1:C:464:PHE:CE2	2.34	0.63
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.34	0.63
1:A:41:LYS:NZ	1:C:562:PHE:HB2	2.13	0.63
1:A:404:GLY:HA2	1:A:508:TYR:CD2	2.34	0.63
1:B:158:ARG:HH11	1:B:158:ARG:CG	2.04	0.63
1:B:316:SER:OG	1:B:317:ASN:N	2.32	0.63
1:B:426:PRO:HD3	1:B:464:PHE:CE2	2.34	0.63
1:A:118:LEU:HD11	1:A:135:PHE:HZ	1.63	0.63
1:B:403:ARG:HH12	1:B:506:GLN:C	2.06	0.63
1:A:316:SER:OG	1:A:317:ASN:N	2.32	0.63
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.79	0.63
1:C:453:TYR:CD2	1:C:495:TYR:HE1	2.10	0.63
1:C:993:ILE:O	1:C:997:ILE:HD12	1.98	0.63
1:A:97:LYS:HZ3	1:A:188:ASN:H	1.47	0.62
1:A:737:ASP:CG	1:C:317:ASN:HD21	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:VAL:HB	1:C:602:THR:HG23	1.80	0.62
1:B:404:GLY:HA2	1:B:508:TYR:CD2	2.34	0.62
1:B:993:ILE:O	1:B:997:ILE:HD12	1.98	0.62
1:C:406:GLU:N	1:C:406:GLU:OE2	2.32	0.62
1:B:105:ILE:HB	1:B:239:GLN:HB3	1.79	0.62
1:B:406:GLU:OE2	1:B:406:GLU:N	2.32	0.62
1:A:426:PRO:HD3	1:A:464:PHE:CE2	2.34	0.62
1:B:970:PHE:CD1	1:B:999:GLY:HA3	2.35	0.62
1:A:970:PHE:CD1	1:A:999:GLY:HA3	2.35	0.62
1:A:984:LEU:HB2	1:A:989:ALA:HB2	1.82	0.62
1:A:303:LEU:HD11	1:A:313:TYR:CE1	2.35	0.62
1:B:317:ASN:HD21	1:C:737:ASP:CG	2.08	0.61
1:A:406:GLU:N	1:A:406:GLU:OE2	2.32	0.61
1:B:984:LEU:HB2	1:B:989:ALA:HB2	1.82	0.61
1:C:309:GLU:O	1:C:313:TYR:OH	2.19	0.61
1:C:970:PHE:CD1	1:C:999:GLY:HA3	2.35	0.61
1:C:303:LEU:HD11	1:C:313:TYR:CE1	2.35	0.61
1:C:496:GLY:O	1:C:505:TYR:OH	2.08	0.61
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.30	0.61
1:B:303:LEU:HD11	1:B:313:TYR:CE1	2.35	0.61
1:C:328:ARG:NE	1:C:533:LEU:HB2	2.07	0.60
1:C:984:LEU:HB2	1:C:989:ALA:HB2	1.82	0.60
1:A:317:ASN:HD21	1:B:737:ASP:CG	2.10	0.60
1:A:317:ASN:ND2	1:B:737:ASP:OD1	2.34	0.60
1:B:231:ILE:HD12	1:B:233:ILE:HB	1.83	0.60
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.84	0.60
1:A:231:ILE:HD12	1:A:233:ILE:HB	1.83	0.60
1:A:451:TYR:HB2	1:A:495:TYR:HB2	1.84	0.60
1:C:316:SER:OG	1:C:317:ASN:N	2.32	0.60
1:B:309:GLU:O	1:B:313:TYR:OH	2.18	0.59
1:B:353:TRP:CZ3	1:B:355:ARG:HG3	2.37	0.59
1:C:725:GLU:OE1	1:C:1028:LYS:NZ	2.30	0.59
1:C:81:ASN:O	1:C:239:GLN:NE2	2.30	0.59
1:C:353:TRP:CZ3	1:C:355:ARG:HG3	2.37	0.59
1:A:725:GLU:OE1	1:A:1028:LYS:NZ	2.30	0.59
1:C:37:TYR:HD1	1:C:37:TYR:H	1.51	0.59
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.84	0.59
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.84	0.59
1:A:326:ILE:HD11	1:A:534:VAL:H	1.68	0.59
1:B:37:TYR:HD1	1:B:37:TYR:H	1.51	0.59
1:B:632:THR:O	1:B:632:THR:OG1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HD11	1:C:266:TYR:CE2	2.38	0.59
1:B:451:TYR:HB2	1:B:495:TYR:HB2	1.84	0.59
1:C:231:ILE:HD12	1:C:233:ILE:HB	1.83	0.59
1:A:277:LEU:HD22	1:A:285:ILE:HD13	1.85	0.58
1:B:312:ILE:C	1:B:313:TYR:HD2	2.11	0.58
1:A:353:TRP:CZ3	1:A:355:ARG:HG3	2.37	0.58
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.30	0.58
1:C:451:TYR:HB2	1:C:495:TYR:HB2	1.84	0.58
1:A:103:GLY:CA	1:A:241:LEU:HB3	2.34	0.58
1:B:1142:GLN:OE1	1:B:1142:GLN:HA	2.03	0.58
1:C:312:ILE:C	1:C:313:TYR:HD2	2.11	0.58
1:C:326:ILE:HD11	1:C:534:VAL:H	1.67	0.58
1:A:312:ILE:C	1:A:313:TYR:HD2	2.11	0.58
1:C:811:LYS:HD2	1:C:813:SER:O	2.04	0.58
1:A:37:TYR:HD1	1:A:37:TYR:H	1.51	0.58
1:A:42:VAL:HG13	1:C:565:PHE:O	2.03	0.58
1:B:216:LEU:HD11	1:B:266:TYR:CE2	2.38	0.58
1:B:811:LYS:HD2	1:B:813:SER:O	2.04	0.58
1:A:216:LEU:HD11	1:A:266:TYR:CE2	2.38	0.58
1:A:811:LYS:HD2	1:A:813:SER:O	2.04	0.58
1:B:158:ARG:HG3	1:B:158:ARG:NH1	1.97	0.58
1:C:158:ARG:HH11	1:C:158:ARG:CG	2.04	0.58
1:C:393:THR:O	1:C:523:THR:OG1	2.22	0.58
1:A:914:ASN:OD1	1:A:915:VAL:N	2.37	0.58
1:B:64:TRP:HD1	1:B:65:PHE:N	2.02	0.58
1:B:562:PHE:HB2	1:C:41:LYS:NZ	2.18	0.58
1:C:103:GLY:CA	1:C:241:LEU:HB3	2.34	0.58
1:A:1090:PRO:HG3	1:A:1095:PHE:CE1	2.39	0.58
1:C:277:LEU:HD22	1:C:285:ILE:HD13	1.86	0.58
1:C:443:SER:C	1:C:444:LYS:HD3	2.29	0.58
1:C:1142:GLN:OE1	1:C:1142:GLN:HA	2.04	0.58
1:B:277:LEU:HD22	1:B:285:ILE:HD13	1.86	0.57
1:B:328:ARG:NE	1:B:533:LEU:HB2	2.07	0.57
1:C:340:GLU:OE1	1:C:340:GLU:N	2.33	0.57
1:C:537:LYS:O	1:C:539:VAL:HG22	2.04	0.57
1:A:1093:GLY:O	1:A:1107:ARG:NH1	2.37	0.57
1:B:91:TYR:CZ	1:B:93:ALA:HB2	2.39	0.57
1:B:103:GLY:CA	1:B:241:LEU:HB3	2.34	0.57
1:B:537:LYS:O	1:B:539:VAL:HG22	2.04	0.57
1:B:1090:PRO:HG3	1:B:1095:PHE:CE1	2.39	0.57
1:C:914:ASN:OD1	1:C:915:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:THR:O	1:B:523:THR:OG1	2.22	0.57
1:B:443:SER:C	1:B:444:LYS:HD3	2.29	0.57
1:C:1090:PRO:HG3	1:C:1095:PHE:CE1	2.39	0.57
1:C:1093:GLY:O	1:C:1107:ARG:NH1	2.37	0.57
1:A:91:TYR:CZ	1:A:93:ALA:HB2	2.39	0.57
1:C:64:TRP:HD1	1:C:65:PHE:N	2.02	0.57
1:A:556:ASN:O	1:A:558:LYS:NZ	2.38	0.57
1:A:1142:GLN:HA	1:A:1142:GLN:OE1	2.04	0.57
1:B:326:ILE:HD11	1:B:534:VAL:H	1.67	0.57
1:B:770:ILE:O	1:B:774:GLN:HG2	2.05	0.57
1:B:914:ASN:OD1	1:B:915:VAL:N	2.37	0.57
1:C:556:ASN:O	1:C:558:LYS:NZ	2.38	0.57
1:C:770:ILE:O	1:C:774:GLN:HG2	2.05	0.57
1:A:41:LYS:HZ1	1:C:562:PHE:HB2	1.69	0.57
1:A:537:LYS:O	1:A:539:VAL:HG22	2.04	0.57
1:B:565:PHE:O	1:C:42:VAL:HG13	2.04	0.57
1:A:443:SER:C	1:A:444:LYS:HD3	2.29	0.57
1:C:91:TYR:CZ	1:C:93:ALA:HB2	2.39	0.57
1:C:632:THR:O	1:C:632:THR:OG1	2.21	0.57
1:A:86:PHE:CE1	1:A:106:PHE:HE2	2.23	0.57
1:A:562:PHE:HB2	1:B:41:LYS:NZ	2.20	0.57
1:A:64:TRP:HD1	1:A:65:PHE:N	2.02	0.57
1:C:33:THR:HA	1:C:58:PHE:CE1	2.40	0.57
1:A:33:THR:HA	1:A:58:PHE:CE1	2.40	0.56
1:B:118:LEU:HD11	1:B:135:PHE:CZ	2.41	0.56
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.87	0.56
1:C:403:ARG:NH2	1:C:505:TYR:HA	2.21	0.56
1:A:131:CYS:HA	1:A:166:CYS:HB3	1.87	0.56
1:A:770:ILE:O	1:A:774:GLN:HG2	2.05	0.56
1:A:393:THR:O	1:A:523:THR:OG1	2.22	0.56
1:B:131:CYS:HA	1:B:166:CYS:HB3	1.87	0.56
1:B:1093:GLY:O	1:B:1107:ARG:NH1	2.37	0.56
1:A:118:LEU:HD11	1:A:135:PHE:CZ	2.41	0.56
1:C:1100:THR:HG22	1:C:1101:HIS:CD2	2.41	0.56
1:A:328:ARG:NE	1:A:533:LEU:HB2	2.08	0.56
1:A:813:SER:O	1:A:815:ARG:N	2.38	0.56
1:A:976:VAL:HG12	1:A:979:ASP:H	1.71	0.56
1:B:33:THR:HA	1:B:58:PHE:CE1	2.40	0.56
1:B:813:SER:O	1:B:815:ARG:N	2.38	0.56
1:C:86:PHE:CE1	1:C:106:PHE:HE2	2.23	0.56
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:C	1:A:380:TYR:HD1	2.14	0.56
1:A:1100:THR:HG22	1:A:1101:HIS:CD2	2.41	0.56
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.88	0.56
1:C:813:SER:O	1:C:815:ARG:N	2.38	0.56
1:C:976:VAL:HG12	1:C:979:ASP:H	1.71	0.56
1:B:86:PHE:CE1	1:B:106:PHE:HE2	2.23	0.56
1:B:403:ARG:NH2	1:B:505:TYR:HA	2.20	0.56
1:C:567:ARG:HH21	1:C:573:THR:HG22	1.71	0.56
1:A:230:PRO:HD3	1:C:357:ARG:NH1	2.21	0.55
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.87	0.55
1:A:392:PHE:N	1:A:392:PHE:CD1	2.74	0.55
1:B:379:CYS:C	1:B:380:TYR:HD1	2.14	0.55
1:B:447:GLY:N	1:B:498:GLN:HE22	2.04	0.55
1:B:556:ASN:O	1:B:558:LYS:NZ	2.38	0.55
1:B:976:VAL:HG12	1:B:979:ASP:H	1.71	0.55
1:A:447:GLY:N	1:A:498:GLN:HE22	2.04	0.55
1:C:418:ILE:HA	1:C:422:ASN:OD1	2.07	0.55
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.88	0.55
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.87	0.55
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.87	0.55
1:C:379:CYS:C	1:C:380:TYR:HD1	2.14	0.55
1:B:1100:THR:HG22	1:B:1101:HIS:CD2	2.41	0.55
1:C:447:GLY:N	1:C:498:GLN:HE22	2.04	0.55
1:A:418:ILE:HA	1:A:422:ASN:OD1	2.07	0.55
1:C:118:LEU:HD11	1:C:135:PHE:CZ	2.41	0.55
1:A:565:PHE:O	1:B:42:VAL:HG13	2.06	0.55
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.42	0.55
1:A:823:PHE:CD1	1:A:1057:PRO:HG3	2.41	0.55
1:B:415:THR:HG1	1:C:369:TYR:HH	1.50	0.55
1:B:567:ARG:HH21	1:B:573:THR:HG22	1.71	0.55
1:B:741:TYR:CZ	1:B:966:LEU:HD21	2.42	0.55
1:B:823:PHE:CD1	1:B:1057:PRO:HG3	2.41	0.55
1:A:403:ARG:NH2	1:A:505:TYR:HA	2.21	0.55
1:B:506:GLN:OE1	1:B:507:PRO:HD2	2.07	0.55
1:A:567:ARG:HH21	1:A:573:THR:HG22	1.71	0.55
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.89	0.54
1:B:110:LEU:N	1:B:114:THR:HG21	2.22	0.54
1:C:392:PHE:CD1	1:C:392:PHE:N	2.74	0.54
1:A:506:GLN:OE1	1:A:507:PRO:HD2	2.07	0.54
1:B:392:PHE:N	1:B:392:PHE:CD1	2.74	0.54
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HE3	1:A:97:LYS:HA	1.89	0.54
1:A:110:LEU:N	1:A:114:THR:HG21	2.22	0.54
1:A:340:GLU:OE1	1:A:340:GLU:N	2.33	0.54
1:B:200:TYR:O	1:B:202:LYS:NZ	2.40	0.54
1:A:376:THR:O	1:A:434:ILE:HA	2.08	0.54
1:C:110:LEU:N	1:C:114:THR:HG21	2.22	0.54
1:C:823:PHE:CD1	1:C:1057:PRO:HG3	2.41	0.54
1:C:506:GLN:OE1	1:C:507:PRO:HD2	2.07	0.54
1:C:741:TYR:CZ	1:C:966:LEU:HD21	2.42	0.54
1:C:97:LYS:HE3	1:C:97:LYS:HA	1.89	0.54
1:B:403:ARG:HD2	1:B:497:PHE:CZ	2.42	0.54
1:B:418:ILE:HA	1:B:422:ASN:OD1	2.07	0.54
1:B:442:ASP:OD1	1:B:451:TYR:OH	2.15	0.54
1:A:422:ASN:ND2	1:A:454:ARG:H	2.06	0.53
1:A:904:TYR:CE2	1:C:1107:ARG:HD2	2.43	0.53
1:A:920:GLN:HE22	1:C:1130:ILE:HB	1.72	0.53
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.90	0.53
1:B:392:PHE:N	1:B:392:PHE:HD1	2.06	0.53
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.89	0.53
1:C:187:LYS:N	1:C:211:ASN:HA	2.24	0.53
1:C:412:PRO:HB3	1:C:426:PRO:O	2.09	0.53
1:A:187:LYS:N	1:A:211:ASN:HA	2.23	0.53
1:C:419:ALA:HA	1:C:423:TYR:O	2.09	0.53
1:A:136:CYS:SG	1:A:158:ARG:NH2	2.82	0.53
1:A:287:ASP:HB3	1:A:306:PHE:CE1	2.44	0.53
1:B:97:LYS:HE3	1:B:97:LYS:HA	1.89	0.53
1:C:392:PHE:N	1:C:392:PHE:HD1	2.06	0.53
1:B:376:THR:O	1:B:434:ILE:HA	2.08	0.53
1:B:454:ARG:HH11	1:B:454:ARG:HB2	1.74	0.53
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.91	0.53
1:C:287:ASP:HB3	1:C:306:PHE:CE1	2.44	0.53
1:A:454:ARG:HB2	1:A:454:ARG:NH1	2.24	0.53
1:A:632:THR:O	1:A:632:THR:OG1	2.21	0.53
1:C:136:CYS:SG	1:C:158:ARG:NH2	2.82	0.53
1:C:376:THR:O	1:C:434:ILE:HA	2.08	0.53
1:C:422:ASN:ND2	1:C:454:ARG:H	2.06	0.53
1:A:115:GLN:HA	1:A:132:GLU:HG3	1.90	0.53
1:B:136:CYS:SG	1:B:158:ARG:NH2	2.82	0.53
1:B:187:LYS:N	1:B:211:ASN:HA	2.24	0.53
1:B:422:ASN:ND2	1:B:454:ARG:H	2.06	0.53
1:C:127:VAL:HG22	1:C:171:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:HD2	1:C:497:PHE:CZ	2.42	0.53
1:A:81:ASN:O	1:A:239:GLN:NE2	2.30	0.53
1:A:454:ARG:HB2	1:A:454:ARG:HH11	1.74	0.53
1:B:419:ALA:HA	1:B:423:TYR:O	2.09	0.53
1:C:340:GLU:O	1:C:344:ALA:HB2	2.09	0.53
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.41	0.53
1:B:563:GLN:NE2	1:C:43:PHE:HA	2.23	0.53
1:B:1050:MET:HE2	1:B:1052:PHE:HE2	1.74	0.53
1:A:340:GLU:O	1:A:344:ALA:HB2	2.09	0.53
1:A:392:PHE:N	1:A:392:PHE:HD1	2.06	0.53
1:B:81:ASN:O	1:B:239:GLN:NE2	2.30	0.53
1:B:115:GLN:HA	1:B:132:GLU:HG3	1.90	0.53
1:B:287:ASP:HB3	1:B:306:PHE:CE1	2.44	0.53
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.90	0.52
1:A:1103:PHE:HZ	2:F:1:NAG:H62	1.74	0.52
1:C:65:PHE:CZ	1:C:84:LEU:HD21	2.45	0.52
1:C:454:ARG:HH11	1:C:454:ARG:HB2	1.74	0.52
1:C:811:LYS:NZ	1:C:813:SER:HB3	2.25	0.52
1:B:454:ARG:HB2	1:B:454:ARG:NH1	2.24	0.52
1:B:818:ILE:HA	1:B:821:LEU:HD12	1.91	0.52
1:C:115:GLN:HA	1:C:132:GLU:HG3	1.90	0.52
1:A:738:CYS:SG	1:A:739:THR:N	2.82	0.52
1:A:818:ILE:HA	1:A:821:LEU:HD12	1.91	0.52
1:B:127:VAL:HG22	1:B:171:VAL:HG23	1.91	0.52
1:B:340:GLU:O	1:B:344:ALA:HB2	2.09	0.52
1:C:303:LEU:HD11	1:C:313:TYR:HE1	1.75	0.52
1:C:454:ARG:HB2	1:C:454:ARG:NH1	2.24	0.52
1:A:127:VAL:HG22	1:A:171:VAL:HG23	1.91	0.52
1:A:412:PRO:HB3	1:A:426:PRO:O	2.09	0.52
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.45	0.52
1:A:919:ASN:O	1:A:923:ILE:HD12	2.10	0.52
1:C:738:CYS:SG	1:C:739:THR:N	2.82	0.52
1:A:65:PHE:CZ	1:A:84:LEU:HD21	2.45	0.52
1:C:395:VAL:HG22	1:C:515:PHE:HD2	1.74	0.52
1:B:738:CYS:SG	1:B:739:THR:N	2.82	0.52
1:C:541:PHE:CZ	1:C:587:ILE:HD13	2.45	0.52
1:C:1050:MET:HE2	1:C:1052:PHE:HE2	1.74	0.52
1:A:419:ALA:HA	1:A:423:TYR:O	2.09	0.52
1:A:758:SER:O	1:A:762:GLN:HG2	2.10	0.52
