



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 08:43 PM EST

PDB ID : 8DZI
EMDB ID : EMD-27799
Title : Structure of SARS-CoV-2 Omicron BA.1.1.529 Spike trimer with one RBD down in complex with the Fab fragment of human neutralizing antibody MB.02
Authors : Hu, Y.; Xiong, Y.
Deposited on : 2022-08-07
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

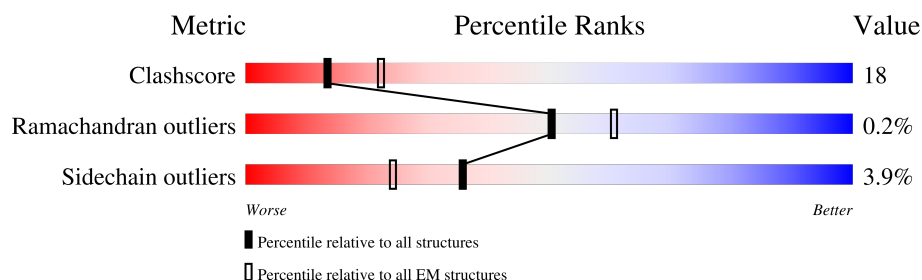
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1285	<div> <div>5%</div> <div>56%</div> <div>27%</div> <div>16%</div> </div>
1	C	1285	<div> <div>9%</div> <div>55%</div> <div>27%</div> <div>16%</div> </div>
1	E	1285	<div> <div>5%</div> <div>53%</div> <div>29%</div> <div>16%</div> </div>
2	B	118	<div> <div>6%</div> <div>47%</div> <div>51%</div> <div>.</div> </div>
2	G	118	<div> <div>44%</div> <div>54%</div> <div>42%</div> <div>.</div> </div>
2	H	118	<div> <div>42%</div> <div>54%</div> <div>.</div> </div>
3	D	109	<div> <div>5%</div> <div>45%</div> <div>50%</div> <div>5%</div> </div>
3	F	109	<div> <div>53%</div> <div>44%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	109	
4	I	2	
4	J	2	
4	K	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
4	c	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1083	Total	C	N	O	S	0	0
			8496	5436	1418	1604	38		
1	A	1080	Total	C	N	O	S	0	0
			8467	5418	1413	1598	38		
1	E	1074	Total	C	N	O	S	0	0
			8420	5391	1403	1588	38		

There are 387 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	140	ASP	TYR	conflict	UNP P0DTC2
C	206	ILE	-	insertion	UNP P0DTC2
C	207	VAL	-	insertion	UNP P0DTC2
C	208	ARG	ASN	conflict	UNP P0DTC2
C	209	GLU	LEU	conflict	UNP P0DTC2
C	210	PRO	VAL	conflict	UNP P0DTC2
C	211	GLU	ARG	conflict	UNP P0DTC2
C	336	ASP	GLY	conflict	UNP P0DTC2
C	368	LEU	SER	conflict	UNP P0DTC2
C	370	PRO	SER	conflict	UNP P0DTC2
C	372	PHE	SER	conflict	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	conflict	UNP P0DTC2
C	443	SER	GLY	conflict	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	490	ARG	GLN	conflict	UNP P0DTC2
C	493	SER	GLY	conflict	UNP P0DTC2
C	495	ARG	GLN	conflict	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	conflict	UNP P0DTC2
C	544	LYS	THR	conflict	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	conflict	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	761	LYS	ASN	conflict	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2
C	814	PRO	PHE	conflict	UNP P0DTC2
C	853	LYS	ASN	conflict	UNP P0DTC2
C	889	PRO	ALA	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	939	PRO	ALA	conflict	UNP P0DTC2
C	951	HIS	GLN	conflict	UNP P0DTC2
C	966	LYS	ASN	conflict	UNP P0DTC2
C	978	PHE	LEU	conflict	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1206	GLY	-	expression tag	UNP P0DTC2
C	1207	SER	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	TYR	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ALA	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	ASP	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	GLN	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	TYR	-	expression tag	UNP P0DTC2
C	1221	VAL	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1223	LYS	-	expression tag	UNP P0DTC2
C	1224	ASP	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	TRP	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	LEU	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	SER	-	expression tag	UNP P0DTC2
C	1232	THR	-	expression tag	UNP P0DTC2
C	1233	PHE	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	PRO	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	SER	-	expression tag	UNP P0DTC2
C	1256	ALA	-	expression tag	UNP P0DTC2
C	1257	TRP	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	PRO	-	expression tag	UNP P0DTC2
C	1261	GLN	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1265	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	SER	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	ALA	-	expression tag	UNP P0DTC2
C	1278	TRP	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	PRO	-	expression tag	UNP P0DTC2
C	1282	GLN	-	expression tag	UNP P0DTC2
C	1283	PHE	-	expression tag	UNP P0DTC2
C	1284	GLU	-	expression tag	UNP P0DTC2
C	1285	LYS	-	expression tag	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	conflict	UNP P0DTC2
A	206	ILE	-	insertion	UNP P0DTC2
A	207	VAL	-	insertion	UNP P0DTC2
A	208	ARG	ASN	conflict	UNP P0DTC2
A	209	GLU	LEU	conflict	UNP P0DTC2
A	210	PRO	VAL	conflict	UNP P0DTC2
A	211	GLU	ARG	conflict	UNP P0DTC2
A	336	ASP	GLY	conflict	UNP P0DTC2
A	368	LEU	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	conflict	UNP P0DTC2
A	490	ARG	GLN	conflict	UNP P0DTC2
A	493	SER	GLY	conflict	UNP P0DTC2
A	495	ARG	GLN	conflict	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	conflict	UNP P0DTC2
A	544	LYS	THR	conflict	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	conflict	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	761	LYS	ASN	conflict	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	853	LYS	ASN	conflict	UNP P0DTC2
A	889	PRO	ALA	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	939	PRO	ALA	conflict	UNP P0DTC2
A	951	HIS	GLN	conflict	UNP P0DTC2
A	966	LYS	ASN	conflict	UNP P0DTC2
A	978	PHE	LEU	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1206	GLY	-	expression tag	UNP P0DTC2
A	1207	SER	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	TYR	-	expression tag	UNP P0DTC2
A	1210	ILE	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ALA	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	ASP	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	GLN	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	TYR	-	expression tag	UNP P0DTC2
A	1221	VAL	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	LYS	-	expression tag	UNP P0DTC2
A	1224	ASP	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2
A	1227	TRP	-	expression tag	UNP P0DTC2
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	LEU	-	expression tag	UNP P0DTC2
A	1230	LEU	-	expression tag	UNP P0DTC2
A	1231	SER	-	expression tag	UNP P0DTC2
A	1232	THR	-	expression tag	UNP P0DTC2
A	1233	PHE	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	PRO	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	ALA	-	expression tag	UNP P0DTC2
A	1257	TRP	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	PRO	-	expression tag	UNP P0DTC2
A	1261	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	LYS	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	SER	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	ALA	-	expression tag	UNP P0DTC2
A	1278	TRP	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	PRO	-	expression tag	UNP P0DTC2
A	1282	GLN	-	expression tag	UNP P0DTC2
A	1283	PHE	-	expression tag	UNP P0DTC2
A	1284	GLU	-	expression tag	UNP P0DTC2
A	1285	LYS	-	expression tag	UNP P0DTC2
E	67	VAL	ALA	variant	UNP P0DTC2
E	?	-	HIS	deletion	UNP P0DTC2
E	?	-	VAL	deletion	UNP P0DTC2
E	93	ILE	THR	variant	UNP P0DTC2
E	?	-	GLY	deletion	UNP P0DTC2
E	?	-	VAL	deletion	UNP P0DTC2
E	?	-	TYR	deletion	UNP P0DTC2
E	140	ASP	TYR	conflict	UNP P0DTC2
E	206	ILE	-	insertion	UNP P0DTC2
E	207	VAL	-	insertion	UNP P0DTC2
E	208	ARG	ASN	conflict	UNP P0DTC2
E	209	GLU	LEU	conflict	UNP P0DTC2
E	210	PRO	VAL	conflict	UNP P0DTC2
E	211	GLU	ARG	conflict	UNP P0DTC2
E	336	ASP	GLY	conflict	UNP P0DTC2
E	368	LEU	SER	conflict	UNP P0DTC2
E	370	PRO	SER	conflict	UNP P0DTC2
E	372	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	414	ASN	LYS	variant	UNP P0DTC2
E	437	LYS	ASN	conflict	UNP P0DTC2
E	443	SER	GLY	conflict	UNP P0DTC2
E	474	ASN	SER	variant	UNP P0DTC2
E	475	LYS	THR	variant	UNP P0DTC2
E	481	ALA	GLU	conflict	UNP P0DTC2
E	490	ARG	GLN	conflict	UNP P0DTC2
E	493	SER	GLY	conflict	UNP P0DTC2
E	495	ARG	GLN	conflict	UNP P0DTC2
E	498	TYR	ASN	variant	UNP P0DTC2
E	502	HIS	TYR	conflict	UNP P0DTC2
E	544	LYS	THR	conflict	UNP P0DTC2
E	611	GLY	ASP	variant	UNP P0DTC2
E	652	TYR	HIS	variant	UNP P0DTC2
E	676	LYS	ASN	conflict	UNP P0DTC2
E	678	HIS	PRO	variant	UNP P0DTC2
E	679	GLY	ARG	conflict	UNP P0DTC2
E	680	SER	ARG	conflict	UNP P0DTC2
E	682	SER	ARG	conflict	UNP P0DTC2
E	761	LYS	ASN	conflict	UNP P0DTC2
E	793	TYR	ASP	variant	UNP P0DTC2
E	814	PRO	PHE	conflict	UNP P0DTC2
E	853	LYS	ASN	conflict	UNP P0DTC2
E	889	PRO	ALA	conflict	UNP P0DTC2
E	896	PRO	ALA	conflict	UNP P0DTC2
E	939	PRO	ALA	conflict	UNP P0DTC2
E	951	HIS	GLN	conflict	UNP P0DTC2
E	966	LYS	ASN	conflict	UNP P0DTC2
E	978	PHE	LEU	conflict	UNP P0DTC2
E	983	PRO	LYS	conflict	UNP P0DTC2
E	984	PRO	VAL	conflict	UNP P0DTC2
E	1206	GLY	-	expression tag	UNP P0DTC2
E	1207	SER	-	expression tag	UNP P0DTC2
E	1208	GLY	-	expression tag	UNP P0DTC2
E	1209	TYR	-	expression tag	UNP P0DTC2
E	1210	ILE	-	expression tag	UNP P0DTC2
E	1211	PRO	-	expression tag	UNP P0DTC2
E	1212	GLU	-	expression tag	UNP P0DTC2
E	1213	ALA	-	expression tag	UNP P0DTC2
E	1214	PRO	-	expression tag	UNP P0DTC2
E	1215	ARG	-	expression tag	UNP P0DTC2
E	1216	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1217	GLY	-	expression tag	UNP P0DTC2
E	1218	GLN	-	expression tag	UNP P0DTC2
E	1219	ALA	-	expression tag	UNP P0DTC2
E	1220	TYR	-	expression tag	UNP P0DTC2
E	1221	VAL	-	expression tag	UNP P0DTC2
E	1222	ARG	-	expression tag	UNP P0DTC2
E	1223	LYS	-	expression tag	UNP P0DTC2
E	1224	ASP	-	expression tag	UNP P0DTC2
E	1225	GLY	-	expression tag	UNP P0DTC2
E	1226	GLU	-	expression tag	UNP P0DTC2
E	1227	TRP	-	expression tag	UNP P0DTC2
E	1228	VAL	-	expression tag	UNP P0DTC2
E	1229	LEU	-	expression tag	UNP P0DTC2
E	1230	LEU	-	expression tag	UNP P0DTC2
E	1231	SER	-	expression tag	UNP P0DTC2
E	1232	THR	-	expression tag	UNP P0DTC2
E	1233	PHE	-	expression tag	UNP P0DTC2
E	1234	LEU	-	expression tag	UNP P0DTC2
E	1235	GLY	-	expression tag	UNP P0DTC2
E	1236	ARG	-	expression tag	UNP P0DTC2
E	1237	SER	-	expression tag	UNP P0DTC2
E	1238	LEU	-	expression tag	UNP P0DTC2
E	1239	GLU	-	expression tag	UNP P0DTC2
E	1240	VAL	-	expression tag	UNP P0DTC2
E	1241	LEU	-	expression tag	UNP P0DTC2
E	1242	PHE	-	expression tag	UNP P0DTC2
E	1243	GLN	-	expression tag	UNP P0DTC2
E	1244	GLY	-	expression tag	UNP P0DTC2
E	1245	PRO	-	expression tag	UNP P0DTC2
E	1246	GLY	-	expression tag	UNP P0DTC2
E	1247	HIS	-	expression tag	UNP P0DTC2
E	1248	HIS	-	expression tag	UNP P0DTC2
E	1249	HIS	-	expression tag	UNP P0DTC2
E	1250	HIS	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	HIS	-	expression tag	UNP P0DTC2
E	1254	HIS	-	expression tag	UNP P0DTC2
E	1255	SER	-	expression tag	UNP P0DTC2
E	1256	ALA	-	expression tag	UNP P0DTC2
E	1257	TRP	-	expression tag	UNP P0DTC2
E	1258	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1259	HIS	-	expression tag	UNP P0DTC2
E	1260	PRO	-	expression tag	UNP P0DTC2
E	1261	GLN	-	expression tag	UNP P0DTC2
E	1262	PHE	-	expression tag	UNP P0DTC2
E	1263	GLU	-	expression tag	UNP P0DTC2
E	1264	LYS	-	expression tag	UNP P0DTC2
E	1265	GLY	-	expression tag	UNP P0DTC2
E	1266	GLY	-	expression tag	UNP P0DTC2
E	1267	GLY	-	expression tag	UNP P0DTC2
E	1268	SER	-	expression tag	UNP P0DTC2
E	1269	GLY	-	expression tag	UNP P0DTC2
E	1270	GLY	-	expression tag	UNP P0DTC2
E	1271	GLY	-	expression tag	UNP P0DTC2
E	1272	GLY	-	expression tag	UNP P0DTC2
E	1273	SER	-	expression tag	UNP P0DTC2
E	1274	GLY	-	expression tag	UNP P0DTC2
E	1275	GLY	-	expression tag	UNP P0DTC2
E	1276	SER	-	expression tag	UNP P0DTC2
E	1277	ALA	-	expression tag	UNP P0DTC2
E	1278	TRP	-	expression tag	UNP P0DTC2
E	1279	SER	-	expression tag	UNP P0DTC2
E	1280	HIS	-	expression tag	UNP P0DTC2
E	1281	PRO	-	expression tag	UNP P0DTC2
E	1282	GLN	-	expression tag	UNP P0DTC2
E	1283	PHE	-	expression tag	UNP P0DTC2
E	1284	GLU	-	expression tag	UNP P0DTC2
E	1285	LYS	-	expression tag	UNP P0DTC2

