



Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:24 PM JST

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

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

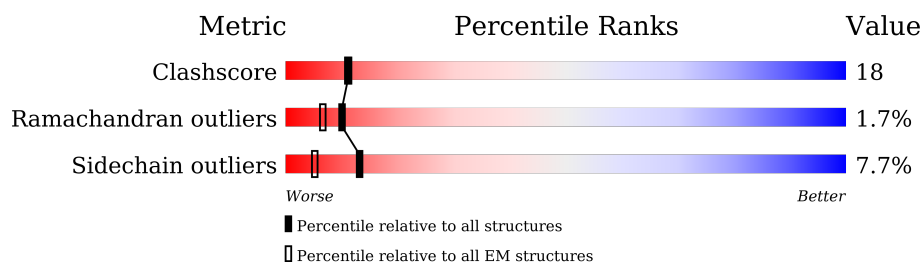
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 Å.

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












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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	E	124	68% 31% .
1	G	124	61% 35% .
1	I	124	48% 48% .
2	A	1288	53% 28% . 16%
2	B	1288	50% 29% . . 16%
2	C	1288	54% 26% . 16%
3	K	2	50% 50%
3	L	2	100%
3	M	2	100%

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Mol	Chain	Length	Quality of chain
3	N	2	 100%
3	R	2	 50%50%
3	S	2	 100%
3	T	2	 50%50%
3	U	2	 100%
3	X	2	 50%50%
3	Y	2	 100%
3	Z	2	 50%50%
3	a	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 28908 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called nanobody Nb4.

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

- Molecule 2 is a protein called Spike glycoprotein.

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

There are 354 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	658	SER	ASN	conflict	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	19	ILE	THR	conflict	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	655	TYR	HIS	variant	UNP P0DTC2
B	658	SER	ASN	conflict	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	conflict	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	658	SER	ASN	conflict	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2

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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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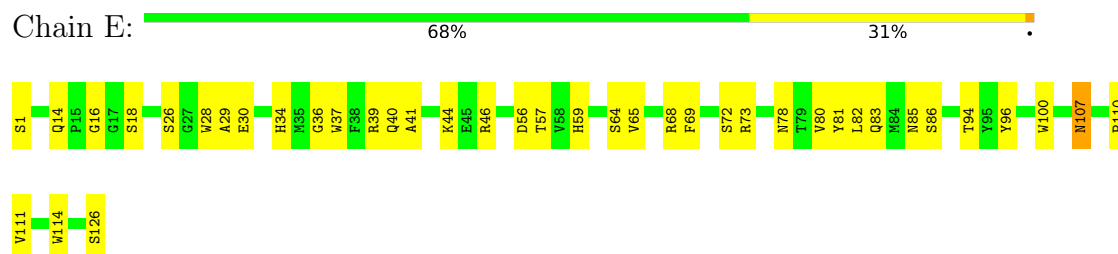
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

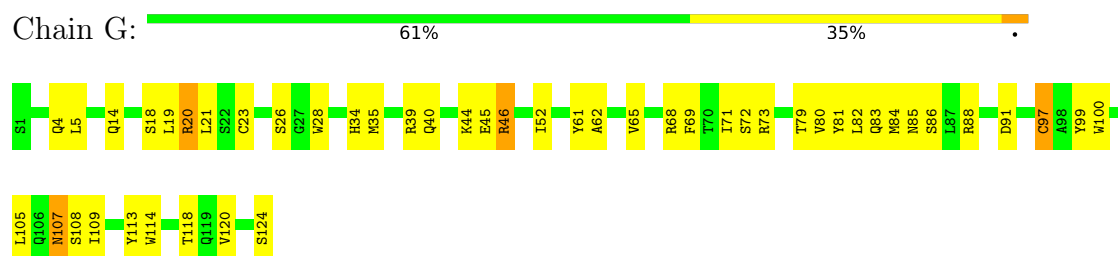
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

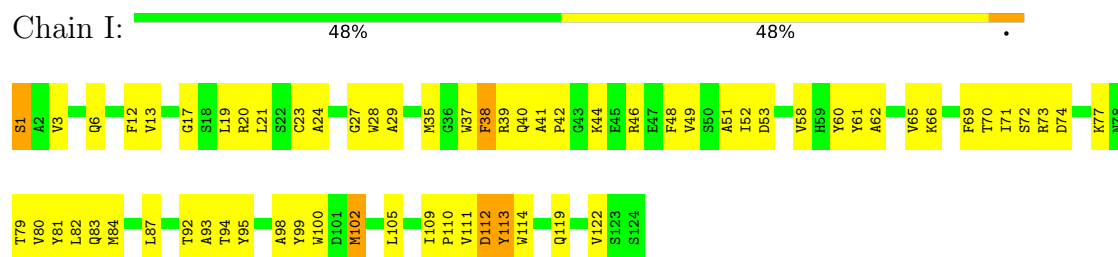
• Molecule 1: nanobody Nb4



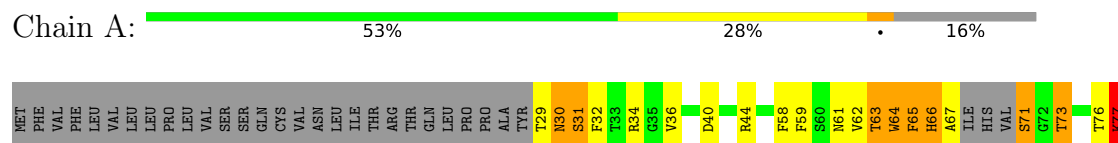
• Molecule 1: nanobody Nb4



• Molecule 1: nanobody Nb4



• Molecule 2: Spike glycoprotein

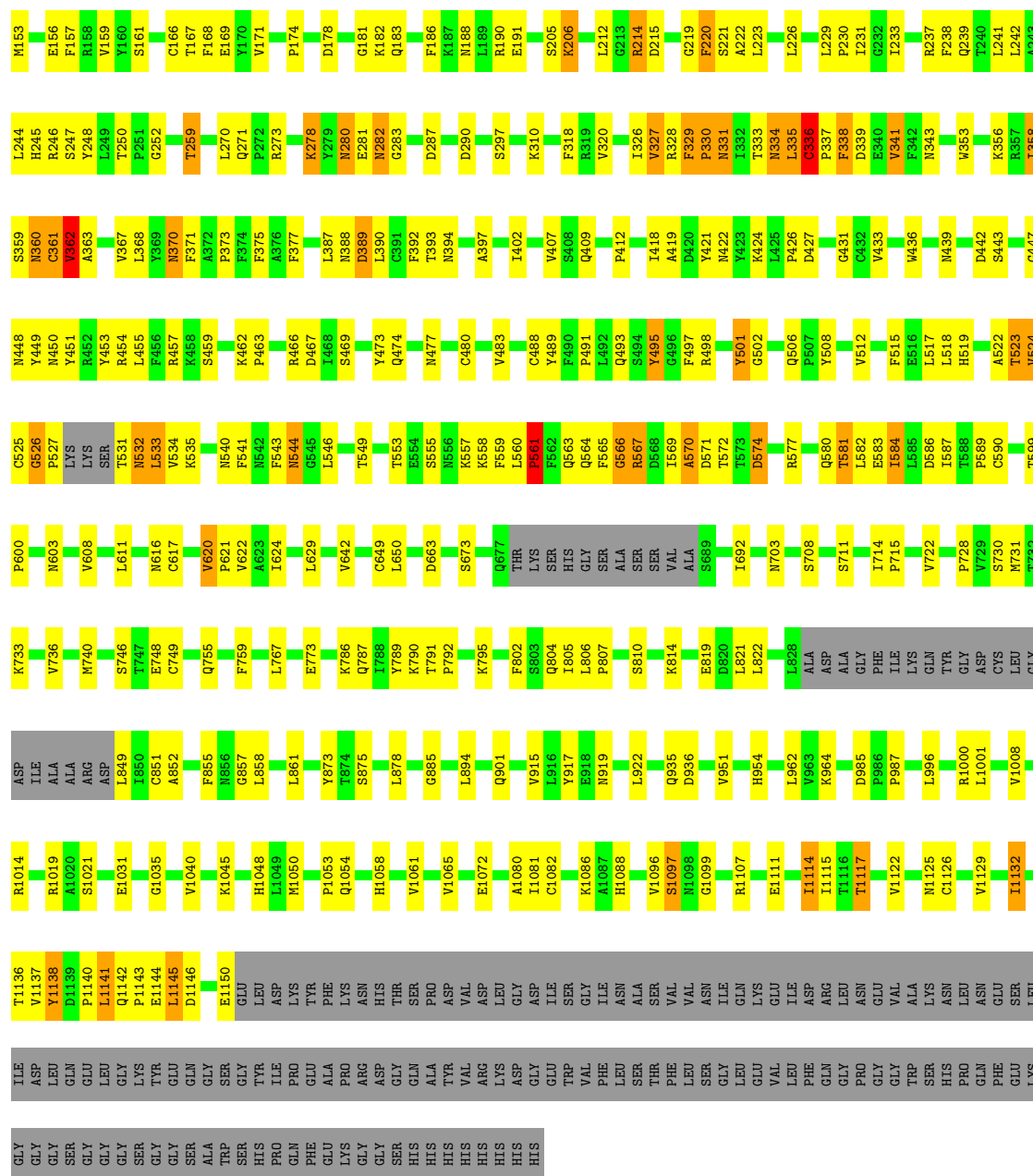


TRP	SER	E1150	L894	F759	N544	P463	L390	Q314	I233	Y144
	GLY	Y1047	P899	Q762	T553	F464	C391	F318	N234	Y145
SER	TYR	H1048	L894	L763	T553	L629	F392	I235	H146	
GLY	ASP	M1050	Q901	L763	S555	T630	R466	T393	T236	
PHE	TRP			E773	N556	T632	N394	V320		
GLU	ALA	V1065	Y904	Q774	K557	W633	V395	S325	Q239	
LYS	PHE	T1066	R905		K558		F400	S325	T240	
GLY	ASN	Y1067		N777	F559	Y473	V401	I326	L241	
GLY	ARG		V915	S637	L560	A475	I402	R328	L242	
SER	GLY	THR	Y916	Q784	F561		R403	F329	A243	
GLN	SER	K1073	Y917		F562		G404	P330	L244	
HIS	ALA	K1074	E918	Y789	Q563		N405	T333	R246	
HIS	TYR	F1075	N919		Q564		E406	N334	S247	
HIS	VAL	T1076		G798	F565		V407	N334	Y248	
HIS	ASP	T1077	L922		S566		S408	L335	L249	
HIS	ARG	A1078		F802	B567		Q409	C336	T250	
HIS	LYS						I410	P337	P251	
HIS	ASP	GLY	K933	L806	A570		I411	F338	P251	
HIS	GLY	ASP	T934	P807			A411	D339	S255	
HIS	ILE	TRP	Q935		A575		Q414	E340	S255	
	GLY	VAL	L945	K811	THR		T415	V341	T259	
	GLY	PHE		LYS	LYS		G496	F342	A260	
	ILE	V1096		SER	SER		R498	N343	G961	
	ASN	S1097	N955	L821	HIS		P499		A262	
	ALA	N1098	A956	L822	GLY		T500			
	SER	G1099			SER		I418			
	THR	VAL	L959	L828	GLY		A419			
	VAL	VAL		ALA	ALA		D420			
	LEU	VAL	V963	ASP	SER		Y421			
	SER	ASN	K964	ALA	SER		N422			
	GLY	ILE	F1103	GLY	SER		Y423			
	LEU	GLY	V1104	VAL	VAL		Q506			
	GLY	GLN	S967	PHE	ALA		P426			
	VAL	GLY		ILE	S689		D427			
	LEU	ILE	S975	LYS	Q690		D428			
	ASP	ASP	V976	GLN	S691		F429			
	GLY	ARG	L977	TRP	I692					
	GLY	LEU		GLY						
	PRO	ASN	R983	ASP	Y695					
	GLY	GLY	L984	CYS	P600		C432			
	VAL	VAL	D985	LEU	G601		V433			
	ALA	ALA	P986	GLY	N710		I434			
	TRP	VAL	S1123	GLY	N603		A435			
	SER	LYS	G1124	ASP	T604		W436			
	ASN	ASN	N1125	ILE	A713		N437			
	PRO	GLN	C1126	ALA	P715		S438			
	GLN	ASN	D1127	ALA	I714					
	PHE	GLY		ARG	V722		V445			
	GLY	SER	I1132	ASP	V608		T523			
	LYS	LEU	V1133	L849	A609		V524			
	GLY	ILE	L1004	I950	L611		CYS			
	GLY	ASP	Q1005	V736	Y612		GLY			
	GLY	LEU	D1139	Q853	Q613		PRO			
	SER	GLN	R1019	K854	G614		LYS			
	GLY	GLY	Q1142	F855	V615		S530			
	GLY	LEU	P1143		N616					
	GLY	GLY	E1144	L858	C617		V534			
	SER	LYS	L1145	Y873	T618		F456			
	GLY	TRP	D1146	Y756	F619		R457			
	GLY	GLY	S1147	W886	P621		K458			
	SER	GLN	F1149	S758	V539					
	ALA	GLY	V1040				L461			
							K462			

• Molecule 2: Spike glycoprotein

Chain C:  54% 26% 16%

																												MET																											
																												PHE																											
																												VAL																											
																												PHE																											
																												LEU																											
																												VAL																											
																												LEU																											
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																												VAL																											
																												SER																											
																												SER																											
																												GLN																											
																												CYS																											
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																												PRO																											
																												ALA																											
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																												V36																											
																												Y37																											
																												L54																											
																												F58																											
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																												V62																											
																												T63																											
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																												F65																											
																												H66																											
																												A67																											
																												T68																											
																												HIS																											
																												VAL																											
																												SER																											
																												GLY																											
																												T73																											
																												N74																											
																												Y78																											
																												F79																											
																												D80																											





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

Chain M:  100%



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

Chain N:  100%



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

Chain R:  50% 50%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain U:  100%



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

Chain X:  50% 50%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  50% 50%

MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.25	0/1016	0.50	0/1382
1	G	0.33	0/1006	0.51	0/1371
1	I	0.31	0/1016	0.52	0/1382
2	A	0.37	0/8612	0.54	0/11736
2	B	0.41	0/8616	0.56	0/11737
2	C	0.36	0/8652	0.54	0/11785
All	All	0.37	0/28918	0.54	0/39393

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	987	0	906	29	0
1	G	977	0	884	34	0
1	I	987	0	906	51	0
2	A	8410	0	8146	325	0
2	B	8413	0	8147	331	0
2	C	8448	0	8203	291	0
3	K	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	X	28	0	25	1	0
3	Y	28	0	25	0	0
3	Z	28	0	25	1	0
3	a	28	0	25	0	0
4	A	112	0	104	4	0
4	B	140	0	130	2	0
4	C	98	0	91	0	0
All	All	28908	0	27817	1016	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 18.