1:B:357:ARG:NH1	1:C:230:PRO:HD3	2.25	0.52
1:B:412:PRO:HB3	1:B:426:PRO:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:ILE:HD12	1:B:923:ILE:H	1.75	0.52
1:C:758:SER:O	1:C:762:GLN:HG2	2.10	0.52
1:C:1032:CYS:SG	1:C:1048:HIS:HE1	2.33	0.52
1:C:1103:PHE:HZ	2:N:1:NAG:H62	1.74	0.52
1:A:1002:GLN:HE21	1:B:1005:GLN:HE22	1.58	0.52
1:B:340:GLU:OE1	1:B:340:GLU:N	2.33	0.52
1:B:1032:CYS:SG	1:B:1048:HIS:HE1	2.33	0.52
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.92	0.52
1:B:1103:PHE:HZ	2:J:1:NAG:H62	1.74	0.52
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.43	0.52
1:A:719:THR:HA	1:A:926:GLN:NE2	2.24	0.51
1:B:380:TYR:CD1	1:B:380:TYR:N	2.78	0.51
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.45	0.51
1:A:562:PHE:HB2	1:B:41:LYS:HZ2	1.73	0.51
1:A:923:ILE:HD12	1:A:923:ILE:H	1.75	0.51
1:B:395:VAL:HG22	1:B:515:PHE:HD2	1.75	0.51
1:B:758:SER:O	1:B:762:GLN:HG2	2.10	0.51
1:A:1050:MET:HE2	1:A:1052:PHE:HE2	1.74	0.51
1:B:65:PHE:CZ	1:B:84:LEU:HD21	2.45	0.51
1:C:736:VAL:HG22	1:C:858:LEU:HD23	1.92	0.51
1:A:381:GLY:O	1:B:983:ARG:NH1	2.43	0.51
1:A:809:PRO:O	1:A:814:LYS:NZ	2.43	0.51
1:A:811:LYS:NZ	1:A:813:SER:HB3	2.25	0.51
1:A:1032:CYS:SG	1:A:1048:HIS:HE1	2.33	0.51
1:B:736:VAL:HG22	1:B:858:LEU:HD23	1.92	0.51
1:B:811:LYS:NZ	1:B:813:SER:HB3	2.25	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
1:C:811:LYS:HZ3	1:C:813:SER:HB3	1.76	0.51
1:C:919:ASN:O	1:C:923:ILE:HD12	2.10	0.51
1:A:792:PRO:HG3	1:C:707:TYR:HD2	1.76	0.51
1:B:439:ASN:N	1:B:506:GLN:HE22	2.09	0.51
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.41	0.51
1:B:919:ASN:O	1:B:923:ILE:HD12	2.10	0.51
1:B:1130:ILE:HB	1:C:920:GLN:HE22	1.76	0.51
1:C:439:ASN:N	1:C:506:GLN:HE22	2.09	0.51
1:C:790:LYS:HB2	1:C:790:LYS:NZ	2.26	0.51
1:A:33:THR:HA	1:A:58:PHE:HE1	1.75	0.51
1:B:303:LEU:HD11	1:B:313:TYR:HE1	1.75	0.51
1:C:33:THR:HA	1:C:58:PHE:HE1	1.75	0.51
1:C:380:TYR:N	1:C:380:TYR:CD1	2.78	0.51
1:C:818:ILE:HA	1:C:821:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:O	1:A:202:LYS:NZ	2.40	0.51
1:A:303:LEU:HD11	1:A:313:TYR:HE1	1.75	0.51
1:A:395:VAL:HG22	1:A:515:PHE:HD2	1.75	0.51
1:A:581:THR:O	1:A:583:GLU:N	2.44	0.51
1:A:1045:LYS:NZ	1:B:890:ALA:O	2.44	0.51
1:A:380:TYR:CD1	1:A:380:TYR:N	2.78	0.51
1:B:402:ILE:HD11	1:B:407:VAL:HA	1.93	0.51
1:B:33:THR:HA	1:B:58:PHE:HE1	1.75	0.51
1:B:37:TYR:HD2	1:B:204:TYR:CZ	2.29	0.51
1:B:790:LYS:HB2	1:B:790:LYS:NZ	2.26	0.51
1:C:60:SER:HA	1:C:634:ARG:NH2	2.26	0.50
1:A:60:SER:HA	1:A:634:ARG:NH2	2.26	0.50
1:A:439:ASN:N	1:A:506:GLN:HE22	2.09	0.50
1:B:36:VAL:HG11	1:B:220:PHE:CZ	2.47	0.50
1:C:402:ILE:HD11	1:C:407:VAL:HA	1.93	0.50
1:C:453:TYR:HD2	1:C:495:TYR:CE1	2.18	0.50
1:C:37:TYR:HD2	1:C:204:TYR:CZ	2.29	0.50
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.92	0.50
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.94	0.50
1:B:498:GLN:HB2	1:B:501:ASN:OD1	2.12	0.50
1:C:923:ILE:HD12	1:C:923:ILE:H	1.75	0.50
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.93	0.50
1:A:438:SER:HB3	1:A:509:ARG:HG3	1.94	0.50
1:A:498:GLN:HB2	1:A:501:ASN:OD1	2.12	0.50
1:A:1102:TRP:CD1	1:A:1135:ASN:HD22	2.29	0.50
1:B:60:SER:HA	1:B:634:ARG:NH2	2.26	0.50
1:B:100:ILE:HG22	1:B:242:LEU:CD1	2.42	0.50
1:B:287:ASP:HB3	1:B:306:PHE:HE1	1.77	0.50
1:A:37:TYR:HD2	1:A:204:TYR:CZ	2.29	0.50
1:A:402:ILE:HD11	1:A:407:VAL:HA	1.93	0.50
1:A:1138:TYR:OH	1:A:1143:PRO:HG3	2.12	0.50
1:B:1102:TRP:CD1	1:B:1135:ASN:HD22	2.29	0.50
1:B:1138:TYR:OH	1:B:1143:PRO:HG3	2.12	0.50
1:C:809:PRO:O	1:C:814:LYS:NZ	2.43	0.50
1:A:97:LYS:NZ	1:A:188:ASN:H	2.09	0.50
1:A:789:TYR:HA	1:C:703:ASN:O	2.12	0.50
1:B:37:TYR:HE1	1:B:55:PHE:CD2	2.30	0.50
1:C:438:SER:HB3	1:C:509:ARG:HG3	1.94	0.50
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.47	0.50
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.47	0.50
1:A:37:TYR:HE1	1:A:55:PHE:CD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HA	1:A:272:PRO:HA	1.94	0.49
1:B:707:TYR:HD2	1:C:792:PRO:HG3	1.77	0.49
1:B:809:PRO:O	1:B:814:LYS:NZ	2.43	0.49
1:C:498:GLN:HB2	1:C:501:ASN:OD1	2.12	0.49
1:B:54:LEU:HA	1:B:272:PRO:HA	1.94	0.49
1:B:581:THR:O	1:B:583:GLU:N	2.44	0.49
1:C:100:ILE:HG22	1:C:242:LEU:CD1	2.42	0.49
1:C:380:TYR:HD1	1:C:380:TYR:N	2.11	0.49
1:A:521:PRO:HB3	1:A:564:GLN:HE21	1.78	0.49
1:C:800:PHE:CE2	1:C:924:ALA:HA	2.48	0.49
1:C:954:GLN:OE1	1:C:1014:ARG:HD3	2.12	0.49
1:C:1102:TRP:CD1	1:C:1135:ASN:HD22	2.29	0.49
1:A:733:LYS:HE3	1:A:771:ALA:HB1	1.95	0.49
1:A:790:LYS:HD3	1:C:702:GLU:OE2	2.13	0.49
1:A:1048:HIS:HD2	1:A:1049:LEU:N	2.11	0.49
1:B:380:TYR:HD1	1:B:380:TYR:N	2.11	0.49
1:B:521:PRO:HB3	1:B:564:GLN:HE21	1.78	0.49
1:B:954:GLN:OE1	1:B:1014:ARG:HD3	2.12	0.49
1:C:102:ARG:HG3	1:C:141:LEU:HD12	1.94	0.49
1:C:581:THR:O	1:C:583:GLU:N	2.44	0.49
1:C:37:TYR:HE1	1:C:55:PHE:CD2	2.30	0.49
1:C:54:LEU:HA	1:C:272:PRO:HA	1.94	0.49
1:C:97:LYS:NZ	1:C:188:ASN:H	2.09	0.49
1:C:431:GLY:HA2	1:C:515:PHE:CE1	2.48	0.49
1:C:733:LYS:HE3	1:C:771:ALA:HB1	1.95	0.49
1:A:403:ARG:HD2	1:A:497:PHE:CZ	2.43	0.49
1:A:560:LEU:O	1:A:562:PHE:N	2.45	0.49
1:A:914:ASN:HD22	1:C:1123:SER:CB	2.26	0.49
1:C:90:VAL:HG13	1:C:267:VAL:HG23	1.95	0.49
1:C:741:TYR:CE1	1:C:966:LEU:HD21	2.48	0.49
1:A:205:SER:OG	1:A:206:LYS:N	2.46	0.49
1:A:431:GLY:HA2	1:A:515:PHE:CE1	2.48	0.49
1:A:790:LYS:HB2	1:A:790:LYS:NZ	2.26	0.49
1:B:733:LYS:HE3	1:B:771:ALA:HB1	1.94	0.49
1:B:1048:HIS:HD2	1:B:1049:LEU:N	2.11	0.49
1:A:200:TYR:CD2	1:A:200:TYR:N	2.80	0.49
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.12	0.49
1:A:1011:GLN:OE1	1:A:1011:GLN:HA	2.12	0.49
1:B:205:SER:OG	1:B:206:LYS:N	2.46	0.49
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.95	0.49
1:B:381:GLY:O	1:C:983:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLY:HA2	1:B:515:PHE:CE1	2.48	0.49
1:B:741:TYR:CE1	1:B:966:LEU:HD21	2.48	0.49
1:B:1107:ARG:HD2	1:C:904:TYR:CE2	2.47	0.49
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.12	0.49
1:A:355:ARG:HH22	1:A:396:TYR:CA	2.26	0.49
1:B:97:LYS:NZ	1:B:188:ASN:H	2.09	0.49
1:C:521:PRO:HB3	1:C:564:GLN:HE21	1.78	0.49
1:C:560:LEU:O	1:C:562:PHE:N	2.45	0.49
1:C:1048:HIS:HD2	1:C:1049:LEU:N	2.11	0.49
1:A:37:TYR:N	1:A:37:TYR:CD1	2.81	0.49
1:A:800:PHE:CE2	1:A:924:ALA:HA	2.48	0.49
1:B:90:VAL:HG13	1:B:267:VAL:HG23	1.95	0.49
1:B:811:LYS:HZ3	1:B:813:SER:HB3	1.77	0.49
1:B:1002:GLN:HE21	1:C:1005:GLN:HE22	1.61	0.49
1:A:43:PHE:HA	1:C:563:GLN:NE2	2.27	0.48
1:A:102:ARG:HG3	1:A:141:LEU:HD12	1.94	0.48
1:A:134:GLN:HA	1:A:134:GLN:OE1	2.13	0.48
1:A:380:TYR:HD1	1:A:380:TYR:N	2.11	0.48
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.48	0.48
1:A:954:GLN:OE1	1:A:1014:ARG:HD3	2.12	0.48
1:B:102:ARG:HG3	1:B:141:LEU:HD12	1.94	0.48
1:B:355:ARG:HG2	1:B:398:ASP:OD2	2.13	0.48
1:B:560:LEU:O	1:B:562:PHE:N	2.45	0.48
1:C:205:SER:OG	1:C:206:LYS:N	2.46	0.48
1:C:355:ARG:HH22	1:C:396:TYR:CA	2.26	0.48
1:B:1011:GLN:OE1	1:B:1011:GLN:HA	2.12	0.48
1:C:37:TYR:N	1:C:37:TYR:CD1	2.81	0.48
1:C:636:TYR:OH	1:C:638:THR:HB	2.14	0.48
1:C:1090:PRO:HG3	1:C:1095:PHE:CD1	2.48	0.48
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.43	0.48
1:B:134:GLN:OE1	1:B:134:GLN:HA	2.13	0.48
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.41	0.48
1:C:1011:GLN:HA	1:C:1011:GLN:OE1	2.12	0.48
1:A:100:ILE:HG22	1:A:242:LEU:CD1	2.42	0.48
1:B:355:ARG:HH22	1:B:396:TYR:CA	2.26	0.48
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.12	0.48
1:C:620:VAL:O	1:C:624:ILE:HG13	2.14	0.48
1:C:1138:TYR:OH	1:C:1143:PRO:HG3	2.12	0.48
1:A:355:ARG:HG2	1:A:398:ASP:OD2	2.13	0.48
1:A:620:VAL:O	1:A:624:ILE:HG13	2.14	0.48
1:B:816:SER:OG	1:B:819:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:TYR:O	1:C:202:LYS:NZ	2.40	0.48
1:C:403:ARG:HH22	1:C:506:GLN:H	1.61	0.48
1:A:816:SER:OG	1:A:819:GLU:HG3	2.14	0.48
1:B:457:ARG:HH21	1:B:460:ASN:C	2.21	0.48
1:B:1090:PRO:HG3	1:B:1095:PHE:CD1	2.48	0.48
1:C:355:ARG:NH2	1:C:396:TYR:HB3	2.26	0.48
1:A:287:ASP:HB3	1:A:306:PHE:HE1	1.77	0.48
1:A:313:TYR:HD2	1:A:313:TYR:N	2.12	0.48
1:A:403:ARG:HH22	1:A:506:GLN:H	1.61	0.48
1:A:1090:PRO:HG3	1:A:1095:PHE:CD1	2.48	0.48
1:B:355:ARG:NH2	1:B:396:TYR:HB3	2.25	0.48
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.95	0.48
1:A:143:VAL:HA	1:A:154:GLU:HA	1.95	0.48
1:A:403:ARG:CZ	1:A:404:GLY:H	2.27	0.48
1:A:702:GLU:OE2	1:B:790:LYS:HD3	2.14	0.48
1:A:1130:ILE:HB	1:B:920:GLN:HE22	1.79	0.48
1:B:800:PHE:CE2	1:B:924:ALA:HA	2.48	0.48
1:C:355:ARG:HG2	1:C:398:ASP:OD2	2.13	0.48
1:A:90:VAL:HG13	1:A:267:VAL:HG23	1.95	0.47
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.95	0.47
1:A:707:TYR:HD2	1:B:792:PRO:HG3	1.79	0.47
1:B:200:TYR:N	1:B:200:TYR:CD2	2.80	0.47
1:C:117:LEU:HD21	1:C:119:ILE:HG13	1.96	0.47
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	1.95	0.47
1:B:403:ARG:HH22	1:B:506:GLN:H	1.61	0.47
1:B:719:THR:HA	1:B:926:GLN:NE2	2.24	0.47
1:A:403:ARG:HH11	1:A:497:PHE:HZ	1.61	0.47
1:A:416:GLY:O	1:A:420:ASP:HB2	2.14	0.47
1:A:457:ARG:HH21	1:A:460:ASN:C	2.21	0.47
1:A:636:TYR:OH	1:A:638:THR:HB	2.14	0.47
1:B:446:GLY:C	1:B:498:GLN:HE22	2.23	0.47
1:C:134:GLN:OE1	1:C:134:GLN:HA	2.13	0.47
1:C:327:VAL:H	1:C:531:THR:CG2	2.27	0.47
1:C:438:SER:OG	1:C:507:PRO:HB2	2.15	0.47
1:B:312:ILE:HD12	1:B:666:ILE:HD13	1.96	0.47
1:B:403:ARG:HH11	1:B:497:PHE:HZ	1.61	0.47
1:B:1045:LYS:NZ	1:C:890:ALA:O	2.47	0.47
1:C:37:TYR:HD1	1:C:37:TYR:N	2.13	0.47
1:C:143:VAL:HA	1:C:154:GLU:HA	1.95	0.47
1:C:274:THR:O	1:C:274:THR:OG1	2.32	0.47
1:C:457:ARG:HH21	1:C:460:ASN:C	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:SER:OG	1:A:507:PRO:HB2	2.15	0.47
1:A:560:LEU:N	1:A:563:GLN:HE21	2.05	0.47
1:B:438:SER:OG	1:B:507:PRO:HB2	2.15	0.47
1:B:636:TYR:OH	1:B:638:THR:HB	2.14	0.47
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.97	0.47
1:C:287:ASP:HB3	1:C:306:PHE:HE1	1.77	0.47
1:C:312:ILE:HD12	1:C:666:ILE:HD13	1.96	0.47
1:C:416:GLY:O	1:C:420:ASP:HB2	2.14	0.47
1:A:357:ARG:NH1	1:B:230:PRO:HD3	2.30	0.47
1:A:970:PHE:HE1	1:B:759:PHE:HE2	1.60	0.47
1:A:1048:HIS:CD2	1:A:1049:LEU:N	2.83	0.47
1:B:56:LEU:HD22	1:B:91:TYR:CD2	2.50	0.47
1:B:416:GLY:O	1:B:420:ASP:HB2	2.14	0.47
1:C:790:LYS:HB2	1:C:790:LYS:HZ3	1.80	0.47
1:A:37:TYR:HD1	1:A:37:TYR:N	2.13	0.47
1:A:366:SER:HG	1:A:388:ASN:CG	2.23	0.47
1:B:313:TYR:N	1:B:313:TYR:CD2	2.83	0.47
1:B:702:GLU:OE2	1:C:790:LYS:HD3	2.14	0.47
1:B:1048:HIS:CD2	1:B:1049:LEU:N	2.83	0.47
1:C:313:TYR:HD2	1:C:313:TYR:N	2.12	0.47
1:C:446:GLY:C	1:C:498:GLN:HE22	2.23	0.47
1:C:1048:HIS:CD2	1:C:1049:LEU:N	2.83	0.47
1:A:274:THR:O	1:A:274:THR:OG1	2.32	0.47
1:A:720:ILE:H	1:A:926:GLN:NE2	2.13	0.47
1:A:902:MET:CE	1:A:1049:LEU:HD13	2.45	0.47
1:B:313:TYR:HD2	1:B:313:TYR:N	2.12	0.47
1:B:1086:LYS:HB3	1:B:1122:VAL:HG13	1.97	0.47
1:C:403:ARG:HH11	1:C:497:PHE:HZ	1.61	0.47
1:C:403:ARG:CZ	1:C:404:GLY:H	2.27	0.47
1:C:816:SER:OG	1:C:819:GLU:HG3	2.14	0.47
1:A:393:THR:HG21	1:A:518:LEU:HB2	1.97	0.47
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.45	0.47
1:B:37:TYR:N	1:B:37:TYR:CD1	2.81	0.47
1:B:130:VAL:O	1:B:130:VAL:HG22	2.15	0.47
1:B:421:TYR:HE2	1:B:457:ARG:N	2.13	0.47
1:B:620:VAL:O	1:B:624:ILE:HG13	2.14	0.47
1:C:56:LEU:HD22	1:C:91:TYR:CD2	2.50	0.47
1:C:313:TYR:N	1:C:313:TYR:CD2	2.83	0.47
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.97	0.47
1:C:900:MET:HE2	1:C:900:MET:HB3	1.75	0.47
1:A:37:TYR:HD2	1:A:204:TYR:CE2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:C	1:A:55:PHE:HD2	2.23	0.47
1:A:56:LEU:HD22	1:A:91:TYR:CD2	2.50	0.47
1:A:131:CYS:HA	1:A:166:CYS:CB	2.45	0.47
1:B:131:CYS:HA	1:B:166:CYS:CB	2.45	0.47
1:B:193:VAL:HG23	1:B:223:LEU:HD23	1.96	0.47
1:A:312:ILE:HD12	1:A:666:ILE:HD13	1.96	0.46