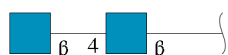
- Molecule 2 is a protein called antibody MB.02 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	118	Total	C	N	O	S	0	0
			912	581	146	179	6		
2	B	118	Total	C	N	O	S	0	0
			912	581	146	179	6		
2	G	118	Total	C	N	O	S	0	0
			912	581	146	179	6		

- Molecule 3 is a protein called antibody MB.02 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	109	Total	C	N	O	S	0	0
			823	515	142	164	2		
3	D	109	Total	C	N	O	S	0	0
			823	515	142	164	2		
3	F	109	Total	C	N	O	S	0	0
			823	515	142	164	2		

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



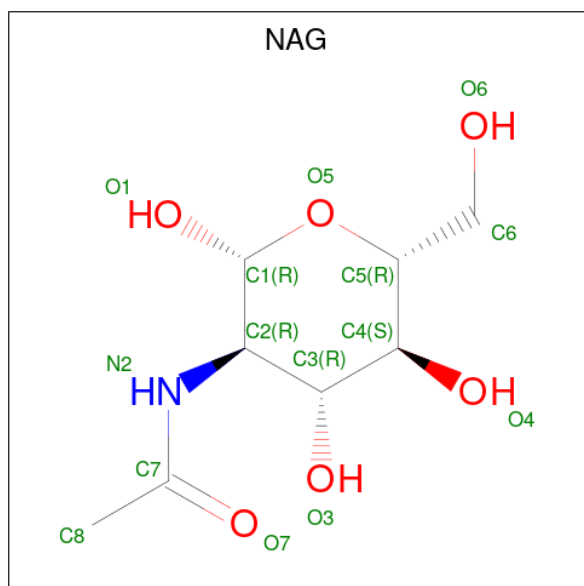
Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			70	40	5	25	
5	C	1	Total	C	N	O	0
			70	40	5	25	
5	C	1	Total	C	N	O	0
			70	40	5	25	
5	C	1	Total	C	N	O	0
			70	40	5	25	
5	C	1	Total	C	N	O	0
			70	40	5	25	