All (1016) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:CYS:HA	2:B:432:CYS:HA	1.42	1.02
2:A:71:SER:HA	2:A:79:PHE:HA	1.42	1.01
2:A:617:CYS:HA	2:A:621:PRO:HD2	1.46	0.95
2:B:44:ARG:HH21	2:B:49:HIS:CG	1.86	0.93
2:C:393:THR:HA	2:C:522:ALA:HA	1.50	0.92
2:A:620:VAL:HG13	2:A:621:PRO:HD3	1.52	0.92
2:A:617:CYS:C	2:A:619:GLU:H	1.74	0.90
2:C:337:PRO:HA	2:C:358:ILE:HD12	1.51	0.90
1:G:73:ARG:HA	1:G:80:VAL:HA	1.52	0.88
2:B:44:ARG:NH2	2:B:49:HIS:CE1	2.43	0.87
2:C:139:PRO:HA	2:C:157:PHE:HA	1.56	0.86
2:C:331:ASN:HA	2:C:580:GLN:HG3	1.57	0.85
2:C:519:HIS:CD2	2:C:567:ARG:HH21	1.95	0.84
2:B:337:PRO:HG2	2:B:358:ILE:HG23	1.60	0.83
1:E:1:SER:HB3	1:E:30:GLU:HB2	1.59	0.83
2:A:621:PRO:HA	2:A:624:ILE:HG23	1.59	0.82
2:B:79:PHE:HD1	2:B:242:LEU:HD12	1.42	0.81
2:A:617:CYS:HB2	2:A:621:PRO:HB2	1.63	0.81
2:B:426:PRO:HG2	2:B:429:PHE:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ARG:NH2	2:B:49:HIS:ND1	2.32	0.77
2:B:624:ILE:HD11	2:B:637:SER:HA	1.66	0.77
2:A:61:ASN:HB3	2:A:258:TRP:HA	1.65	0.77
2:A:96:GLU:HB2	2:A:100:ILE:HB	1.67	0.76
2:B:102:ARG:HD3	2:B:244:LEU:HD13	1.67	0.76
2:C:336:CYS:HB3	2:C:362:VAL:H	1.49	0.76
2:B:107:GLY:H	2:B:235:ILE:HG23	1.49	0.76
2:A:403:ARG:HD2	2:A:505:HIS:HA	1.67	0.75
2:C:83:VAL:HG23	2:C:239:GLN:HB2	1.69	0.75
2:B:44:ARG:NH2	2:B:49:HIS:CG	2.55	0.74
2:B:129:LYS:HE3	2:B:166:CYS:HB3	1.70	0.74
1:I:73:ARG:HA	1:I:80:VAL:HA	1.69	0.74
2:A:617:CYS:O	2:A:619:GLU:N	2.20	0.74
2:B:44:ARG:HH22	2:B:49:HIS:CE1	2.04	0.74
2:B:362:VAL:HA	2:B:524:VAL:HG11	1.69	0.74
2:B:336:CYS:HA	2:B:361:CYS:HA	1.69	0.73
2:A:126:VAL:HG13	2:A:174:PRO:HA	1.71	0.73
2:A:335:LEU:HB3	2:A:361:CYS:HB3	1.68	0.73
1:E:40:GLN:HB2	1:E:46:ARG:HG3	1.70	0.73
2:A:106:PHE:HB3	2:A:235:ILE:HD12	1.70	0.73
2:A:617:CYS:C	2:A:619:GLU:N	2.42	0.73
2:B:405:ASN:N	2:B:504:GLY:O	2.22	0.73
1:E:65:VAL:HB	1:E:69:PHE:HB2	1.69	0.72
2:A:335:LEU:HB3	2:A:361:CYS:CB	2.21	0.71
2:C:858:LEU:HD11	2:C:962:LEU:HD22	1.72	0.71
2:B:105:ILE:HD11	2:B:241:LEU:HD21	1.73	0.71
2:C:454:ARG:NH2	2:C:469:SER:O	2.24	0.71
2:B:42:VAL:CG2	2:B:44:ARG:HH11	2.03	0.71
2:B:112:SER:HB3	2:B:134:GLN:HA	1.72	0.71
2:B:303:LEU:HD22	2:B:308:VAL:HG12	1.73	0.71
2:A:193:VAL:HB	2:A:204:TYR:HB2	1.73	0.71
2:A:102:ARG:NH2	2:A:121:ASN:O	2.24	0.70
2:A:395:VAL:HG22	2:A:515:PHE:HB3	1.74	0.70
2:B:64:TRP:HE1	2:B:260:ALA:HA	1.55	0.70
2:A:263:ALA:HB3	2:A:266:TYR:CZ	2.27	0.70
2:A:740:MET:HG2	2:B:319:ARG:HE	1.57	0.69
2:B:905:ARG:NH1	2:B:1049:LEU:O	2.24	0.69
2:B:40:ASP:CG	2:B:44:ARG:HH12	1.96	0.69
2:A:770:ILE:HD12	2:A:1012:LEU:HD22	1.75	0.69
1:G:61:TYR:HE1	1:G:71:ILE:H	1.38	0.69
2:B:422:ASN:ND2	2:B:454:ARG:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:437:ASN:ND2	2:A:507:PRO:O	2.27	0.68
2:A:401:VAL:HG22	2:A:509:ARG:HG2	1.74	0.68
2:B:773:GLU:OE1	2:B:774:GLN:NE2	2.26	0.68
2:C:519:HIS:HD2	2:C:567:ARG:HH21	1.41	0.68
2:C:624:ILE:HG21	2:C:629:LEU:HD13	1.76	0.68
2:B:451:TYR:HB3	2:B:495:TYR:HD2	1.57	0.68
2:A:378:LYS:HG3	2:A:433:VAL:HB	1.75	0.68
2:B:139:PRO:HB3	2:B:243:ALA:HB2	1.76	0.68
2:C:83:VAL:HG21	2:C:237:ARG:HH21	1.56	0.68
2:C:1053:PRO:O	2:C:1054:GLN:NE2	2.26	0.68
2:B:29:THR:OG1	2:B:30:ASN:N	2.26	0.67
2:C:491:PRO:O	2:C:493:GLN:NE2	2.27	0.67
1:I:39:ARG:HG3	1:I:95:TYR:HD1	1.60	0.67
2:A:105:ILE:HG12	2:A:241:LEU:HD21	1.77	0.67
2:B:335:LEU:HG	2:B:360:ASN:HB2	1.77	0.67
2:B:100:ILE:O	2:B:242:LEU:HA	1.95	0.67
2:C:1138:TYR:HE1	2:C:1143:PRO:HG2	1.59	0.67
2:B:44:ARG:HG2	2:B:47:VAL:HG11	1.77	0.67
2:C:455:LEU:H	2:C:493:GLN:HE22	1.43	0.67
2:C:328:ARG:HH11	2:C:533:LEU:HB3	1.59	0.66
2:B:458:LYS:HG3	2:B:473:TYR:HD1	1.61	0.66
2:A:1053:PRO:O	2:A:1054:GLN:NE2	2.29	0.66
2:B:64:TRP:HE1	2:B:260:ALA:CA	2.09	0.66
2:B:336:CYS:CA	2:B:361:CYS:HA	2.25	0.66
2:B:821:LEU:HD22	2:B:935:GLN:HG3	1.78	0.66
2:A:328:ARG:HH21	2:A:533:LEU:HA	1.61	0.66
2:C:81:ASN:O	2:C:239:GLN:NE2	2.28	0.66
1:G:20:ARG:HE	1:G:81:TYR:HB3	1.61	0.65
2:A:393:THR:HB	2:A:520:ALA:HB3	1.78	0.65
2:A:444:LYS:H	2:A:448:ASN:HB2	1.62	0.65
2:C:98:SER:O	2:C:102:ARG:NH2	2.29	0.65
2:A:350:VAL:HG11	2:A:418:ILE:HD11	1.78	0.65
2:C:73:THR:HB	2:C:141:LEU:HD13	1.78	0.65
2:C:951:VAL:HA	2:C:954:HIS:CE1	2.32	0.65
2:B:454:ARG:HD3	2:B:457:ARG:HG3	1.79	0.65
1:E:36:GLY:HA3	1:E:100:TRP:HE1	1.62	0.65
2:C:326:ILE:HD11	2:C:534:VAL:HG13	1.79	0.65
2:A:100:ILE:HG23	2:A:244:LEU:HD23	1.77	0.65
2:A:434:ILE:HB	2:A:511:VAL:HB	1.79	0.65
2:B:401:VAL:HG13	2:B:509:ARG:HG2	1.79	0.65
2:B:426:PRO:HB3	2:B:463:PRO:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:64:TRP:CD2	2:A:259:THR:HB	2.32	0.65
2:A:91:TYR:N	2:A:268:GLY:O	2.26	0.65
2:B:176:LEU:HA	2:B:190:ARG:HH12	1.62	0.65
2:B:295:PRO:HG2	2:B:636:TYR:CE2	2.32	0.65
2:A:398:ASP:O	2:A:512:VAL:N	2.30	0.64
2:B:964:LYS:NZ	2:C:570:ALA:HA	2.11	0.64
2:A:147:LYS:HA	2:A:246:ARG:HA	1.79	0.64
2:C:985:ASP:HB2	2:C:987:PRO:HD2	1.79	0.64
2:C:74:ASN:HB2	2:C:78:ARG:HH21	1.63	0.64
2:A:175:PHE:O	2:A:207:HIS:NE2	2.27	0.64
2:A:615:VAL:HG21	2:A:621:PRO:HG2	1.80	0.64
2:B:271:GLN:HG2	2:B:272:PRO:HD2	1.78	0.64
2:A:620:VAL:CG1	2:A:621:PRO:HD3	2.26	0.64
2:C:553:THR:HG23	2:C:586:ASP:HB3	1.79	0.64
2:B:392:PHE:CB	2:B:515:PHE:HB3	2.28	0.64
2:A:738:CYS:HB3	2:A:742:ILE:HD12	1.80	0.64
2:B:379:CYS:HA	2:B:432:CYS:CA	2.25	0.64
2:A:485:GLY:H	2:A:488:CYS:HB2	1.62	0.64
2:B:133:PHE:CG	2:B:160:TYR:HA	2.32	0.63
2:C:418:ILE:HA	2:C:422:ASN:HB2	1.80	0.63
2:C:559:PHE:HB3	2:C:577:ARG:NH1	2.11	0.63
2:A:538:CYS:HB3	2:A:551:VAL:HG22	1.80	0.63
2:B:407:VAL:HA	2:B:410:ILE:HD12	1.78	0.63
2:C:68:ILE:HG12	2:C:252:GLY:HA2	1.80	0.63
1:E:68:ARG:NH1	1:E:86:SER:O	2.32	0.63
2:B:624:ILE:HG22	2:B:628:GLN:HB3	1.79	0.63
2:A:134:GLN:HB3	2:A:161:SER:HA	1.80	0.63
2:B:922:LEU:HD11	3:R:1:NAG:H5	1.81	0.63
2:B:452:ARG:HA	2:B:494:SER:HA	1.79	0.63
2:A:293:LEU:HD23	2:A:294:ASP:HB2	1.80	0.63
2:C:1138:TYR:CE1	2:C:1143:PRO:HG2	2.34	0.63
2:C:280:ASN:HD21	2:C:282:ASN:HD22	1.47	0.63
2:A:118:LEU:HB2	2:A:120:VAL:HG23	1.80	0.62
1:I:38:PHE:HE2	1:I:100:TRP:HE1	1.47	0.62
1:E:56:ASP:OD1	1:E:59:HIS:NE2	2.32	0.62
2:C:108:THR:HG22	2:C:109:THR:HG23	1.80	0.62
2:A:432:CYS:HB2	2:A:513:LEU:HG	1.81	0.62
2:B:42:VAL:HG21	2:B:44:ARG:HH11	1.63	0.62
2:B:79:PHE:CD1	2:B:242:LEU:HD12	2.32	0.62
2:B:886:TRP:HE1	2:C:1107:ARG:HH12	1.45	0.62
2:A:66:HIS:HA	2:A:263:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:387:LEU:HA	2:A:390:LEU:HB2	1.82	0.62
2:B:43:PHE:O	2:B:44:ARG:C	2.37	0.62
2:C:244:LEU:O	2:C:246:ARG:N	2.30	0.62
2:C:792:PRO:O	2:C:795:LYS:NZ	2.32	0.62
2:A:403:ARG:HG3	2:A:495:TYR:HE1	1.64	0.61
2:B:456:PHE:H	2:B:491:PRO:HA	1.65	0.61
2:B:806:LEU:HD13	2:B:807:PRO:HD2	1.82	0.61
2:C:102:ARG:NH1	2:C:121:ASN:OD1	2.33	0.61
2:C:356:LYS:HB2	2:C:397:ALA:HB3	1.82	0.61
2:B:44:ARG:HH21	2:B:49:HIS:CD2	2.17	0.61
2:B:1142:GLN:HB3	2:B:1143:PRO:HD3	1.82	0.61
2:A:65:PHE:O	2:A:67:ALA:N	2.34	0.61
2:B:418:ILE:HD12	2:B:422:ASN:HD22	1.65	0.61
2:A:365:TYR:HD2	2:A:388:ASN:HA	1.66	0.61
2:B:600:PRO:HD3	2:B:692:ILE:HD11	1.83	0.61
2:A:821:LEU:HD13	2:A:935:GLN:HG3	1.83	0.61
2:A:34:ARG:HH22	2:A:221:SER:H	1.48	0.60
2:A:263:ALA:HB3	2:A:266:TYR:CE1	2.36	0.60
2:A:534:VAL:HG22	2:A:535:LYS:H	1.66	0.60
2:C:68:ILE:H	2:C:80:ASP:HB3	1.66	0.60
2:C:310:LYS:HG3	2:C:600:PRO:HA	1.82	0.60
1:G:107:ASN:HB2	1:G:109:ILE:HG12	1.83	0.60
2:B:1143:PRO:HA	2:B:1146:ASP:HB2	1.82	0.60
2:A:106:PHE:HD2	2:A:235:ILE:HG21	1.64	0.60
2:C:359:SER:HA	2:C:523:THR:HB	1.82	0.60
2:C:915:VAL:O	2:C:919:ASN:ND2	2.34	0.60
2:B:196:ASN:HD21	2:B:233:ILE:HG23	1.67	0.60
2:B:850:ILE:O	2:B:854:LYS:NZ	2.35	0.60
2:C:791:THR:HG21	2:C:806:LEU:HD11	1.83	0.60
2:A:135:PHE:N	2:A:161:SER:OG	2.33	0.60
1:I:74:ASP:OD2	1:I:77:LYS:N	2.25	0.60
2:A:244:LEU:O	2:A:246:ARG:N	2.34	0.60
2:A:578:ASP:N	2:A:583:GLU:O	2.25	0.60
1:G:65:VAL:HB	1:G:69:PHE:HB2	1.83	0.60
1:E:68:ARG:O	1:E:85:ASN:ND2	2.34	0.60
2:B:567:ARG:NE	2:B:570:ALA:O	2.35	0.60
2:B:95:THR:HG21	2:B:212:LEU:HD22	1.83	0.59
2:B:915:VAL:O	2:B:919:ASN:ND2	2.34	0.59
2:C:804:GLN:NE2	2:C:935:GLN:OE1	2.29	0.59
2:A:403:ARG:HG3	2:A:495:TYR:CE1	2.36	0.59
2:C:338:PHE:HD2	2:C:356:LYS:HE3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:HIS:HB2	1:E:100:TRP:HB2	1.85	0.59
2:B:1139:ASP:OD2	2:B:1142:GLN:N	2.33	0.59
2:A:66:HIS:HA	2:A:263:ALA:CB	2.32	0.59
2:A:71:SER:HA	2:A:79:PHE:CA	2.26	0.59
2:B:144:TYR:O	2:B:145:TYR:C	2.41	0.59
2:C:34:ARG:HH12	2:C:219:GLY:H	1.50	0.59
2:C:167:THR:HG22	2:C:168:PHE:H	1.67	0.59
2:C:442:ASP:O	2:C:448:ASN:ND2	2.35	0.59
2:A:34:ARG:NH1	2:A:219:GLY:O	2.36	0.59
2:A:142:ASP:HB2	2:A:146:HIS:HB3	1.84	0.59
2:B:393:THR:HG21	2:B:518:LEU:HB2	1.84	0.59
2:A:177:MET:O	2:A:190:ARG:NH2	2.34	0.59
2:A:365:TYR:CD2	2:A:388:ASN:HA	2.38	0.59
2:B:204:TYR:HA	2:B:225:PRO:HA	1.85	0.59
2:B:597:VAL:HG22	2:B:610:VAL:HG12	1.83	0.59
2:B:353:TRP:HB3	2:B:400:PHE:HD2	1.68	0.59
2:C:205:SER:HB3	2:C:226:LEU:HG	1.85	0.59
2:C:1142:GLN:HG3	2:C:1143:PRO:HD3	1.85	0.59
2:A:401:VAL:HA	2:A:509:ARG:HA	1.83	0.59
2:C:339:ASP:C	2:C:341:VAL:H	2.05	0.59
1:I:83:GLN:NE2	1:I:84:MET:O	2.36	0.59
2:B:894:LEU:HD13	2:C:715:PRO:HD3	1.85	0.59
2:C:111:ASP:OD2	2:C:113:LYS:NZ	2.28	0.59
2:C:122:ASN:HD21	2:C:153:MET:HG3	1.67	0.59
1:I:41:ALA:HB3	1:I:44:LYS:HG3	1.84	0.58
1:I:92:THR:HG22	1:I:122:VAL:H	1.68	0.58
2:B:353:TRP:NE1	2:B:465:GLU:O	2.32	0.58
2:C:337:PRO:C	2:C:339:ASP:H	2.07	0.58
1:I:17:GLY:O	1:I:87:LEU:N	2.34	0.58
2:C:624:ILE:HB	2:C:629:LEU:HD22	1.85	0.58
2:B:128:ILE:H	2:B:128:ILE:HD12	1.68	0.58
1:I:98:ALA:HA	1:I:114:TRP:HA	1.86	0.58
2:A:295:PRO:HG3	2:A:633:TRP:CE2	2.38	0.58
2:B:273:ARG:NH1	2:B:290:ASP:OD2	2.37	0.58
2:B:336:CYS:N	2:B:361:CYS:HA	2.18	0.58
2:B:353:TRP:HB3	2:B:400:PHE:CD2	2.38	0.58
2:C:157:PHE:HD2	2:C:159:VAL:HG13	1.69	0.58
2:A:83:VAL:HA	2:A:239:GLN:HG2	1.86	0.58
2:A:83:VAL:HG11	2:A:237:ARG:HH21	1.67	0.58
2:A:414:GLN:O	2:A:424:LYS:NZ	2.37	0.58
2:A:973:ILE:HG22	2:A:992:GLN:HE21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:187:LYS:O	2:A:189:LEU:N	2.37	0.57
2:C:335:LEU:HD12	2:C:525:CYS:H	1.69	0.57
1:I:65:VAL:HB	1:I:69:PHE:HB2	1.86	0.57
2:A:1126:CYS:HB2	2:A:1132:ILE:HD13	1.85	0.57
2:C:106:PHE:HB2	2:C:117:LEU:HB2	1.85	0.57
2:A:64:TRP:HE1	2:A:262:ALA:N	2.02	0.57
2:B:448:ASN:HB3	2:B:497:PHE:HB2	1.85	0.57
2:B:118:LEU:HD11	2:B:131:CYS:O	2.04	0.57
2:B:289:VAL:HG21	2:B:300:LYS:HD2	1.87	0.57
2:B:295:PRO:HD3	2:B:633:TRP:CD1	2.39	0.57
2:A:429:PHE:HE1	2:A:514:SER:HB3	1.70	0.57
1:I:6:GLN:HB2	1:I:24:ALA:HB3	1.87	0.57
2:A:738:CYS:O	2:A:742:ILE:N	2.35	0.57
2:B:48:LEU:HD12	2:B:276:LEU:HD21	1.87	0.57
2:C:103:GLY:HA3	2:C:120:VAL:HA	1.86	0.57
2:C:736:VAL:HG12	2:C:858:LEU:HD22	1.84	0.57
2:A:139:PRO:HA	2:A:157:PHE:HA	1.87	0.57
2:C:86:PHE:HB2	2:C:238:PHE:HB3	1.86	0.57
2:C:422:ASN:ND2	2:C:454:ARG:O	2.34	0.57
2:C:622:VAL:HG22	2:C:642:VAL:HG11	1.87	0.57
1:E:37:TRP:CD1	1:E:82:LEU:HD22	2.40	0.56
2:A:271:GLN:HG3	2:A:272:PRO:HD2	1.87	0.56
2:B:904:TYR:CE2	2:C:1107:ARG:HD3	2.40	0.56
1:E:16:GLY:HA2	1:E:86:SER:H	1.69	0.56
2:A:396:TYR:N	2:A:514:SER:O	2.37	0.56
2:A:1051:SER:OG	2:A:1064:HIS:ND1	2.33	0.56
1:I:3:VAL:HG21	1:I:99:TYR:HE2	1.71	0.56
2:A:397:ALA:HA	2:A:513:LEU:HA	1.87	0.56
2:A:534:VAL:HG21	2:A:539:VAL:HG21	1.87	0.56
2:B:133:PHE:HA	2:B:163:ALA:HB2	1.85	0.56
2:C:1142:GLN:O	2:C:1146:ASP:N	2.31	0.56
2:A:62:VAL:O	2:A:64:TRP:N	2.37	0.56
2:C:96:GLU:HB2	2:C:100:ILE:HB	1.88	0.56
2:C:580:GLN:O	2:C:582:LEU:N	2.38	0.56
2:B:115:GLN:HA	2:B:132:GLU:HB3	1.86	0.56
1:I:46:ARG:HD2	1:I:114:TRP:CH2	2.40	0.56
2:B:110:LEU:HB3	2:B:136:CYS:SG	2.46	0.56
2:B:964:LYS:HZ3	2:C:570:ALA:HA	1.69	0.56
2:C:146:HIS:HB2	2:C:246:ARG:HA	1.86	0.56
2:A:76:THR:O	2:A:77:LYS:C	2.44	0.56
2:B:523:THR:OG1	2:B:524:VAL:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:TRP:O	2:C:65:PHE:C	2.44	0.56
2:B:351:TYR:HB2	2:B:467:ASP:HB2	1.88	0.56
2:C:985:ASP:OD1	2:C:985:ASP:N	2.39	0.56
2:A:248:TYR:O	2:A:249:LEU:C	2.44	0.55
2:A:592:PHE:HZ	2:C:857:GLY:H	1.54	0.55
2:B:34:ARG:NH1	2:B:219:GLY:O	2.39	0.55
2:C:338:PHE:CD2	2:C:356:LYS:HE3	2.41	0.55
2:A:226:LEU:HD23	2:A:227:VAL:HG23	1.88	0.55
2:A:369:TYR:OH	2:A:384:PRO:O	2.23	0.55
2:B:784:GLN:OE1	2:B:1030:SER:OG	2.23	0.55
2:C:392:PHE:HB3	2:C:515:PHE:HB3	1.87	0.55
2:C:620:VAL:HB	2:C:621:PRO:HD3	1.87	0.55
2:B:104:TRP:HB2	2:B:106:PHE:CE1	2.41	0.55
2:C:773:GLU:OE1	2:C:1019:ARG:NH1	2.38	0.55
2:C:922:LEU:HD11	3:K:1:NAG:H5	1.88	0.55
2:C:1048:HIS:NE2	2:C:1050:MET:O	2.39	0.55
2:C:439:ASN:O	2:C:443:SER:OG	2.20	0.55
2:C:599:THR:HB	2:C:608:VAL:HG12	1.89	0.55
2:C:1086:LYS:HD2	2:C:1122:VAL:HG11	1.87	0.55
1:E:73:ARG:HA	1:E:80:VAL:HA	1.87	0.55
2:C:954:HIS:CD2	2:C:1014:ARG:HH11	2.24	0.55
1:I:51:ALA:HB3	1:I:60:TYR:HD2	1.71	0.55
2:B:356:LYS:HG3	2:B:358:ILE:HG13	1.88	0.55
1:E:28:TRP:HB3	2:A:375:PHE:HE1	1.70	0.55
1:I:62:ALA:O	1:I:66:LYS:N	2.39	0.55
2:A:1101:HIS:ND1	3:Z:1:NAG:H5	2.22	0.55
2:B:36:VAL:HG11	2:B:220:PHE:CE2	2.42	0.55
2:B:102:ARG:NH1	2:B:243:ALA:O	2.40	0.55
2:A:102:ARG:HG3	2:A:243:ALA:HB3	1.88	0.55
2:B:277:LEU:HD23	2:B:285:ILE:HD13	1.89	0.55
2:B:362:VAL:O	2:B:364:ASP:N	2.40	0.55
2:A:453:TYR:HB3	2:A:495:TYR:CZ	2.41	0.55
2:B:318:PHE:HE2	2:B:615:VAL:HG11	1.73	0.55
2:B:318:PHE:CD1	2:B:629:LEU:HA	2.42	0.55
2:C:29:THR:HA	2:C:61:ASN:HA	1.87	0.55
2:C:115:GLN:HG3	2:C:233:ILE:HG12	1.89	0.55
2:A:629:LEU:HD21	2:A:634:ARG:HA	1.89	0.54
2:B:621:PRO:HA	2:B:624:ILE:HG23	1.88	0.54
2:C:29:THR:HA	2:C:62:VAL:N	2.22	0.54
2:A:65:PHE:CZ	2:A:82:PRO:HD2	2.42	0.54
2:B:736:VAL:HG23	2:B:858:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:TYR:HB3	1:G:113:TYR:HB2	1.89	0.54
1:G:18:SER:OG	1:G:83:GLN:OE1	2.25	0.54
2:A:93:ALA:O	2:A:266:TYR:HD2	1.91	0.54
2:A:174:PRO:HG2	2:A:177:MET:HG3	1.89	0.54
2:A:326:ILE:HG23	2:A:541:PHE:HA	1.90	0.54
1:G:4:GLN:HB3	2:C:489:TYR:HE1	1.72	0.54
2:A:29:THR:O	2:A:61:ASN:HA	2.08	0.54
2:A:1040:VAL:HG21	2:C:1035:GLY:HA3	1.88	0.54
2:B:157:PHE:HD1	2:B:158:ARG:N	2.05	0.54
2:B:328:ARG:O	2:B:329:PHE:C	2.45	0.54
2:B:566:GLY:HA3	2:B:575:ALA:HB3	1.88	0.54
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.89	0.54
2:A:1077:THR:OG1	2:A:1078:ALA:N	2.41	0.54
2:C:178:ASP:N	2:C:178:ASP:OD1	2.39	0.54
1:I:61:TYR:HE1	1:I:70:THR:HA	1.72	0.54
2:B:418:ILE:HA	2:B:422:ASN:HB3	1.88	0.54
2:B:676:THR:HB	2:B:690:GLN:HG2	1.89	0.54
2:C:519:HIS:HB3	2:C:565:PHE:CD2	2.43	0.54
2:A:93:ALA:HB1	2:A:189:LEU:HG	1.90	0.54
2:A:811:LYS:NZ	2:A:820:ASP:OD2	2.33	0.54
2:B:617:CYS:O	2:B:621:PRO:HD2	2.08	0.54
2:B:106:PHE:HB3	2:B:235:ILE:CG2	2.38	0.54
2:B:555:SER:HB3	2:B:584:ILE:O	2.08	0.54
2:C:457:ARG:NE	2:C:459:SER:O	2.41	0.53
2:C:748:GLU:OE1	2:C:748:GLU:N	2.38	0.53
2:A:642:VAL:HG22	2:A:651:ILE:HG12	1.90	0.53
2:B:140:PHE:CE1	2:B:158:ARG:HB2	2.44	0.53
2:C:64:TRP:HB2	2:C:66:HIS:NE2	2.23	0.53
2:C:336:CYS:O	2:C:336:CYS:SG	2.66	0.53
2:A:724:THR:HB	2:A:934:ILE:HD11	1.89	0.53
2:C:206:LYS:HD2	2:C:221:SER:HB3	1.90	0.53
2:C:330:PRO:O	2:C:331:ASN:C	2.46	0.53
2:A:904:TYR:OH	2:B:1094:VAL:HB	2.07	0.53
2:B:763:LEU:HD11	2:B:1005:GLN:HE22	1.74	0.53
1:E:57:THR:HG21	2:A:405:ASN:HD21	1.74	0.53