1:A:446:GLY:C	1:A:498:GLN:HE22	2.23	0.46
1:A:568:ASP:HB3	1:A:572:THR:O	2.16	0.46
1:B:129:LYS:HE2	1:B:131:CYS:HB2	1.97	0.46
1:B:133:PHE:HE2	1:B:160:TYR:CG	2.33	0.46
1:B:143:VAL:HA	1:B:154:GLU:HA	1.95	0.46
1:B:327:VAL:H	1:B:531:THR:CG2	2.28	0.46
1:B:403:ARG:CZ	1:B:404:GLY:H	2.27	0.46
1:C:130:VAL:HG22	1:C:130:VAL:O	2.15	0.46
1:C:133:PHE:HE2	1:C:160:TYR:CG	2.33	0.46
1:C:393:THR:HG21	1:C:518:LEU:HB2	1.97	0.46
1:A:193:VAL:HG23	1:A:223:LEU:HD23	1.96	0.46
1:C:1086:LYS:HB3	1:C:1122:VAL:HG13	1.97	0.46
1:A:130:VAL:HG22	1:A:130:VAL:O	2.15	0.46
1:A:230:PRO:HG3	1:C:357:ARG:NE	2.29	0.46
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.51	0.46
1:A:421:TYR:HE2	1:A:457:ARG:N	2.13	0.46
1:B:37:TYR:HD2	1:B:204:TYR:CE2	2.33	0.46
1:C:54:LEU:C	1:C:55:PHE:HD2	2.23	0.46
1:C:168:PHE:CD2	1:C:169:GLU:N	2.84	0.46
1:C:193:VAL:HG23	1:C:223:LEU:HD23	1.96	0.46
1:A:27:ALA:C	1:A:28:TYR:HD1	2.24	0.46
1:A:102:ARG:HD3	1:A:102:ARG:HA	1.68	0.46
1:A:117:LEU:HD21	1:A:119:ILE:HG13	1.96	0.46
1:B:164:ASN:HB2	3:B:1319:NAG:C7	2.45	0.46
1:B:435:ALA:HB2	1:B:510:VAL:HG22	1.98	0.46
1:B:902:MET:CE	1:B:1049:LEU:HD13	2.45	0.46
1:C:61:ASN:HD22	3:C:1301:NAG:C7	2.29	0.46
1:C:310:LYS:HB3	1:C:310:LYS:HE2	1.70	0.46
1:C:666:ILE:HB	1:C:670:ILE:O	2.16	0.46
1:A:61:ASN:HD22	3:A:1301:NAG:C7	2.29	0.46
1:A:164:ASN:HB2	3:A:1319:NAG:C7	2.46	0.46
1:A:310:LYS:HB3	1:A:310:LYS:HE2	1.70	0.46
1:A:917:TYR:HD2	1:C:1089:PHE:CE1	2.34	0.46
1:B:55:PHE:C	1:B:270:LEU:HG	2.41	0.46
1:B:414:GLN:HA	1:B:414:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:PHE:HB2	1:C:41:LYS:HZ2	1.79	0.46
1:B:720:ILE:H	1:B:926:GLN:NE2	2.13	0.46
1:B:736:VAL:HG22	1:B:858:LEU:CD2	2.45	0.46
1:C:37:TYR:HD2	1:C:204:TYR:CE2	2.33	0.46
1:C:131:CYS:HA	1:C:166:CYS:CB	2.45	0.46
1:A:358:ILE:HB	1:A:395:VAL:HB	1.97	0.46
1:A:453:TYR:HD2	1:A:495:TYR:CE1	2.18	0.46
1:B:358:ILE:HB	1:B:395:VAL:HB	1.97	0.46
1:C:102:ARG:HA	1:C:102:ARG:HD3	1.68	0.46
1:C:129:LYS:HE2	1:C:131:CYS:HB2	1.97	0.46
1:C:568:ASP:HB3	1:C:572:THR:O	2.16	0.46
1:B:1144:GLU:OE2	1:B:1144:GLU:N	2.49	0.46
1:C:164:ASN:HB2	3:C:1319:NAG:C7	2.45	0.46
1:C:200:TYR:N	1:C:200:TYR:CD2	2.80	0.46
1:C:366:SER:HG	1:C:388:ASN:CG	2.23	0.46
1:C:414:GLN:OE1	1:C:414:GLN:HA	2.15	0.46
1:C:716:THR:HG22	1:C:1110:TYR:HB3	1.98	0.46
1:C:736:VAL:HG22	1:C:858:LEU:CD2	2.45	0.46
1:A:129:LYS:HE2	1:A:131:CYS:HB2	1.97	0.46
1:A:168:PHE:CD2	1:A:169:GLU:N	2.84	0.46
1:B:54:LEU:C	1:B:55:PHE:HD2	2.23	0.46
1:B:117:LEU:HD21	1:B:119:ILE:HG13	1.96	0.46
1:B:666:ILE:HB	1:B:670:ILE:O	2.16	0.46
1:B:703:ASN:O	1:C:789:TYR:HA	2.16	0.46
1:C:55:PHE:C	1:C:270:LEU:HG	2.41	0.46
1:C:1144:GLU:N	1:C:1144:GLU:OE2	2.49	0.46
1:A:133:PHE:HE2	1:A:160:TYR:CG	2.33	0.46
1:A:1005:GLN:HE22	1:C:1002:GLN:HE21	1.63	0.46
1:A:1086:LYS:HB3	1:A:1122:VAL:HG13	1.97	0.46
1:B:168:PHE:CD2	1:B:169:GLU:N	2.84	0.46
1:B:403:ARG:NH2	1:B:404:GLY:H	2.14	0.46
1:B:568:ASP:HB3	1:B:572:THR:O	2.16	0.46
1:B:970:PHE:HE1	1:C:759:PHE:HE2	1.63	0.46
1:C:719:THR:HA	1:C:926:GLN:NE2	2.24	0.46
1:A:403:ARG:NH2	1:A:404:GLY:H	2.14	0.46
1:C:624:ILE:HG12	1:C:629:LEU:CD2	2.46	0.46
1:C:776:LYS:HB2	1:C:776:LYS:HE3	1.74	0.46
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.98	0.45
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.97	0.45
1:A:819:GLU:OE2	1:A:1055:SER:N	2.30	0.45
1:B:377:PHE:CD1	1:B:434:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	1.98	0.45
1:C:720:ILE:H	1:C:926:GLN:NE2	2.13	0.45
1:B:27:ALA:C	1:B:28:TYR:HD1	2.24	0.45
1:B:278:LYS:HB3	1:B:278:LYS:HE3	1.61	0.45
1:A:666:ILE:HB	1:A:670:ILE:O	2.15	0.45
1:B:1123:SER:CB	1:C:914:ASN:HD22	2.29	0.45
1:C:902:MET:CE	1:C:1049:LEU:HD13	2.45	0.45
1:C:1049:LEU:HA	1:C:1049:LEU:HD23	1.61	0.45
1:A:55:PHE:C	1:A:270:LEU:HG	2.41	0.45
1:A:201:PHE:HE1	1:A:203:ILE:HB	1.82	0.45
1:A:327:VAL:H	1:A:531:THR:CG2	2.28	0.45
1:A:421:TYR:CE2	1:A:457:ARG:HG2	2.52	0.45
1:B:620:VAL:HB	1:B:621:PRO:HD3	1.99	0.45
1:C:358:ILE:HB	1:C:395:VAL:HB	1.97	0.45
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.51	0.45
1:C:388:ASN:O	1:C:526:GLY:HA3	2.17	0.45
1:C:403:ARG:NH2	1:C:404:GLY:H	2.14	0.45
1:A:234:ASN:OD1	3:A:1302:NAG:N2	2.50	0.45
1:A:388:ASN:O	1:A:526:GLY:HA3	2.17	0.45
1:B:102:ARG:HA	1:B:102:ARG:HD3	1.68	0.45
1:B:453:TYR:HD2	1:B:495:TYR:CE1	2.18	0.45
1:B:625:HIS:CE1	1:B:638:THR:HG21	2.52	0.45
1:B:800:PHE:CD2	1:B:924:ALA:HA	2.52	0.45
1:C:36:VAL:HG21	1:C:220:PHE:HZ	1.82	0.45
1:C:393:THR:HA	1:C:522:ALA:HA	1.99	0.45
1:C:421:TYR:CE2	1:C:457:ARG:HG2	2.52	0.45
1:C:435:ALA:HB2	1:C:510:VAL:HG22	1.98	0.45
1:A:36:VAL:HG21	1:A:220:PHE:HZ	1.82	0.45
1:A:313:TYR:N	1:A:313:TYR:CD2	2.83	0.45
1:A:393:THR:HA	1:A:522:ALA:HA	1.99	0.45
1:A:414:GLN:OE1	1:A:414:GLN:HA	2.15	0.45
1:A:529:LYS:HA	1:A:529:LYS:HD3	1.74	0.45
1:B:201:PHE:HE1	1:B:203:ILE:HB	1.82	0.45
1:B:234:ASN:OD1	3:B:1302:NAG:N2	2.50	0.45
1:C:27:ALA:C	1:C:28:TYR:HD1	2.24	0.45
1:A:620:VAL:HB	1:A:621:PRO:HD3	1.99	0.45
1:A:624:ILE:HG12	1:A:629:LEU:CD2	2.46	0.45
1:A:1144:GLU:OE2	1:A:1144:GLU:N	2.49	0.45
1:B:393:THR:HG21	1:B:518:LEU:HB2	1.97	0.45
1:B:768:THR:O	1:B:772:VAL:HG12	2.17	0.45
1:C:421:TYR:HE2	1:C:457:ARG:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:O	1:A:313:TYR:OH	2.19	0.45
1:A:983:ARG:NH1	1:C:381:GLY:O	2.49	0.45
1:B:36:VAL:HG21	1:B:220:PHE:HZ	1.82	0.45
1:B:64:TRP:CD1	1:B:64:TRP:C	2.95	0.45
1:B:1129:VAL:HG13	1:C:917:TYR:HB3	1.98	0.45
1:C:303:LEU:HD11	1:C:313:TYR:CD1	2.52	0.45
1:C:529:LYS:HA	1:C:529:LYS:HD3	1.74	0.45
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	1.98	0.45
1:A:800:PHE:CD2	1:A:924:ALA:HA	2.52	0.45
1:B:388:ASN:O	1:B:526:GLY:HA3	2.17	0.45
1:B:393:THR:HA	1:B:522:ALA:HA	1.99	0.45
1:C:234:ASN:OD1	3:C:1302:NAG:N2	2.50	0.45
1:C:768:THR:O	1:C:772:VAL:HG12	2.17	0.45
1:A:625:HIS:CE1	1:A:638:THR:HG21	2.52	0.45
1:A:716:THR:HG22	1:A:1110:TYR:HB3	1.98	0.45
1:A:870:ILE:O	1:A:874:THR:HG23	2.17	0.45
1:B:350:VAL:HG21	1:B:402:ILE:HG22	1.99	0.45
1:B:790:LYS:HB2	1:B:790:LYS:HZ3	1.82	0.45
1:C:224:GLU:N	1:C:224:GLU:OE1	2.50	0.45
1:A:746:SER:OG	1:A:981:LEU:HD11	2.17	0.44
1:B:403:ARG:HH22	1:B:506:GLN:N	2.16	0.44
1:B:421:TYR:CE2	1:B:457:ARG:HG2	2.52	0.44
1:B:494:SER:OG	1:B:495:TYR:N	2.50	0.44
1:C:403:ARG:HH22	1:C:506:GLN:N	2.16	0.44
1:C:494:SER:OG	1:C:495:TYR:N	2.50	0.44
1:C:620:VAL:HB	1:C:621:PRO:HD3	1.99	0.44
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.16	0.44
1:B:35:GLY:HA3	1:B:56:LEU:HB3	1.99	0.44
1:B:746:SER:OG	1:B:981:LEU:HD11	2.17	0.44
1:C:64:TRP:CD1	1:C:64:TRP:C	2.95	0.44
1:C:870:ILE:O	1:C:874:THR:HG23	2.17	0.44
1:C:968:SER:HB2	1:C:970:PHE:CE2	2.52	0.44
1:A:444:LYS:HD3	1:A:444:LYS:N	2.33	0.44
1:A:968:SER:HB2	1:A:970:PHE:CE2	2.52	0.44
1:B:37:TYR:HD1	1:B:37:TYR:N	2.13	0.44
1:B:303:LEU:HD11	1:B:313:TYR:CD1	2.52	0.44
1:B:444:LYS:HD3	1:B:444:LYS:N	2.33	0.44
1:C:96:GLU:HG2	1:C:98:SER:H	1.83	0.44
1:A:768:THR:O	1:A:772:VAL:HG12	2.17	0.44
1:B:224:GLU:N	1:B:224:GLU:OE1	2.50	0.44
1:B:380:TYR:CE2	1:B:412:PRO:HD2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:PHE:HE1	1:C:203:ILE:HB	1.82	0.44
1:C:624:ILE:HG23	1:C:629:LEU:HD22	1.99	0.44
1:A:96:GLU:HG2	1:A:98:SER:H	1.82	0.44
1:A:624:ILE:HG23	1:A:629:LEU:HD22	1.99	0.44
1:A:914:ASN:OD1	1:A:914:ASN:C	2.60	0.44
1:B:414:GLN:O	1:B:424:LYS:NZ	2.47	0.44
1:B:624:ILE:HG23	1:B:629:LEU:HD22	1.99	0.44
1:B:716:THR:HG22	1:B:1110:TYR:HB3	1.98	0.44
1:B:914:ASN:OD1	1:B:914:ASN:C	2.60	0.44
1:C:444:LYS:HD3	1:C:444:LYS:N	2.32	0.44
1:C:625:HIS:CE1	1:C:638:THR:HG21	2.52	0.44
1:A:224:GLU:N	1:A:224:GLU:OE1	2.51	0.44
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	1.98	0.44
1:B:321:GLN:OE1	1:B:321:GLN:HA	2.18	0.44
1:B:533:LEU:HD11	1:B:585:LEU:HD11	2.00	0.44
1:C:278:LYS:HB3	1:C:278:LYS:HE3	1.62	0.44
1:B:61:ASN:HD22	3:B:1301:NAG:C7	2.28	0.44
1:B:870:ILE:O	1:B:874:THR:HG23	2.17	0.44
1:C:800:PHE:CD2	1:C:924:ALA:HA	2.52	0.44
1:A:403:ARG:HH22	1:A:506:GLN:N	2.16	0.44
1:A:494:SER:OG	1:A:495:TYR:N	2.50	0.44
1:A:621:PRO:HB3	1:A:625:HIS:NE2	2.33	0.44
1:A:714:ILE:HG22	1:A:1110:TYR:HB2	1.99	0.44
1:A:790:LYS:HB2	1:A:790:LYS:HZ3	1.82	0.44
1:A:917:TYR:HD2	1:C:1089:PHE:HE1	1.64	0.44
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.78	0.44
1:B:357:ARG:NE	1:C:230:PRO:HG3	2.33	0.44
1:B:559:PHE:CB	1:B:577:ARG:HH21	2.28	0.44
1:B:714:ILE:HG22	1:B:1110:TYR:HB2	1.99	0.44
1:C:52:GLN:HA	1:C:274:THR:HA	2.00	0.44
1:C:1143:PRO:HG2	1:C:1144:GLU:OE2	2.17	0.44
1:A:1143:PRO:HG2	1:A:1144:GLU:OE2	2.17	0.44
1:C:321:GLN:HA	1:C:321:GLN:OE1	2.18	0.44
1:C:449:TYR:O	1:C:494:SER:OG	2.31	0.44
1:C:452:LEU:HA	1:C:494:SER:HA	2.00	0.44
1:C:903:ALA:HB1	1:C:913:GLN:HB2	2.00	0.44
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.99	0.43
1:A:303:LEU:HD11	1:A:313:TYR:CD1	2.52	0.43
1:A:439:ASN:O	1:A:443:SER:OG	2.36	0.43
1:A:759:PHE:HE2	1:C:970:PHE:HE1	1.66	0.43
1:B:1143:PRO:HG2	1:B:1144:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLY:HA3	1:C:56:LEU:HB3	1.99	0.43
1:C:382:VAL:HG22	1:C:387:LEU:HB3	2.00	0.43
1:C:714:ILE:HG22	1:C:1110:TYR:HB2	1.99	0.43
1:C:746:SER:OG	1:C:981:LEU:HD11	2.17	0.43
1:A:64:TRP:CD1	1:A:65:PHE:N	2.85	0.43
1:A:533:LEU:HD11	1:A:585:LEU:HD11	2.00	0.43
1:A:644:GLN:NE2	1:A:645:THR:O	2.51	0.43
1:A:880:GLY:O	1:A:884:SER:OG	2.31	0.43
1:B:563:GLN:HE22	1:C:43:PHE:HA	1.82	0.43
1:C:621:PRO:HB3	1:C:625:HIS:NE2	2.33	0.43
1:C:914:ASN:OD1	1:C:914:ASN:C	2.60	0.43
1:A:754:LEU:HD23	1:A:754:LEU:HA	1.76	0.43
1:B:345:THR:O	1:B:346:ARG:NH1	2.51	0.43
1:C:754:LEU:HA	1:C:754:LEU:HD23	1.76	0.43
1:A:382:VAL:HG22	1:A:387:LEU:HB3	2.00	0.43
1:A:725:GLU:CD	1:A:1028:LYS:HZ2	2.22	0.43
1:B:452:LEU:HA	1:B:494:SER:HA	2.00	0.43
1:B:968:SER:HB2	1:B:970:PHE:CE2	2.52	0.43
1:C:142:GLY:HA3	1:C:156:GLU:HB2	2.00	0.43
1:C:328:ARG:NH1	1:C:580:GLN:HG3	2.34	0.43
1:A:111:ASP:H	1:A:114:THR:HG22	1.83	0.43
1:A:345:THR:O	1:A:346:ARG:NH1	2.51	0.43
1:A:617:CYS:HA	1:A:620:VAL:HG23	2.01	0.43
1:A:669:GLY:N	1:B:864:LEU:O	2.51	0.43
1:B:142:GLY:HA3	1:B:156:GLU:HB2	2.01	0.43
1:B:644:GLN:NE2	1:B:645:THR:O	2.52	0.43
1:B:903:ALA:HB1	1:B:913:GLN:HB2	2.00	0.43
1:C:36:VAL:O	1:C:223:LEU:HB2	2.19	0.43
1:C:586:ASP:OD1	1:C:587:ILE:N	2.52	0.43
1:C:644:GLN:NE2	1:C:645:THR:O	2.52	0.43
1:B:586:ASP:OD1	1:B:587:ILE:N	2.52	0.43
1:B:629:LEU:HB3	1:B:631:PRO:HD2	2.01	0.43
1:B:880:GLY:O	1:B:884:SER:OG	2.31	0.43
1:B:1089:PHE:HE1	1:C:917:TYR:HD2	1.67	0.43
1:A:39:PRO:HG3	1:A:51:THR:HG21	2.00	0.43
1:A:230:PRO:HD3	1:C:357:ARG:HH11	1.84	0.43
1:A:355:ARG:NH2	1:A:396:TYR:HB3	2.25	0.43
1:A:1049:LEU:HA	1:A:1049:LEU:HD23	1.61	0.43
1:B:39:PRO:HG3	1:B:51:THR:HG21	2.00	0.43
1:B:624:ILE:HG12	1:B:629:LEU:CD2	2.46	0.43
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:N	1:C:491:PRO:O	2.40	0.43
1:C:462:LYS:HE3	1:C:462:LYS:HB2	1.85	0.43
1:A:64:TRP:CD1	1:A:64:TRP:C	2.95	0.43
1:A:142:GLY:HA3	1:A:156:GLU:HB2	2.00	0.43
1:A:321:GLN:HA	1:A:321:GLN:OE1	2.18	0.43
1:A:811:LYS:HZ3	1:A:813:SER:HB3	1.83	0.43
1:B:111:ASP:H	1:B:114:THR:HG22	1.83	0.43
1:B:621:PRO:HB3	1:B:625:HIS:NE2	2.33	0.43
1:B:661:GLU:HG2	1:B:662:CYS:N	2.34	0.43
1:C:111:ASP:H	1:C:114:THR:HG22	1.83	0.43
1:C:661:GLU:HG2	1:C:662:CYS:N	2.34	0.43
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.34	0.43
1:A:36:VAL:O	1:A:223:LEU:HB2	2.19	0.43
1:A:776:LYS:HE3	1:A:776:LYS:HB2	1.74	0.43
1:A:864:LEU:O	1:C:669:GLY:N	2.52	0.43
1:B:96:GLU:HG2	1:B:98:SER:H	1.82	0.43
1:B:115:GLN:OE1	1:B:115:GLN:N	2.50	0.43
1:C:345:THR:O	1:C:346:ARG:NH1	2.51	0.43
1:C:345:THR:HG23	1:C:346:ARG:H	1.84	0.43
1:A:158:ARG:HA	1:A:158:ARG:HD2	1.28	0.43
1:A:350:VAL:HG21	1:A:402:ILE:HG22	1.99	0.43
1:A:1048:HIS:HD2	1:A:1049:LEU:C	2.27	0.43
1:A:1107:ARG:HD2	1:B:904:TYR:CE2	2.51	0.43