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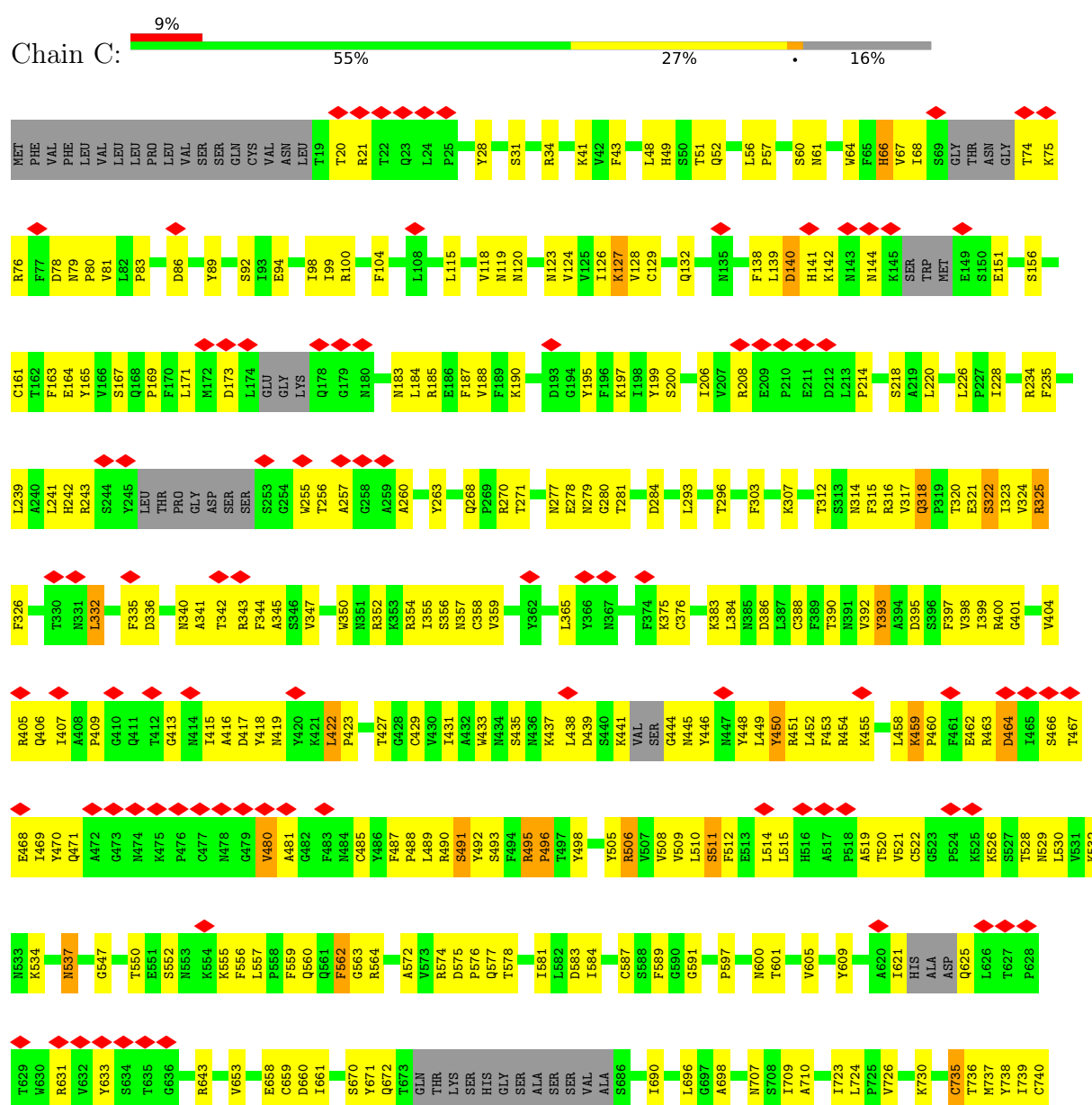
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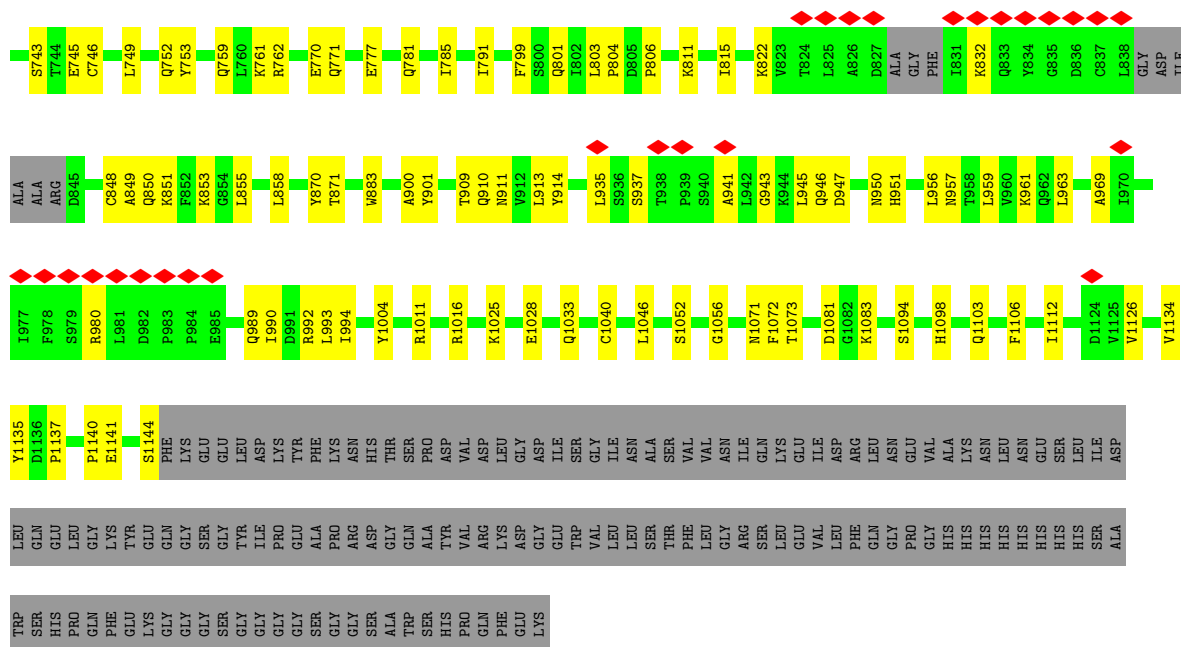
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0
5	E	1	Total 126	C 72	N 9	O 45	0

3 Residue-property plots

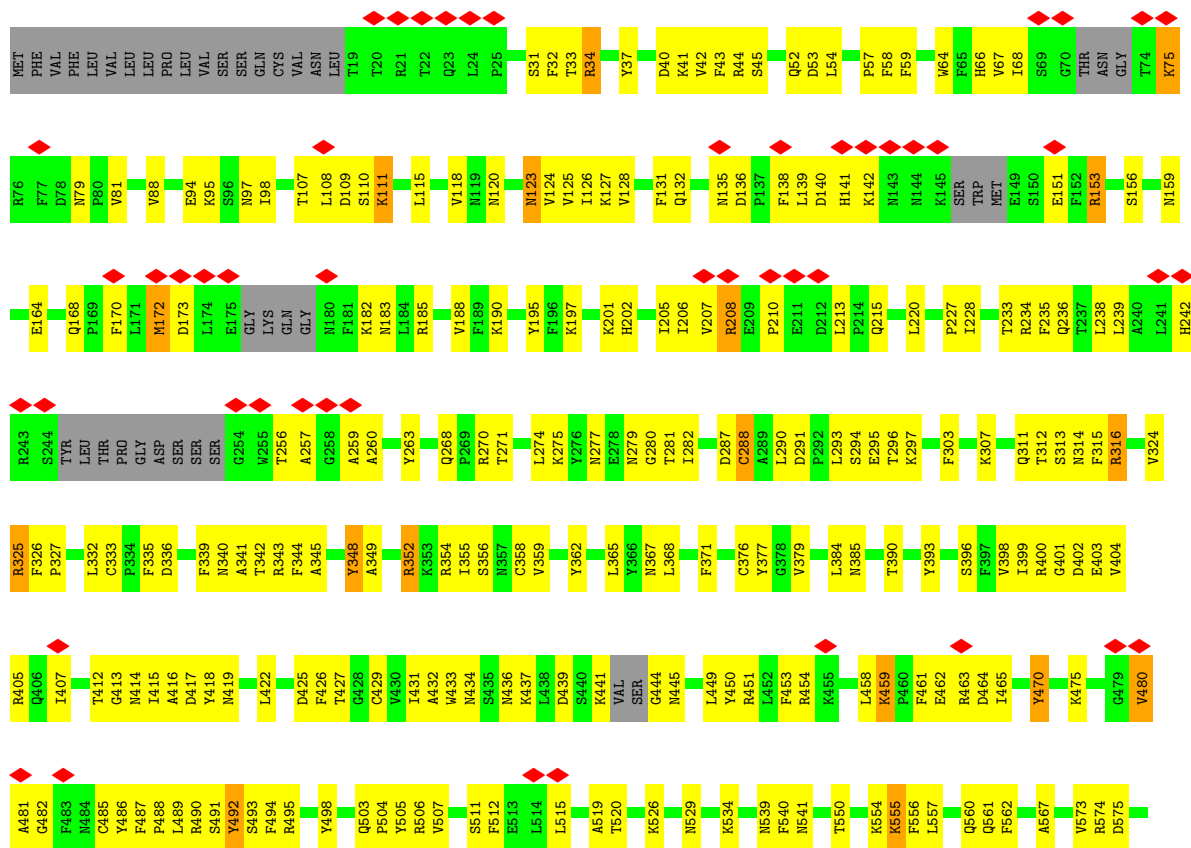
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