2:B:106:PHE:HB2	2:B:117:LEU:HB2	1.90	0.53
2:B:320:VAL:HG13	2:B:628:GLN:HE22	1.72	0.53
2:B:617:CYS:O	2:B:619:GLU:N	2.38	0.53
2:C:110:LEU:HD13	2:C:136:CYS:SG	2.49	0.53
2:C:112:SER:HA	2:C:134:GLN:HA	1.91	0.53
1:G:34:HIS:HB2	1:G:100:TRP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:36:VAL:HG11	2:A:220:PHE:CZ	2.44	0.53
2:A:120:VAL:HG13	2:A:157:PHE:HZ	1.74	0.53
2:B:42:VAL:O	2:C:563:GLN:NE2	2.40	0.53
2:B:339:ASP:HA	2:B:343:ASN:H	1.73	0.53
2:B:538:CYS:SG	2:B:590:CYS:HB3	2.48	0.53
2:A:63:THR:O	2:A:64:TRP:C	2.46	0.53
2:A:454:ARG:NH1	2:A:469:SER:O	2.42	0.53
2:A:966:LEU:O	2:A:975:SER:OG	2.26	0.53
2:B:42:VAL:HG22	2:B:44:ARG:HH11	1.72	0.53
2:C:821:LEU:HD22	2:C:935:GLN:HG3	1.91	0.53
2:A:788:ILE:HG23	2:A:876:ALA:HB2	1.91	0.53
2:B:158:ARG:NH1	2:B:160:TYR:OH	2.42	0.53
2:B:294:ASP:H	2:B:297:SER:HB2	1.74	0.53
2:B:473:TYR:HB3	2:B:491:PRO:HD3	1.90	0.53
2:C:278:LYS:HG2	2:C:287:ASP:H	1.72	0.53
2:C:327:VAL:O	2:C:328:ARG:C	2.47	0.53
2:C:337:PRO:HD3	2:C:363:ALA:O	2.09	0.53
2:C:802:PHE:HD1	2:C:805:ILE:HD11	1.74	0.53
2:C:806:LEU:HG	2:C:807:PRO:HD2	1.91	0.53
2:B:73:THR:O	2:B:144:TYR:N	2.41	0.52
2:C:182:LYS:O	2:C:183:GLN:HG3	2.09	0.52
2:A:375:PHE:HB3	2:A:436:TRP:HB3	1.90	0.52
2:A:624:ILE:HG13	2:A:637:SER:HA	1.91	0.52
2:B:244:LEU:O	2:B:246:ARG:N	2.41	0.52
2:B:393:THR:HB	2:B:516:GLU:O	2.09	0.52
2:C:426:PRO:HD3	2:C:463:PRO:HB3	1.90	0.52
2:A:258:TRP:CE3	4:A:1302:NAG:H5	2.45	0.52
2:A:434:ILE:N	2:A:511:VAL:O	2.27	0.52
2:B:44:ARG:NH2	2:B:49:HIS:CD2	2.76	0.52
2:B:106:PHE:HB3	2:B:235:ILE:HG23	1.92	0.52
2:C:336:CYS:HB3	2:C:362:VAL:N	2.23	0.52
2:A:120:VAL:HB	2:A:127:VAL:HB	1.91	0.52
2:B:175:PHE:O	2:B:190:ARG:NH1	2.42	0.52
2:C:581:THR:O	2:C:582:LEU:C	2.48	0.52
2:A:754:LEU:HD12	2:A:755:GLN:HG3	1.91	0.52
2:B:318:PHE:HD1	2:B:629:LEU:HA	1.74	0.52
2:B:448:ASN:HD21	2:B:451:TYR:HD2	1.58	0.52
2:B:777:ASN:OD1	2:B:1019:ARG:NH1	2.40	0.52
2:C:502:GLY:O	2:C:506:GLN:N	2.43	0.52
2:C:580:GLN:C	2:C:582:LEU:H	2.13	0.52
2:A:444:LYS:HE2	2:A:448:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:GLY:N	2:C:373:PRO:O	2.43	0.52
2:A:629:LEU:HD23	2:A:629:LEU:H	1.75	0.52
2:B:91:TYR:HB3	2:B:268:GLY:HA3	1.92	0.52
2:B:445:VAL:HA	2:B:499:PRO:HG3	1.91	0.52
2:B:727:LEU:HD11	2:B:1028:LYS:HD3	1.92	0.52
2:B:295:PRO:HD3	2:B:633:TRP:HD1	1.75	0.51
1:G:4:GLN:O	1:G:26[A]:SER:OG	2.24	0.51
2:B:133:PHE:CD2	2:B:160:TYR:HA	2.45	0.51
2:C:115:GLN:HB2	2:C:233:ILE:HG12	1.91	0.51
2:A:762:GLN:OE1	2:A:765:ARG:NH1	2.33	0.51
2:C:64:TRP:HD1	2:C:66:HIS:CD2	2.29	0.51
2:C:708:SER:HB3	2:C:711:SER:HB3	1.92	0.51
2:B:215:ASP:O	2:B:216:LEU:C	2.49	0.51
2:C:318:PHE:HZ	2:C:620:VAL:HG12	1.76	0.51
2:C:759:PHE:CD2	2:C:1001:LEU:HD21	2.46	0.51
2:B:187:LYS:CB	2:B:212:LEU:HB2	2.40	0.51
1:G:39:ARG:NH1	1:G:91:ASP:OD1	2.42	0.51
1:G:72:SER:O	1:G:81:TYR:N	2.44	0.51
2:A:244:LEU:HB2	2:A:247:SER:HB3	1.93	0.51
2:B:434:ILE:HG22	2:B:511:VAL:HB	1.92	0.51
2:B:480:CYS:HB3	2:B:483:VAL:O	2.11	0.51
2:A:91:TYR:OH	2:A:191:GLU:HG2	2.11	0.51
2:A:849:LEU:HD21	2:A:852:ALA:HB3	1.93	0.51
2:B:409:GLN:HB3	2:B:419:ALA:HB2	1.91	0.51
2:A:65:PHE:O	2:A:66:HIS:C	2.46	0.51
2:A:258:TRP:HE3	4:A:1302:NAG:HN2	1.58	0.51
2:A:326:ILE:HD11	2:A:328:ARG:HB2	1.93	0.51
2:A:661:GLU:OE2	2:A:662:CYS:N	2.42	0.51
1:E:37:TRP:HH2	1:E:80:VAL:HG13	1.76	0.51
2:A:436:TRP:O	2:A:509:ARG:N	2.44	0.51
2:A:457:ARG:NH1	2:A:467:ASP:HB3	2.26	0.51
2:B:855:PHE:HB3	2:C:589:PRO:HG2	1.92	0.51
2:C:29:THR:CA	2:C:61:ASN:HA	2.40	0.51
1:G:21:LEU:HD12	1:G:82:LEU:HD23	1.93	0.51
1:I:42:PRO:HD3	1:I:93:ALA:HB2	1.93	0.51
2:A:91:TYR:HE1	2:A:191:GLU:HB3	1.76	0.51
2:A:134:GLN:N	2:A:161:SER:OG	2.44	0.51
2:A:894:LEU:HD13	2:B:715:PRO:HD3	1.93	0.51
2:B:822:LEU:HD22	2:B:945:LEU:HD21	1.92	0.51
2:C:453:TYR:HB3	2:C:495:TYR:CE2	2.45	0.51
2:C:565:PHE:CB	2:C:567:ARG:HH22	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1035:GLY:HA3	2:B:1040:VAL:HG21	1.92	0.50
2:B:42:VAL:CG2	2:B:44:ARG:NH1	2.73	0.50
2:B:450:ASN:O	2:B:452:ARG:NH1	2.45	0.50
2:C:335:LEU:HB3	2:C:524:VAL:HG12	1.93	0.50
2:A:63:THR:O	2:A:65:PHE:HB2	2.12	0.50
2:A:452:ARG:HG2	2:A:494:SER:HA	1.94	0.50
2:B:93:ALA:O	2:B:265:TYR:HA	2.10	0.50
2:B:359:SER:HB3	2:B:522:ALA:HB1	1.93	0.50
2:B:1126:CYS:HB2	2:B:1132:ILE:HD13	1.93	0.50
1:I:100:TRP:CD1	1:I:105:LEU:HD11	2.46	0.50
2:A:426:PRO:HB3	2:A:463:PRO:HB3	1.93	0.50
2:A:624:ILE:HD12	2:A:629:LEU:HD22	1.94	0.50
2:B:392:PHE:HB2	2:B:515:PHE:HB3	1.92	0.50
2:C:389:ASP:OD1	2:C:527:PRO:HD2	2.12	0.50
2:A:541:PHE:HB3	2:A:552:LEU:HD11	1.94	0.50
2:B:387:LEU:HA	2:B:390:LEU:HB2	1.93	0.50
2:B:752:LEU:HD23	2:B:993:ILE:HG22	1.94	0.50
2:C:134:GLN:HG2	2:C:161:SER:HB3	1.93	0.50
2:C:543:PHE:O	2:C:544:ASN:C	2.50	0.50
1:G:14:GLN:HG3	1:G:124:SER:HA	1.94	0.50
2:B:29:THR:N	2:B:260:ALA:HA	2.27	0.50
2:B:115:GLN:NE2	2:B:130:VAL:O	2.45	0.50
2:C:1082:CYS:HB2	2:C:1132:ILE:HG12	1.93	0.50
2:B:798:GLY:HA3	2:B:899:PRO:HG3	1.94	0.50
2:C:29:THR:CB	2:C:259:THR:HA	2.41	0.50
2:C:37:TYR:HA	2:C:223:LEU:H	1.76	0.50
2:C:714:ILE:HD12	2:C:1096:VAL:HG11	1.93	0.50
1:I:40:GLN:NE2	1:I:94:THR:O	2.45	0.50
2:A:190:ARG:HB3	2:A:192:PHE:CE2	2.47	0.50
2:A:206:LYS:HB3	2:A:223:LEU:HD22	1.94	0.50
2:A:762:GLN:HE22	2:A:765:ARG:HH22	1.58	0.50
2:B:43:PHE:H	2:C:566:GLY:HA2	1.76	0.50
2:B:72:GLY:O	2:B:73:THR:C	2.50	0.50
2:B:79:PHE:CE2	2:B:139:PRO:HB2	2.47	0.50
2:B:119:ILE:HG12	2:B:128:ILE:HG23	1.93	0.50
2:B:448:ASN:O	2:B:498:ARG:NH1	2.45	0.50
2:A:748:GLU:HG3	2:A:981:LEU:HD11	1.93	0.49
2:B:62:VAL:HG22	2:B:266:TYR:HB3	1.94	0.49
2:C:454:ARG:HE	2:C:491:PRO:HB2	1.77	0.49
2:A:328:ARG:NH1	2:A:578:ASP:OD2	2.45	0.49
2:A:393:THR:OG1	2:A:394:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:VAL:HG22	2:B:174:PRO:HA	1.93	0.49
2:B:802:PHE:HB3	2:B:806:LEU:HD23	1.93	0.49
2:C:1125:ASN:OD1	2:C:1126:CYS:N	2.45	0.49
2:B:967:SER:O	2:B:975:SER:HB2	2.12	0.49
2:B:1116:THR:HA	2:B:1138:TYR:O	2.12	0.49
1:E:28:TRP:HB3	2:A:375:PHE:CE1	2.48	0.49
2:A:77:LYS:O	2:A:78:ARG:C	2.50	0.49
2:C:281:GLU:C	2:C:283:GLY:H	2.16	0.49
1:G:40:GLN:HB2	1:G:46:ARG:HG3	1.94	0.49
2:A:392:PHE:H	2:A:524:VAL:HG23	1.77	0.49
2:B:131:CYS:HB3	2:B:133:PHE:CE2	2.47	0.49
2:B:595:VAL:HG21	2:B:631:PRO:HG2	1.94	0.49
2:C:431:GLY:HA2	2:C:515:PHE:CD2	2.47	0.49
2:C:409:GLN:HB3	2:C:419:ALA:HB2	1.95	0.49
2:C:1097:SER:C	2:C:1099:GLY:H	2.15	0.49
2:A:31:SER:O	2:A:32:PHE:C	2.51	0.49
2:A:40:ASP:OD1	2:A:40:ASP:N	2.46	0.49
2:A:77:LYS:O	2:A:79:PHE:N	2.45	0.49
2:A:157:PHE:HB3	2:A:243:ALA:HB2	1.94	0.49
2:C:359:SER:HA	2:C:523:THR:CB	2.42	0.49
2:A:78:ARG:CB	2:A:251:PRO:HA	2.42	0.49
2:A:399:SER:HA	2:A:511:VAL:HA	1.95	0.49
2:B:789:TYR:HA	2:C:703:ASN:O	2.12	0.49
2:C:393:THR:HG21	2:C:519:HIS:O	2.12	0.49
1:E:41:ALA:HB3	1:E:44:LYS:HB2	1.95	0.49
2:C:807:PRO:HG3	2:C:875:SER:HB2	1.95	0.49
1:E:41:ALA:HA	1:E:94:THR:H	1.78	0.48
2:A:365:TYR:CE2	2:A:524:VAL:HG11	2.48	0.48
2:B:339:ASP:O	2:B:340:GLU:C	2.51	0.48
2:C:328:ARG:HH12	2:C:533:LEU:CD2	2.26	0.48
2:C:565:PHE:HB2	2:C:567:ARG:HH22	1.78	0.48
2:C:616:ASN:OD1	2:C:616:ASN:N	2.42	0.48
1:G:68:ARG:NH1	1:G:85:ASN:O	2.46	0.48
2:A:337:PRO:C	2:A:339:ASP:H	2.15	0.48
2:A:677:GLN:O	2:A:689:SER:OG	2.31	0.48
2:B:42:VAL:HG22	2:B:44:ARG:NH1	2.27	0.48
2:C:519:HIS:HD2	2:C:567:ARG:NH2	2.09	0.48
2:B:392:PHE:HB3	2:B:515:PHE:HB3	1.94	0.48
2:C:480:CYS:HB3	2:C:483:VAL:O	2.14	0.48
2:C:600:PRO:HD3	2:C:692:ILE:HD11	1.94	0.48
2:A:553:THR:HG23	2:A:586:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:VAL:HA	2:B:514:SER:O	2.13	0.48
2:B:503:VAL:HA	2:B:506:GLN:HE21	1.78	0.48
2:A:273:ARG:HA	2:A:273:ARG:HD3	1.52	0.48
2:A:452:ARG:HA	2:A:495:TYR:H	1.78	0.48
2:B:983:ARG:HG2	2:C:517:LEU:HD22	1.94	0.48
2:B:1145:LEU:HA	2:B:1148:PHE:HB3	1.95	0.48
2:A:457:ARG:HG2	2:A:458:LYS:H	1.79	0.48
2:C:457:ARG:NH1	2:C:467:ASP:OD2	2.46	0.48
2:A:809:PRO:O	2:A:814:LYS:NZ	2.40	0.48
2:C:328:ARG:HH12	2:C:533:LEU:HD23	1.79	0.48
2:A:61:ASN:HB3	2:A:258:TRP:CA	2.37	0.48
2:A:109:THR:HG21	2:A:113:LYS:HB2	1.96	0.48
2:A:635:VAL:HG23	2:A:636:TYR:HD1	1.79	0.48
2:B:599:THR:HB	2:B:608:VAL:HG12	1.96	0.48
1:E:46:ARG:HD3	1:E:114:TRP:CZ2	2.49	0.48
1:I:109:ILE:HG13	1:I:110:PRO:HD3	1.94	0.48
2:A:379:CYS:HA	2:A:432:CYS:HA	1.96	0.48
2:B:121:ASN:ND2	2:B:176:LEU:HB2	2.29	0.48
2:B:435:ALA:HA	2:B:509:ARG:O	2.14	0.48
2:C:328:ARG:NH1	2:C:533:LEU:HB3	2.27	0.48
2:C:329:PHE:CG	2:C:330:PRO:HD2	2.49	0.48
2:A:702:GLU:HG3	2:C:790:LYS:HE2	1.96	0.47
2:C:767:LEU:HD13	2:C:1008:VAL:HG22	1.96	0.47
1:G:68:ARG:NH1	1:G:86:SER:O	2.47	0.47
1:I:28:TRP:HB3	2:C:375:PHE:CZ	2.49	0.47
1:I:98:ALA:HB1	1:I:111:VAL:HG11	1.97	0.47
2:A:131:CYS:SG	2:A:165:ASN:O	2.72	0.47
2:A:336:CYS:N	2:A:361:CYS:HB2	2.29	0.47
2:B:379:CYS:CA	2:B:432:CYS:HA	2.28	0.47
2:B:452:ARG:HG3	2:B:494:SER:HA	1.96	0.47
1:E:111:VAL:HG21	1:E:114:TRP:CZ2	2.49	0.47
2:A:176:LEU:HD23	2:A:190:ARG:HG2	1.96	0.47
2:A:335:LEU:HB3	2:A:361:CYS:HB2	1.97	0.47
2:A:402:ILE:HG21	2:A:410:ILE:HG13	1.94	0.47
2:B:164:ASN:O	2:B:166:CYS:SG	2.72	0.47
1:I:1:SER:HB2	1:I:29:ALA:HA	1.96	0.47
2:A:568:ASP:OD1	2:A:570:ALA:N	2.40	0.47
2:B:715:PRO:HA	2:B:1072:GLU:HA	1.96	0.47
2:A:328:ARG:HD3	2:A:531:THR:OG1	2.14	0.47
2:A:355:ARG:HH12	2:A:464:PHE:HB3	1.80	0.47
2:A:761:THR:OG1	2:A:762:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:767:LEU:O	2:A:770:ILE:HG22	2.14	0.47
2:B:560:LEU:O	2:B:561:PRO:C	2.53	0.47
2:C:498:ARG:HG3	2:C:501:TYR:HE2	1.80	0.47
1:I:23:CYS:HB2	1:I:37:TRP:CH2	2.49	0.47
2:A:29:THR:HA	2:A:259:THR:C	2.34	0.47
2:A:44:ARG:O	2:A:283:GLY:HA2	2.14	0.47
2:B:325:SER:HB2	2:B:539:VAL:HG12	1.94	0.47
2:C:102:ARG:O	2:C:121:ASN:HB3	2.15	0.47
1:E:14:GLN:HG3	1:E:126:SER:HA	1.97	0.47
1:I:20:ARG:HG3	1:I:83:GLN:HB2	1.96	0.47
2:A:448:ASN:HB3	2:A:497:PHE:HB2	1.96	0.47
2:A:534:VAL:HG11	2:A:552:LEU:HD22	1.96	0.47
2:A:922:LEU:HD11	3:X:1:NAG:H5	1.95	0.47
2:B:451:TYR:HB3	2:B:495:TYR:CD2	2.45	0.47
2:B:453:TYR:CE1	2:B:455:LEU:HB2	2.49	0.47
2:C:106:PHE:CE1	2:C:119:ILE:HD12	2.49	0.47
2:C:819:GLU:HA	2:C:822:LEU:HD12	1.96	0.47
2:A:80:ASP:OD1	2:A:252:GLY:HA2	2.13	0.47
2:A:117:LEU:O	2:A:119:ILE:N	2.48	0.47
2:A:372:ALA:N	2:A:375:PHE:HE2	2.13	0.47
2:A:589:PRO:HB3	2:C:855:PHE:HD1	1.80	0.47
2:C:36:VAL:HG13	2:C:222:ALA:HA	1.97	0.47
1:G:69:PHE:HB3	1:G:82:LEU:HD11	1.97	0.47
1:I:13:VAL:HG23	1:I:122:VAL:HG13	1.96	0.47
2:A:65:PHE:HZ	2:A:82:PRO:HD2	1.79	0.47
2:A:339:ASP:HA	2:A:343:ASN:HB2	1.97	0.47
2:C:449:TYR:OH	2:C:498:ARG:NH2	2.47	0.47
2:C:474:GLN:HA	2:C:488:CYS:SG	2.55	0.47
2:C:555:SER:HB2	2:C:586:ASP:HB2	1.97	0.47
2:A:103:GLY:O	2:A:241:LEU:N	2.48	0.46
2:A:157:PHE:HD1	2:A:157:PHE:H	1.62	0.46
2:A:283:GLY:HA3	2:B:560:LEU:HD11	1.97	0.46
2:A:1117:THR:HG22	2:A:1140:PRO:HD2	1.97	0.46
2:B:131:CYS:HB2	2:B:166:CYS:HB3	1.75	0.46
2:C:421:TYR:HB3	2:C:457:ARG:HB3	1.97	0.46
1:I:112:ASP:OD1	1:I:112:ASP:N	2.46	0.46
2:B:40:ASP:CG	2:B:44:ARG:NH1	2.68	0.46
2:B:299:THR:OG1	2:B:308:VAL:HG11	2.15	0.46
2:B:454:ARG:NH2	2:B:469:SER:O	2.48	0.46
2:C:181:GLY:HA3	2:C:186:PHE:CE2	2.51	0.46
2:C:247:SER:OG	2:C:247:SER:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:34:ARG:NH2	2:A:221:SER:OG	2.48	0.46
2:A:71:SER:N	2:A:80:ASP:OD1	2.48	0.46
2:A:319:ARG:HD3	2:C:740:MET:HE1	1.96	0.46
2:B:758:SER:O	2:B:762:GLN:NE2	2.38	0.46
2:C:731:MET:O	2:C:733:LYS:NZ	2.42	0.46
1:G:19:LEU:HD12	1:G:19:LEU:HA	1.79	0.46
2:B:986:PRO:N	2:B:987:PRO:HD2	2.30	0.46
2:B:1107:ARG:H	2:B:1107:ARG:HD2	1.80	0.46
1:I:19:LEU:H	1:I:84:MET:HG2	1.79	0.46
1:I:94:THR:OG1	1:I:119:GLN:OE1	2.29	0.46
2:B:75:GLY:O	2:B:77:LYS:N	2.49	0.46
2:C:212:LEU:HD13	2:C:215:ASP:HA	1.97	0.46
2:C:290:ASP:O	2:C:297:SER:HB3	2.15	0.46
1:I:35:MET:N	1:I:35:MET:SD	2.89	0.46
2:A:104:TRP:CD1	2:A:240:THR:HG23	2.50	0.46
2:A:713:ALA:HB3	2:C:894:LEU:HB3	1.96	0.46
2:A:1082:CYS:HB2	2:A:1126:CYS:HB2	1.90	0.46
2:C:242:LEU:HD12	2:C:242:LEU:HA	1.79	0.46
1:G:68:ARG:HD3	1:G:88:ARG:HH21	1.80	0.46
2:A:372:ALA:H	2:A:375:PHE:HE2	1.62	0.46
2:C:36:VAL:HG11	2:C:220:PHE:CE2	2.50	0.46
2:C:387:LEU:HD23	2:C:392:PHE:CZ	2.50	0.46
2:C:746:SER:HB2	2:C:749:CYS:HB3	1.98	0.46
1:I:72:SER:O	1:I:81:TYR:N	2.42	0.46
2:A:337:PRO:O	2:A:339:ASP:N	2.46	0.46
2:B:983:ARG:HA	2:C:390:LEU:HD11	1.98	0.46
2:C:433:VAL:HG12	2:C:512:VAL:HG13	1.98	0.46
2:B:190:ARG:HB3	2:B:192:PHE:CZ	2.50	0.46
2:B:290:ASP:O	2:B:297:SER:HB3	2.16	0.46
2:B:404:GLY:HA2	2:B:407:VAL:HG23	1.97	0.46
2:B:1035:GLY:HA3	2:C:1040:VAL:HG21	1.97	0.46
2:B:1102:TRP:CZ2	2:B:1133:VAL:HG11	2.51	0.46
2:C:339:ASP:O	2:C:341:VAL:N	2.45	0.46
1:I:48:PHE:HZ	1:I:60:TYR:HB3	1.81	0.46
2:A:136:CYS:SG	2:A:138:ASP:HB2	2.56	0.46
2:A:167:THR:HG22	2:A:168:PHE:H	1.79	0.46
2:A:715:PRO:HA	2:A:1072:GLU:HA	1.98	0.46
2:B:97:LYS:HA	2:B:97:LYS:HD2	1.75	0.46
2:B:176:LEU:O	2:B:178:ASP:N	2.49	0.46
2:B:1077:THR:OG1	2:B:1078:ALA:N	2.49	0.46
2:C:153:MET:SD	2:C:156:GLU:HG3	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:559:PHE:HB2	2:C:584:ILE:HD12	1.98	0.46
2:C:878:LEU:HD12	2:C:878:LEU:HA	1.76	0.46
1:I:71:ILE:HG13	1:I:81:TYR:O	2.16	0.45
2:A:147:LYS:HE3	2:A:248:TYR:HB2	1.98	0.45
2:A:382:VAL:HG21	2:A:390:LEU:HD12	1.97	0.45
2:A:675:GLN:O	2:A:677:GLN:NE2	2.46	0.45
2:A:756:TYR:OH	2:A:998:THR:HG22	2.16	0.45
2:B:406:GLU:O	2:B:410:ILE:N	2.50	0.45
2:C:519:HIS:HB3	2:C:565:PHE:HD2	1.81	0.45
1:G:34:HIS:HB3	1:G:100:TRP:HE3	1.82	0.45
2:A:462:LYS:HB2	2:A:465:GLU:HB2	1.98	0.45
2:A:894:LEU:HB3	2:B:713:ALA:HB3	1.98	0.45
2:B:118:LEU:HD12	2:B:118:LEU:H	1.80	0.45
2:B:352:ALA:O	2:B:466:ARG:NH2	2.49	0.45
2:B:629:LEU:HG	2:B:632:THR:H	1.80	0.45
2:C:131:CYS:HB3	2:C:133:PHE:CE1	2.52	0.45
2:C:334:ASN:HB2	2:C:361:CYS:C	2.37	0.45
2:C:402:ILE:O	2:C:508:TYR:N	2.39	0.45
1:G:118:THR:HG22	1:G:120:VAL:HG23	1.98	0.45
2:A:996:LEU:HD21	2:A:1000:ARG:CZ	2.46	0.45
2:A:1104:VAL:HG11	2:A:1119:ASN:OD1	2.17	0.45
2:C:650:LEU:HD12	2:C:650:LEU:HA	1.79	0.45
2:A:119:ILE:HG22	2:A:175:PHE:CZ	2.52	0.45
2:A:543:PHE:O	2:A:546:LEU:HB2	2.16	0.45
2:A:798:GLY:HA3	2:A:899:PRO:HG3	1.96	0.45
2:B:236:THR:HG21	4:B:1302:NAG:H5	1.99	0.45
2:B:320:VAL:HB	2:B:590:CYS:HB2	1.98	0.45
2:B:602:THR:O	2:B:603:ASN:C	2.54	0.45
2:C:457:ARG:NH2	2:C:459:SER:OG	2.49	0.45
2:C:786:LYS:HG3	2:C:787:GLN:HG3	1.98	0.45
2:A:32:PHE:HD2	2:A:218:GLN:HG2	1.82	0.45
2:A:190:ARG:HE	2:A:207:HIS:CG	2.35	0.45
2:A:191:GLU:O	2:A:223:LEU:HD13	2.16	0.45
2:A:589:PRO:HG3	2:C:855:PHE:HB2	1.99	0.45
2:A:931:ILE:O	2:A:934:ILE:HG22	2.17	0.45
2:B:33:THR:OG1	2:B:219:GLY:O	2.23	0.45
2:B:853:GLN:HB2	2:B:854:LYS:HZ2	1.81	0.45
2:C:137:ASN:H	2:C:159:VAL:HA	1.81	0.45
1:E:107:ASN:HB2	1:E:110:PRO:HD3	1.98	0.45
2:A:289:VAL:HG21	2:A:300:LYS:HD2	1.99	0.45
2:A:451:TYR:HD2	2:A:495:TYR:CD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:794:ILE:HG21	4:B:1308:NAG:H61	1.99	0.45
2:B:147:LYS:HA	2:B:147:LYS:HD3	1.78	0.45
2:C:128:ILE:HG13	2:C:229:LEU:HD11	1.99	0.45
2:C:1088:HIS:CE1	2:C:1137:VAL:HG11	2.52	0.45
1:G:45:GLU:OE2	2:C:450:ASN:ND2	2.50	0.45
2:A:294:ASP:HB3	2:A:297:SER:H	1.82	0.45
2:B:139:PRO:HA	2:B:157:PHE:HA	1.97	0.45
2:B:387:LEU:O	2:B:388:ASN:C	2.54	0.45