1:B:52:GLN:HA	1:B:274:THR:HA	2.00	0.43
1:B:382:VAL:HG22	1:B:387:LEU:HB3	2.00	0.43
1:B:617:CYS:HA	1:B:620:VAL:HG23	2.01	0.43
1:C:84:LEU:HD22	1:C:267:VAL:HG11	2.01	0.43
1:C:617:CYS:HA	1:C:620:VAL:HG23	2.01	0.43
1:A:52:GLN:HA	1:A:274:THR:HA	2.00	0.42
1:A:337:PRO:HB2	1:A:340:GLU:OE1	2.19	0.42
1:A:983:ARG:O	1:A:984:LEU:HD23	2.19	0.42
1:B:345:THR:HG23	1:B:346:ARG:H	1.84	0.42
1:C:629:LEU:HB3	1:C:631:PRO:HD2	2.01	0.42
1:C:705:VAL:O	1:C:707:TYR:N	2.52	0.42
1:C:983:ARG:O	1:C:984:LEU:HD23	2.19	0.42
1:C:1048:HIS:HD2	1:C:1049:LEU:C	2.27	0.42
1:A:449:TYR:CE1	1:A:496:GLY:HA2	2.54	0.42
1:A:825:LYS:HE3	1:A:938:LEU:O	2.19	0.42
1:A:903:ALA:HB1	1:A:913:GLN:HB2	2.00	0.42
1:C:39:PRO:HG3	1:C:51:THR:HG21	2.00	0.42
1:A:328:ARG:NH1	1:A:580:GLN:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:HE3	1:A:462:LYS:HB2	1.85	0.42
1:A:1139:ASP:HA	1:A:1140:PRO:HD3	1.90	0.42
1:B:328:ARG:NH1	1:B:580:GLN:HG3	2.34	0.42
1:B:338:PHE:HD1	1:B:342:PHE:HE1	1.67	0.42
1:B:439:ASN:OD1	1:B:440:ASN:N	2.52	0.42
1:B:1089:PHE:CE1	1:C:917:TYR:HD2	2.37	0.42
1:C:64:TRP:CD1	1:C:65:PHE:N	2.85	0.42
1:C:337:PRO:HB2	1:C:340:GLU:OE1	2.19	0.42
1:C:1073:LYS:HB3	1:C:1073:LYS:HE2	1.78	0.42
1:A:586:ASP:OD1	1:A:587:ILE:N	2.52	0.42
1:A:629:LEU:HB3	1:A:631:PRO:HD2	2.01	0.42
1:A:703:ASN:O	1:B:789:TYR:HA	2.19	0.42
1:A:1123:SER:CB	1:B:914:ASN:HD22	2.32	0.42
1:B:378:LYS:HE2	1:B:380:TYR:CE1	2.55	0.42
1:C:115:GLN:OE1	1:C:115:GLN:N	2.50	0.42
1:C:533:LEU:HD11	1:C:585:LEU:HD11	2.00	0.42
1:C:713:ALA:HA	1:C:1073:LYS:O	2.20	0.42
1:A:414:GLN:O	1:A:424:LYS:NZ	2.47	0.42
1:A:439:ASN:OD1	1:A:440:ASN:N	2.52	0.42
1:A:452:LEU:HA	1:A:494:SER:HA	2.00	0.42
1:A:455:LEU:N	1:A:491:PRO:O	2.40	0.42
1:A:518:LEU:HD23	1:A:518:LEU:HA	1.91	0.42
1:A:559:PHE:CB	1:A:577:ARG:HH21	2.28	0.42
1:A:786:LYS:H	1:A:786:LYS:HG2	1.64	0.42
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	2.01	0.42
1:B:189:LEU:HB2	1:B:210:ILE:CG2	2.49	0.42
1:B:366:SER:HG	1:B:388:ASN:CG	2.27	0.42
1:B:449:TYR:O	1:B:494:SER:OG	2.31	0.42
1:B:1043:CYS:O	1:B:1064:HIS:CD2	2.73	0.42
1:C:350:VAL:HG21	1:C:402:ILE:HG22	1.99	0.42
1:C:439:ASN:OD1	1:C:440:ASN:N	2.52	0.42
1:C:1116:THR:HA	1:C:1138:TYR:O	2.20	0.42
1:A:705:VAL:O	1:A:707:TYR:N	2.52	0.42
1:B:325:SER:HA	1:B:540:ASN:O	2.20	0.42
1:B:900:MET:HE2	1:B:900:MET:HB3	1.75	0.42
1:B:1116:THR:HA	1:B:1138:TYR:O	2.20	0.42
1:B:1130:ILE:HD12	1:C:920:GLN:HE21	1.85	0.42
1:C:120:VAL:HG12	1:C:122:ASN:ND2	2.34	0.42
1:C:449:TYR:CE1	1:C:496:GLY:HA2	2.55	0.42
1:C:718:PHE:HD2	1:C:1067:TYR:HE2	1.68	0.42
1:C:825:LYS:HE3	1:C:938:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1043:CYS:O	1:C:1064:HIS:CD2	2.73	0.42
1:A:356:LYS:HG2	1:A:357:ARG:O	2.19	0.42
1:A:667:GLY:HA2	1:B:864:LEU:HA	2.02	0.42
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.34	0.42
1:B:84:LEU:HD22	1:B:267:VAL:HG11	2.01	0.42
1:B:120:VAL:HG12	1:B:122:ASN:ND2	2.34	0.42
1:B:337:PRO:HB2	1:B:340:GLU:OE1	2.19	0.42
1:B:562:PHE:HB2	1:C:41:LYS:HZ1	1.85	0.42
1:B:586:ASP:OD1	1:B:586:ASP:C	2.63	0.42
1:B:716:THR:OG1	1:B:1071:GLN:O	2.35	0.42
1:C:356:LYS:HG2	1:C:357:ARG:O	2.19	0.42
1:C:378:LYS:HE2	1:C:380:TYR:CE1	2.55	0.42
1:C:439:ASN:O	1:C:443:SER:OG	2.36	0.42
1:C:559:PHE:CB	1:C:577:ARG:HH21	2.28	0.42
1:C:748:GLU:OE2	1:C:981:LEU:HD13	2.19	0.42
1:A:325:SER:HA	1:A:540:ASN:O	2.20	0.42
1:A:353:TRP:HB3	1:A:400:PHE:HD1	1.85	0.42
1:A:713:ALA:HA	1:A:1073:LYS:O	2.20	0.42
1:A:790:LYS:NZ	1:C:704:SER:HB3	2.35	0.42
1:A:917:TYR:CD2	1:C:1089:PHE:HE1	2.37	0.42
1:B:36:VAL:O	1:B:223:LEU:HB2	2.19	0.42
1:B:356:LYS:HG2	1:B:357:ARG:O	2.19	0.42
1:B:1028:LYS:O	1:B:1032:CYS:HB2	2.16	0.42
1:B:1048:HIS:HD2	1:B:1049:LEU:C	2.27	0.42
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.78	0.42
1:A:1116:THR:HA	1:A:1138:TYR:O	2.20	0.42
1:B:983:ARG:O	1:B:984:LEU:HD23	2.19	0.42
1:B:1012:LEU:HD23	1:B:1012:LEU:HA	1.81	0.42
1:C:725:GLU:CD	1:C:1028:LYS:HZ2	2.23	0.42
1:C:1012:LEU:HD23	1:C:1012:LEU:HA	1.81	0.42
1:A:718:PHE:HD2	1:A:1067:TYR:HE2	1.68	0.42
1:B:201:PHE:O	1:B:228:ASP:HA	2.20	0.42
1:B:449:TYR:CE1	1:B:496:GLY:HA2	2.55	0.42
1:C:189:LEU:HB2	1:C:210:ILE:CG2	2.49	0.42
1:C:543:PHE:CD1	1:C:576:VAL:HG11	2.55	0.42
1:A:115:GLN:OE1	1:A:115:GLN:N	2.50	0.41
1:A:345:THR:HG23	1:A:346:ARG:H	1.84	0.41
1:A:748:GLU:OE2	1:A:981:LEU:HD13	2.19	0.41
1:A:890:ALA:O	1:C:1045:LYS:NZ	2.51	0.41
1:A:902:MET:HE1	1:A:1049:LEU:HD13	2.02	0.41
1:B:713:ALA:HA	1:B:1073:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:GLU:OE2	1:B:981:LEU:HD13	2.19	0.41
1:B:786:LYS:H	1:B:786:LYS:HG2	1.64	0.41
1:C:140:PHE:HA	1:C:241:LEU:HD11	2.02	0.41
1:C:189:LEU:HD23	1:C:190:ARG:N	2.35	0.41
1:C:983:ARG:C	1:C:984:LEU:HD23	2.45	0.41
1:C:1028:LYS:O	1:C:1032:CYS:HB2	2.16	0.41
1:A:189:LEU:HB2	1:A:210:ILE:CG2	2.50	0.41
1:B:38:TYR:CE2	1:B:222:ALA:HB1	2.55	0.41
1:B:353:TRP:CD1	1:B:423:TYR:CD1	3.08	0.41
1:B:825:LYS:HE3	1:B:938:LEU:O	2.19	0.41
1:B:983:ARG:C	1:B:984:LEU:HD23	2.45	0.41
1:C:38:TYR:CE2	1:C:222:ALA:HB1	2.55	0.41
1:C:560:LEU:HB2	1:C:562:PHE:CE1	2.55	0.41
1:A:43:PHE:HA	1:C:563:GLN:HE22	1.84	0.41
1:A:920:GLN:HE21	1:C:1130:ILE:HD12	1.85	0.41
1:B:103:GLY:HA3	1:B:241:LEU:HD23	2.02	0.41
1:B:158:ARG:HA	1:B:158:ARG:HD2	1.28	0.41
1:B:726:ILE:O	1:B:947:LYS:HE2	2.20	0.41
1:B:1139:ASP:HA	1:B:1140:PRO:HD3	1.90	0.41
1:C:505:TYR:O	1:C:505:TYR:CG	2.73	0.41
1:C:666:ILE:HD13	1:C:666:ILE:HA	1.85	0.41
1:C:902:MET:HE1	1:C:1049:LEU:HD13	2.02	0.41
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.56	0.41
1:A:345:THR:HG23	1:A:346:ARG:N	2.35	0.41
1:A:1073:LYS:HB3	1:A:1073:LYS:HE2	1.78	0.41
1:B:560:LEU:HB2	1:B:562:PHE:CE1	2.55	0.41
1:B:902:MET:HE1	1:B:1049:LEU:HD13	2.02	0.41
1:C:537:LYS:HE3	1:C:537:LYS:HB3	1.91	0.41
1:C:981:LEU:HD21	1:C:993:ILE:HD11	2.03	0.41
1:A:84:LEU:HD22	1:A:267:VAL:HG11	2.01	0.41
1:A:103:GLY:HA3	1:A:241:LEU:HD23	2.02	0.41
1:A:268:GLY:C	1:A:269:TYR:HD1	2.29	0.41
1:A:748:GLU:O	1:A:752:LEU:HD23	2.20	0.41
1:A:914:ASN:HD22	1:C:1123:SER:HB2	1.86	0.41
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.56	0.41
1:B:345:THR:HG23	1:B:346:ARG:N	2.35	0.41
1:B:710:ASN:OD1	1:B:710:ASN:C	2.64	0.41
1:B:718:PHE:HD2	1:B:1067:TYR:HE2	1.68	0.41
1:C:201:PHE:O	1:C:228:ASP:HA	2.20	0.41
1:C:268:GLY:C	1:C:269:TYR:HD1	2.29	0.41
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:THR:HG23	1:C:346:ARG:N	2.35	0.41
1:C:353:TRP:CD1	1:C:423:TYR:CD1	3.08	0.41
1:C:743:CYS:SG	1:C:749:CYS:C	3.04	0.41
1:A:103:GLY:HA3	1:A:241:LEU:HB3	2.03	0.41
1:A:110:LEU:H	1:A:114:THR:HG21	1.86	0.41
1:A:120:VAL:HG12	1:A:122:ASN:ND2	2.34	0.41
1:A:378:LYS:HE2	1:A:380:TYR:CE1	2.55	0.41
1:A:710:ASN:OD1	1:A:710:ASN:C	2.64	0.41
1:A:726:ILE:O	1:A:947:LYS:HE2	2.21	0.41
1:A:743:CYS:SG	1:A:749:CYS:C	3.04	0.41
1:B:568:ASP:HB2	1:B:574:ASP:HB2	2.03	0.41
1:B:776:LYS:HE3	1:B:776:LYS:HB2	1.74	0.41
1:C:353:TRP:HB3	1:C:400:PHE:HD1	1.85	0.41
1:C:531:THR:OG1	1:C:532:ASN:N	2.54	0.41
1:A:568:ASP:HB2	1:A:574:ASP:HB2	2.03	0.41
1:A:707:TYR:HE1	1:B:897:PRO:HA	1.85	0.41
1:A:983:ARG:C	1:A:984:LEU:HD23	2.45	0.41
1:B:189:LEU:HD23	1:B:190:ARG:N	2.35	0.41
1:B:353:TRP:HB3	1:B:400:PHE:HD1	1.85	0.41
1:B:452:LEU:HG	1:B:492:LEU:HD12	2.02	0.41
1:C:36:VAL:HG21	1:C:220:PHE:CZ	2.55	0.41
1:C:443:SER:HB2	1:C:498:GLN:C	2.46	0.41
1:C:726:ILE:O	1:C:947:LYS:HE2	2.20	0.41
1:C:804:GLN:HE22	1:C:935:GLN:HE22	1.69	0.41
1:A:38:TYR:CE2	1:A:222:ALA:HB1	2.56	0.41
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.56	0.41
1:A:353:TRP:CD1	1:A:423:TYR:CD1	3.08	0.41
1:A:443:SER:HB2	1:A:498:GLN:C	2.46	0.41
1:A:543:PHE:CD1	1:A:576:VAL:HG11	2.55	0.41
1:A:981:LEU:HD21	1:A:993:ILE:HD11	2.03	0.41
1:B:743:CYS:SG	1:B:749:CYS:C	3.04	0.41
1:B:981:LEU:HD21	1:B:993:ILE:HD11	2.03	0.41
1:B:1029:MET:HE2	1:B:1053:PRO:HB3	2.03	0.41
1:C:241:LEU:HD12	1:C:242:LEU:N	2.36	0.41
1:C:338:PHE:HD1	1:C:342:PHE:HE1	1.67	0.41
1:C:452:LEU:HG	1:C:492:LEU:HD12	2.02	0.41
1:A:164:ASN:CG	1:A:165:ASN:N	2.79	0.41
1:A:189:LEU:HD23	1:A:190:ARG:N	2.35	0.41
1:A:338:PHE:HD1	1:A:342:PHE:HE1	1.67	0.41
1:A:426:PRO:HD3	1:A:464:PHE:HE2	1.85	0.41
1:A:586:ASP:OD1	1:A:586:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:GLU:HG2	1:A:662:CYS:N	2.34	0.41
1:A:1043:CYS:O	1:A:1064:HIS:CD2	2.73	0.41
1:B:229:LEU:CD2	1:B:231:ILE:HG22	2.51	0.41
1:B:268:GLY:C	1:B:269:TYR:HD1	2.29	0.41
1:B:748:GLU:O	1:B:752:LEU:HD23	2.20	0.41
1:B:754:LEU:HA	1:B:754:LEU:HD23	1.76	0.41
1:C:164:ASN:CG	1:C:165:ASN:N	2.79	0.41
1:C:748:GLU:O	1:C:752:LEU:HD23	2.20	0.41
1:C:811:LYS:HD3	1:C:813:SER:H	1.85	0.41
1:C:1050:MET:HE2	1:C:1052:PHE:CE2	2.55	0.41
1:A:87:ASN:OD1	1:A:87:ASN:N	2.54	0.41
1:A:531:THR:OG1	1:A:532:ASN:N	2.54	0.41
1:A:560:LEU:HB2	1:A:562:PHE:CE1	2.55	0.41
1:A:1050:MET:HE2	1:A:1052:PHE:CE2	2.55	0.41
1:B:443:SER:HB2	1:B:498:GLN:C	2.46	0.41
1:B:487:ASN:OD1	1:B:487:ASN:C	2.64	0.41
1:B:531:THR:OG1	1:B:532:ASN:N	2.54	0.41
1:B:669:GLY:N	1:C:864:LEU:O	2.51	0.41
1:C:103:GLY:HA3	1:C:241:LEU:HD23	2.02	0.41
1:C:229:LEU:CD2	1:C:231:ILE:HG22	2.51	0.41
1:C:568:ASP:HB2	1:C:574:ASP:HB2	2.03	0.41
1:C:586:ASP:OD1	1:C:586:ASP:C	2.63	0.41
1:A:140:PHE:HA	1:A:241:LEU:HD11	2.02	0.40
1:A:811:LYS:HD3	1:A:813:SER:H	1.85	0.40
1:B:64:TRP:CD1	1:B:65:PHE:N	2.85	0.40
1:B:462:LYS:HE3	1:B:462:LYS:HB2	1.85	0.40
1:B:543:PHE:CD1	1:B:576:VAL:HG11	2.55	0.40
1:C:325:SER:HA	1:C:540:ASN:O	2.20	0.40
1:C:796:ASP:OD2	1:C:796:ASP:N	2.46	0.40
1:A:241:LEU:HD12	1:A:242:LEU:N	2.36	0.40
1:A:410:ILE:HD13	1:A:410:ILE:HA	1.86	0.40
1:A:1029:MET:HE2	1:A:1053:PRO:HB3	2.03	0.40
1:B:63:THR:HG22	1:B:65:PHE:CE2	2.57	0.40
1:C:63:THR:HG22	1:C:65:PHE:CE2	2.57	0.40
1:C:596:SER:OG	1:C:611:LEU:HB3	2.22	0.40
1:C:716:THR:OG1	1:C:1071:GLN:O	2.35	0.40
1:A:55:PHE:CD2	1:A:55:PHE:N	2.90	0.40
1:A:201:PHE:O	1:A:228:ASP:HA	2.20	0.40
1:A:229:LEU:CD2	1:A:231:ILE:HG22	2.51	0.40
1:A:505:TYR:O	1:A:505:TYR:CG	2.74	0.40
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLY:HA3	1:B:241:LEU:HB3	2.02	0.40
1:B:110:LEU:H	1:B:114:THR:HG21	1.86	0.40
1:B:164:ASN:CG	1:B:165:ASN:N	2.79	0.40
1:B:310:LYS:HE2	1:B:310:LYS:HB3	1.70	0.40
1:B:559:PHE:HZ	1:B:566:GLY:H	1.70	0.40
1:B:1049:LEU:HD23	1:B:1049:LEU:HA	1.61	0.40
1:B:1073:LYS:HE2	1:B:1073:LYS:HB3	1.78	0.40
1:C:86:PHE:HD2	1:C:86:PHE:O	2.04	0.40
1:C:158:ARG:HD2	1:C:158:ARG:HA	1.28	0.40
1:A:452:LEU:HG	1:A:492:LEU:HD12	2.02	0.40
1:A:559:PHE:HZ	1:A:566:GLY:H	1.70	0.40
1:B:140:PHE:HA	1:B:241:LEU:HD11	2.02	0.40
1:B:241:LEU:HD12	1:B:242:LEU:N	2.36	0.40
1:C:403:ARG:HD2	1:C:403:ARG:HH11	1.73	0.40
1:C:430:THR:O	1:C:515:PHE:HD1	2.05	0.40
1:C:710:ASN:OD1	1:C:710:ASN:C	2.64	0.40
1:C:1029:MET:HE2	1:C:1053:PRO:HB3	2.03	0.40
1:C:1139:ASP:HA	1:C:1140:PRO:HD3	1.90	0.40
1:A:28:TYR:HD2	1:A:61:ASN:OD1	2.05	0.40
1:A:96:GLU:OE2	1:A:99:ASN:N	2.55	0.40
1:A:201:PHE:CD1	1:A:201:PHE:C	3.00	0.40
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.92	0.40
1:A:823:PHE:HD1	1:A:1057:PRO:HG3	1.86	0.40
1:A:914:ASN:ND2	1:C:1123:SER:OG	2.55	0.40
1:A:920:GLN:NE2	1:C:1130:ILE:HD12	2.37	0.40
1:A:986:PRO:O	1:A:990:GLU:HB2	2.22	0.40
1:B:92:PHE:HB3	1:B:194:PHE:HE1	1.87	0.40
1:B:100:ILE:HD13	1:B:100:ILE:HA	1.92	0.40
1:C:433:VAL:C	1:C:434:ILE:HG13	2.47	0.40
1:C:559:PHE:HZ	1:C:566:GLY:H	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	999/1274 (78%)	928 (93%)	71 (7%)	0	100	100
1	B	999/1274 (78%)	928 (93%)	71 (7%)	0	100	100
1	C	999/1274 (78%)	929 (93%)	70 (7%)	0	100	100
All	All	2997/3822 (78%)	2785 (93%)	212 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	888/1099 (81%)	861 (97%)	27 (3%)	36	64
1	B	888/1099 (81%)	861 (97%)	27 (3%)	36	64
1	C	888/1099 (81%)	861 (97%)	27 (3%)	36	64
All	All	2664/3297 (81%)	2583 (97%)	81 (3%)	37	64