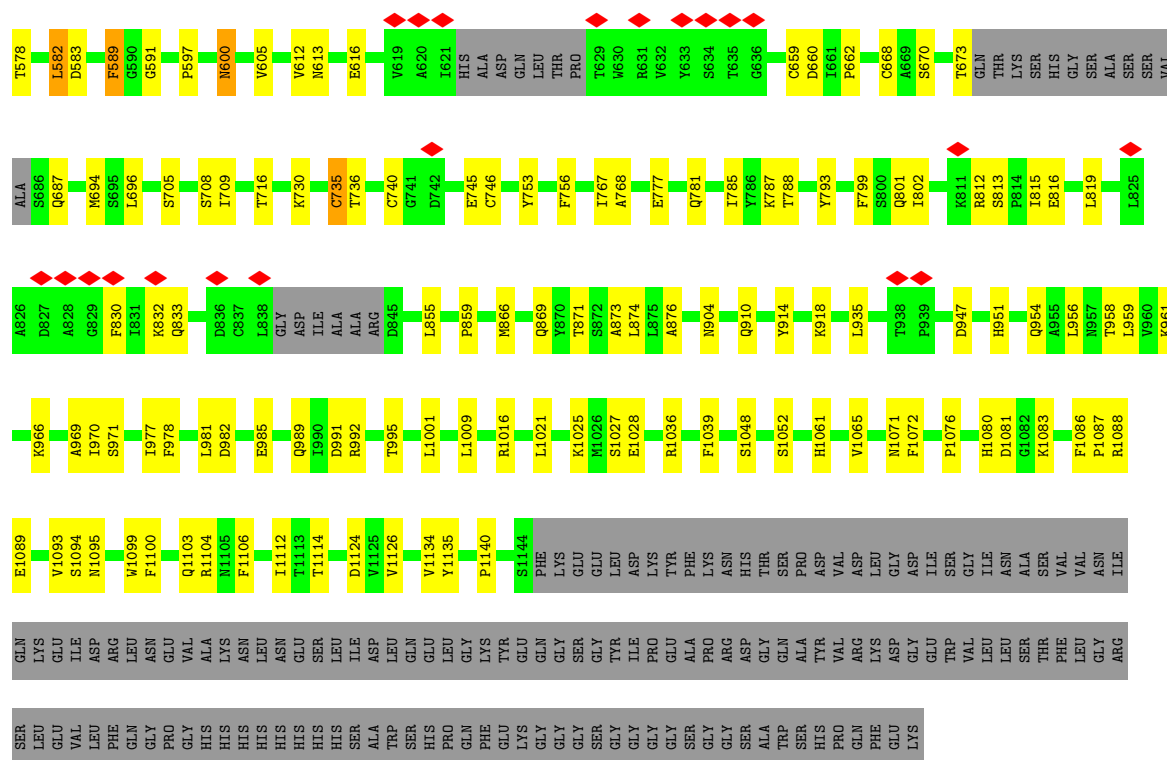
• Molecule 1: Spike glycoprotein



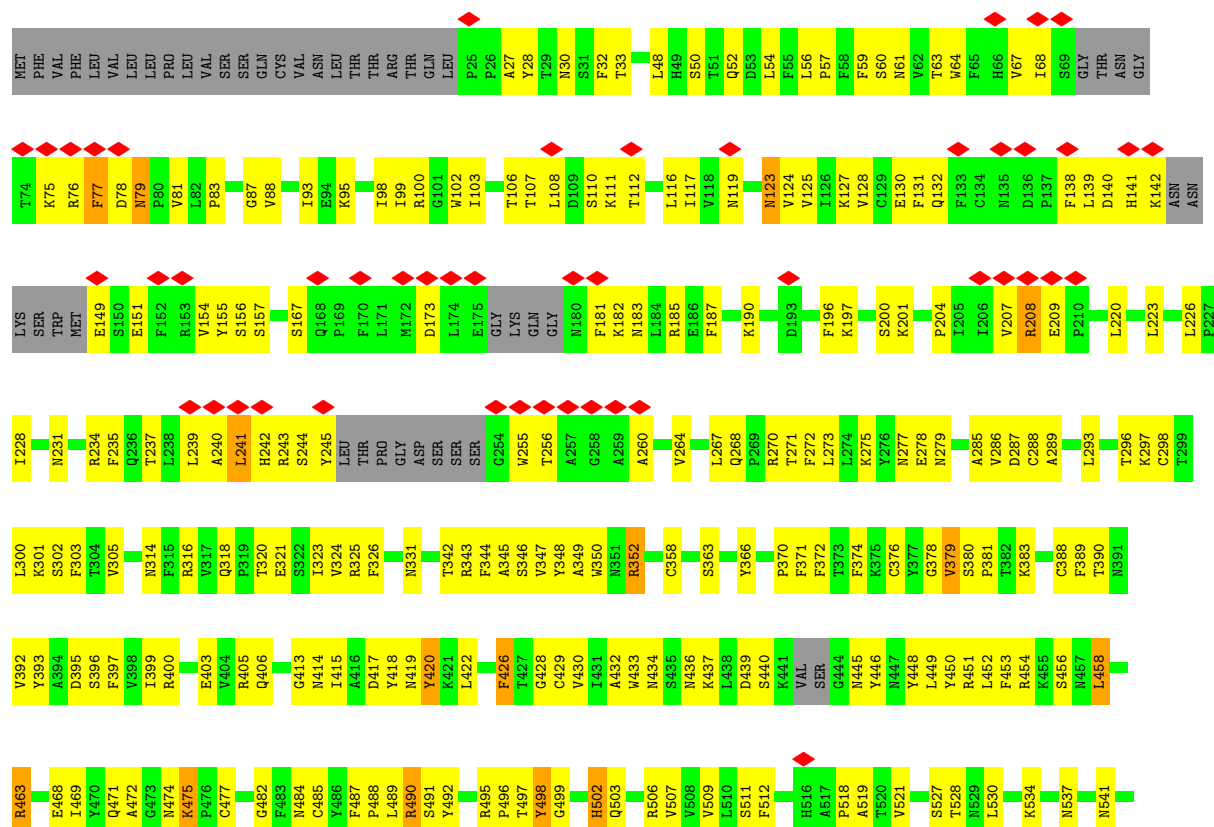


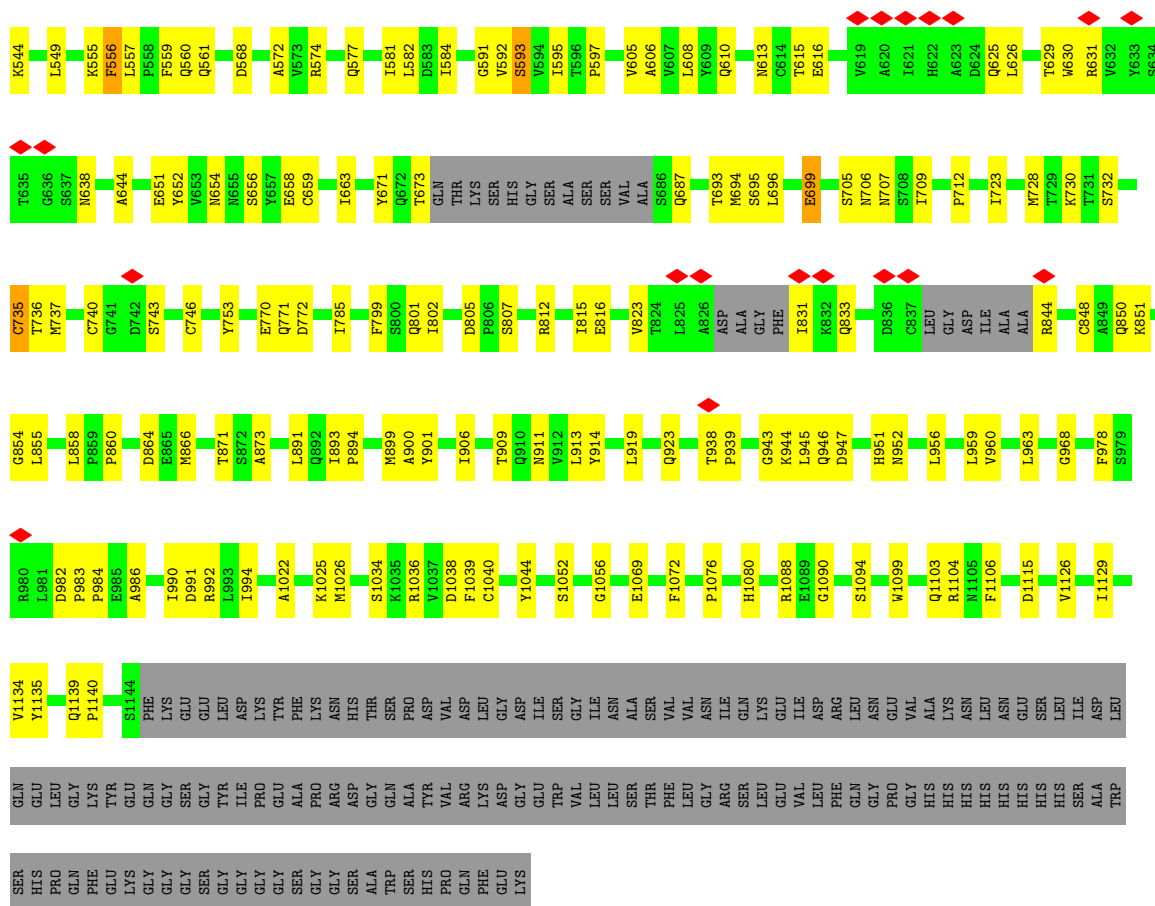
• Molecule 1: Spike glycoprotein



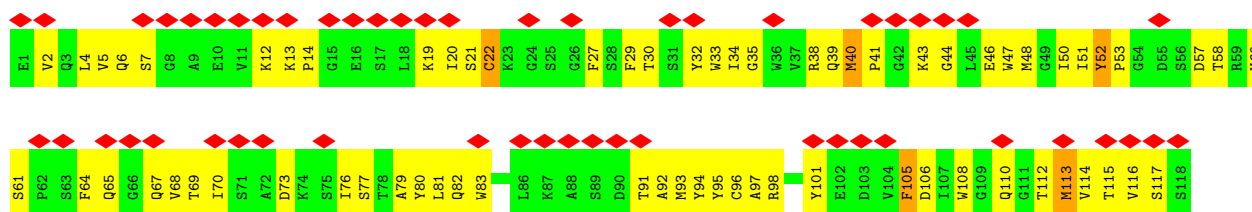


• Molecule 1: Spike glycoprotein

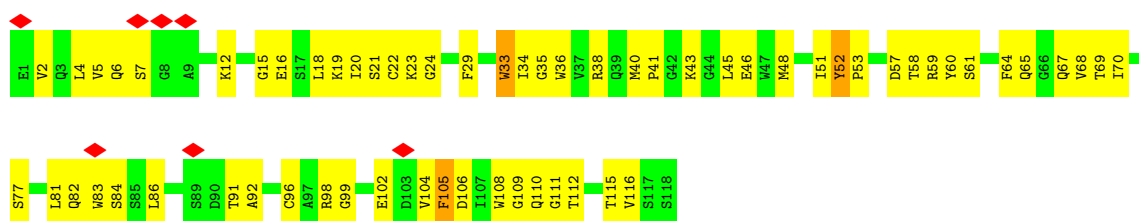




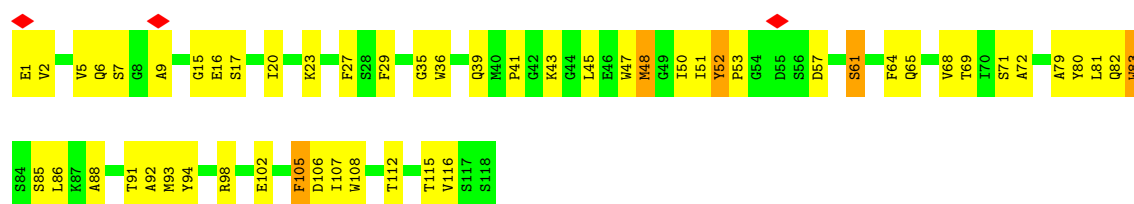
• Molecule 2: antibody MB.02 heavy chain