2:B:516:GLU:H	2:B:516:GLU:HG3	1.44	0.45
2:B:612:TYR:OH	2:B:629:LEU:HD13	2.16	0.45
2:C:30:ASN:HB3	2:C:32:PHE:CE1	2.52	0.45
1:I:39:ARG:HG3	1:I:95:TYR:CD1	2.47	0.45
2:A:118:LEU:H	2:A:118:LEU:HG	1.40	0.45
2:A:451:TYR:HD2	2:A:495:TYR:HD2	1.64	0.45
2:B:1138:TYR:HE1	2:B:1143:PRO:HG2	1.81	0.45
2:C:320:VAL:HG23	2:C:590:CYS:HB2	1.98	0.45
2:C:802:PHE:CD1	2:C:805:ILE:HD11	2.52	0.45
2:A:802:PHE:O	2:A:803:SER:C	2.55	0.45
2:B:43:PHE:HA	2:C:563:GLN:OE1	2.17	0.45
2:B:64:TRP:HD1	2:B:259:THR:HG23	1.82	0.45
2:B:449:TYR:O	2:B:494:SER:OG	2.35	0.45
2:C:964:LYS:HB2	2:C:964:LYS:HE2	1.82	0.45
1:E:73:ARG:HG3	1:E:80:VAL:HB	1.98	0.45
2:B:64:TRP:CZ3	2:B:262:ALA:HA	2.52	0.45
2:B:130:VAL:HG11	2:B:231:ILE:HG12	1.98	0.45
2:B:339:ASP:O	2:B:341:VAL:N	2.50	0.45
2:B:558:LYS:HE3	2:B:558:LYS:HB3	1.33	0.45
2:B:620:VAL:HB	2:B:621:PRO:HD3	1.98	0.45
2:B:917:TYR:HB3	2:C:1129:VAL:HG13	1.99	0.45
2:C:524:VAL:O	2:C:525:CYS:SG	2.74	0.45
2:C:728:PRO:O	2:C:1021:SER:OG	2.31	0.45
1:G:68:ARG:HB3	1:G:85:ASN:O	2.17	0.44
2:A:490:PHE:CE2	2:A:492:LEU:HB2	2.52	0.44
2:B:49:HIS:CE1	2:B:51:THR:HB	2.52	0.44
2:B:63:THR:HG1	2:B:65:PHE:HD1	1.63	0.44
2:B:502:GLY:O	2:B:506:GLN:N	2.50	0.44
2:B:616:ASN:O	2:B:617:CYS:C	2.55	0.44
2:B:673:SER:HB3	2:B:695:TYR:HE2	1.80	0.44
2:A:431:GLY:HA3	2:A:514:SER:HA	1.98	0.44
2:B:553:THR:HG23	2:B:586:ASP:HB3	1.99	0.44
2:B:1125:ASN:OD1	2:B:1125:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:PHE:CZ	2:C:89:GLY:HA2	2.52	0.44
2:C:339:ASP:C	2:C:341:VAL:N	2.71	0.44
2:C:443:SER:HB2	2:C:498:ARG:C	2.38	0.44
1:G:69:PHE:CE2	1:G:84:MET:HG2	2.52	0.44
2:A:150:LYS:HD2	2:A:150:LYS:HA	1.68	0.44
2:B:133:PHE:O	2:B:134:GLN:C	2.55	0.44
2:B:411:ALA:O	2:B:414:GLN:HG2	2.18	0.44
2:B:537:LYS:HG3	2:B:539:VAL:HG13	1.99	0.44
2:C:337:PRO:C	2:C:339:ASP:N	2.71	0.44
2:A:204:TYR:HA	2:A:225:PRO:HA	1.99	0.44
2:B:955:ASN:OD1	2:B:956:ALA:N	2.50	0.44
2:C:111:ASP:OD1	2:C:114:THR:OG1	2.35	0.44
1:G:44:LYS:HD2	1:G:44:LYS:HA	1.77	0.44
1:I:99:TYR:HB3	1:I:113:TYR:HB3	1.99	0.44
2:B:106:PHE:HD2	2:B:235:ILE:HG21	1.82	0.44
2:B:206:LYS:HB3	2:B:223:LEU:HD22	2.00	0.44
2:B:178:ASP:N	2:B:178:ASP:OD1	2.42	0.44
2:B:543:PHE:O	2:B:544:ASN:C	2.55	0.44
2:A:709:ASN:ND2	4:A:1307:NAG:O5	2.49	0.44
2:B:157:PHE:CD1	2:B:158:ARG:N	2.85	0.44
2:B:318:PHE:CE2	2:B:615:VAL:HG11	2.52	0.44
1:G:61:TYR:CE1	1:G:71:ILE:HG22	2.53	0.44
1:G:109:ILE:HD12	2:C:501:TYR:HA	2.00	0.44
2:A:105:ILE:HD12	2:A:116:SER:HB2	1.98	0.44
2:A:357:ARG:HD2	2:A:359:SER:HB2	1.99	0.44
2:B:722:VAL:HG22	2:B:1065:VAL:HG22	2.00	0.44
2:C:29:THR:HA	2:C:61:ASN:CA	2.48	0.44
2:C:329:PHE:O	2:C:331:ASN:N	2.50	0.44
2:C:560:LEU:O	2:C:561:PRO:C	2.56	0.44
2:A:59:PHE:HB2	2:A:293:LEU:HD11	1.99	0.44
2:A:676:THR:HG1	2:A:689:SER:HG	1.60	0.44
2:C:125:ASN:OD1	2:C:171:VAL:HG23	2.17	0.44
2:B:78:ARG:HD2	2:B:78:ARG:HA	1.36	0.43
2:B:613:GLN:HE21	2:B:613:GLN:HB2	1.57	0.43
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.77	0.43
2:B:1050:MET:HB2	2:B:1065:VAL:HB	2.00	0.43
2:C:128:ILE:HG21	2:C:229:LEU:HD11	1.99	0.43
2:C:555:SER:HB3	2:C:584:ILE:O	2.18	0.43
1:E:29:ALA:O	2:A:377:PHE:N	2.51	0.43
1:G:105:LEU:HD11	1:G:108:SER:HA	2.00	0.43
2:A:325:SER:HB2	2:A:540:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:715:PRO:HD3	2:C:894:LEU:HD13	1.99	0.43
2:A:927:PHE:O	2:A:928:ASN:C	2.56	0.43
2:B:858:LEU:HD13	2:B:959:LEU:HD22	1.99	0.43
2:C:168:PHE:CZ	2:C:230:PRO:HG2	2.53	0.43
2:C:733:LYS:HB2	2:C:861:LEU:HB2	1.99	0.43
1:I:38:PHE:HE2	1:I:100:TRP:NE1	2.16	0.43
2:A:44:ARG:HH11	2:B:567:ARG:HH11	1.65	0.43
2:A:58:PHE:HB2	2:A:290:ASP:HB2	2.00	0.43
2:A:121:ASN:CG	2:A:176:LEU:HB2	2.38	0.43
2:A:147:LYS:HA	2:A:147:LYS:HD3	1.86	0.43
2:A:603:ASN:N	2:A:603:ASN:OD1	2.51	0.43
2:A:1129:VAL:HG13	2:C:917:TYR:HB3	2.01	0.43
2:B:1145:LEU:O	2:B:1149:LYS:N	2.41	0.43
2:C:335:LEU:HD23	2:C:363:ALA:HA	2.00	0.43
2:A:597:VAL:HG22	2:A:610:VAL:HG12	2.00	0.43
2:A:1097:SER:C	2:A:1099:GLY:H	2.20	0.43
2:B:1123:SER:O	2:B:1123:SER:OG	2.31	0.43
2:C:54:LEU:HB3	2:C:270:LEU:HB3	2.01	0.43
2:C:146:HIS:CG	2:C:247:SER:H	2.37	0.43
2:C:328:ARG:HA	2:C:328:ARG:HD2	1.76	0.43
2:C:885:GLY:HA2	2:C:901:GLN:NE2	2.33	0.43
2:C:1117:THR:HG22	2:C:1140:PRO:HD2	2.01	0.43
2:A:540:ASN:HA	2:A:549:THR:HA	2.00	0.43
2:A:612:TYR:HE1	2:A:651:ILE:HD12	1.83	0.43
2:A:703:ASN:O	2:C:789:TYR:HA	2.18	0.43
2:A:1148:PHE:CE2	2:B:1145:LEU:HD13	2.53	0.43
1:E:68:ARG:HD2	1:E:86:SER:HB3	2.00	0.43
1:I:49:VAL:HG13	1:I:65:VAL:HG11	1.99	0.43
1:I:53:ASP:HB3	1:I:58:VAL:H	1.83	0.43
2:A:531:THR:OG1	2:A:532:ASN:N	2.52	0.43
2:A:644:GLN:HG2	4:A:1305:NAG:H82	2.00	0.43
2:B:75:GLY:O	2:B:76:THR:C	2.56	0.43
2:B:191:GLU:O	2:B:223:LEU:HD13	2.18	0.43
2:B:563:GLN:H	2:B:563:GLN:HG2	1.68	0.43
2:B:224:GLU:OE1	2:B:224:GLU:N	2.49	0.43
2:B:501:TYR:HB3	2:B:505:HIS:HB2	2.01	0.43
2:B:853:GLN:OE1	2:B:854:LYS:NZ	2.44	0.43
2:B:964:LYS:HZ2	2:C:570:ALA:HA	1.83	0.43
2:B:1073:LYS:HD3	2:B:1075:PHE:CZ	2.54	0.43
2:C:525:CYS:O	2:C:526:GLY:C	2.56	0.43
2:A:97:LYS:HD3	2:A:97:LYS:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:434:ILE:O	2:A:511:VAL:N	2.35	0.43
2:B:37:TYR:OH	2:B:53:ASP:OD1	2.37	0.43
2:B:320:VAL:HA	2:B:628:GLN:OE1	2.19	0.43
2:B:756:TYR:OH	2:B:994:ASP:OD1	2.35	0.43
2:C:519:HIS:CD2	2:C:567:ARG:NH2	2.75	0.43
2:A:30:ASN:O	2:A:32:PHE:N	2.51	0.43
2:A:490:PHE:HE2	2:A:492:LEU:HB2	1.84	0.43
2:A:1039:ARG:NE	2:C:1031:GLU:OE2	2.49	0.43
2:B:366:SER:O	2:B:369:TYR:HB2	2.19	0.43
2:C:125:ASN:OD1	2:C:127:VAL:N	2.52	0.43
2:C:454:ARG:HD3	2:C:457:ARG:HB2	2.00	0.43
1:I:74:ASP:HB2	1:I:81:TYR:CZ	2.53	0.43
2:A:421:TYR:O	2:A:457:ARG:NE	2.52	0.43
2:B:73:THR:OG1	2:B:247:SER:HB3	2.19	0.43
2:B:77:LYS:O	2:B:78:ARG:C	2.57	0.43
2:C:119:ILE:HG23	2:C:128:ILE:HD12	2.00	0.43
2:C:131:CYS:SG	2:C:166:CYS:N	2.91	0.43
2:C:191:GLU:H	2:C:191:GLU:HG2	1.61	0.43
2:C:572:THR:O	2:C:574:ASP:N	2.52	0.43
2:A:71:SER:O	2:A:250:THR:HB	2.19	0.42
2:A:559:PHE:HB3	2:A:577:ARG:HH21	1.84	0.42
2:A:1045:LYS:HE3	2:A:1045:LYS:HB2	1.80	0.42
2:B:1114:ILE:O	2:B:1119:ASN:ND2	2.52	0.42
1:I:19:LEU:HD13	1:I:87:LEU:HD13	2.01	0.42
2:A:117:LEU:O	2:A:119:ILE:HG12	2.19	0.42
2:A:314:GLN:OE1	2:A:315:THR:N	2.52	0.42
2:A:442:ASP:O	2:A:448:ASN:ND2	2.52	0.42
2:A:866:THR:HG23	2:A:869:MET:HE2	2.02	0.42
2:A:969:LYS:HD2	2:C:755:GLN:HE22	1.84	0.42
2:B:416:GLY:O	2:B:420:ASP:N	2.50	0.42
2:B:421:TYR:HB3	2:B:457:ARG:HB3	2.01	0.42
2:B:534:VAL:HG21	2:B:539:VAL:HG21	2.01	0.42
2:C:30:ASN:O	2:C:32:PHE:N	2.53	0.42
2:C:88:ASP:O	2:C:270:LEU:HB2	2.19	0.42
2:C:447:GLY:HA2	2:C:498:ARG:HG2	2.01	0.42
1:G:62:ALA:HB3	1:G:65:VAL:HG22	2.00	0.42
2:A:248:TYR:O	2:A:250:THR:N	2.51	0.42
2:A:546:LEU:HD23	2:A:546:LEU:HA	1.77	0.42
2:A:1018:ILE:O	2:A:1022:ALA:N	2.41	0.42
2:B:318:PHE:HA	2:B:630:THR:OG1	2.19	0.42
2:B:416:GLY:O	2:B:420:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:624:ILE:H	2:B:624:ILE:HG12	1.40	0.42
2:B:650:LEU:HD12	2:B:650:LEU:HA	1.89	0.42
2:C:567:ARG:HH11	2:C:567:ARG:H	1.65	0.42
1:I:52:ILE:HB	1:I:71:ILE:HG23	2.01	0.42
2:A:790:LYS:HD3	2:A:790:LYS:HA	1.84	0.42
2:C:188:ASN:O	2:C:190:ARG:HG3	2.19	0.42
2:A:36:VAL:HG11	2:A:220:PHE:CE2	2.55	0.42
2:A:392:PHE:C	2:A:522:ALA:HA	2.40	0.42
2:A:985:ASP:HB2	2:A:987:PRO:HD2	2.00	0.42
2:B:37:TYR:OH	2:B:195:LYS:NZ	2.52	0.42
2:B:37:TYR:HA	2:B:223:LEU:H	1.83	0.42
2:C:533:LEU:HG	2:C:533:LEU:O	2.18	0.42
1:G:23:CYS:HB2	1:G:97:CYS:HB2	1.81	0.42
1:I:40:GLN:H	1:I:40:GLN:CD	2.21	0.42
2:A:64:TRP:HB2	2:A:259:THR:H	1.84	0.42
2:A:309:GLU:OE1	2:A:310:LYS:N	2.52	0.42
2:A:422:ASN:OD1	2:A:454:ARG:HB3	2.20	0.42
2:A:748:GLU:H	2:A:748:GLU:CD	2.22	0.42
2:A:751:ASN:O	2:A:755:GLN:NE2	2.38	0.42
2:B:977:LEU:HD23	2:B:977:LEU:H	1.85	0.42
2:B:1047:TYR:O	2:B:1067:TYR:N	2.46	0.42
2:C:68:ILE:HA	2:C:250:THR:HB	2.01	0.42
2:C:462:LYS:HA	2:C:462:LYS:HD2	1.65	0.42
1:E:18:SER:HB3	1:E:83:GLN:HE21	1.84	0.42
1:I:40:GLN:HE22	1:I:94:THR:HB	1.85	0.42
2:A:78:ARG:HA	2:A:252:GLY:N	2.35	0.42
2:A:126:VAL:O	2:A:171:VAL:HA	2.19	0.42
2:A:350:VAL:HG22	2:A:422:ASN:HB3	2.02	0.42
2:C:214:ARG:NH1	2:C:215:ASP:OD1	2.52	0.42
2:C:1114:ILE:HD13	2:C:1114:ILE:HA	1.80	0.42
2:C:1144:GLU:OE1	2:C:1144:GLU:N	2.51	0.42
2:A:133:PHE:CD2	2:A:136:CYS:HA	2.54	0.42
2:A:146:HIS:CD2	2:A:147:LYS:H	2.38	0.42
2:A:998:THR:O	2:A:1002:GLN:HB2	2.20	0.42
2:B:36:VAL:O	2:B:223:LEU:HG	2.20	0.42
2:B:197:ILE:HG13	2:B:202:LYS:HZ3	1.84	0.42
2:B:376:ALA:N	2:B:435:ALA:O	2.50	0.42
2:B:993:ILE:HD13	2:B:993:ILE:HA	1.91	0.42
2:C:137:ASN:HB2	2:C:159:VAL:HA	2.00	0.42
2:C:451:TYR:HD2	2:C:497:PHE:HD2	1.68	0.42
1:G:65:VAL:HB	1:G:69:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:993:ILE:HD13	2:A:993:ILE:HA	1.87	0.42
2:B:121:ASN:CG	2:B:176:LEU:HB2	2.40	0.42
2:B:1125:ASN:ND2	2:B:1127:ASP:OD1	2.53	0.42
2:C:157:PHE:CD2	2:C:159:VAL:HG13	2.52	0.42
2:C:518:LEU:HD12	2:C:518:LEU:HA	1.84	0.42
2:C:523:THR:HG23	2:C:524:VAL:HG22	2.02	0.42
1:I:37:TRP:CD2	1:I:82:LEU:HD22	2.54	0.42
2:A:117:LEU:HD13	2:A:130:VAL:HG13	2.01	0.42
2:A:170:TYR:CE1	2:A:231:ILE:HD11	2.54	0.42
2:A:390:LEU:HB3	2:A:392:PHE:CZ	2.54	0.42
2:B:190:ARG:O	2:B:192:PHE:N	2.52	0.42
2:B:201:PHE:HB3	2:B:229:LEU:HB3	2.02	0.42
2:B:234:ASN:OD1	2:B:234:ASN:N	2.52	0.42
2:C:100:ILE:H	2:C:100:ILE:HG13	1.63	0.42
1:I:100:TRP:CD1	1:I:111:VAL:HG13	2.54	0.41
2:A:190:ARG:O	2:A:192:PHE:N	2.49	0.41
2:A:802:PHE:HZ	2:A:898:PHE:CZ	2.38	0.41
2:B:64:TRP:CD1	2:B:259:THR:HG23	2.55	0.41
2:B:143:VAL:HG13	2:B:245:HIS:CE1	2.54	0.41
2:B:559:PHE:HE2	2:B:564:GLN:O	2.03	0.41
2:B:1004:LEU:HD23	2:B:1004:LEU:HA	1.89	0.41
2:C:278:LYS:HE3	2:C:278:LYS:HB2	1.93	0.41
2:C:353:TRP:O	2:C:466:ARG:NE	2.39	0.41
2:C:580:GLN:C	2:C:582:LEU:N	2.73	0.41
2:A:169:GLU:OE2	2:A:171:VAL:HB	2.20	0.41
2:A:248:TYR:HD2	2:A:249:LEU:HG	1.84	0.41
2:A:707:TYR:HB3	2:C:792:PRO:HG2	2.00	0.41
2:B:157:PHE:HD1	2:B:158:ARG:H	1.66	0.41
2:C:67:ALA:O	2:C:250:THR:HB	2.19	0.41
2:C:129:LYS:HE3	2:C:129:LYS:HB2	1.83	0.41
2:C:728:PRO:HB3	2:C:951:VAL:HG21	2.01	0.41
1:E:39:ARG:NH2	1:E:64:SER:OG	2.52	0.41
1:G:71:ILE:HA	1:G:82:LEU:HA	2.03	0.41
2:A:138:ASP:OD1	2:A:139:PRO:HD2	2.21	0.41
2:B:131:CYS:HB3	2:B:133:PHE:CZ	2.55	0.41
2:C:371:PHE:HZ	2:C:436:TRP:CE3	2.38	0.41
2:C:1045:LYS:HB2	2:C:1045:LYS:HE2	1.72	0.41
1:E:73:ARG:HH12	1:E:78:ASN:HA	1.85	0.41
1:I:24:ALA:HB2	1:I:79:THR:HG22	2.01	0.41
2:B:176:LEU:HA	2:B:190:ARG:HH22	1.85	0.41
2:B:335:LEU:HD13	2:B:335:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:LEU:HA	2:B:461:LEU:HD23	1.81	0.41
2:C:540:ASN:OD1	2:C:549:THR:OG1	2.38	0.41
2:C:849:LEU:HG	2:C:851:CYS:H	1.85	0.41
2:C:1054:GLN:N	2:C:1061:VAL:O	2.50	0.41
1:I:69:PHE:HA	1:I:84:MET:HB3	2.01	0.41
2:A:29:THR:HA	2:A:260:ALA:N	2.35	0.41
2:A:83:VAL:HG11	2:A:237:ARG:NH2	2.35	0.41
2:A:811:LYS:HE3	2:A:811:LYS:HB2	1.80	0.41
2:B:73:THR:HG23	2:B:79:PHE:CZ	2.55	0.41
2:B:189:LEU:O	2:B:191:GLU:HG3	2.21	0.41
2:B:375:PHE:HA	2:B:436:TRP:HB3	2.03	0.41
2:C:127:VAL:HG23	2:C:169:GLU:HB3	2.02	0.41
2:C:402:ILE:HD11	2:C:407:VAL:HA	2.01	0.41
1:I:100:TRP:HB3	1:I:102:MET:SD	2.60	0.41
2:A:34:ARG:HH22	2:A:221:SER:N	2.14	0.41
2:A:144:TYR:HA	2:A:146:HIS:CE1	2.56	0.41
2:A:423:TYR:HA	2:A:461:LEU:HD12	2.02	0.41
2:A:433:VAL:HG22	2:A:512:VAL:HG22	2.03	0.41
2:A:986:PRO:N	2:A:987:PRO:HD2	2.35	0.41
2:B:473:TYR:CZ	2:B:475:ALA:HB2	2.56	0.41
2:C:126:VAL:HG13	2:C:174:PRO:HA	2.03	0.41
2:C:715:PRO:HA	2:C:1072:GLU:HA	2.03	0.41
2:C:996:LEU:HD21	2:C:1000:ARG:CZ	2.50	0.41
2:B:347:PHE:HE2	2:B:511:VAL:HG22	1.86	0.41
2:B:559:PHE:O	2:B:560:LEU:C	2.59	0.41
2:B:1114:ILE:HD12	2:B:1114:ILE:HA	1.75	0.41
2:C:412:PRO:HB3	2:C:427:ASP:HA	2.02	0.41
1:I:21:LEU:HD23	1:I:21:LEU:HA	1.94	0.41
2:A:409:GLN:O	2:A:419:ALA:HB2	2.21	0.41
2:A:420:ASP:O	2:A:460:ASN:HA	2.20	0.41
2:A:1104:VAL:HG21	2:A:1119:ASN:OD1	2.21	0.41
2:B:122:ASN:HB3	2:B:153:MET:SD	2.61	0.41
2:B:222:ALA:HB2	2:B:285:ILE:HB	2.02	0.41
2:C:141:LEU:HD12	2:C:144:TYR:HA	2.03	0.41
2:C:663:ASP:HB3	2:C:673:SER:HB3	2.03	0.41
1:E:40:GLN:HB3	1:E:96:TYR:CE1	2.56	0.41
1:G:5:LEU:HD13	1:G:114:TRP:O	2.21	0.41
2:A:141:LEU:HD23	2:A:141:LEU:HA	1.85	0.41
2:A:375:PHE:HB3	2:A:436:TRP:CB	2.50	0.41
2:A:417:ASN:HA	2:A:421:TYR:CD2	2.55	0.41
2:A:449:TYR:O	2:A:494:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:578:ASP:HB2	2:A:585:LEU:HD23	2.02	0.41
2:A:722:VAL:HG22	2:A:1065:VAL:HG22	2.03	0.41
2:A:1093:GLY:HA2	2:A:1107:ARG:HD2	2.02	0.41
2:B:117:LEU:CD2	2:B:233:ILE:HD13	2.50	0.41
2:B:242:LEU:O	2:B:243:ALA:C	2.59	0.41
2:B:246:ARG:O	2:B:247:SER:C	2.59	0.41
2:B:273:ARG:HD3	2:B:273:ARG:HA	1.91	0.41
2:B:314:GLN:HA	2:B:596:SER:HA	2.02	0.41
2:B:369:TYR:HD1	2:B:369:TYR:HA	1.79	0.41
2:B:555:SER:HB3	2:B:584:ILE:C	2.42	0.41
2:C:124:THR:O	2:C:124:THR:OG1	2.38	0.41
2:C:730:SER:O	2:C:1058:HIS:HB3	2.20	0.41
2:A:320:VAL:HG21	2:A:620:VAL:HG21	2.03	0.41
2:B:117:LEU:HD23	2:B:233:ILE:HD13	2.03	0.41
2:B:242:LEU:O	2:B:244:LEU:N	2.54	0.41
2:B:454:ARG:HG3	2:B:491:PRO:HB2	2.03	0.41
2:C:584:ILE:H	2:C:584:ILE:HG12	1.53	0.41
2:C:852:ALA:O	2:C:855:PHE:HB3	2.21	0.41
2:C:1080:ALA:HB3	2:C:1132:ILE:HD12	2.03	0.41
1:E:72:SER:O	1:E:81:TYR:N	2.28	0.40
2:A:63:THR:HA	2:A:257:GLY:HA2	2.04	0.40
2:A:170:TYR:OH	2:A:230:PRO:HD2	2.21	0.40
2:A:559:PHE:CD1	2:A:584:ILE:HD12	2.57	0.40
2:A:805:ILE:HD13	2:A:931:ILE:HD11	2.03	0.40
2:B:359:SER:HB3	2:B:522:ALA:CB	2.51	0.40
2:C:281:GLU:O	2:C:283:GLY:N	2.53	0.40
2:A:133:PHE:HA	2:A:162:SER:HA	2.02	0.40
2:A:631:PRO:O	2:A:633:TRP:NE1	2.54	0.40
2:B:164:ASN:HB3	2:B:165:ASN:H	1.59	0.40
2:B:350:VAL:CG1	2:B:422:ASN:HD21	2.34	0.40
2:B:985:ASP:N	2:B:985:ASP:OD1	2.52	0.40
2:B:1097:SER:C	2:B:1099:GLY:H	2.25	0.40
2:C:64:TRP:CD1	2:C:66:HIS:CD2	3.08	0.40
2:C:541:PHE:CZ	2:C:587:ILE:HD13	2.57	0.40
2:C:1146:ASP:O	2:C:1150:GLU:N	2.42	0.40
2:A:167:THR:HG22	2:A:168:PHE:N	2.36	0.40
2:A:425:LEU:HD23	2:A:425:LEU:HA	1.93	0.40
2:A:867:ASP:OD1	2:A:867:ASP:N	2.52	0.40
2:A:1054:GLN:N	2:A:1061:VAL:O	2.53	0.40
2:B:195:LYS:HB3	2:B:195:LYS:HE2	1.84	0.40
2:B:453:TYR:HB3	2:B:495:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:THR:C	2:C:61:ASN:HA	2.42	0.40
2:C:271:GLN:O	2:C:273:ARG:N	2.55	0.40
2:C:473:TYR:H	2:C:491:PRO:HD3	1.85	0.40
2:C:814:LYS:HA	2:C:814:LYS:HD3	1.84	0.40
2:C:1141:LEU:O	2:C:1145:LEU:N	2.55	0.40
1:I:111:VAL:O	1:I:112:ASP:C	2.60	0.40
2:B:54:LEU:HB3	2:B:270:LEU:HD23	2.03	0.40
2:B:387:LEU:HA	2:B:387:LEU:HD22	1.90	0.40
2:B:453:TYR:OH	2:B:455:LEU:HD22	2.21	0.40
2:C:58:PHE:HD1	2:C:58:PHE:HA	1.75	0.40
2:C:105:ILE:HB	2:C:241:LEU:HD11	2.03	0.40
2:C:393:THR:OG1	2:C:394:ASN:N	2.55	0.40
2:C:611:LEU:HD12	2:C:649:CYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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	E	123/124 (99%)	112 (91%)	11 (9%)	0	100	100
1	G	123/124 (99%)	113 (92%)	10 (8%)	0	100	100
1	I	123/124 (99%)	115 (94%)	8 (6%)	0	100	100
2	A	1073/1288 (83%)	949 (88%)	104 (10%)	20 (2%)	6	26
2	B	1071/1288 (83%)	903 (84%)	147 (14%)	21 (2%)	6	25
2	C	1074/1288 (83%)	932 (87%)	121 (11%)	21 (2%)	6	25
All	All	3587/4236 (85%)	3124 (87%)	401 (11%)	62 (2%)	10	27