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	TYR
1	A	94	SER
1	A	101	ILE
1	A	155	SER
1	A	158	ARG
1	A	198	ASP
1	A	200	TYR
1	A	278	LYS
1	A	313	TYR
1	A	376	THR
1	A	380	TYR
1	A	392	PHE
1	A	445	VAL

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Mol	Chain	Res	Type
1	A	458	LYS
1	A	464	PHE
1	A	509	ARG
1	A	539	VAL
1	A	546	LEU
1	A	583	GLU
1	A	607	GLN
1	A	632	THR
1	A	718	PHE
1	A	902	MET
1	A	907	ASN
1	A	1068	VAL
1	A	1107	ARG
1	A	1142	GLN
1	B	37	TYR
1	B	94	SER
1	B	101	ILE
1	B	155	SER
1	B	158	ARG
1	B	198	ASP
1	B	200	TYR
1	B	278	LYS
1	B	313	TYR
1	B	376	THR
1	B	380	TYR
1	B	392	PHE
1	B	445	VAL
1	B	458	LYS
1	B	464	PHE
1	B	509	ARG
1	B	539	VAL
1	B	546	LEU
1	B	583	GLU
1	B	607	GLN
1	B	632	THR
1	B	718	PHE
1	B	902	MET
1	B	907	ASN
1	B	1068	VAL
1	B	1107	ARG
1	B	1142	GLN
1	C	37	TYR