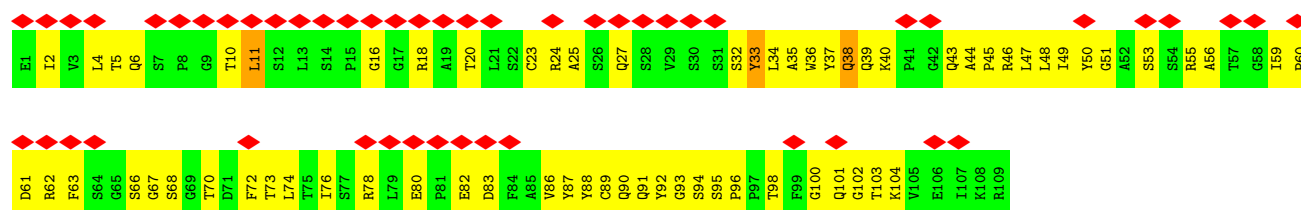
• Molecule 2: antibody MB.02 heavy chain



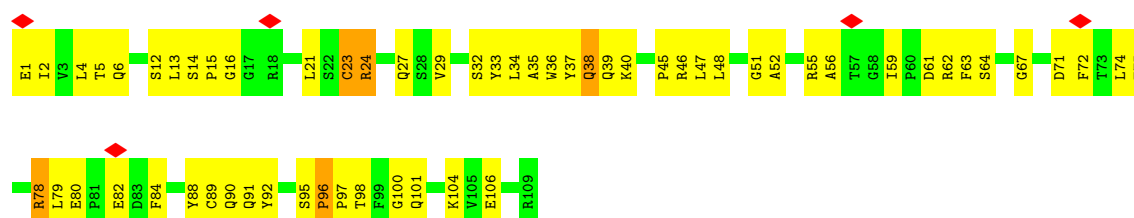
• Molecule 2: antibody MB.02 heavy chain



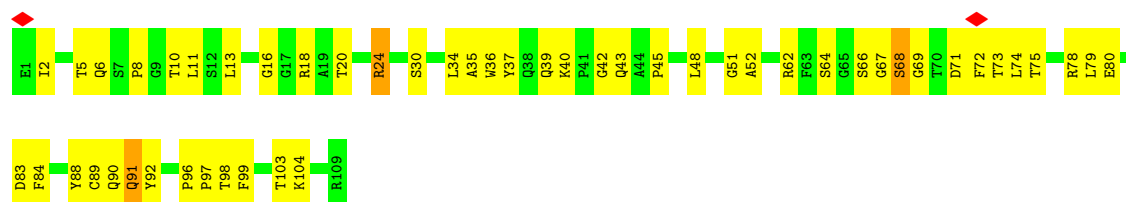
- Chain L:  46% 38% 60%



- Chain D: 