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	77	LYS
2	A	78	ARG
2	A	245	HIS
2	A	333	THR
2	A	618	THR
2	B	44	ARG
2	B	251	PRO
2	B	363	ALA
2	C	231	ILE
2	C	330	PRO
2	C	370	ASN
2	C	570	ALA
2	A	31	SER
2	A	64	TRP
2	A	73	THR
2	A	118	LEU
2	A	332	ILE
2	B	73	THR
2	B	76	THR
2	B	145	TYR
2	B	163	ALA
2	B	248	TYR
2	B	330	PRO
2	B	619	GLU
2	C	245	HIS
2	C	282	ASN
2	C	526	GLY
2	C	544	ASN
2	C	571	ASP
2	C	581	THR
2	A	30	ASN
2	A	63	THR
2	A	260	ALA
2	B	78	ARG
2	B	243	ALA
2	B	340	GLU
2	B	561	PRO
2	B	617	CYS
2	C	331	ASN
2	A	66	HIS
2	A	249	LEU
2	A	336	CYS
2	A	393	THR

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Mol	Chain	Res	Type
2	B	329	PHE
2	B	360	ASN
2	B	618	THR
2	C	336	CYS
2	C	532	ASN
2	C	546	LEU
2	C	564	GLN
2	A	534	VAL
2	B	381	GLY
2	C	360	ASN
2	C	361	CYS
2	C	620	VAL
2	A	285	ILE
2	B	245	HIS
2	C	362	VAL
2	A	233	ILE
2	B	336	CYS
2	C	566	GLY
2	C	561	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	102/101 (101%)	99 (97%)	3 (3%)	37	62
1	G	100/101 (99%)	92 (92%)	8 (8%)	10	32
1	I	102/101 (101%)	96 (94%)	6 (6%)	16	42
2	A	931/1113 (84%)	877 (94%)	54 (6%)	17	43
2	B	934/1113 (84%)	829 (89%)	105 (11%)	5	18
2	C	939/1113 (84%)	874 (93%)	65 (7%)	13	38
All	All	3108/3642 (85%)	2867 (92%)	241 (8%)	13	33