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Mol	Chain	Res	Type
1	C	94	SER
1	C	101	ILE
1	C	155	SER
1	C	158	ARG
1	C	198	ASP
1	C	200	TYR
1	C	278	LYS
1	C	313	TYR
1	C	376	THR
1	C	380	TYR
1	C	392	PHE
1	C	445	VAL
1	C	458	LYS
1	C	464	PHE
1	C	509	ARG
1	C	539	VAL
1	C	546	LEU
1	C	583	GLU
1	C	607	GLN
1	C	632	THR
1	C	718	PHE
1	C	902	MET
1	C	907	ASN
1	C	1068	VAL
1	C	1107	ARG
1	C	1142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	66	HIS
1	A	245	HIS
1	A	422	ASN
1	A	437	ASN
1	A	563	GLN
1	A	644	GLN
1	A	804	GLN
1	A	920	GLN
1	A	926	GLN
1	A	935	GLN
1	A	957	GLN

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Mol	Chain	Res	Type
1	A	1005	GLN
1	A	1048	HIS
1	B	49	HIS
1	B	66	HIS
1	B	245	HIS
1	B	422	ASN
1	B	437	ASN
1	B	644	GLN
1	B	804	GLN
1	B	920	GLN
1	B	926	GLN
1	B	935	GLN
1	B	957	GLN
1	B	1005	GLN
1	B	1048	HIS
1	C	49	HIS
1	C	66	HIS
1	C	245	HIS
1	C	422	ASN
1	C	437	ASN
1	C	644	GLN
1	C	804	GLN
1	C	920	GLN
1	C	926	GLN
1	C	935	GLN
1	C	957	GLN
1	C	1005	GLN
1	C	1048	HIS
1	C	1113	GLN
1	C	1119	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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
2	NAG	D	1	1,2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.39	0
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.65	1 (5%)
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.49	0
2	NAG	F	1	1,2	14,14,15	0.54	0	17,19,21	0.47	0
2	NAG	F	2	2	14,14,15	0.21	0	17,19,21	0.37	0
2	NAG	G	1	1,2	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	G	2	2	14,14,15	0.21	0	17,19,21	0.56	0
2	NAG	H	1	1,2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.38	0
2	NAG	I	1	1,2	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.48	0
2	NAG	J	1	1,2	14,14,15	0.53	0	17,19,21	0.47	0
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.37	0
2	NAG	K	1	1,2	14,14,15	0.36	0	17,19,21	0.49	0
2	NAG	K	2	2	14,14,15	0.19	0	17,19,21	0.56	0
2	NAG	L	1	1,2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	L	2	2	14,14,15	0.30	0	17,19,21	0.38	0
2	NAG	M	1	1,2	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
2	NAG	M	2	2	14,14,15	0.18	0	17,19,21	0.49	0
2	NAG	N	1	1,2	14,14,15	0.53	0	17,19,21	0.47	0
2	NAG	N	2	2	14,14,15	0.20	0	17,19,21	0.37	0
2	NAG	O	1	1,2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	O	2	2	14,14,15	0.20	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	2.07	114.96	112.19
2	M	1	NAG	C1-O5-C5	2.07	114.95	112.19
2	I	1	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6

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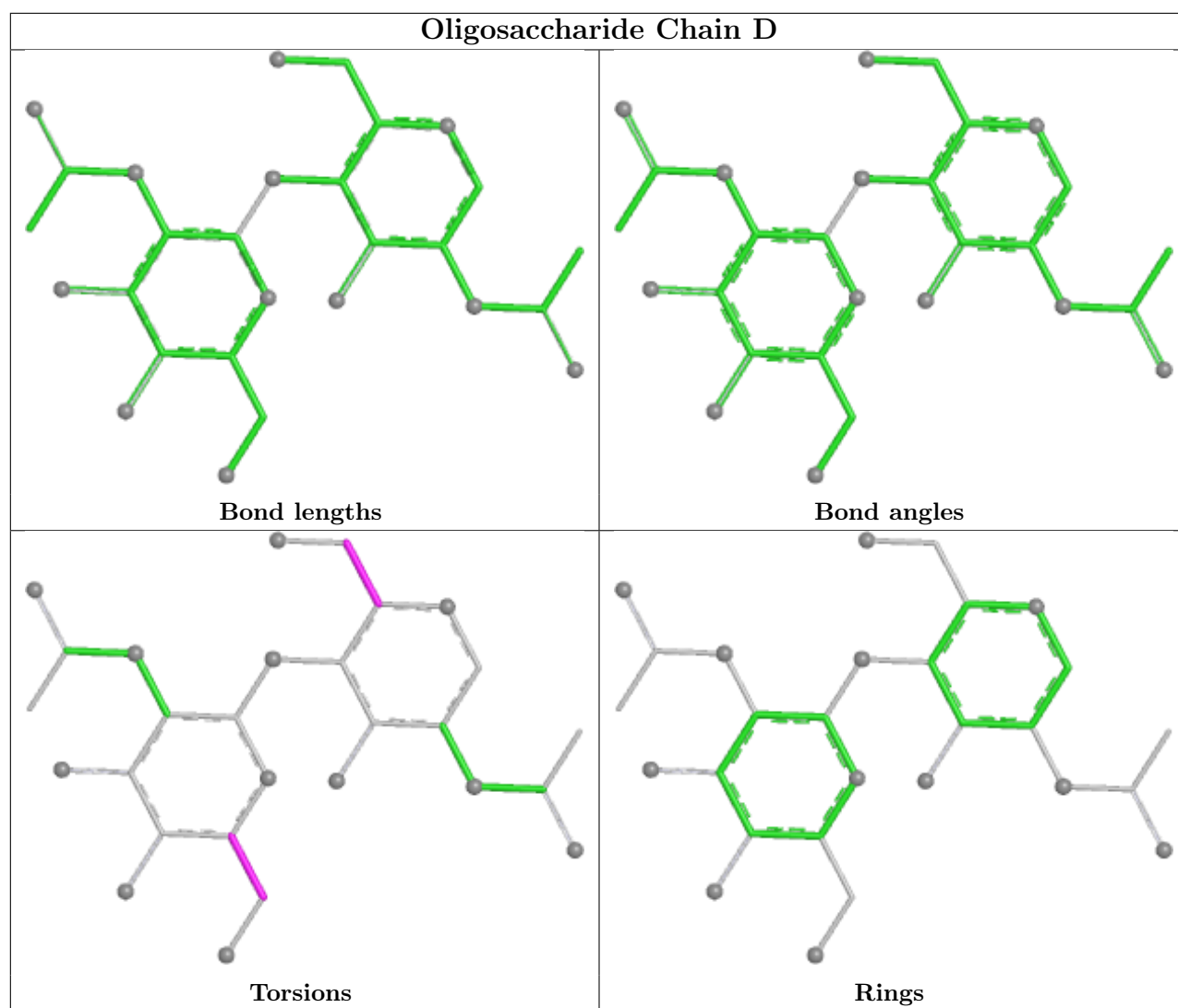
Mol	Chain	Res	Type	Atoms
2	O	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C1-C2-N2-C7
2	J	1	NAG	C1-C2-N2-C7
2	N	1	NAG	C1-C2-N2-C7

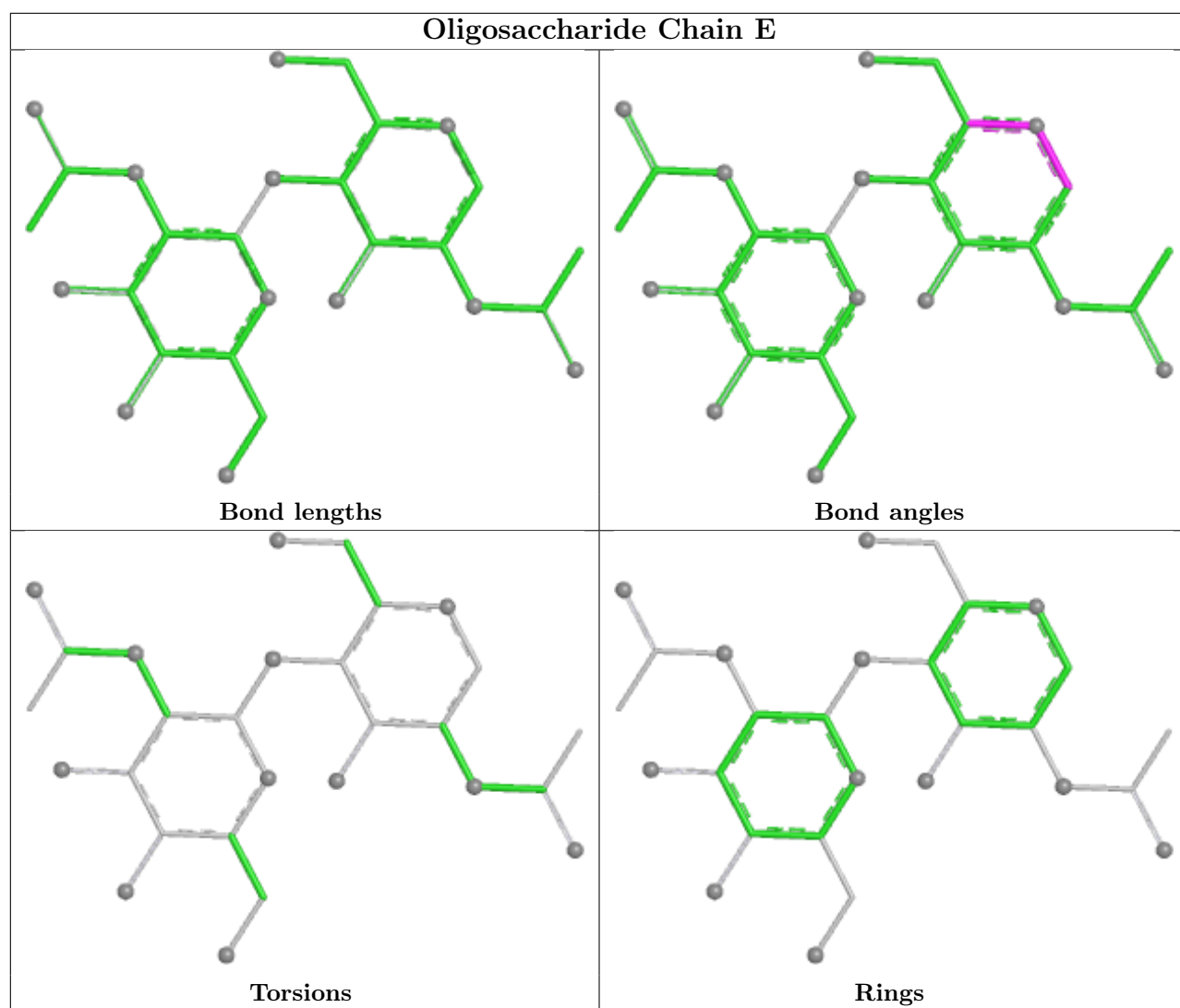
There are no ring outliers.

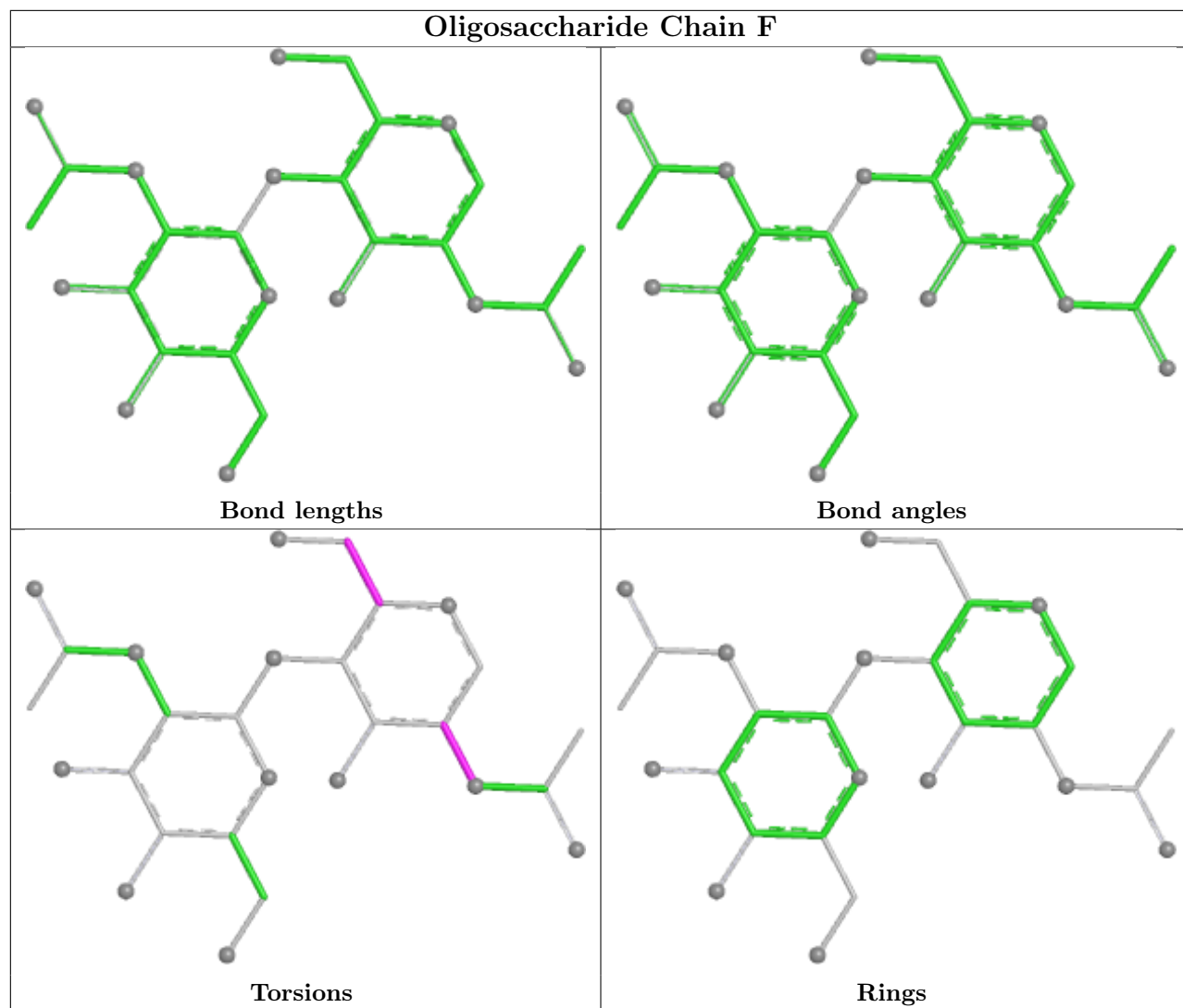
3 monomers are involved in 3 short contacts:

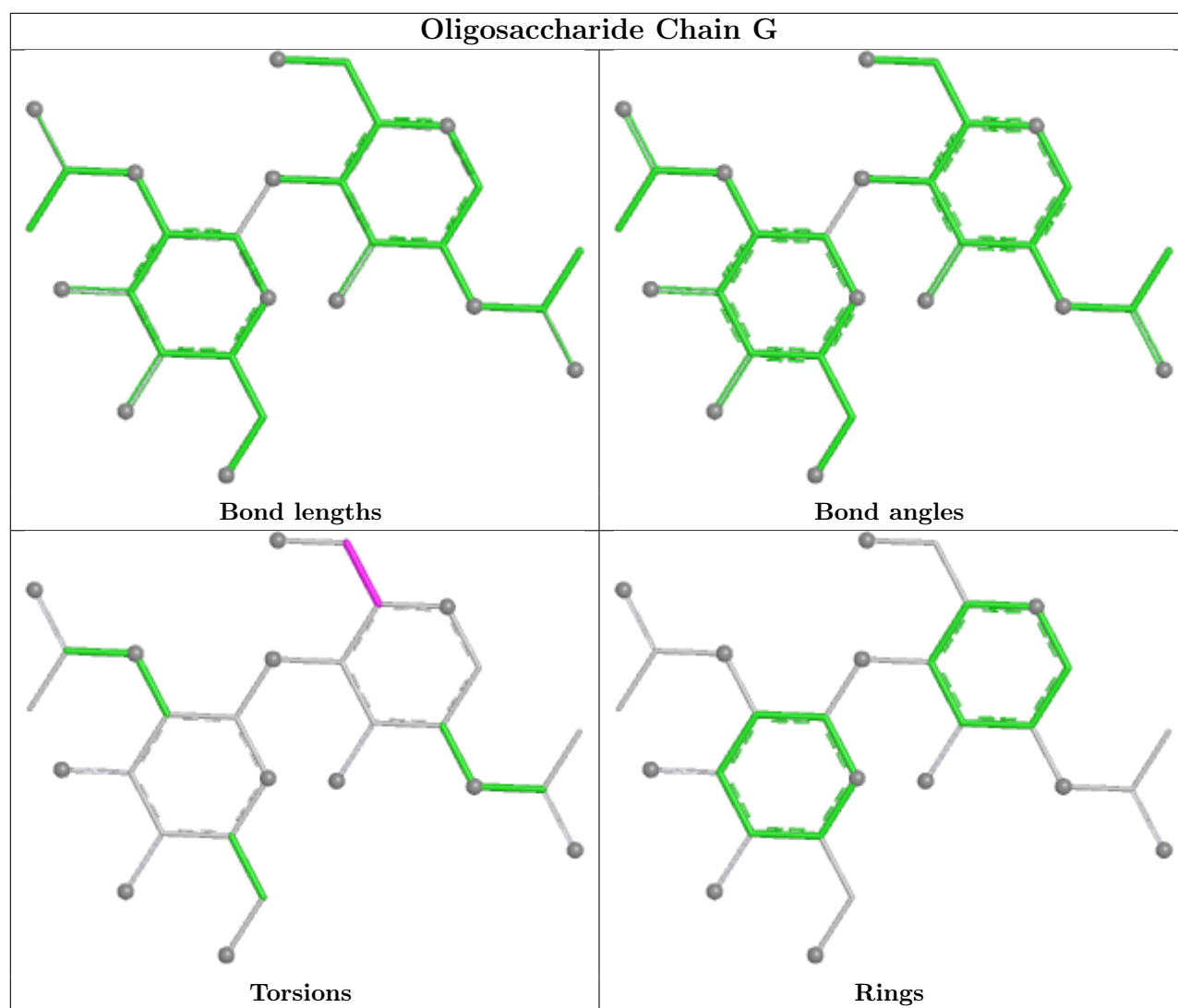
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	N	1	NAG	1	0
2	J	1	NAG	1	0

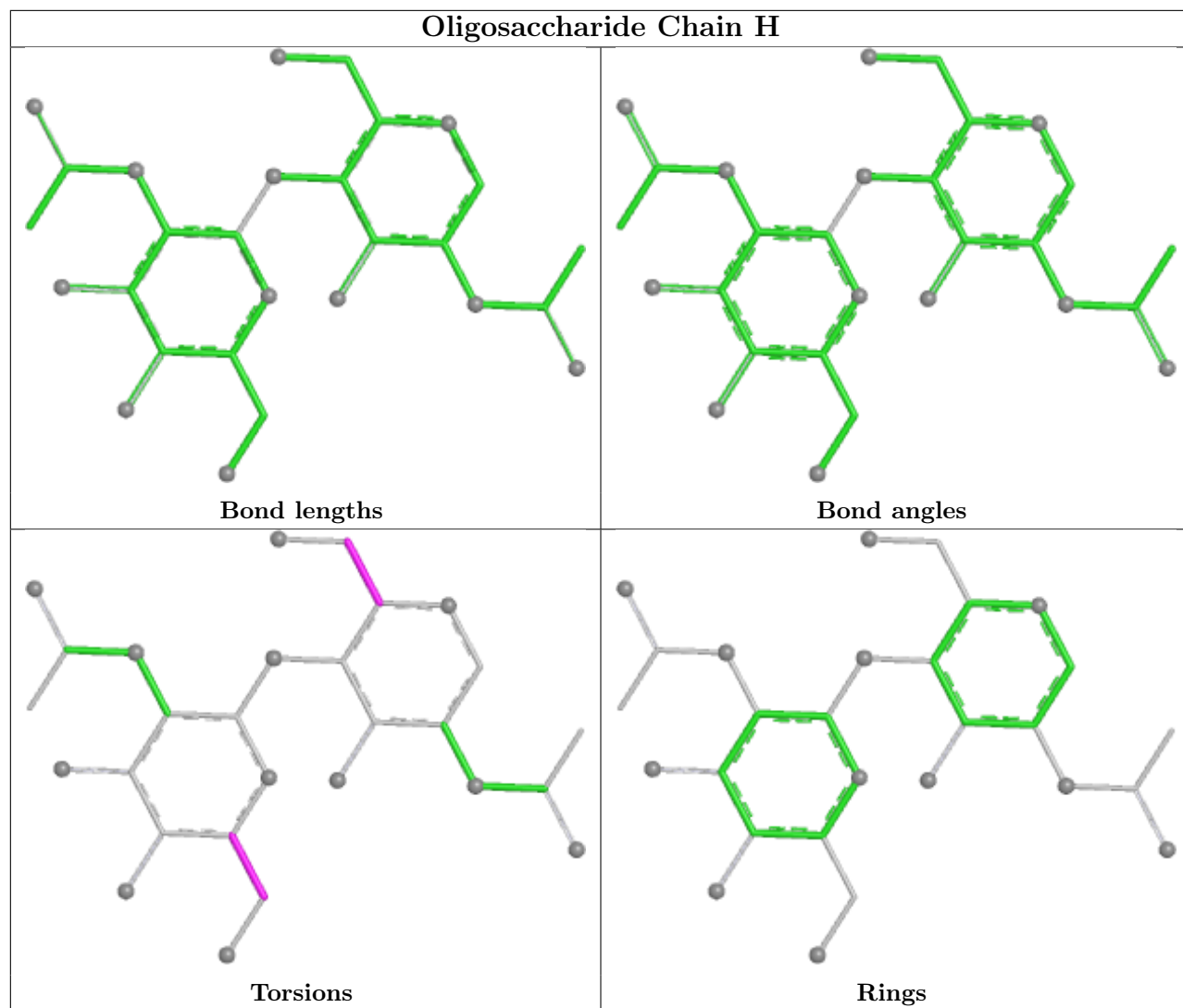
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