- Chain F:  53% 44%



- Chain I:  50% 50%



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



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



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



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



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



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



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

Chain Q:  50% 50%



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

Chain R:  50% 100%



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

Chain S:  50% 50% 50%



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

Chain T:  50% 100%



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

Chain U:  100% 50% 50%



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

Chain V:  50% 50% 50%



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

Chain W:  100%
100%



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

Chain X:  100%
100%



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

Chain Y:  50%
100%



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

Chain Z:  50%
100%



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

Chain a:  100%



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

Chain b:  50%
50%



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

Chain c: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176861	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/8667	0.48	0/11789
1	C	0.26	0/8696	0.49	1/11829 (0.0%)
1	E	0.26	0/8621	0.48	0/11729
2	B	0.28	0/936	0.55	0/1265
2	G	0.26	0/936	0.53	0/1265
2	H	0.26	0/936	0.54	0/1265
3	D	0.26	0/842	0.55	0/1141
3	F	0.26	0/842	0.56	0/1141
3	L	0.25	0/842	0.59	1/1141 (0.1%)
All	All	0.26	0/31318	0.50	2/42565 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	422	LEU	CA-CB-CG	5.82	128.68	115.30
3	L	11	LEU	CA-CB-CG	5.42	127.76	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	95	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8467	0	8261	269	0
1	C	8496	0	8295	293	0
1	E	8420	0	8209	283	0
2	B	912	0	873	54	0
2	G	912	0	873	38	0
2	H	912	0	873	65	0
3	D	823	0	805	50	0
3	F	823	0	805	37	0
3	L	823	0	805	66	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	1	0
4	V	28	0	25	1	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	3	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
5	A	126	0	117	4	0
5	C	70	0	65	2	0
5	E	126	0	117	3	0
All	All	31470	0	30598	1115	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 (1115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:CYS:HA	1:C:522:CYS:HB3	1.57	0.87
1:A:279:ASN:HD22	1:E:555:LYS:HE3	1.41	0.83
1:E:436:ASN:HB2	1:E:503:GLN:HE21	1.44	0.83
1:C:451:ARG:HH12	1:C:468:GLU:H	1.27	0.82
1:A:557:LEU:H	1:A:560:GLN:HE21	1.24	0.81
1:C:1103:GLN:HE21	1:C:1106:PHE:HB3	1.44	0.80
3:L:49:ILE:HA	3:L:56:ALA:HB2	1.64	0.80
1:A:575:ASP:HB2	1:A:582:LEU:HD11	1.64	0.79
2:B:34:ILE:HA	2:B:98:ARG:HA	1.65	0.77
1:A:413:GLY:H	1:A:416:ALA:HB3	1.50	0.77
1:C:184:LEU:HD22	1:C:214:PRO:HG2	1.65	0.76
1:A:140:ASP:H	1:A:151:GLU:HG2	1.51	0.76
1:C:75:LYS:HE3	1:C:257:ALA:HB1	1.68	0.76
2:H:112:THR:HG22	2:H:114:VAL:HG23	1.67	0.75
1:A:400:ARG:HA	1:A:494:PHE:HZ	1.51	0.75
1:C:552:SER:HB3	1:C:581:ILE:HG22	1.67	0.75
1:E:289:ALA:HB1	1:E:629:THR:HG21	1.69	0.75
1:E:499:GLY:HA2	1:E:503:GLN:HG2	1.68	0.75
1:C:141:HIS:HB3	1:C:242:HIS:HB2	1.69	0.74
2:H:69:THR:HB	2:H:82:GLN:HB2	1.70	0.74
1:C:419:ASN:ND2	1:C:451:ARG:O	2.22	0.73
1:A:139:LEU:HD11	1:A:238:LEU:HB3	1.68	0.73
1:C:355:ILE:HB	1:C:392:VAL:HB	1.70	0.73
2:B:5:VAL:O	2:B:23:LYS:N	2.22	0.72
1:C:413:GLY:H	1:C:416:ALA:HB3	1.55	0.72
1:A:127:LYS:HG2	1:A:164:GLU:HG2	1.72	0.72
1:A:293:LEU:HB2	1:A:605:VAL:HG11	1.71	0.72
1:C:562:PHE:HB2	1:C:564:ARG:HH12	1.53	0.72
1:E:325:ARG:HE	1:E:530:LEU:HD23	1.55	0.71
1:E:652:TYR:HH	1:E:693:THR:HG1	1.27	0.71
1:A:128:VAL:HG11	1:A:228:ILE:HG21	1.71	0.71
1:C:451:ARG:HG3	1:C:488:PRO:HB2	1.71	0.71
1:C:352:ARG:H	1:C:463:ARG:HH21	1.40	0.70
1:E:380:SER:HB3	1:E:383:LYS:HB2	1.74	0.70
3:F:90:GLN:HG2	3:F:99:PHE:HA	1.73	0.69
3:F:6:GLN:HB3	3:F:103:THR:HG23	1.73	0.69
1:C:31:SER:HB3	1:C:60:SER:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:812:ARG:HG2	1:E:816:GLU:HB3	1.74	0.69
1:C:100:ARG:HD3	1:C:119:ASN:HB3	1.75	0.69
1:C:458:LEU:HD12	1:C:462:GLU:HG2	1.75	0.69
1:C:959:LEU:HD21	1:C:1004:TYR:HB2	1.75	0.69
3:L:91:GLN:HG3	3:L:98:THR:H	1.58	0.69
1:E:349:ALA:O	1:E:352:ARG:NH2	2.25	0.69
2:B:98:ARG:HE	2:B:106:ASP:HB3	1.55	0.68
3:L:40:LYS:HB2	3:L:43:GLN:HB2	1.74	0.68
1:A:441:LYS:HE3	2:B:104:VAL:HG11	1.76	0.68
1:E:638:ASN:HD21	1:E:651:GLU:HA	1.57	0.68
2:G:105:PHE:HB2	2:G:108:TRP:HE1	1.58	0.68
2:B:23:LYS:NZ	2:B:77:SER:OG	2.27	0.68
1:C:126:ILE:HB	1:C:165:TYR:HB3	1.76	0.68
3:L:6:GLN:HA	3:L:23:CYS:HA	1.76	0.67
1:C:791:ILE:HG23	4:R:2:NAG:H82	1.76	0.67
1:E:396:SER:HB2	1:E:506:ARG:HH22	1.58	0.67
3:L:67:GLY:HA3	3:L:73:THR:H	1.60	0.67
1:A:866:MET:HB2	1:E:696:LEU:HD21	1.77	0.67
3:D:95:SER:HB2	3:D:96:PRO:HD2	1.76	0.67
1:C:848:CYS:HA	1:C:851:LYS:HG2	1.76	0.66
1:A:613:ASN:HB3	1:A:616:GLU:HB2	1.76	0.66
1:E:454:ARG:HE	1:E:456:SER:H	1.41	0.66
3:D:12:SER:HA	3:D:106:GLU:H	1.60	0.66
1:E:128:VAL:HG11	1:E:228:ILE:HG12	1.76	0.66
1:C:325:ARG:NH1	1:C:528:THR:O	2.29	0.66
1:C:57:PRO:HB2	1:C:60:SER:HB3	1.78	0.66
1:A:1028:GLU:OE2	1:E:1036:ARG:NH1	2.28	0.66
3:L:16:GLY:HA2	3:L:78:ARG:HG2	1.78	0.66
3:D:82:GLU:OE2	3:D:82:GLU:N	2.28	0.66
2:B:51:ILE:HD12	2:B:58:THR:OG1	1.95	0.66
1:C:34:ARG:NH1	1:C:218:SER:OG	2.29	0.66
1:C:491:SER:OG	1:C:493:SER:OG	2.14	0.65
1:C:574:ARG:HG2	1:C:581:ILE:HG12	1.78	0.65
1:E:428:GLY:HA3	1:E:511:SER:HA	1.77	0.65
1:C:495:ARG:H	1:C:498:TYR:HB2	1.62	0.65
1:C:850:GLN:HB3	1:C:855:LEU:HB2	1.79	0.65
3:L:40:LYS:HD3	3:L:46:ARG:HB3	1.78	0.65
2:B:110:GLN:NE2	2:B:111:GLY:O	2.29	0.65
1:A:463:ARG:HD2	1:A:465:ILE:HD11	1.78	0.65
1:E:50:SER:HB2	1:E:301:LYS:HZ1	1.61	0.65
1:E:54:LEU:HD13	1:E:190:LYS:HZ2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:PHE:HB3	1:C:490:ARG:HH12	1.60	0.65
1:A:75:LYS:HE3	1:A:257:ALA:HB1	1.78	0.65
3:D:39:GLN:HA	3:D:45:PRO:HA	1.78	0.65
1:C:735:CYS:SG	1:C:736:THR:N	2.70	0.65
3:L:6:GLN:OE1	3:L:6:GLN:N	2.30	0.65
1:E:331:ASN:HB3	1:E:358:CYS:HA	1.78	0.64
1:E:1103:GLN:HE21	1:E:1106:PHE:HB3	1.62	0.64