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	26[A]	SER
1	E	26[B]	SER
1	E	107	ASN
1	G	20	ARG
1	G	28	TRP
1	G	35	MET
1	G	46	ARG
1	G	52	ILE
1	G	79	THR
1	G	97	CYS
1	G	107	ASN
1	I	1	SER
1	I	12	PHE
1	I	38	PHE
1	I	102	MET
1	I	112	ASP
1	I	113	TYR
2	A	65	PHE
2	A	71	SER
2	A	73	THR
2	A	77	LYS
2	A	80	ASP
2	A	105	ILE
2	A	117	LEU
2	A	118	LEU
2	A	130	VAL
2	A	132	GLU
2	A	134	GLN
2	A	175	PHE
2	A	182	LYS
2	A	186	PHE
2	A	220	PHE
2	A	233	ILE
2	A	244	LEU
2	A	250	THR
2	A	256	SER
2	A	259	THR
2	A	281	GLU
2	A	284	THR
2	A	335	LEU
2	A	336	CYS
2	A	347	PHE
2	A	362	VAL

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Mol	Chain	Res	Type
2	A	375	PHE
2	A	387	LEU
2	A	389	ASP
2	A	390	LEU
2	A	394	ASN
2	A	495	TYR
2	A	523	THR
2	A	524	VAL
2	A	533	LEU
2	A	556	ASN
2	A	558	LYS
2	A	559	PHE
2	A	591	SER
2	A	600	PRO
2	A	605	SER
2	A	618	THR
2	A	619	GLU
2	A	690	GLN
2	A	721	SER
2	A	764	LYS
2	A	811	LYS
2	A	884	SER
2	A	886	TRP
2	A	931	ILE
2	A	967	SER
2	A	1050	MET
2	A	1097	SER
2	A	1111	GLU
2	B	40	ASP
2	B	42	VAL
2	B	44	ARG
2	B	46	SER
2	B	61	ASN
2	B	66	HIS
2	B	73	THR
2	B	77	LYS
2	B	78	ARG
2	B	80	ASP
2	B	126	VAL
2	B	132	GLU
2	B	134	GLN
2	B	157	PHE

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Mol	Chain	Res	Type
2	B	186	PHE
2	B	202	LYS
2	B	212	LEU
2	B	214	ARG
2	B	215	ASP
2	B	220	PHE
2	B	239	GLN
2	B	240	THR
2	B	242	LEU
2	B	247	SER
2	B	248	TYR
2	B	249	LEU
2	B	255	SER
2	B	259	THR
2	B	281	GLU
2	B	307	THR
2	B	308	VAL
2	B	309	GLU
2	B	327	VAL
2	B	329	PHE
2	B	333	THR
2	B	334	ASN
2	B	335	LEU
2	B	336	CYS
2	B	338	PHE
2	B	347	PHE
2	B	359	SER
2	B	360	ASN
2	B	361	CYS
2	B	369	TYR
2	B	375	PHE
2	B	378	LYS
2	B	382	VAL
2	B	383	SER
2	B	386	LYS
2	B	387	LEU
2	B	389	ASP
2	B	390	LEU
2	B	391	CYS
2	B	395	VAL
2	B	400	PHE
2	B	402	ILE

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Mol	Chain	Res	Type
2	B	403	ARG
2	B	423	TYR
2	B	428	ASP
2	B	433	VAL
2	B	434	ILE
2	B	438	SER
2	B	449	TYR
2	B	452	ARG
2	B	495	TYR
2	B	503	VAL
2	B	513	LEU
2	B	516	GLU
2	B	517	LEU
2	B	524	VAL
2	B	537	LYS
2	B	557	LYS
2	B	558	LYS
2	B	561	PRO
2	B	580	GLN
2	B	581	THR
2	B	582	LEU
2	B	584	ILE
2	B	590	CYS
2	B	602	THR
2	B	605	SER
2	B	617	CYS
2	B	618	THR
2	B	619	GLU
2	B	624	ILE
2	B	629	LEU
2	B	640	SER
2	B	657	ASN
2	B	710	ASN
2	B	759	PHE
2	B	811	LYS
2	B	849	LEU
2	B	873	TYR
2	B	901	GLN
2	B	933	LYS
2	B	963	VAL
2	B	967	SER
2	B	1000	ARG

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Mol	Chain	Res	Type
2	B	1081	ILE
2	B	1096	VAL
2	B	1101	HIS
2	B	1104	VAL
2	B	1114	ILE
2	B	1115	ILE
2	B	1119	ASN
2	C	31	SER
2	C	62	VAL
2	C	68	ILE
2	C	73	THR
2	C	74	ASN
2	C	134	GLN
2	C	206	LYS
2	C	214	ARG
2	C	220	PHE
2	C	248	TYR
2	C	259	THR
2	C	278	LYS
2	C	280	ASN
2	C	327	VAL
2	C	329	PHE
2	C	333	THR
2	C	334	ASN
2	C	335	LEU
2	C	336	CYS
2	C	338	PHE
2	C	341	VAL
2	C	343	ASN
2	C	358	ILE
2	C	360	ASN
2	C	362	VAL
2	C	367	VAL
2	C	368	LEU
2	C	370	ASN
2	C	377	PHE
2	C	388	ASN
2	C	389	ASP
2	C	424	LYS
2	C	477	ASN
2	C	495	TYR
2	C	501	TYR

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Mol	Chain	Res	Type
2	C	523	THR
2	C	524	VAL
2	C	531	THR
2	C	532	ASN
2	C	533	LEU
2	C	535	LYS
2	C	557	LYS
2	C	558	LYS
2	C	561	PRO
2	C	567	ARG
2	C	569	ILE
2	C	574	ASP
2	C	583	GLU
2	C	584	ILE
2	C	603	ASN
2	C	617	CYS
2	C	810	SER
2	C	873	TYR
2	C	936	ASP
2	C	1081	ILE
2	C	1097	SER
2	C	1111	GLU
2	C	1114	ILE
2	C	1115	ILE
2	C	1117	THR
2	C	1132	ILE
2	C	1136	THR
2	C	1138	TYR
2	C	1141	LEU
2	C	1145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	121	ASN
2	A	992	GLN
2	B	74	ASN
2	B	81	ASN
2	B	115	GLN
2	B	165	ASN
2	B	196	ASN
2	B	245	HIS

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Mol	Chain	Res	Type
2	B	331	ASN
2	B	422	ASN
2	B	580	GLN
2	C	122	ASN
2	C	245	HIS
2	C	334	ASN
2	C	519	HIS
2	C	542	ASN
2	C	954	HIS
2	C	1101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	K	1	3,2	14,14,15	0.28	0	17,19,21	0.47	0
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	L	1	3,2	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	L	2	3	14,14,15	0.18	0	17,19,21	0.36	0
3	NAG	M	1	3,2	14,14,15	0.39	0	17,19,21	0.40	0
3	NAG	M	2	3	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	N	1	3,2	14,14,15	0.40	0	17,19,21	0.57	0
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	0.43	0
3	NAG	R	1	3,2	14,14,15	0.26	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	R	2	3	14,14,15	0.17	0	17,19,21	0.37	0
3	NAG	S	1	3,2	14,14,15	0.39	0	17,19,21	0.40	0
3	NAG	S	2	3	14,14,15	0.16	0	17,19,21	0.40	0
3	NAG	T	1	3,2	14,14,15	0.39	0	17,19,21	0.90	2 (11%)
3	NAG	T	2	3	14,14,15	0.40	0	17,19,21	0.33	0
3	NAG	U	1	3,2	14,14,15	0.39	0	17,19,21	0.57	0
3	NAG	U	2	3	14,14,15	0.39	0	17,19,21	0.67	0
3	NAG	X	1	3,2	14,14,15	0.38	0	17,19,21	0.40	0
3	NAG	X	2	3	14,14,15	0.19	0	17,19,21	0.36	0
3	NAG	Y	1	3,2	14,14,15	0.42	0	17,19,21	0.56	0
3	NAG	Y	2	3	14,14,15	0.42	0	17,19,21	0.38	0
3	NAG	Z	1	3,2	14,14,15	0.39	0	17,19,21	0.85	2 (11%)
3	NAG	Z	2	3	14,14,15	0.41	0	17,19,21	0.35	0
3	NAG	a	1	3,2	14,14,15	0.59	0	17,19,21	0.44	0
3	NAG	a	2	3	14,14,15	0.22	0	17,19,21	0.39	0

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

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C1-O5-C5	2.25	115.24	112.19
3	T	1	NAG	O5-C1-C2	2.21	114.78	111.29
3	Z	1	NAG	O5-C1-C2	-2.06	108.04	111.29
3	Z	1	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (41) torsion outliers are listed below:

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

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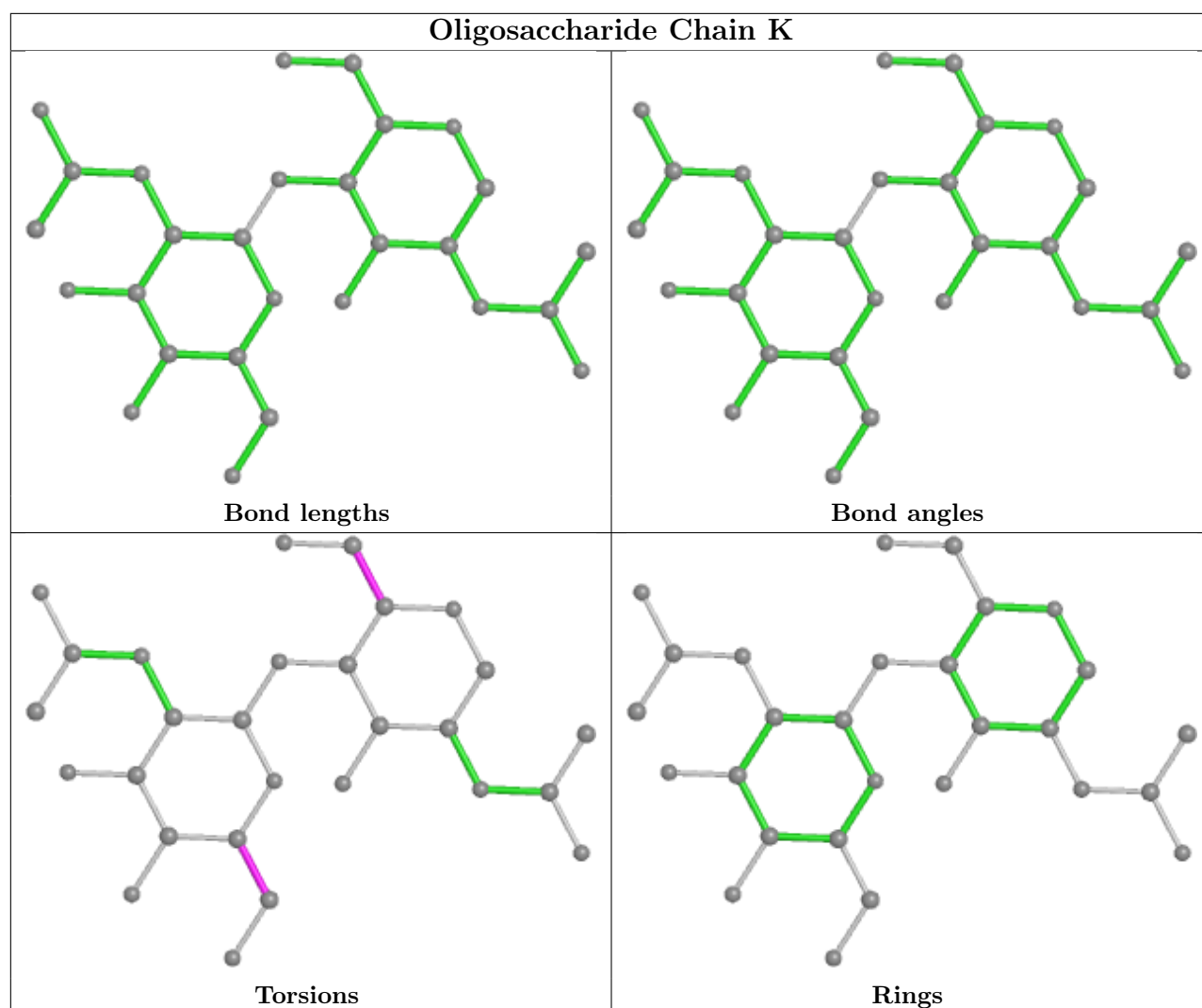
Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O7-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	N	2	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O7-C7-N2-C2
3	X	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	T	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C4-C5-C6-O6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

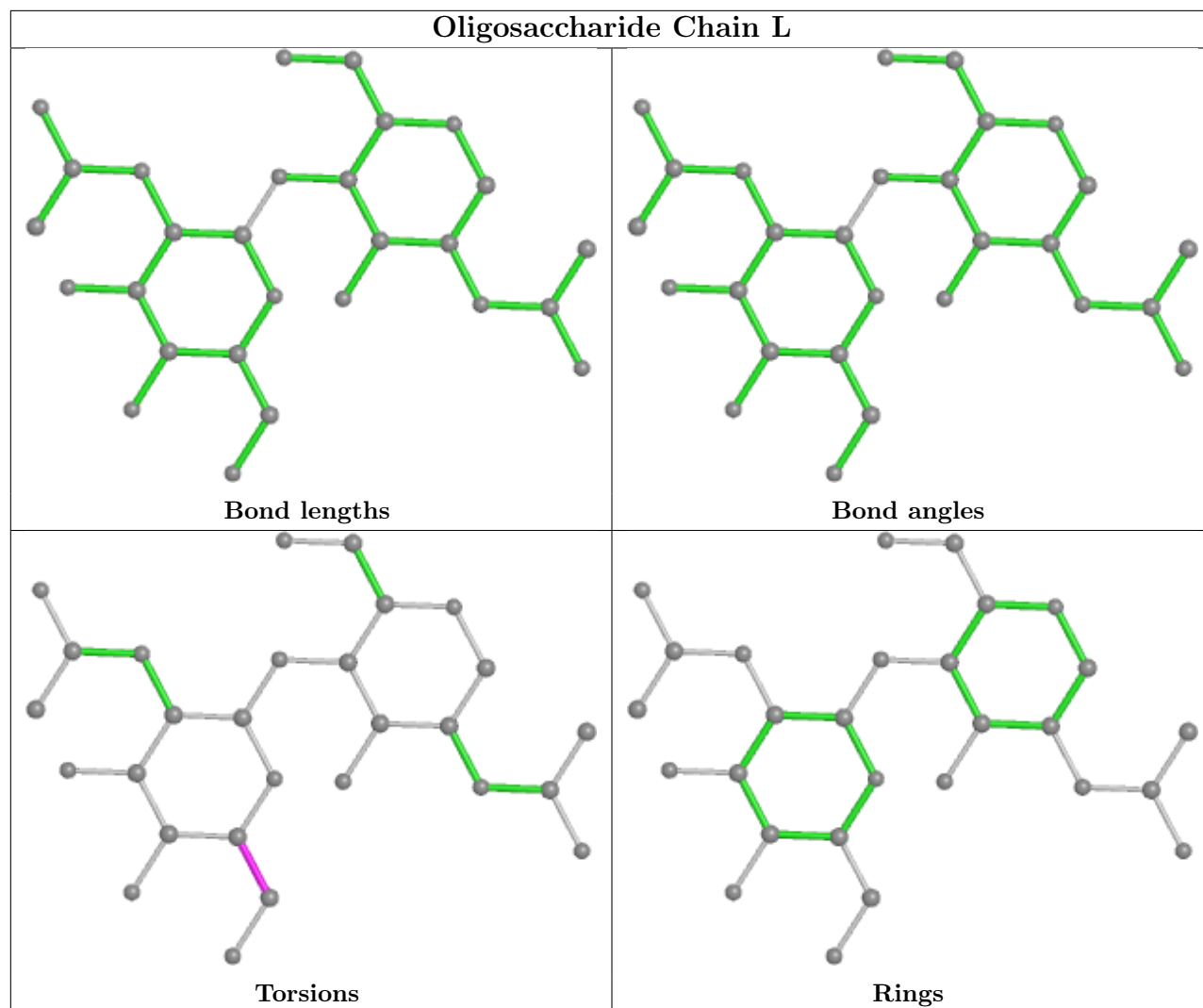
There are no ring outliers.