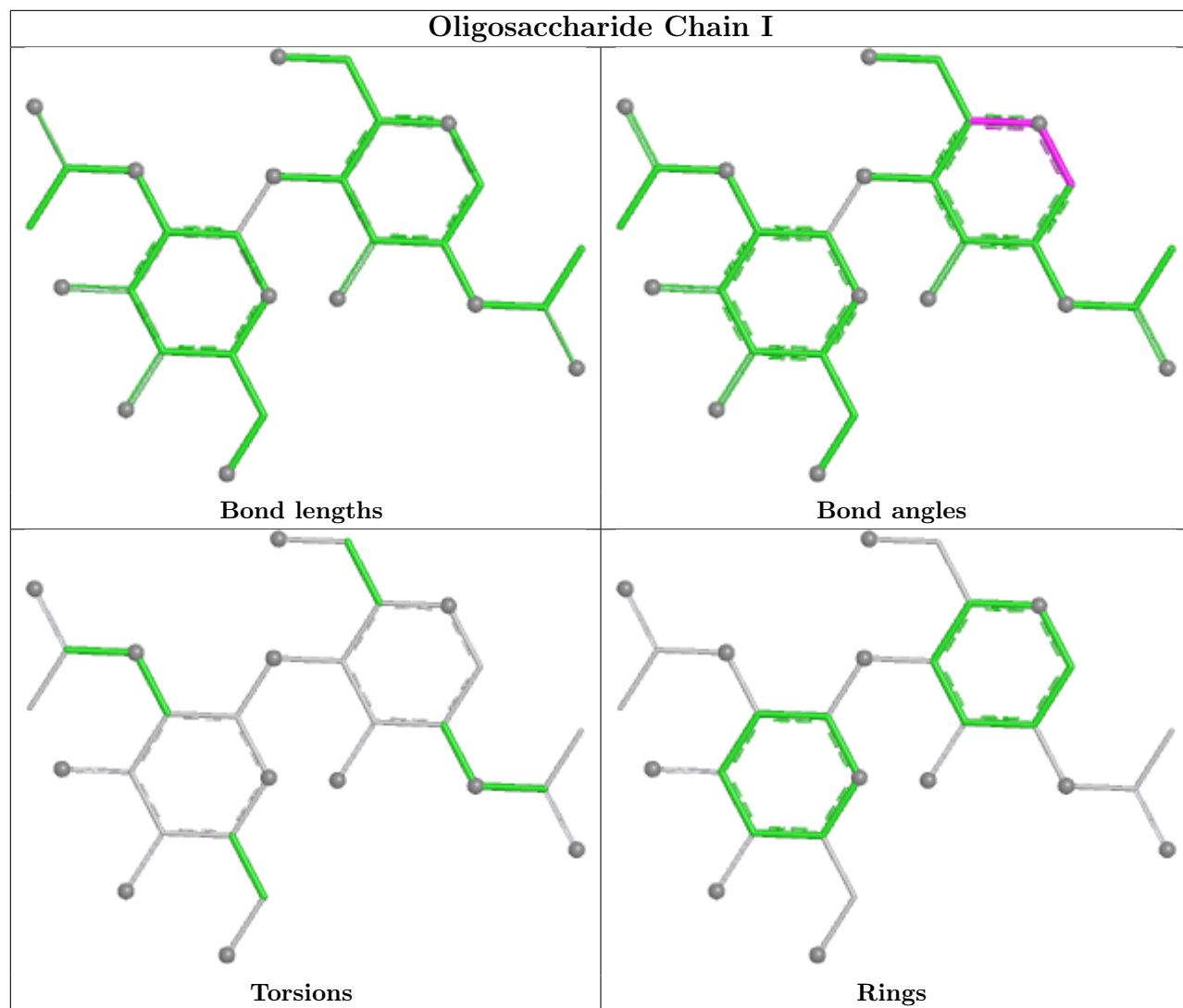


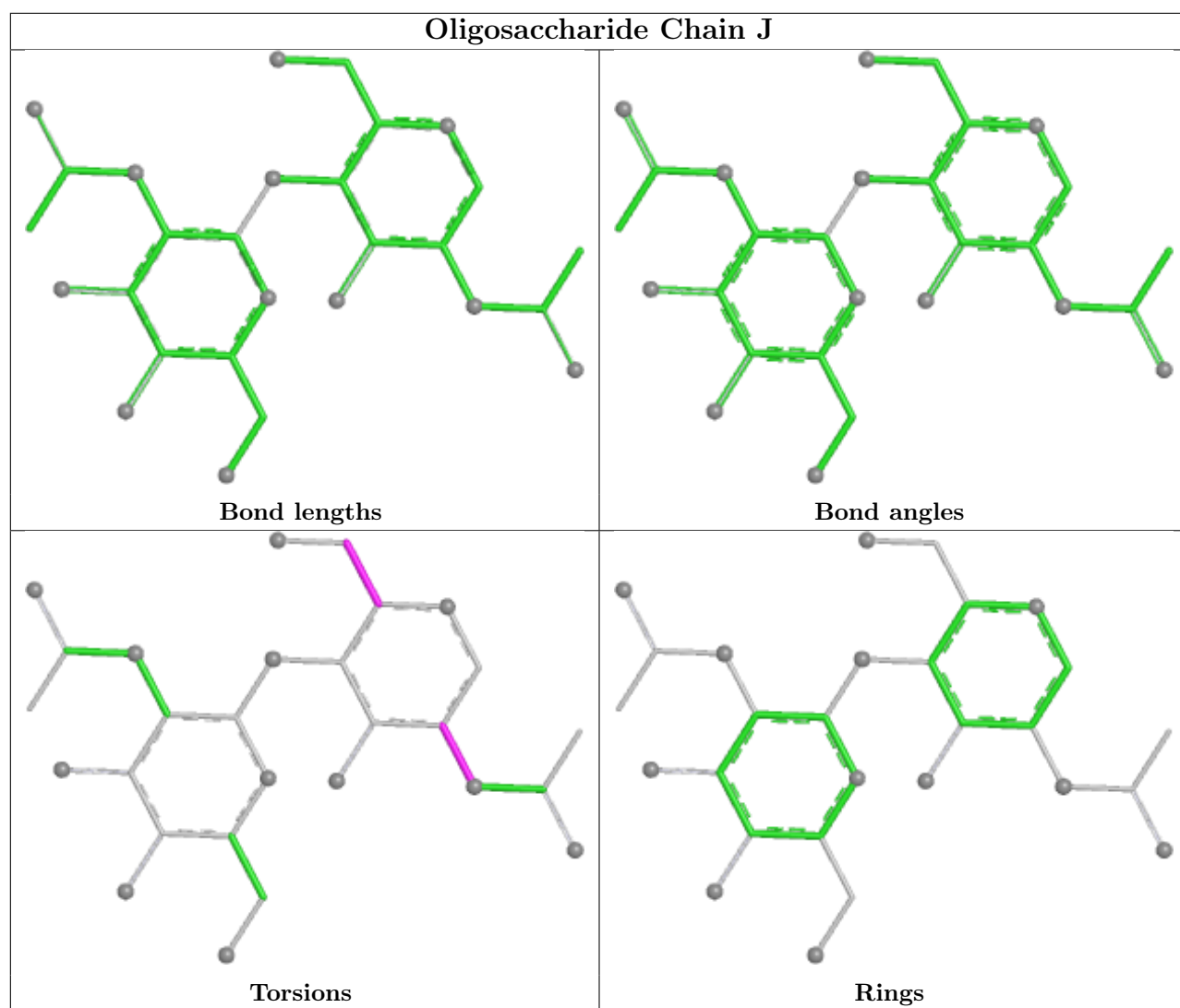


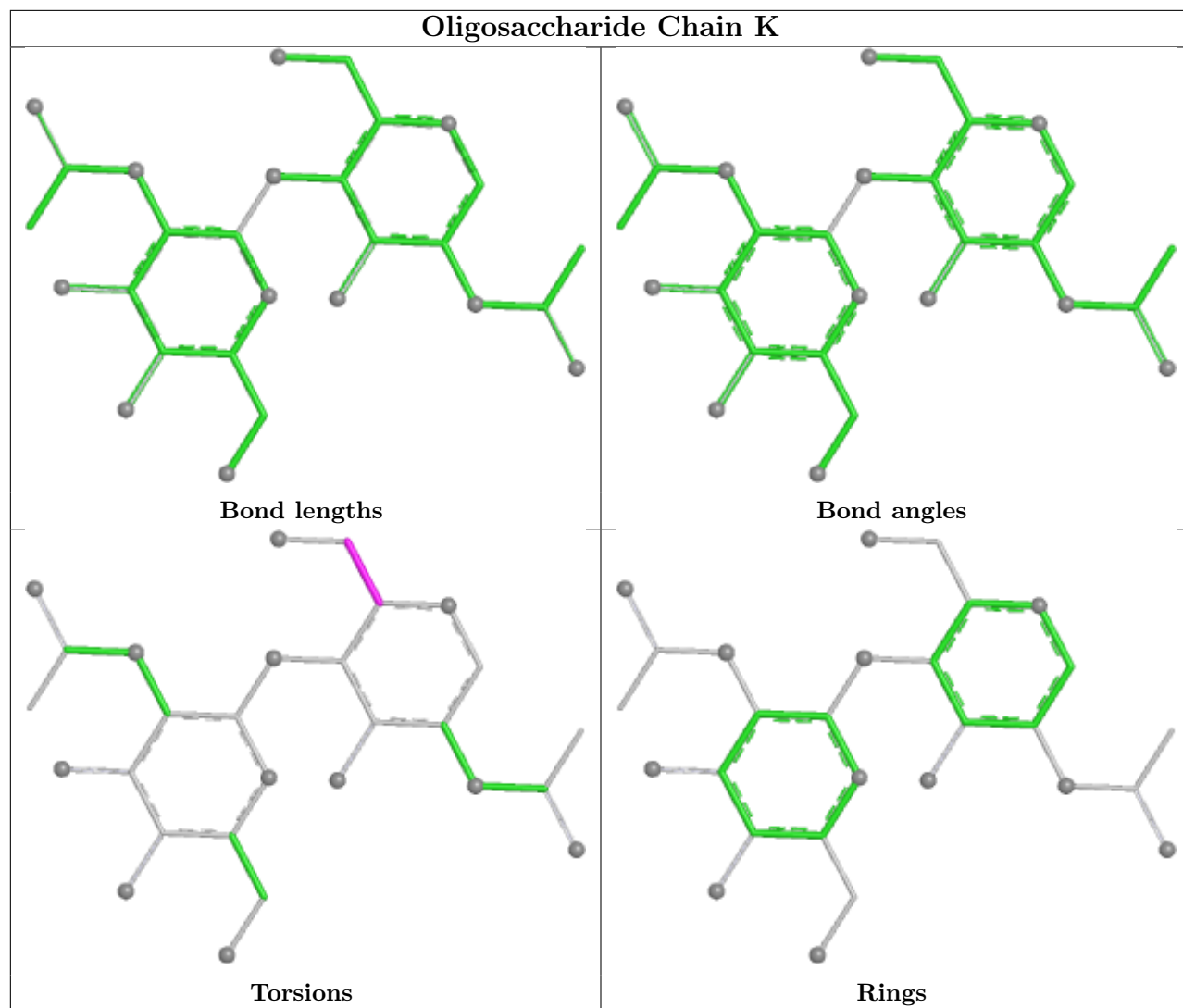


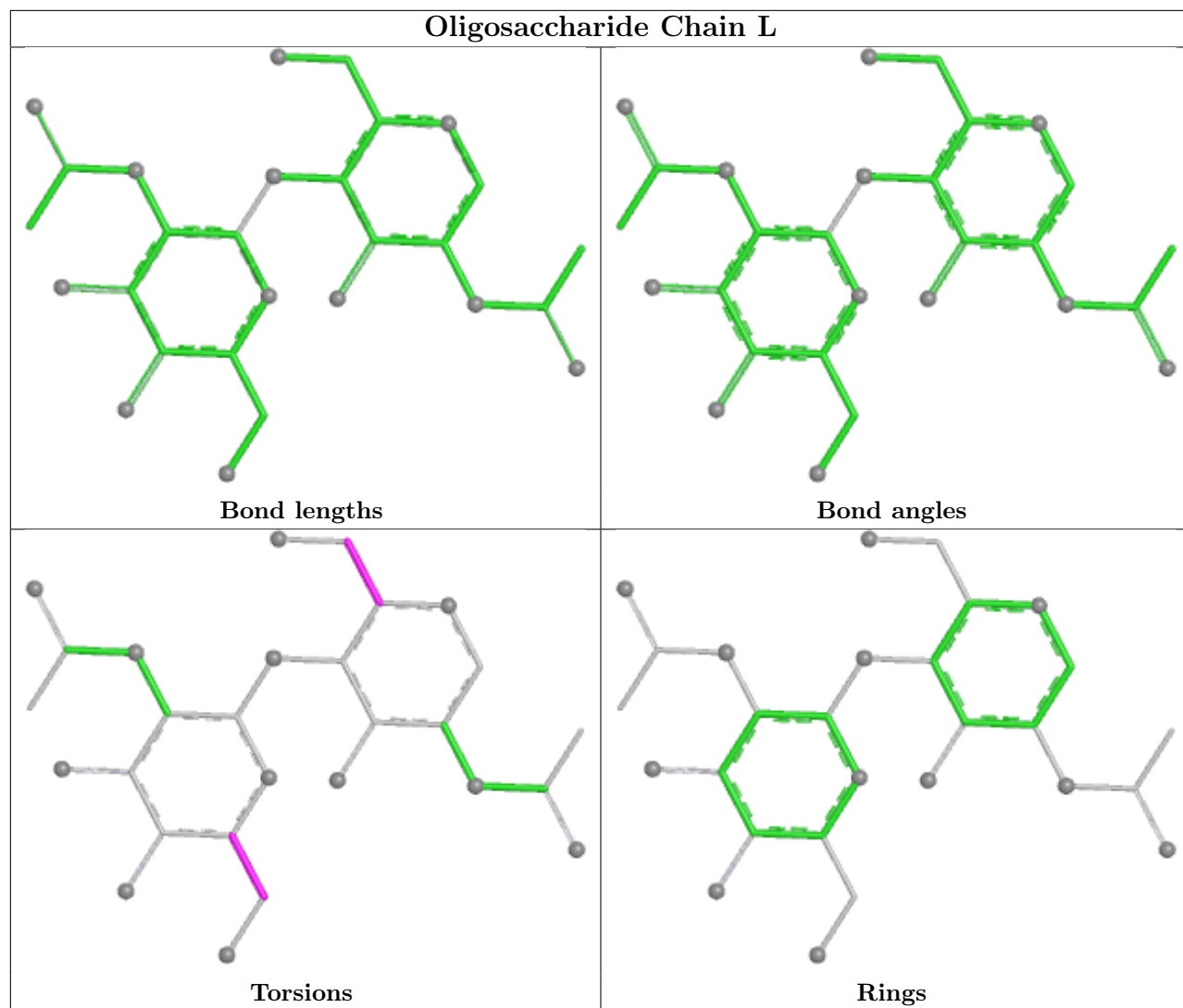


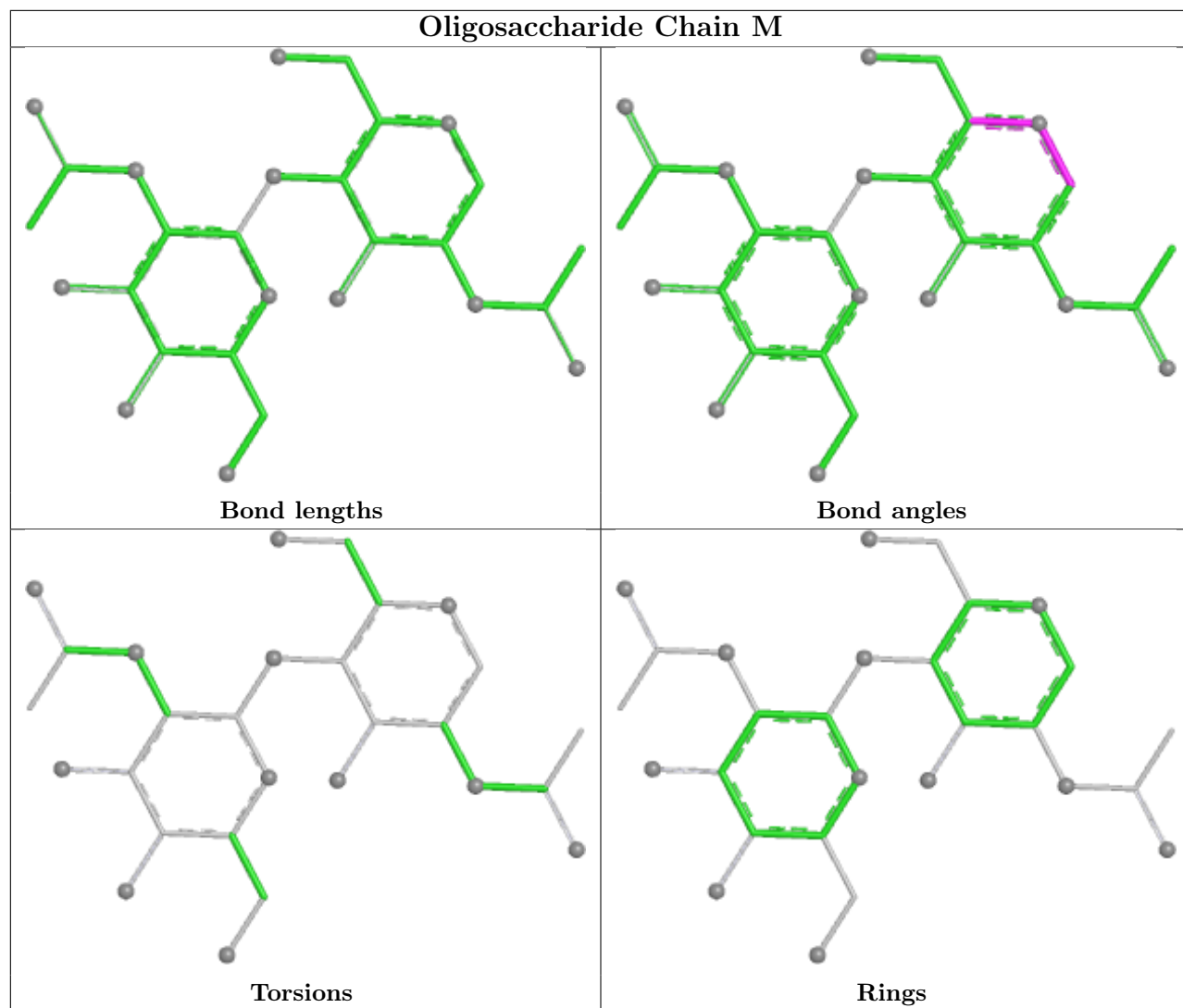


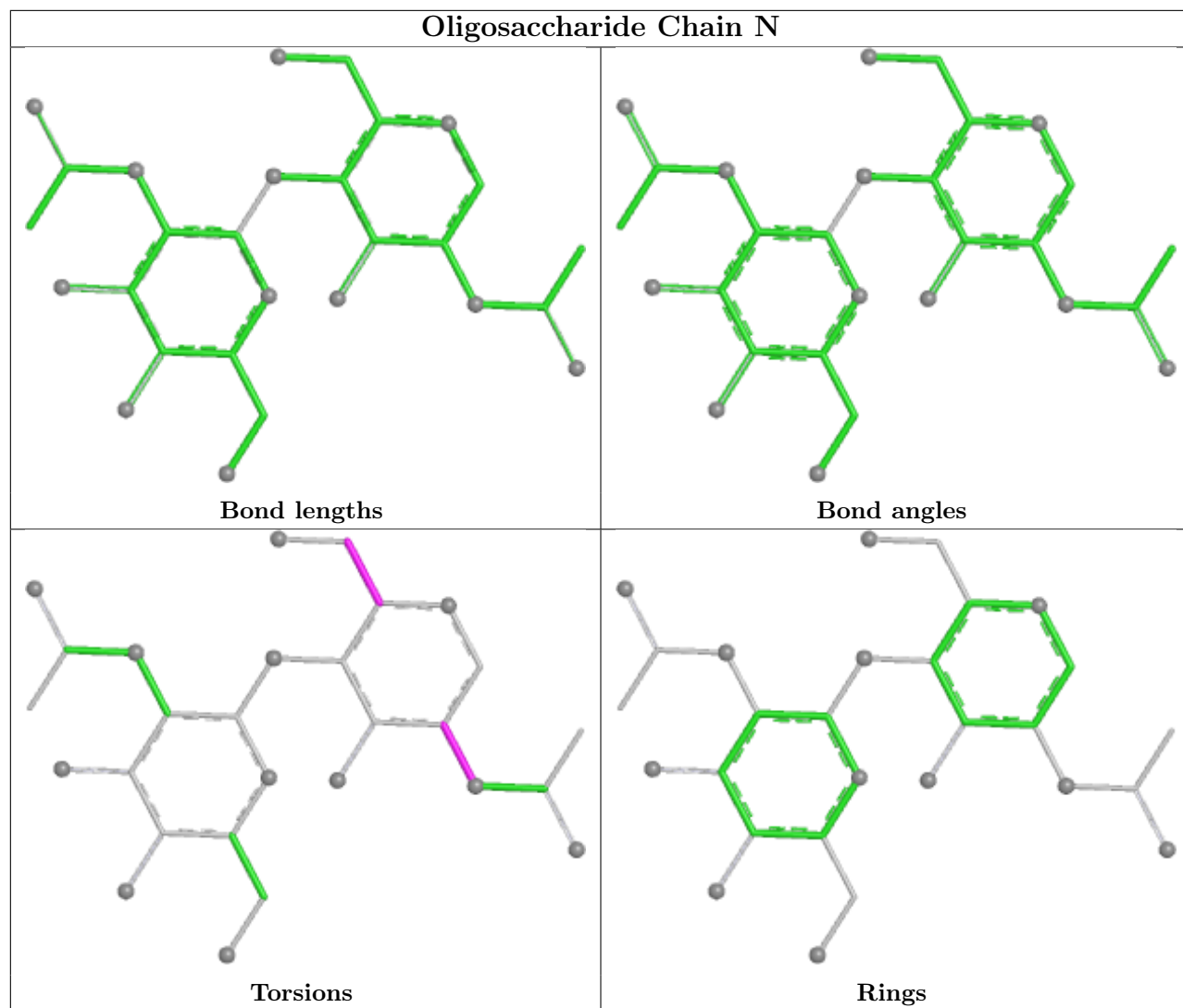


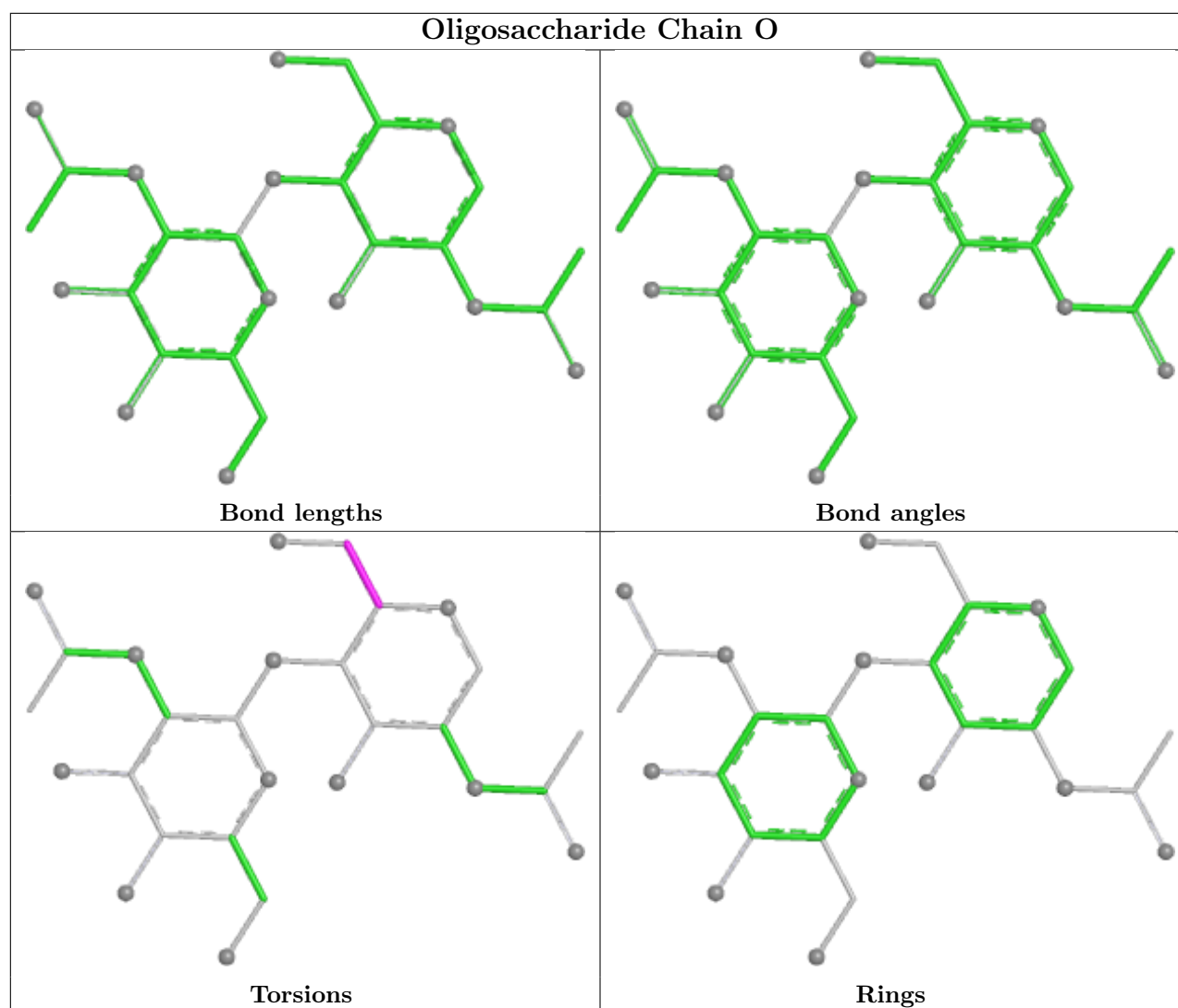












5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1301	1	14,14,15	0.51	0	17,19,21	0.45	0
3	NAG	C	1301	1	14,14,15	0.51	0	17,19,21	0.45	0
3	NAG	C	1306	1	14,14,15	0.43	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1309	1	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	A	1314	1	14,14,15	0.19	0	17,19,21	0.52	0
3	NAG	B	1306	1	14,14,15	0.43	0	17,19,21	0.55	0
3	NAG	C	1308	1	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	A	1309	1	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	A	1306	1	14,14,15	0.44	0	17,19,21	0.55	0
3	NAG	A	1308	1	14,14,15	0.39	0	17,19,21	0.45	0
3	NAG	C	1314	1	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	C	1309	1	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	B	1302	1	14,14,15	0.35	0	17,19,21	0.63	1 (5%)
3	NAG	A	1302	1	14,14,15	0.35	0	17,19,21	0.62	1 (5%)
3	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
3	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	C	1319	1	14,14,15	0.41	0	17,19,21	0.44	0
3	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	A	1319	1	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	B	1305	1	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
3	NAG	B	1304	1	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	B	1314	1	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	A	1301	1	14,14,15	0.51	0	17,19,21	0.46	0
3	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
3	NAG	C	1302	1	14,14,15	0.34	0	17,19,21	0.63	1 (5%)
3	NAG	B	1308	1	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	B	1319	1	14,14,15	0.41	0	17,19,21	0.44	0
3	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1319	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1319	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1319	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1305	NAG	C1-O5-C5	2.30	115.27	112.19
3	C	1305	NAG	C1-O5-C5	2.27	115.23	112.19
3	A	1305	NAG	C1-O5-C5	2.27	115.23	112.19
3	B	1302	NAG	C1-O5-C5	2.05	114.94	112.19
3	C	1302	NAG	C1-O5-C5	2.05	114.93	112.19
3	A	1302	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1314	NAG	O5-C5-C6-O6
3	B	1314	NAG	O5-C5-C6-O6
3	C	1314	NAG	O5-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	A	1319	NAG	C3-C2-N2-C7
3	B	1319	NAG	C3-C2-N2-C7
3	C	1319	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	NAG	1	0
3	C	1301	NAG	1	0
3	B	1302	NAG	1	0
3	A	1302	NAG	1	0
3	C	1319	NAG	1	0
3	A	1319	NAG	1	0
3	A	1301	NAG	1	0
3	C	1302	NAG	1	0
3	B	1319	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.

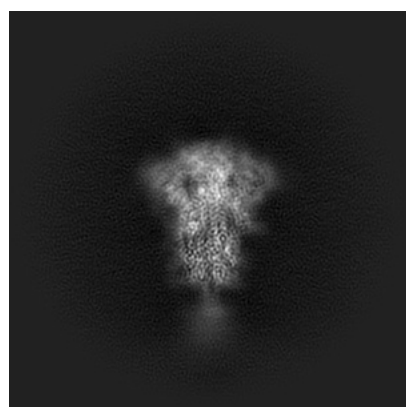
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22078. These allow visual inspection of the internal detail of the map and identification of artifacts.

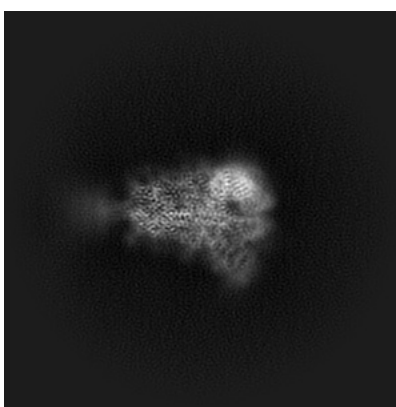
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

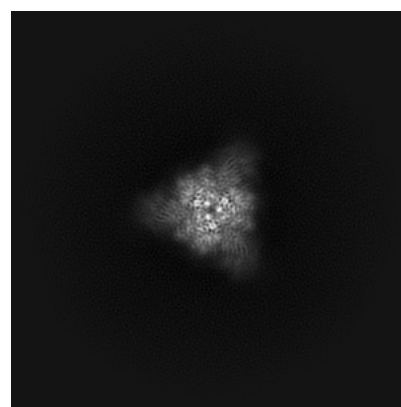
6.1.1 Primary map



X



Y

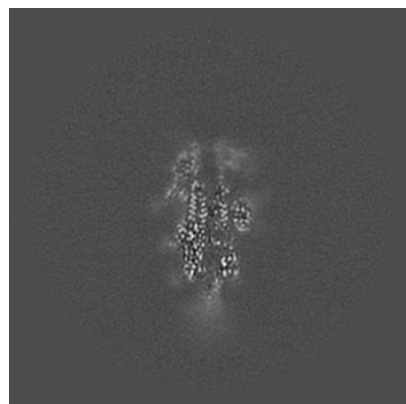


Z

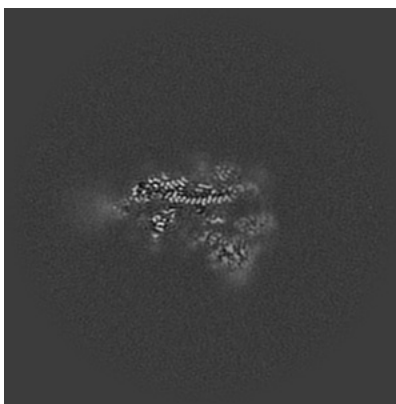
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

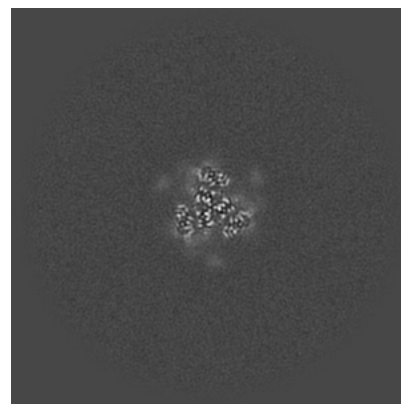
6.2.1 Primary map



X Index: 192



Y Index: 192

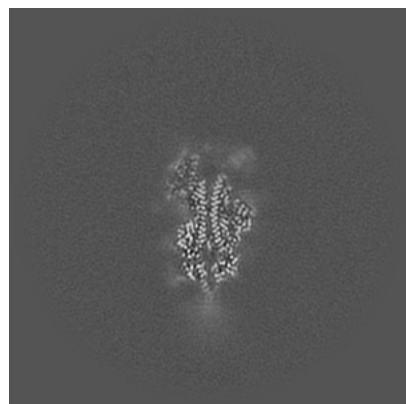


Z Index: 192

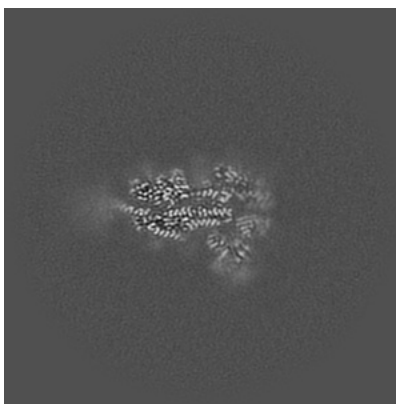
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

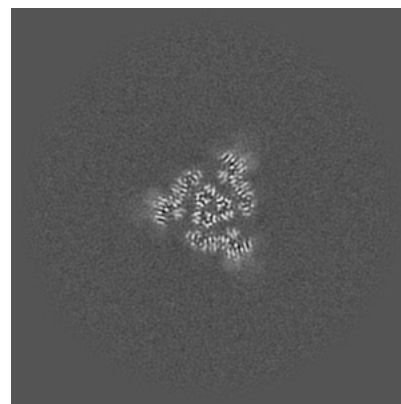
6.3.1 Primary map



X Index: 188



Y Index: 199

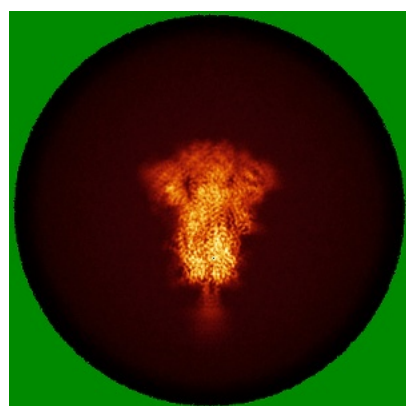


Z Index: 210

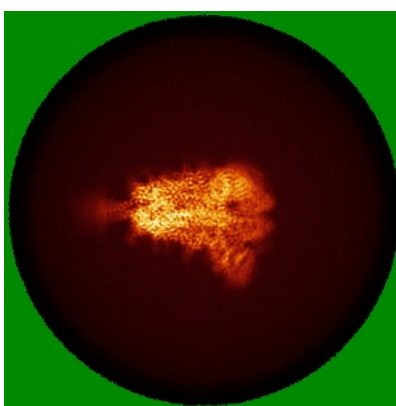
The images above show the largest variance slices of the map in three orthogonal directions.

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

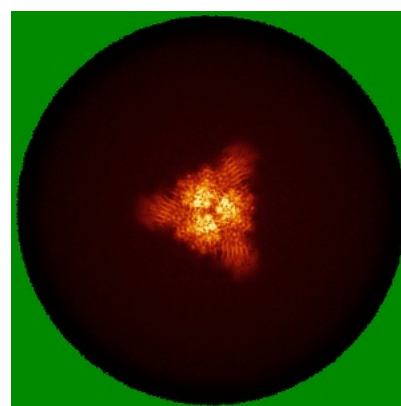
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

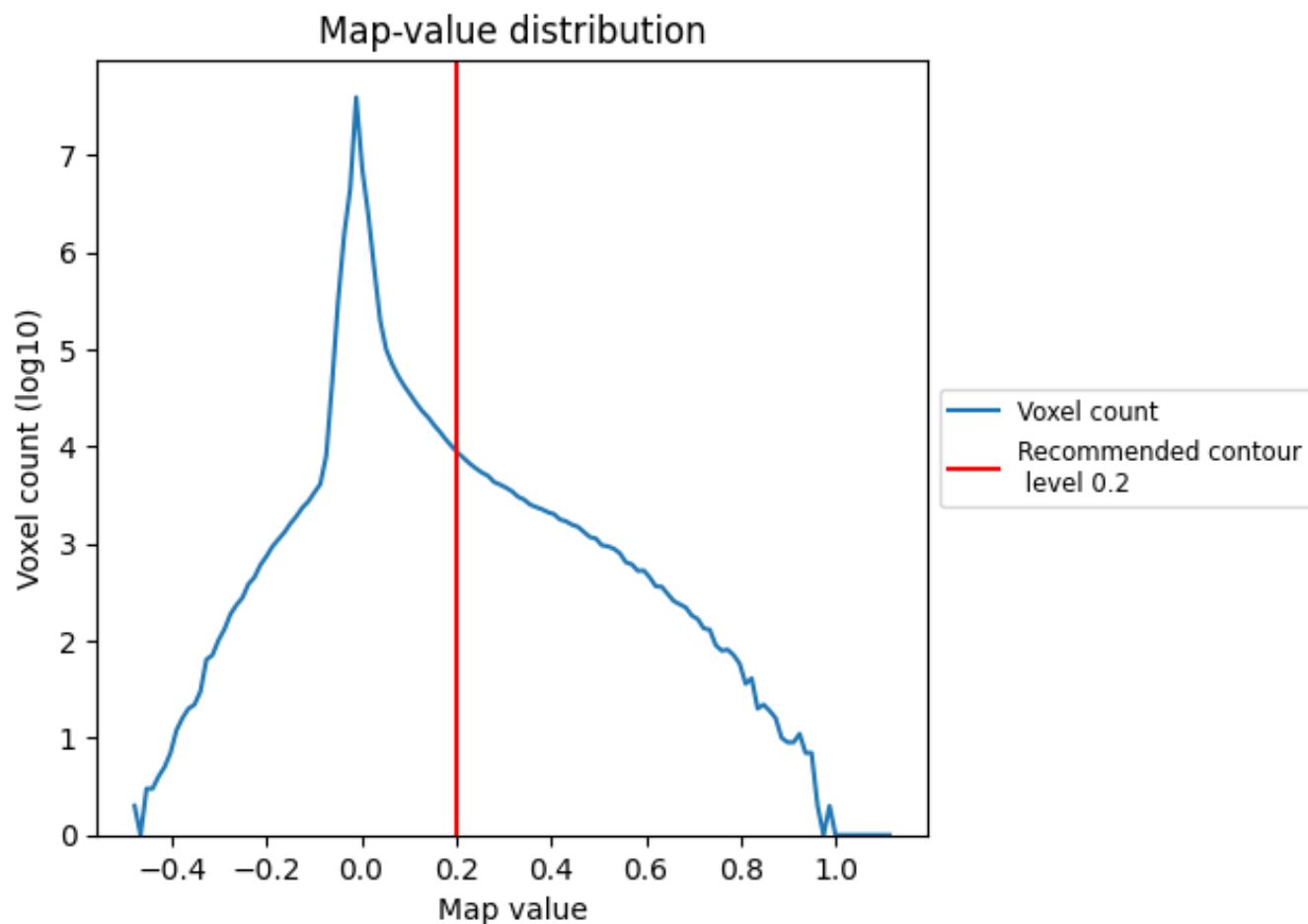
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