2:H:38:ARG:HB3	2:H:48:MET:SD	2.36	0.64
2:H:39:GLN:N	2:H:93:MET:O	2.25	0.64
2:G:17:SER:OG	2:G:82:GLN:OE1	2.15	0.64
1:E:207:VAL:HG22	1:E:209:GLU:H	1.61	0.64
1:A:1093:VAL:O	1:A:1100:PHE:N	2.29	0.64
2:H:6:GLN:H	2:H:110:GLN:HG3	1.63	0.64
2:H:38:ARG:NH1	2:H:46:GLU:OE2	2.31	0.64
2:H:105:PHE:HB2	2:H:108:TRP:HE1	1.61	0.64
1:C:118:VAL:HG22	1:C:120:ASN:H	1.63	0.64
3:F:64:SER:HB2	3:F:75:THR:HB	1.80	0.64
1:A:128:VAL:HG21	1:A:228:ILE:HG13	1.80	0.64
3:F:18:ARG:NH1	3:F:20:THR:OG1	2.24	0.64
1:E:728:MET:HB2	1:E:952:ASN:HD21	1.63	0.63
1:C:1135:TYR:HE1	1:C:1140:PRO:HG2	1.63	0.63
2:H:35:GLY:H	2:H:98:ARG:HA	1.63	0.63
1:A:41:LYS:NZ	1:E:559:PHE:O	2.27	0.63
1:C:139:LEU:HD22	1:C:151:GLU:HA	1.79	0.63
1:C:407:ILE:HD12	1:C:415:ILE:HG12	1.81	0.63
3:L:10:THR:HA	3:L:104:LYS:H	1.63	0.63
1:A:327:PRO:HB3	1:A:541:ASN:HD21	1.64	0.63
3:D:55:ARG:NH2	3:D:63:PHE:O	2.32	0.63
1:A:705:SER:HB3	1:A:708:SER:HB3	1.81	0.63
1:C:206:ILE:O	1:C:208:ARG:NH1	2.32	0.62
1:E:656:SER:HB3	1:E:695:SER:HB3	1.81	0.62
2:H:51:ILE:HA	2:H:58:THR:HA	1.81	0.62
1:A:352:ARG:HB2	1:A:393:TYR:HE1	1.64	0.62
3:D:91:GLN:HE21	3:D:98:THR:H	1.48	0.62
1:E:730:LYS:NZ	1:E:772:ASP:OD2	2.32	0.62
1:C:803:LEU:HD13	1:C:804:PRO:HD2	1.82	0.62
1:E:968:GLY:HA3	1:E:992:ARG:HH21	1.63	0.62
1:C:119:ASN:HD22	1:C:169:PRO:HB2	1.64	0.62
1:C:322:SER:HA	1:C:537:ASN:HB2	1.81	0.62
1:A:41:LYS:HE2	1:E:518:PRO:HD2	1.81	0.62
3:F:30:SER:HB2	3:F:69:GLY:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASN:ND2	1:E:555:LYS:HE3	2.13	0.62
2:B:6:GLN:H	2:B:110:GLN:HB3	1.65	0.62
1:C:242:HIS:HB3	1:C:256:THR:HB	1.81	0.62
3:D:6:GLN:HE22	3:D:88:TYR:HA	1.64	0.62
1:E:799:PHE:HD1	1:E:802:ILE:HD11	1.65	0.62
1:C:390:THR:HG22	1:C:515:LEU:HA	1.82	0.62
2:B:52:TYR:HB3	2:B:57:ASP:HB2	1.82	0.62
1:E:432:ALA:HB2	1:E:507:VAL:HG13	1.82	0.61
2:H:105:PHE:HB3	3:L:47:LEU:HB2	1.82	0.61
3:L:49:ILE:HD12	3:L:74:LEU:HD11	1.81	0.61
1:E:376:CYS:HA	1:E:429:CYS:HA	1.82	0.61
1:C:279:ASN:O	1:A:555:LYS:NZ	2.33	0.61
1:C:406:GLN:HB3	1:C:413:GLY:HA3	1.81	0.61
1:C:469:ILE:HA	1:C:488:PRO:HD3	1.81	0.61
1:C:139:LEU:O	1:C:241:LEU:N	2.28	0.61
1:C:200:SER:HA	1:C:220:LEU:HD23	1.83	0.61
1:C:336:ASP:OD1	1:C:340:ASN:ND2	2.33	0.61
1:C:390:THR:HA	1:C:520:THR:HG22	1.82	0.61
2:H:70:ILE:HG23	2:H:81:LEU:HG	1.81	0.61
1:C:871:THR:HG21	1:C:1052:SER:HB3	1.81	0.61
3:D:32:SER:O	3:D:92:TYR:HB3	2.00	0.61
1:E:270:ARG:NH1	1:E:287:ASP:OD2	2.34	0.61
1:A:793:TYR:HB2	4:Y:2:NAG:H82	1.82	0.61
1:E:498:TYR:HB3	1:E:502:HIS:HB2	1.82	0.61
1:A:415:ILE:HG22	1:A:419:ASN:HD22	1.66	0.60
1:C:128:VAL:HG11	1:C:228:ILE:HG21	1.83	0.60
1:A:556:PHE:HB3	1:A:574:ARG:HH21	1.65	0.60
1:E:615:THR:OG1	1:E:616:GLU:OE2	2.19	0.60
1:A:290:LEU:HD23	1:A:291:ASP:HB3	1.83	0.60
1:C:399:ILE:HG22	1:C:401:GLY:H	1.65	0.60
1:E:286:VAL:HG21	1:E:297:LYS:HD3	1.84	0.60
1:C:455:LYS:HG2	1:C:471:GLN:H	1.66	0.60
1:C:653:VAL:HG21	1:C:690:ILE:HD12	1.84	0.60
3:L:80:GLU:H	3:L:83:ASP:HB2	1.67	0.60
1:A:138:PHE:H	1:A:153:ARG:HH22	1.47	0.60
1:E:737:MET:HE2	1:E:854:GLY:HA2	1.83	0.60
1:A:1081:ASP:O	1:A:1083:LYS:NZ	2.34	0.60
3:D:33:TYR:HB3	3:D:51:GLY:HA2	1.84	0.60
3:D:78:ARG:HH21	3:D:80:GLU:HA	1.66	0.60
3:D:79:LEU:HB3	3:D:84:PHE:HE1	1.65	0.60
1:C:520:THR:HG23	1:C:521:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:CYS:HB2	1:C:521:VAL:HG22	1.84	0.59
1:E:173:ASP:HB3	1:E:185:ARG:HH21	1.67	0.59
1:C:127:LYS:HD3	1:C:164:GLU:HG2	1.83	0.59
3:D:6:GLN:HB2	3:D:21:LEU:HD11	1.82	0.59
1:E:434:ASN:HD21	1:E:436:ASN:HB3	1.66	0.59
1:A:575:ASP:HB3	1:A:578:THR:O	2.02	0.59
1:A:367:ASN:HB3	5:A:1309:NAG:O5	2.02	0.59
3:L:37:TYR:O	3:L:88:TYR:N	2.35	0.59
3:L:55:ARG:HE	3:L:59:ILE:HG22	1.68	0.59
3:D:90:GLN:OE1	3:D:97:PRO:HB2	2.03	0.59
1:E:616:GLU:OE2	1:E:616:GLU:N	2.34	0.59
1:E:1088:ARG:NH1	1:E:1115:ASP:O	2.30	0.59
1:C:449:LEU:HB3	1:C:489:LEU:HB3	1.83	0.59
1:C:469:ILE:HD12	1:C:485:CYS:SG	2.43	0.59
1:C:404:VAL:HG13	1:C:405:ARG:HD2	1.85	0.59
1:C:710:ALA:HB3	1:E:891:LEU:HB3	1.83	0.59
1:E:139:LEU:H	1:E:240:ALA:HA	1.67	0.59
3:F:62:ARG:HD2	3:F:78:ARG:HB2	1.85	0.59
3:F:80:GLU:H	3:F:83:ASP:HB2	1.68	0.59
1:C:144:ASN:ND2	1:C:151:GLU:OE2	2.35	0.58
3:L:32:SER:O	3:L:93:GLY:N	2.34	0.58
1:A:422:LEU:HD23	1:A:461:PHE:HE1	1.68	0.58
1:A:801:GLN:O	1:A:813:SER:OG	2.17	0.58
1:A:414:ASN:OD1	1:A:415:ILE:N	2.36	0.58
2:B:29:PHE:HB3	2:B:53:PRO:HB2	1.85	0.58
1:A:33:THR:O	1:A:34:ARG:NH1	2.36	0.58
1:A:453:PHE:HB3	1:A:470:TYR:CD2	2.37	0.58
1:A:206:ILE:HG13	1:A:208:ARG:HH21	1.66	0.58
1:A:274:LEU:HB3	1:A:282:ILE:HD13	1.86	0.58
2:G:98:ARG:HB2	2:G:106:ASP:HB2	1.85	0.58
2:H:73:ASP:HB3	2:H:76:ILE:HG22	1.84	0.58
1:A:985:GLU:OE2	1:A:985:GLU:N	2.25	0.58
1:A:288:CYS:HB2	1:A:295:GLU:HA	1.85	0.58
2:H:32:TYR:HB3	2:H:98:ARG:HH12	1.67	0.58
2:H:91:THR:OG1	2:H:116:VAL:N	2.35	0.58
1:E:982:ASP:OD2	1:E:984:PRO:HD2	2.04	0.58
1:A:362:TYR:HE2	1:A:385:ASN:HA	1.68	0.58
3:D:62:ARG:HD2	3:D:78:ARG:HB3	1.85	0.58
3:F:16:GLY:N	3:F:79:LEU:O	2.35	0.58
3:F:24:ARG:NH1	3:F:71:ASP:OD1	2.37	0.58
1:A:390:THR:HG22	1:A:515:LEU:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:LEU:HD13	1:A:956:LEU:HD22	1.86	0.58
3:D:6:GLN:HA	3:D:23:CYS:HA	1.86	0.57
1:E:67:VAL:HG22	1:E:77:PHE:HA	1.84	0.57
2:H:41:PRO:HD3	2:H:92:ALA:HA	1.86	0.57
1:E:196:PHE:HB3	1:E:226:LEU:HB2	1.86	0.57
1:C:415:ILE:HG13	1:C:419:ASN:HD22	1.69	0.57
1:A:107:THR:OG1	1:A:109:ASP:OD2	2.14	0.57
1:C:332:LEU:HA	1:C:359:VAL:HB	1.87	0.57
1:E:293:LEU:O	1:E:296:THR:OG1	2.20	0.57
1:A:52:GLN:HG2	1:A:271:THR:HG22	1.85	0.57
1:A:344:PHE:HB2	1:A:506:ARG:HE	1.70	0.57
1:A:437:LYS:HZ2	2:B:33:TRP:HB2	1.69	0.57
1:E:110:SER:HB3	1:E:132:GLN:HB2	1.86	0.57
1:A:142:LYS:HE2	1:A:256:THR:HG21	1.87	0.57
1:A:352:ARG:HG2	1:A:463:ARG:HH21	1.70	0.56
1:E:27:ALA:HB3	1:E:64:TRP:HB3	1.87	0.56
1:C:409:PRO:HG3	1:C:422:LEU:HD21	1.87	0.56
2:H:7:SER:OG	2:H:21:SER:N	2.32	0.56
1:A:451:ARG:NH1	1:A:464:ASP:OD2	2.37	0.56
3:D:62:ARG:HH12	3:D:80:GLU:HB2	1.69	0.56
1:E:54:LEU:HB3	1:E:190:LYS:HZ1	1.69	0.56
1:E:99:ILE:HD11	1:E:237:THR:HB	1.87	0.56
1:E:277:ASN:ND2	1:E:279:ASN:H	2.02	0.56
1:E:289:ALA:O	1:E:629:THR:OG1	2.12	0.56
1:E:390:THR:HG22	1:E:519:ALA:HA	1.87	0.56
1:E:430:VAL:HG22	1:E:509:VAL:HG23	1.85	0.56
1:E:482:GLY:H	1:E:485:CYS:HB2	1.70	0.56
1:C:441:LYS:HD3	1:C:444:GLY:HA2	1.87	0.56
1:E:79:ASN:OD1	1:E:237:THR:OG1	2.24	0.56
1:E:316:ARG:N	1:E:625:GLN:OE1	2.38	0.56