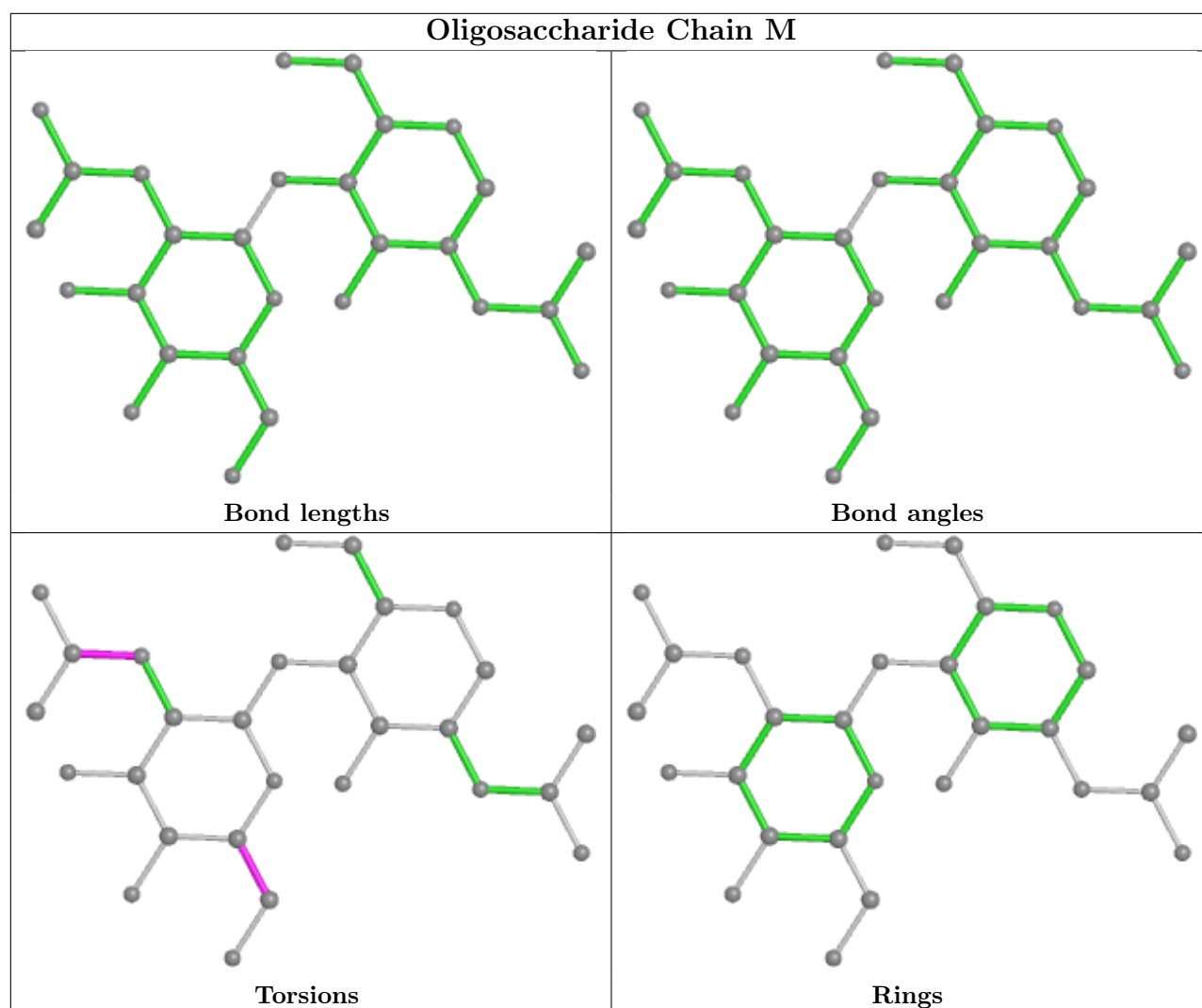
4 monomers are involved in 4 short contacts:

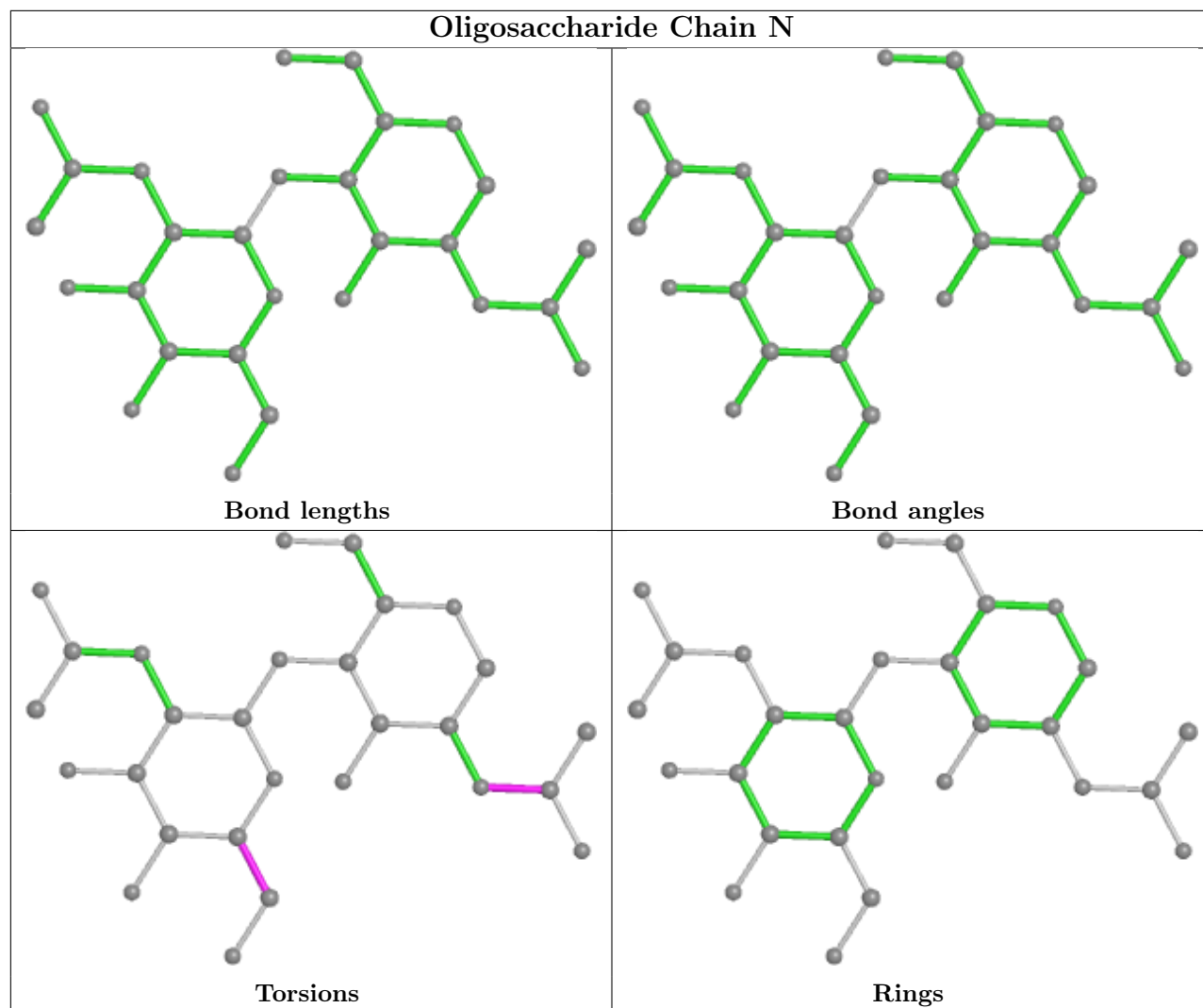
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	1	NAG	1	0
3	R	1	NAG	1	0
3	K	1	NAG	1	0
3	X	1	NAG	1	0

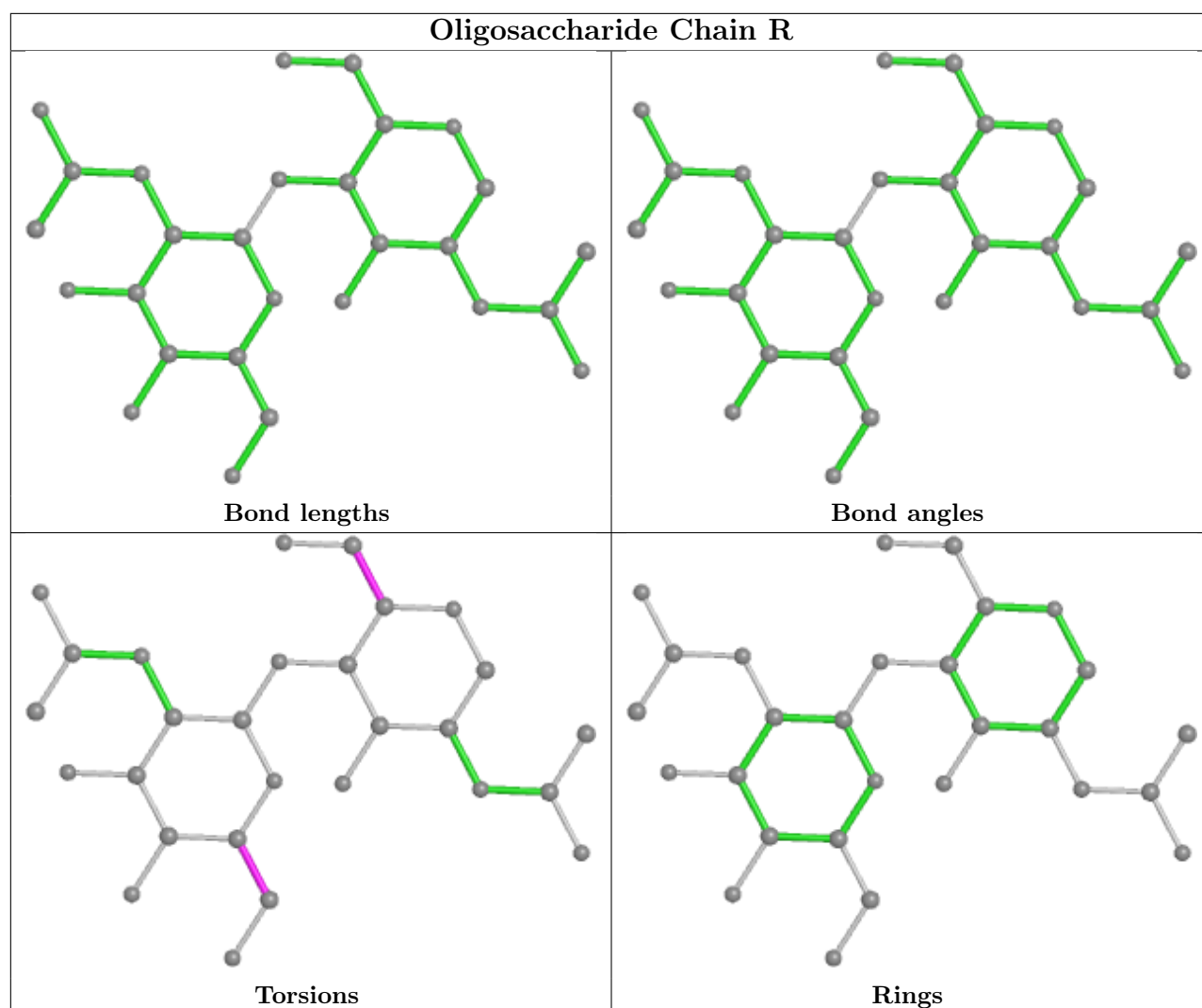
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