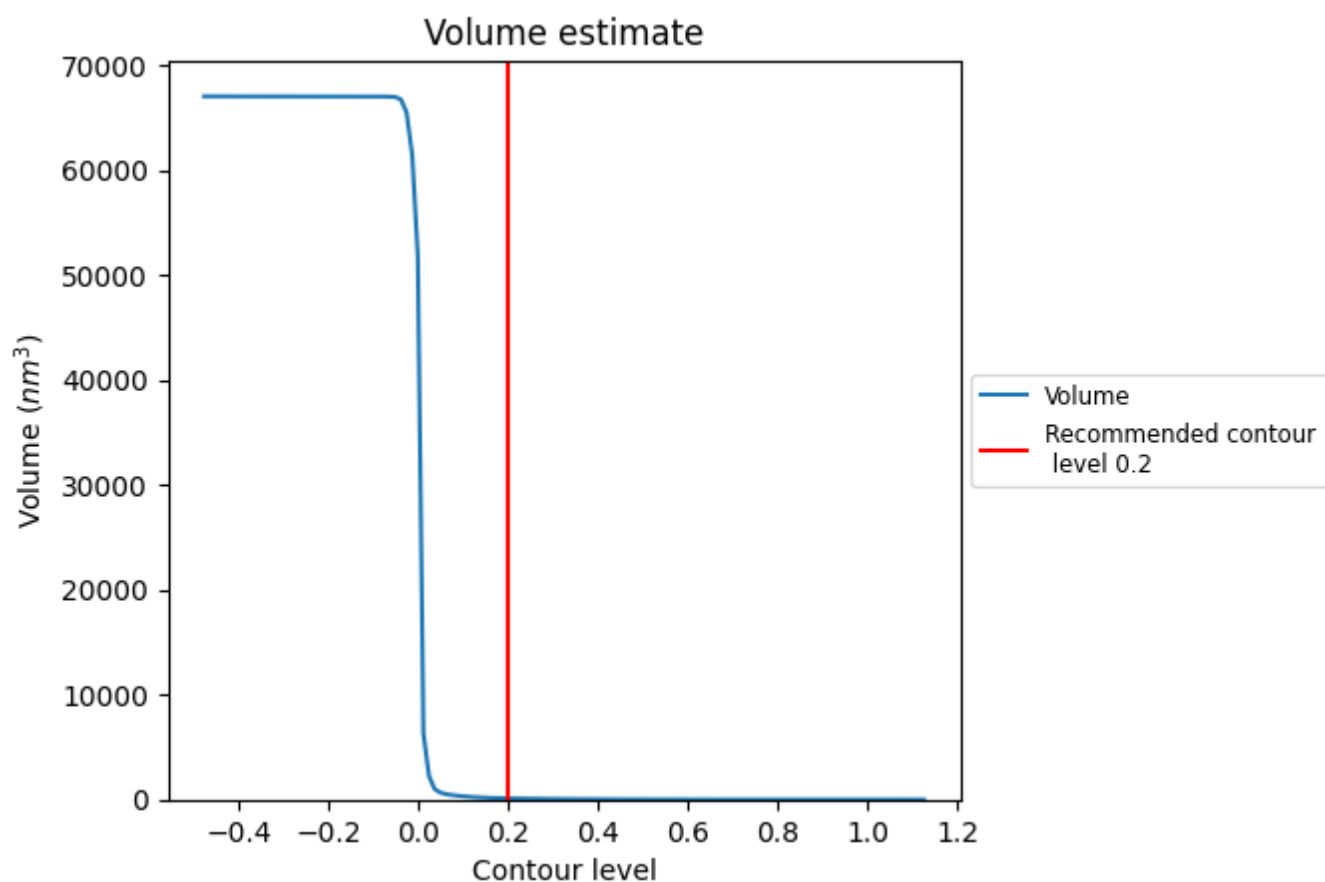
This section contains the results of statistical analysis of the map.

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.

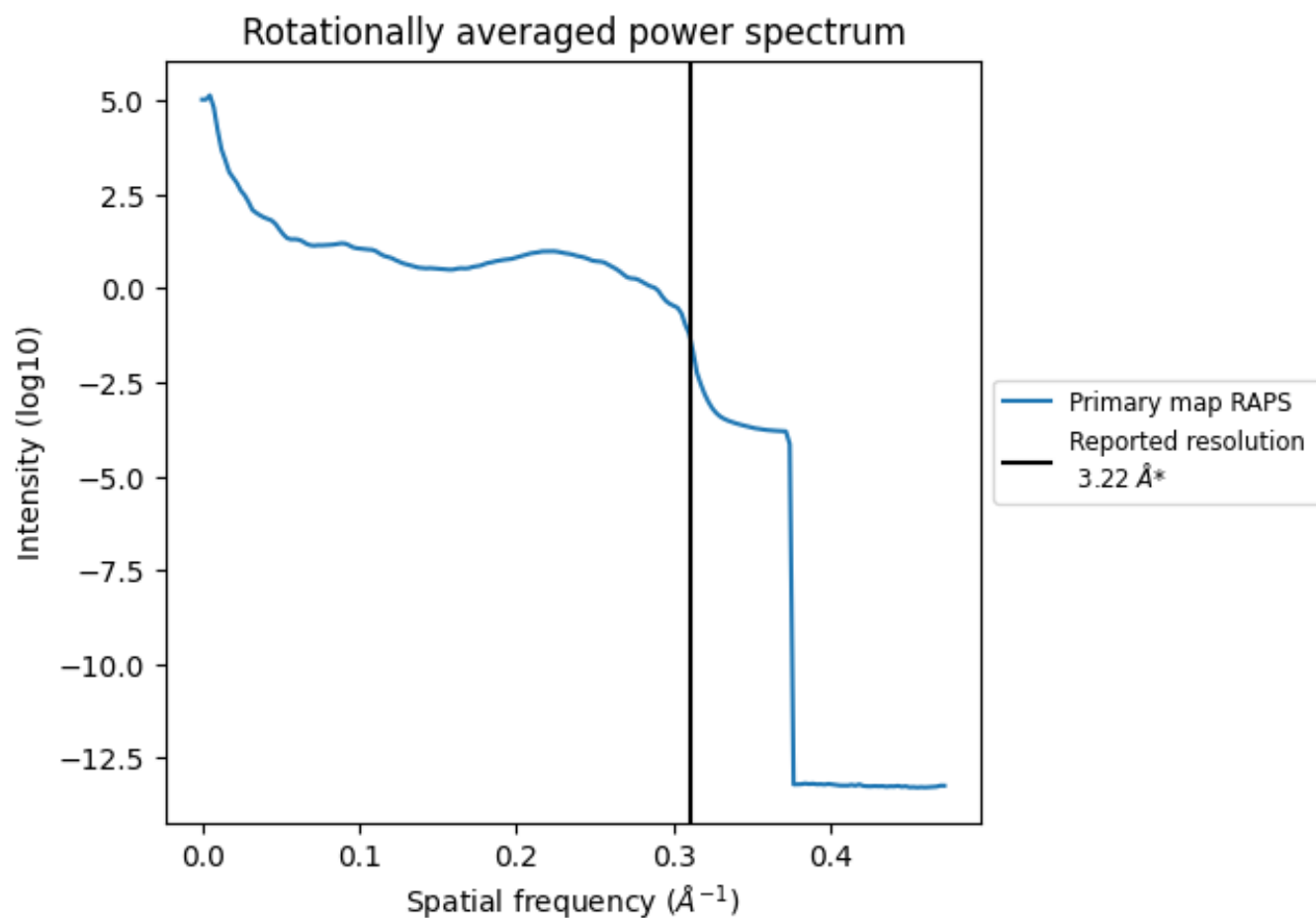
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm^3 ; this corresponds to an approximate mass of 101 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 ⓘ

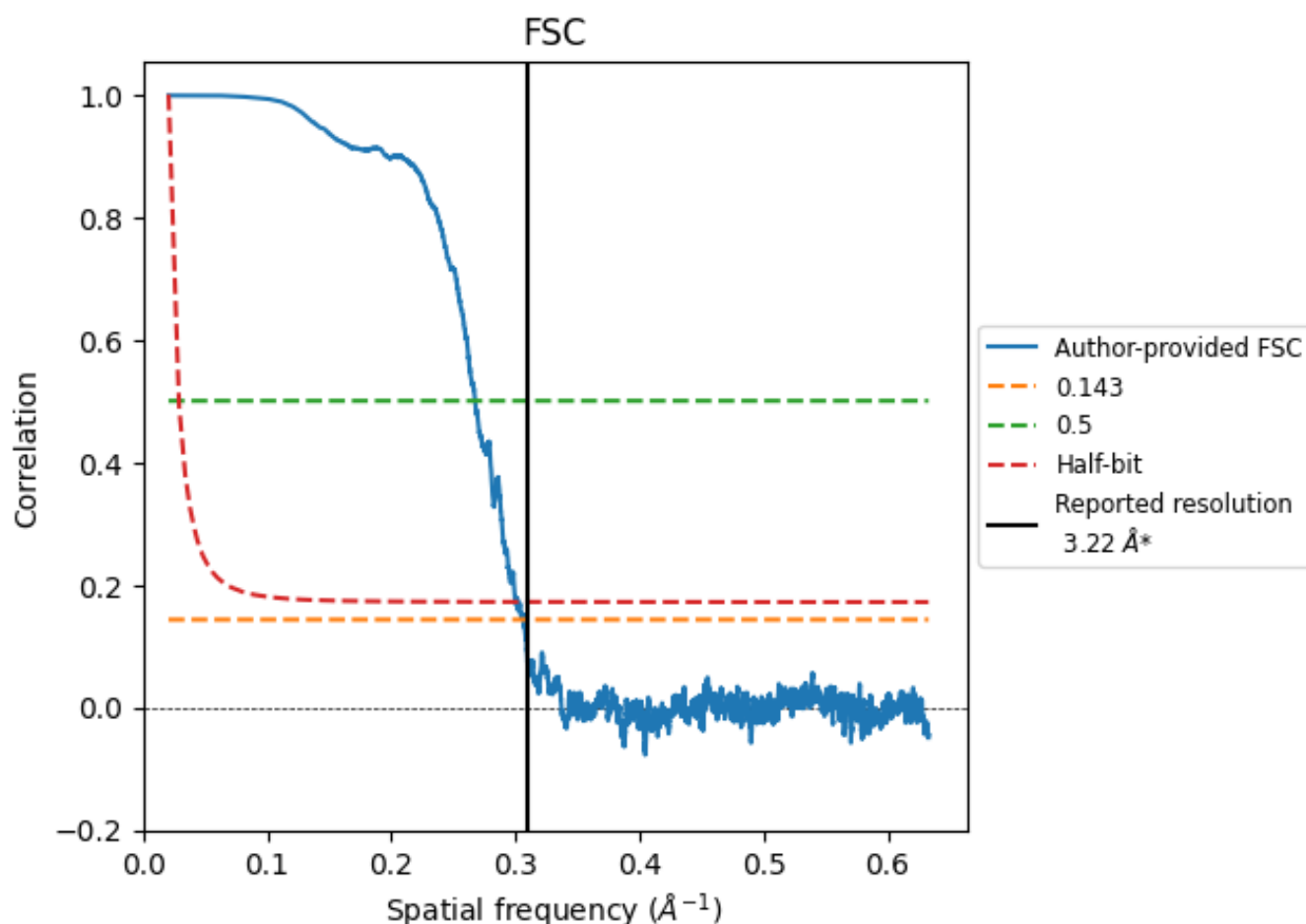


*Reported resolution corresponds to spatial frequency of 0.311 $\text{\AA}^{-1}$

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 0.311 Å⁻¹

8.2 Resolution estimates [i](#)

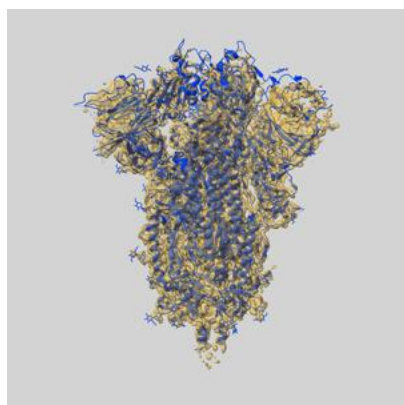
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.26	3.74	3.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

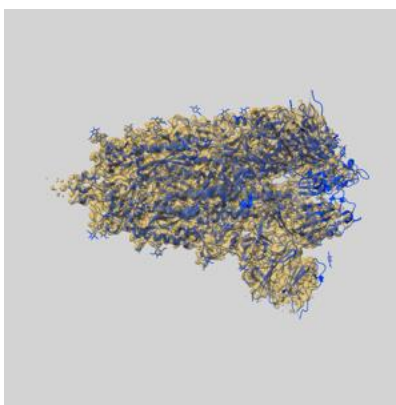
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22078 and PDB model 6X6P. Per-residue inclusion information can be found in section [3](#) on page [14](#).

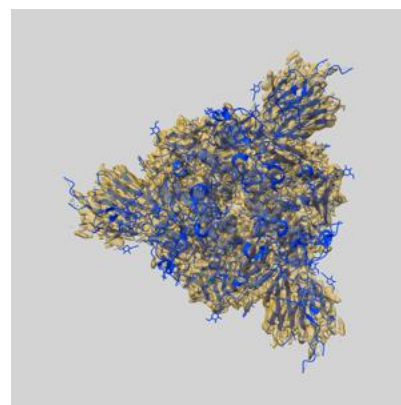
9.1 Map-model overlay [i](#)



X



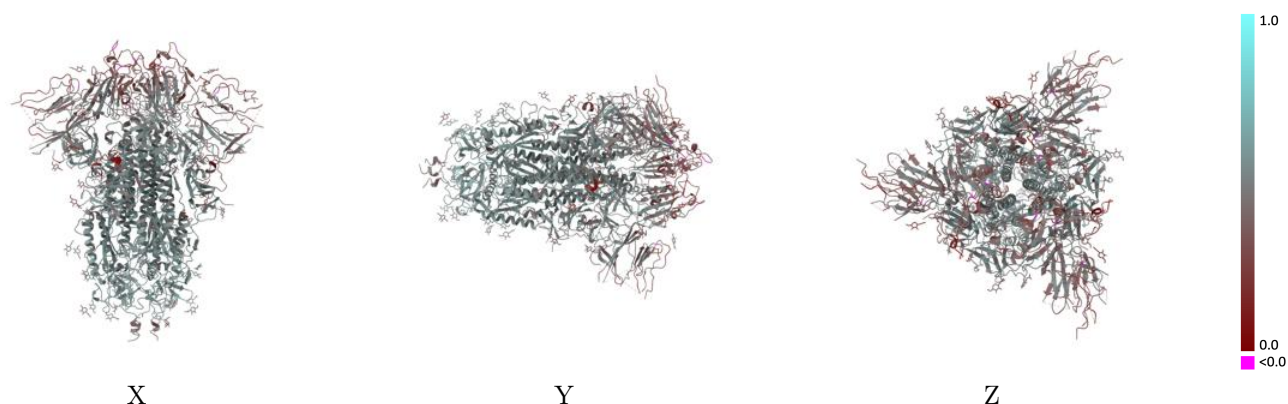
Y



Z

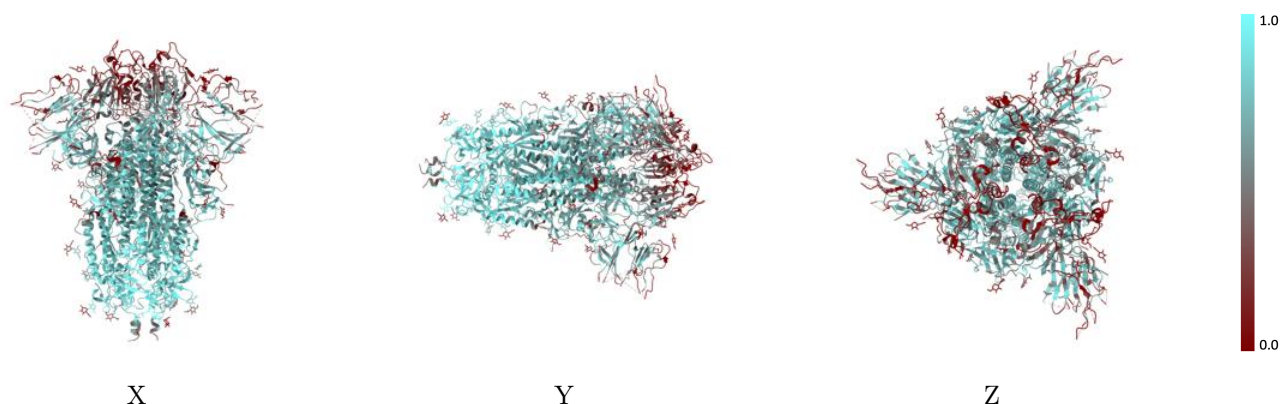
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



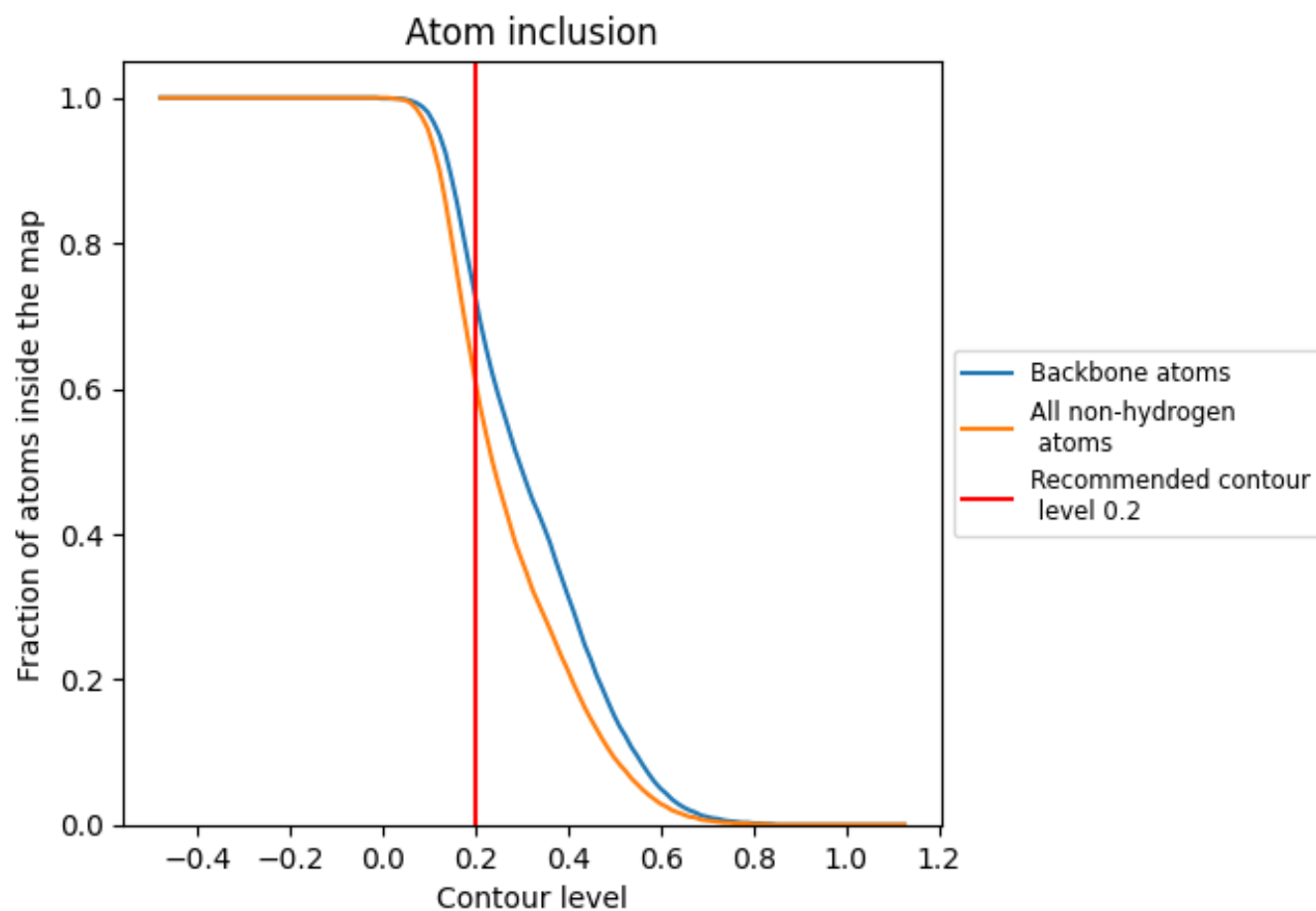
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 61% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.4690
A	0.6130	0.4690
B	0.6140	0.4690
C	0.6130	0.4690
D	0.6790	0.4900
E	0.4640	0.4690
F	0.5710	0.4940
G	0.5000	0.4600
H	0.6790	0.4810
I	0.4640	0.4760
J	0.4640	0.5030
K	0.5000	0.4420
L	0.6430	0.4980
M	0.4640	0.4830
N	0.5000	0.4910
O	0.5000	0.4590

1.0

0.0

<0.0