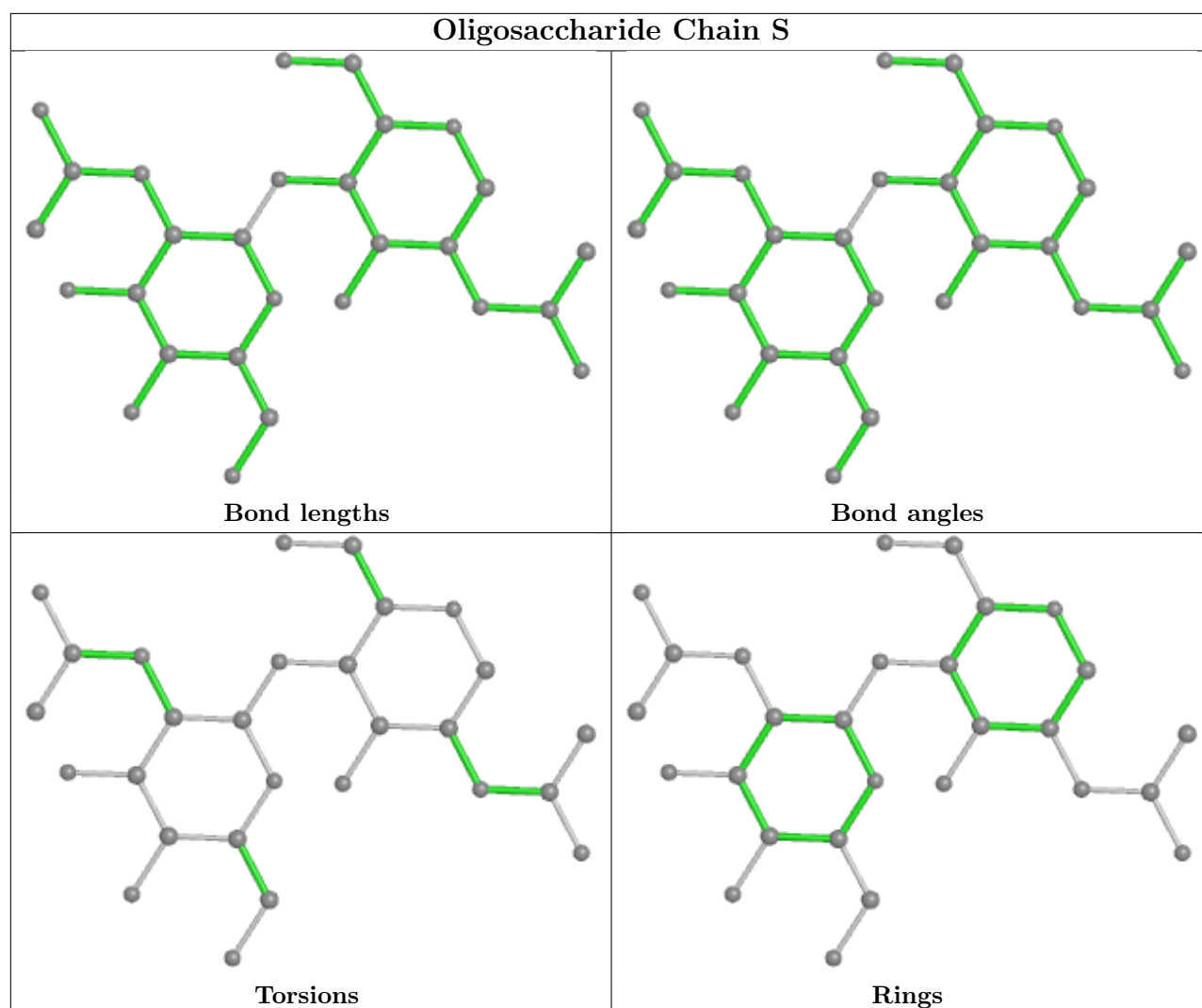


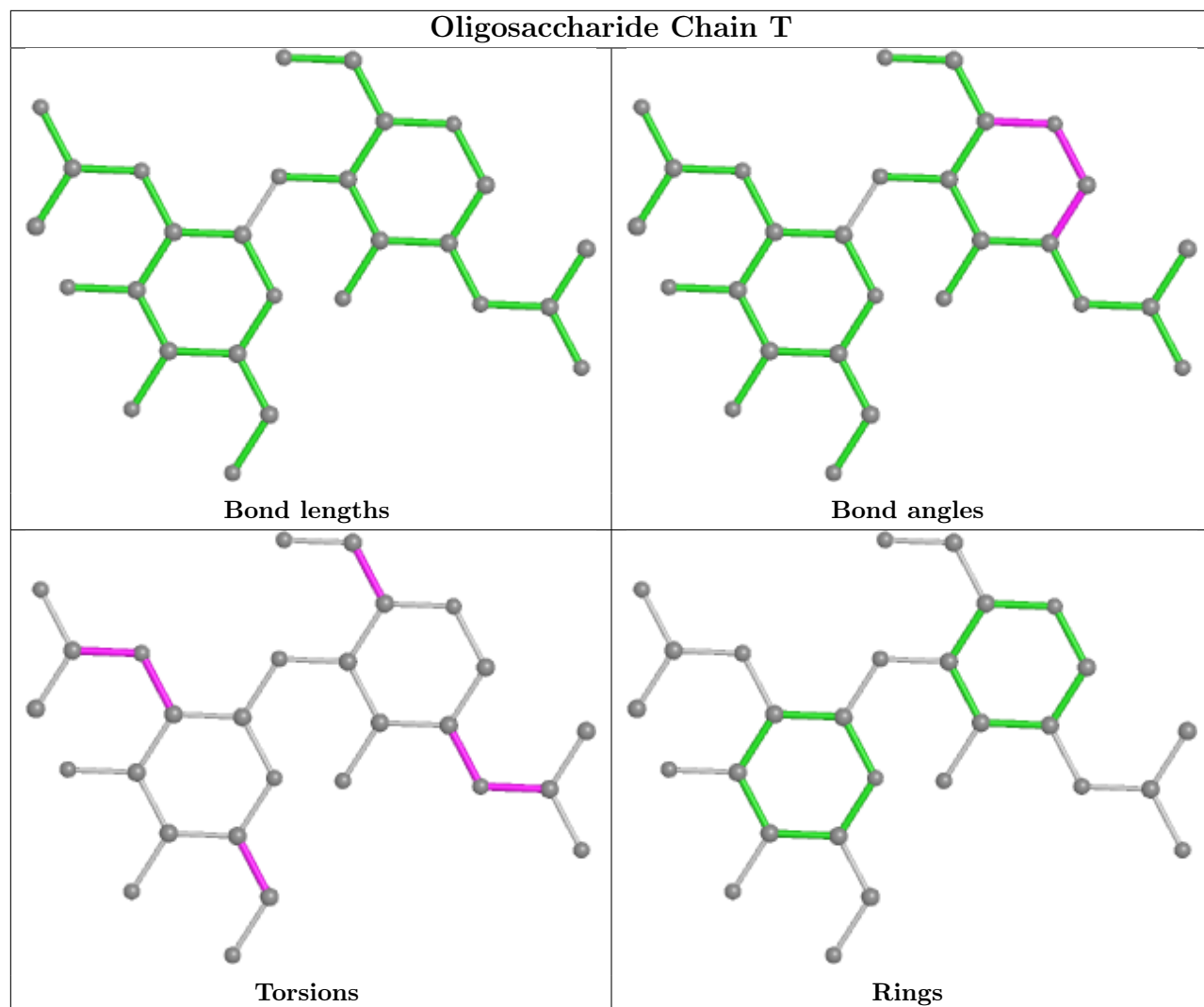


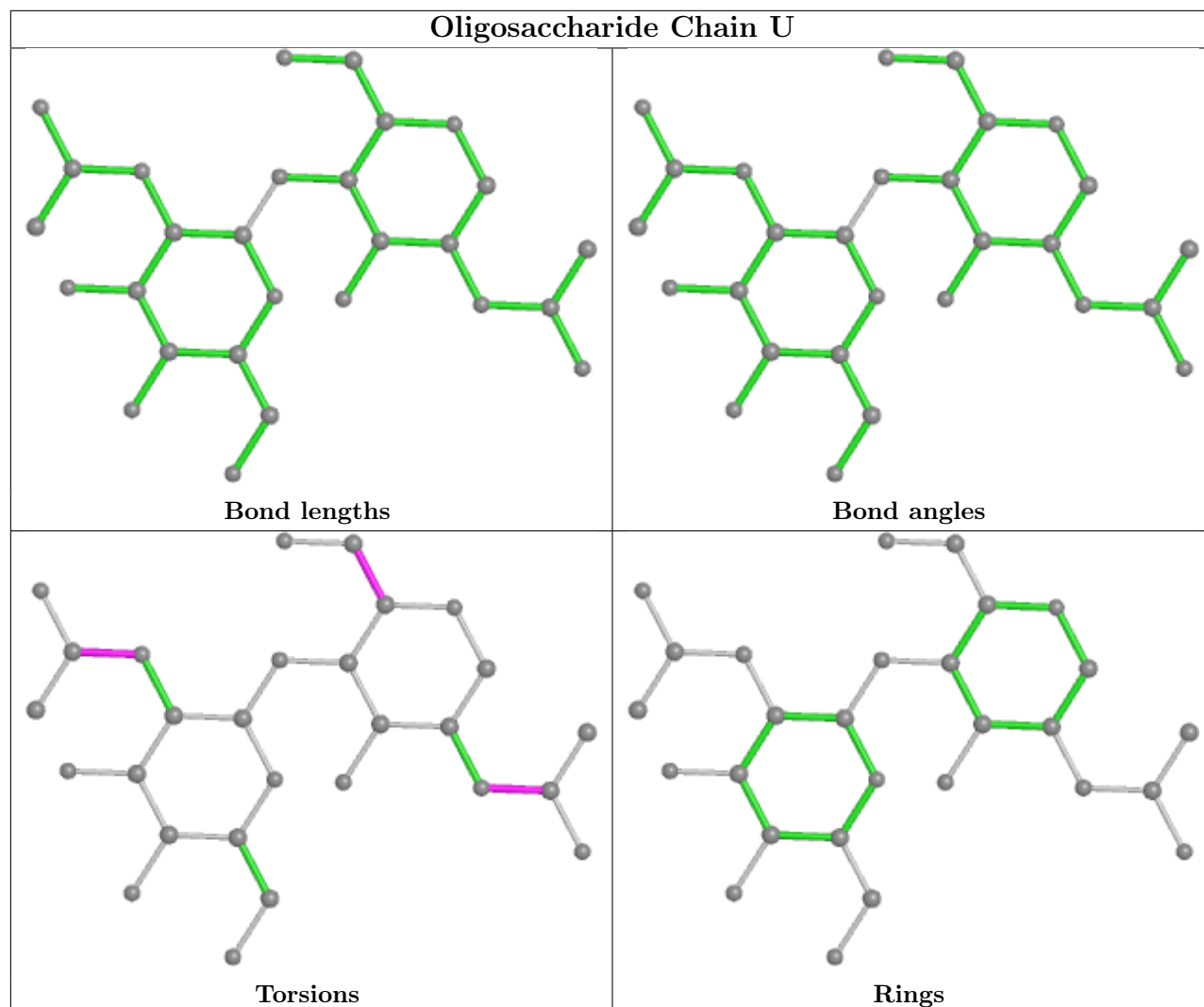


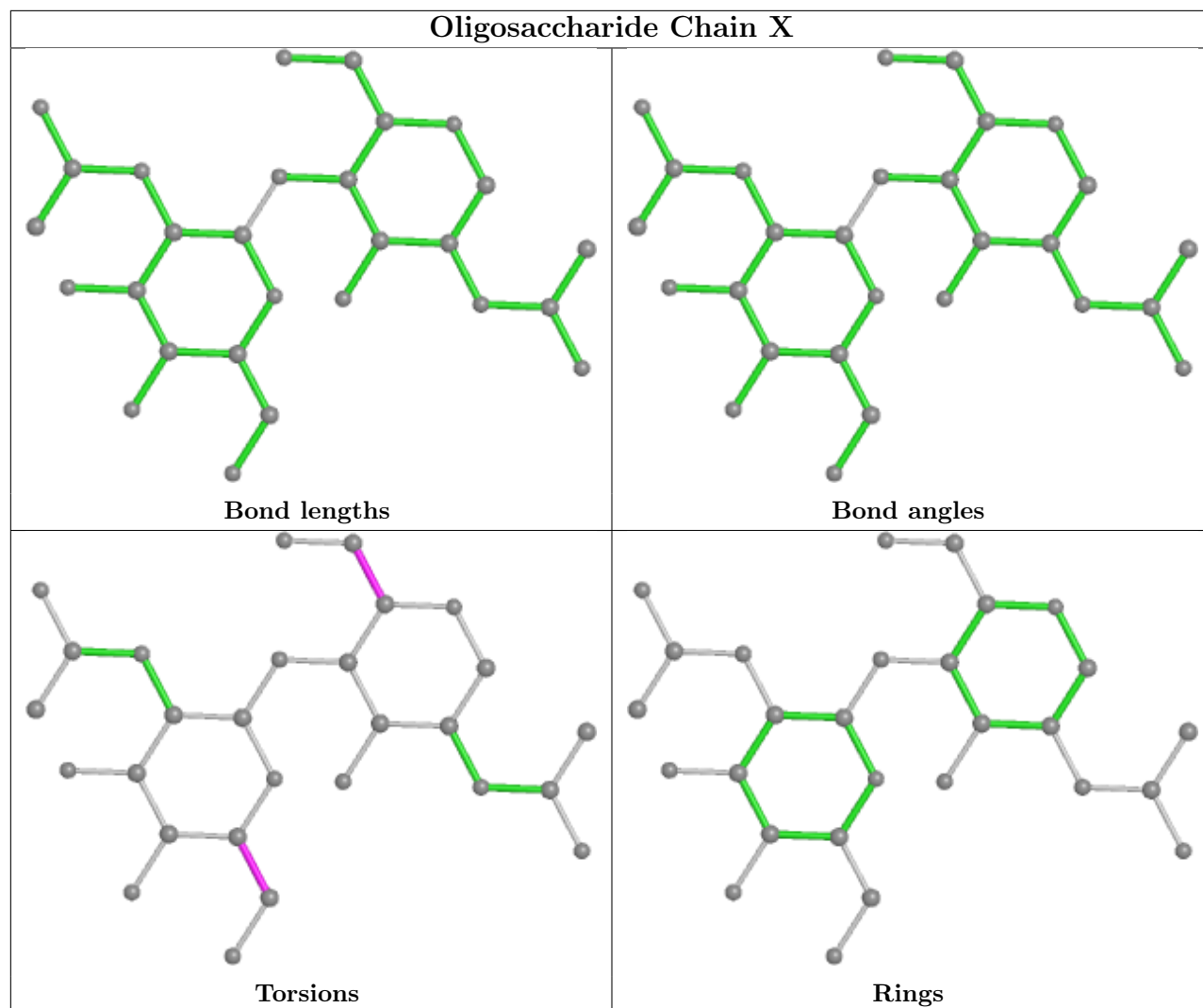


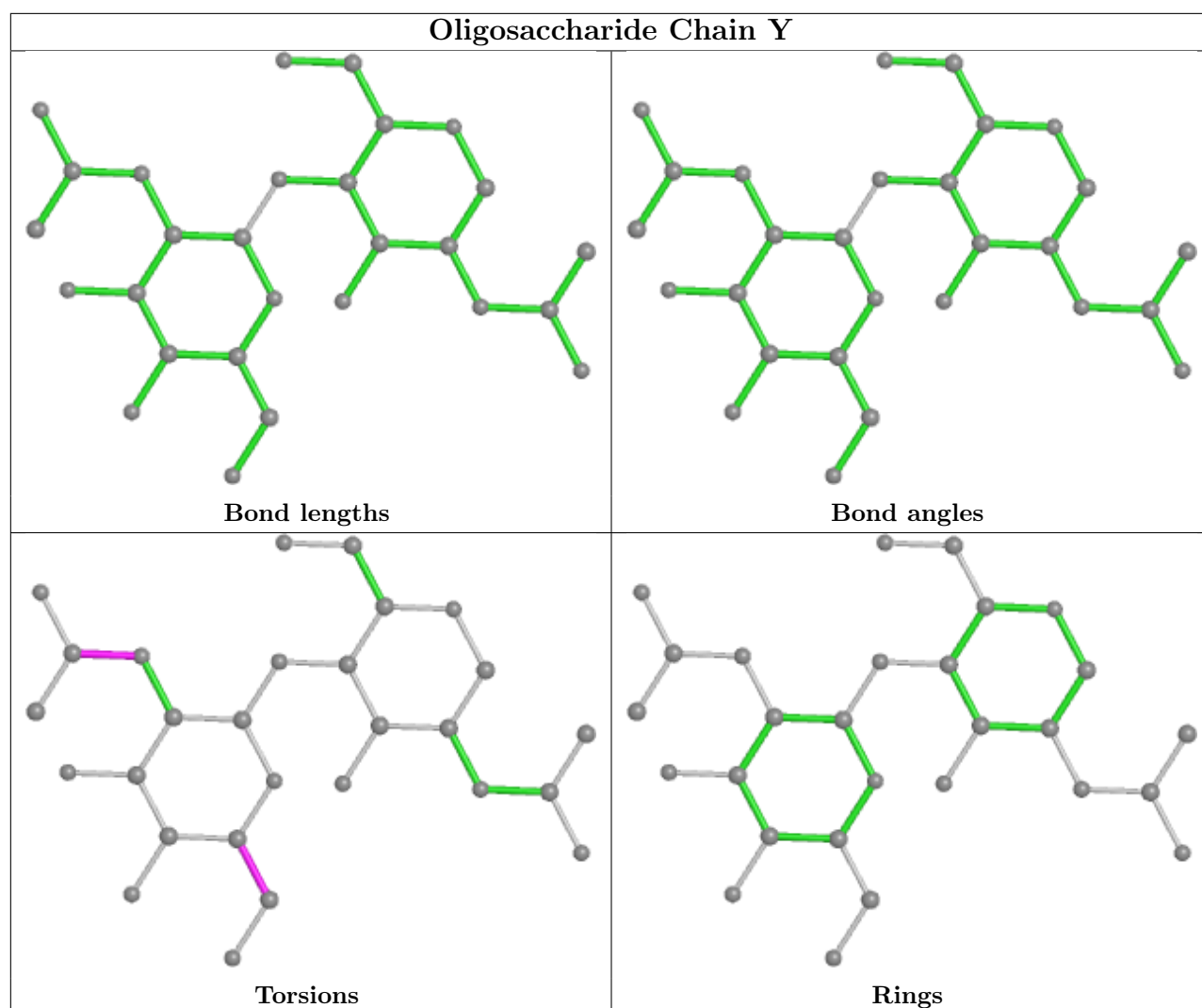


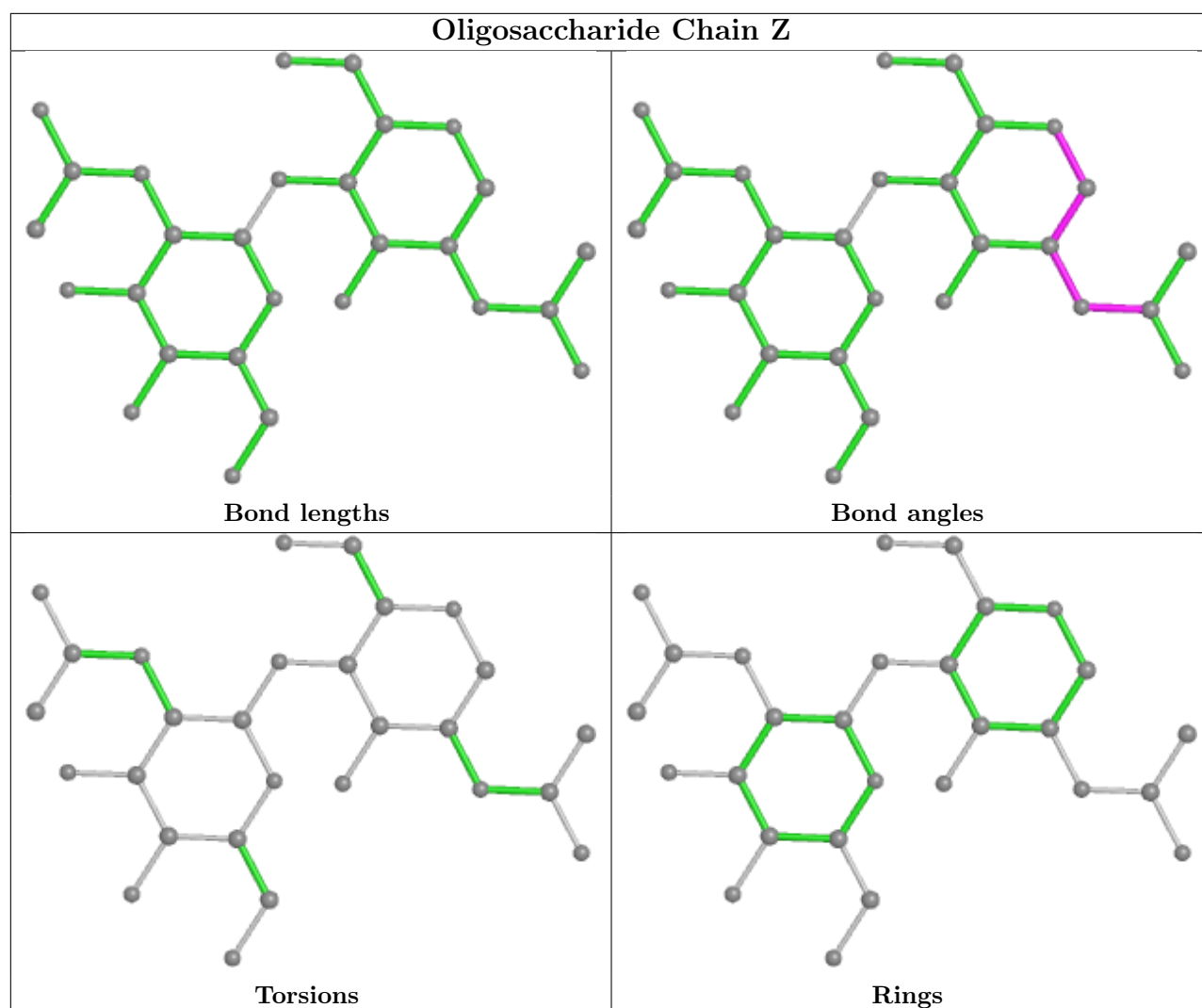


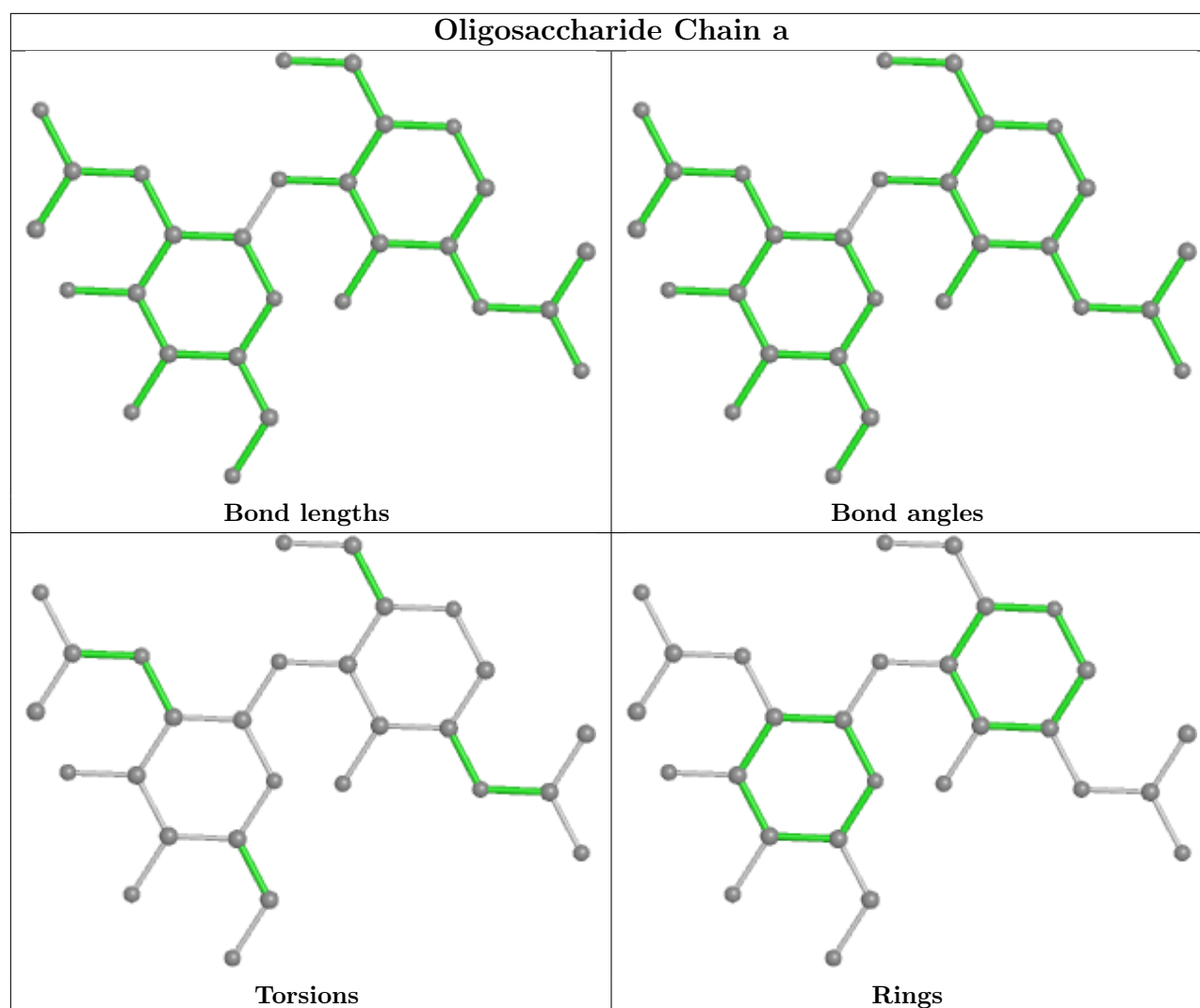












5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1308	2	14,14,15	0.24	0	17,19,21	0.56	0
4	NAG	B	1308	2	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
4	NAG	A	1302	-	14,14,15	0.40	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1306	2	14,14,15	0.41	0	17,19,21	1.60	1 (5%)
4	NAG	C	1303	2	14,14,15	0.41	0	17,19,21	0.51	0
4	NAG	C	1302	2	14,14,15	0.41	0	17,19,21	0.70	0
4	NAG	A	1301	2	14,14,15	0.41	0	17,19,21	0.41	0
4	NAG	A	1307	-	14,14,15	0.23	0	17,19,21	0.62	1 (5%)
4	NAG	B	1309	2	14,14,15	0.21	0	17,19,21	0.55	0
4	NAG	A	1306	-	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	C	1304	-	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	B	1305	2	14,14,15	0.41	0	17,19,21	0.37	0
4	NAG	B	1304	2	14,14,15	0.39	0	17,19,21	0.41	0
4	NAG	C	1306	-	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	B	1303	2	14,14,15	0.42	0	17,19,21	0.63	0
4	NAG	C	1307	2	14,14,15	0.40	0	17,19,21	0.40	0
4	NAG	A	1305	2	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
4	NAG	B	1302	2	14,14,15	0.40	0	17,19,21	0.58	0
4	NAG	C	1301	2	14,14,15	0.38	0	17,19,21	1.22	2 (11%)
4	NAG	C	1305	-	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1303	2	14,14,15	0.40	0	17,19,21	0.34	0
4	NAG	A	1304	2	14,14,15	0.39	0	17,19,21	0.78	1 (5%)
4	NAG	B	1301	2	14,14,15	0.41	0	17,19,21	0.33	0
4	NAG	B	1307	2	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
4	NAG	B	1310	-	14,14,15	0.20	0	17,19,21	0.36	0

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

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1306	NAG	O5-C1-C2	6.17	121.04	111.29
4	C	1301	NAG	O5-C1-C2	4.26	118.01	111.29
4	B	1308	NAG	O5-C1-C2	3.36	116.59	111.29
4	A	1304	NAG	O5-C1-C2	-2.73	106.97	111.29
4	B	1307	NAG	C1-O5-C5	2.33	115.35	112.19
4	A	1307	NAG	C1-O5-C5	2.16	115.12	112.19
4	C	1301	NAG	C1-O5-C5	2.13	115.08	112.19
4	A	1305	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

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

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

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

There are no ring outliers.

5 monomers are involved in 6 short contacts:

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