1:C:341:ALA:HB3	1:C:344:PHE:HE1	1.71	0.56
1:C:354:ARG:HE	1:C:356:SER:HB2	1.70	0.56
2:H:91:THR:HG23	2:H:115:THR:HA	1.88	0.56
1:C:390:THR:HB	1:C:519:ALA:HA	1.88	0.56
1:A:785:ILE:HG23	1:A:873:ALA:HB2	1.88	0.56
2:H:29:PHE:HB3	2:H:53:PRO:HB2	1.87	0.56
2:H:108:TRP:HB2	3:L:44:ALA:HB1	1.87	0.56
3:F:24:ARG:HH12	3:F:71:ASP:HA	1.69	0.56
1:C:318:GLN:HB3	1:C:625:GLN:N	2.21	0.56
2:H:68:VAL:HB	2:H:83:TRP:HA	1.88	0.56
1:A:390:THR:HA	1:A:520:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:ASN:ND2	2:G:102:GLU:OE2	2.33	0.56
1:A:294:SER:HA	1:A:297:LYS:HD2	1.88	0.56
1:E:241:LEU:HB3	1:E:255:TRP:HB3	1.87	0.56
1:C:777:GLU:O	1:C:781:GLN:NE2	2.39	0.55
1:C:909:THR:OG1	1:C:911:ASN:OD1	2.20	0.55
1:A:459:LYS:HG3	1:A:462:GLU:HB2	1.88	0.55
1:A:787:LYS:NZ	1:E:699:GLU:OE1	2.33	0.55
3:F:90:GLN:HE22	3:F:97:PRO:HB2	1.70	0.55
1:E:393:TYR:N	1:E:511:SER:O	2.34	0.55
3:F:64:SER:N	3:F:75:THR:O	2.39	0.55
1:A:139:LEU:HD23	1:A:151:GLU:HB3	1.88	0.55
1:E:658:GLU:OE1	1:E:659:CYS:N	2.38	0.55
1:C:335:PHE:HE2	1:C:365:LEU:HD11	1.71	0.55
3:F:37:TYR:HB2	3:F:88:TYR:HB2	1.88	0.55
1:C:324:VAL:HG22	1:C:526:LYS:HA	1.87	0.55
1:A:40:ASP:OD1	1:A:41:LYS:N	2.35	0.55
1:E:737:MET:CE	1:E:854:GLY:HA2	2.37	0.55
1:A:453:PHE:HB2	1:A:488:PRO:HA	1.88	0.55
1:C:547:GLY:HA3	1:C:584:ILE:HD11	1.89	0.55
1:A:324:VAL:HG23	1:A:539:ASN:HB3	1.87	0.55
1:A:390:THR:HB	1:A:519:ALA:HA	1.87	0.55
1:A:493:SER:HB3	1:A:495:ARG:HH21	1.72	0.55
3:D:16:GLY:H	3:D:79:LEU:HB2	1.70	0.55
1:E:107:THR:O	1:E:234:ARG:NH2	2.40	0.55
3:L:91:GLN:HB3	3:L:94:SER:HB3	1.89	0.55
2:B:91:THR:HG23	2:B:115:THR:HA	1.89	0.55
1:E:245:TYR:N	1:E:256:THR:OG1	2.36	0.55
1:E:293:LEU:HB2	1:E:605:VAL:HG11	1.88	0.55
1:C:404:VAL:HA	1:C:407:ILE:HG22	1.89	0.55
1:A:425:ASP:N	1:A:425:ASP:OD1	2.40	0.55
2:B:98:ARG:NE	2:B:106:ASP:HB3	2.20	0.55
3:D:67:GLY:HA3	3:D:72:PHE:HA	1.89	0.55
1:E:440:SER:HB3	1:E:496:PRO:HG3	1.89	0.55
1:C:52:GLN:HG2	1:C:271:THR:HB	1.88	0.54
3:D:56:ALA:HB3	3:D:59:ILE:HG13	1.88	0.54
1:E:919:LEU:HG	1:E:923:GLN:HE21	1.71	0.54
1:C:376:CYS:HA	1:C:429:CYS:HA	1.89	0.54
2:H:32:TYR:HB3	2:H:98:ARG:NH1	2.22	0.54
1:C:422:LEU:HD12	1:C:423:PRO:HD2	1.89	0.54
1:E:437:LYS:NZ	2:G:53:PRO:HD2	2.21	0.54
1:C:127:LYS:HZ2	1:C:161:CYS:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:TRP:HB2	1:C:395:ASP:OD1	2.06	0.54
2:G:29:PHE:CE2	2:G:53:PRO:HB3	2.42	0.54
3:L:55:ARG:HH22	3:L:61:ASP:HA	1.72	0.54
1:A:480:VAL:HG22	1:A:481:ALA:H	1.71	0.54
1:A:801:GLN:HB3	1:A:815:ILE:HD11	1.88	0.54
1:E:110:SER:OG	1:E:111:LYS:NZ	2.28	0.54
1:E:395:ASP:OD2	1:E:463:ARG:NH2	2.41	0.54
1:E:549:LEU:HD12	1:E:582:LEU:HB3	1.90	0.54
1:C:489:LEU:O	1:C:490:ARG:NH1	2.41	0.54
1:A:1103:GLN:HE21	1:A:1106:PHE:HB3	1.73	0.54
1:C:481:ALA:HB2	1:C:487:PHE:HB2	1.90	0.54
1:A:450:TYR:HE2	1:A:492:TYR:HA	1.72	0.54
1:E:451:ARG:HG3	1:E:488:PRO:HB2	1.89	0.54
1:C:325:ARG:HG2	1:C:576:PRO:HD2	1.90	0.54
1:C:398:VAL:HG13	1:C:506:ARG:HH22	1.72	0.54
1:C:563:GLY:N	1:C:572:ALA:O	2.37	0.54
1:A:449:LEU:HA	1:A:491:SER:HA	1.88	0.54
1:A:562:PHE:HB3	1:A:573:VAL:HG23	1.89	0.54
1:A:67:VAL:HG22	1:A:75:LYS:HD2	1.90	0.54
1:A:1048:SER:OG	1:A:1061:HIS:ND1	2.41	0.54
1:E:61:ASN:OD1	5:E:1302:NAG:N2	2.41	0.54
3:F:90:GLN:NE2	3:F:97:PRO:HB2	2.23	0.54
1:C:127:LYS:NZ	1:C:161:CYS:HB3	2.23	0.53
2:H:52:TYR:HB3	2:H:57:ASP:HB2	1.90	0.53
2:B:68:VAL:HB	2:B:83:TRP:HA	1.89	0.53
1:E:595:ILE:HB	1:E:606:ALA:HB3	1.90	0.53
1:C:455:LYS:NZ	1:C:469:ILE:O	2.37	0.53
1:C:743:SER:HB2	1:C:746:CYS:HB3	1.90	0.53
1:E:106:THR:OG1	1:E:231:ASN:O	2.26	0.53
1:C:185:ARG:HB3	1:C:187:PHE:HE1	1.73	0.53
3:L:5:THR:O	3:L:24:ARG:N	2.31	0.53
1:A:398:VAL:HG13	1:A:506:ARG:HD3	1.89	0.53
2:B:6:GLN:HA	2:B:22:CYS:HA	1.90	0.53
3:D:5:THR:HA	3:D:101:GLN:HG2	1.89	0.53
1:C:609:TYR:CE2	1:C:621:ILE:HD11	2.43	0.53
2:H:93:MET:HB2	2:H:113:MET:SD	2.48	0.53
3:D:36:TRP:O	3:D:48:LEU:N	2.42	0.53
1:E:608:LEU:HD22	1:E:663:ILE:HG23	1.91	0.53
1:C:226:LEU:HB3	1:C:228:ILE:HD12	1.89	0.53
1:C:320:THR:OG1	1:C:321:GLU:OE1	2.26	0.53
1:E:103:ILE:HD12	1:E:116:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:34:LEU:HA	3:F:91:GLN:HA	1.91	0.53
3:F:67:GLY:HA3	3:F:72:PHE:HA	1.90	0.53
1:A:81:VAL:HG23	1:A:108:LEU:HD22	1.91	0.53
1:E:27:ALA:O	1:E:64:TRP:N	2.40	0.53
1:C:41:LYS:HB2	1:A:560:GLN:HA	1.91	0.53
1:C:451:ARG:NH1	1:C:468:GLU:H	2.01	0.53
1:C:1126:VAL:HG23	1:E:914:TYR:HB3	1.91	0.53
1:A:172:MET:SD	1:A:172:MET:N	2.74	0.53
1:C:435:SER:HB3	1:C:506:ARG:HB2	1.91	0.53
2:H:2:VAL:HG22	2:H:27:PHE:HB3	1.91	0.53
3:L:78:ARG:NE	3:L:80:GLU:OE1	2.40	0.53
1:E:342:THR:O	1:E:343:ARG:HD2	2.09	0.53
2:H:5:VAL:HG13	2:H:110:GLN:HG2	1.91	0.53
2:G:105:PHE:HB2	2:G:108:TRP:NE1	2.23	0.53
1:C:550:THR:O	1:C:583:ASP:N	2.42	0.53
1:C:943:GLY:O	1:C:947:ASP:N	2.40	0.53
1:E:801:GLN:HB3	1:E:815:ILE:HD11	1.90	0.53
2:H:61:SER:O	2:H:65:GLN:N	2.42	0.52
2:H:97:ALA:HA	2:H:108:TRP:HA	1.91	0.52
1:E:57:PRO:HB2	1:E:60:SER:HB3	1.91	0.52
1:C:277:ASN:OD1	1:C:281:THR:N	2.40	0.52
1:C:296:THR:HG22	1:C:312:THR:HG21	1.90	0.52
1:C:439:ASP:OD2	1:C:506:ARG:NH2	2.42	0.52
2:H:94:TYR:HB2	2:H:112:THR:HB	1.91	0.52
2:B:20:ILE:HG12	2:B:81:LEU:HB3	1.91	0.52
2:B:23:LYS:NZ	2:B:77:SER:O	2.43	0.52
1:E:141:HIS:CE1	1:E:242:HIS:H	2.27	0.52
1:E:350:TRP:CZ2	1:E:420:TYR:HB2	2.45	0.52
2:G:5:VAL:HB	2:G:23:LYS:HB3	1.91	0.52
1:C:1033:GLN:HE21	1:C:1046:LEU:HA	1.74	0.52
3:D:62:ARG:NH1	3:D:78:ARG:O	2.43	0.52
2:H:20:ILE:HG12	2:H:81:LEU:HB3	1.91	0.52
3:L:36:TRP:N	3:L:49:ILE:O	2.42	0.52
1:A:205:ILE:HG13	1:A:207:VAL:H	1.75	0.52
3:D:37:TYR:HB2	3:D:88:TYR:HB2	1.91	0.52
2:H:48:MET:SD	2:H:48:MET:N	2.83	0.52
1:A:914:TYR:HB3	1:E:1126:VAL:HG23	1.90	0.52
2:B:86:LEU:HD22	2:B:116:VAL:HG21	1.92	0.52
3:D:15:PRO:HA	3:D:79:LEU:HB2	1.91	0.52
1:E:983:PRO:HA	1:E:986:ALA:HB3	1.92	0.52
1:C:142:LYS:HB2	1:C:242:HIS:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:O	1:A:185:ARG:NH1	2.35	0.52
1:A:183:ASN:O	1:A:185:ARG:NH1	2.42	0.52
1:A:399:ILE:HG13	1:A:401:GLY:H	1.75	0.52
3:D:64:SER:OG	3:D:75:THR:O	2.21	0.52
1:E:201:LYS:HB2	1:E:220:LEU:HA	1.90	0.52
3:F:40:LYS:HB2	3:F:43:GLN:HB2	1.92	0.52
1:A:333:CYS:HB3	1:A:335:PHE:HD1	1.75	0.52
1:E:346:SER:OG	1:E:347:VAL:N	2.43	0.52
1:E:730:LYS:HZ3	1:E:860:PRO:HA	1.75	0.52
1:A:34:ARG:NH2	1:A:215:GLN:HA	2.25	0.51
1:E:906:ILE:HD12	1:E:1044:TYR:HB3	1.92	0.51
1:C:345:ALA:O	1:C:397:PHE:HA	2.10	0.51
2:H:92:ALA:HB3	2:H:94:TYR:HE1	1.75	0.51
3:L:36:TRP:O	3:L:48:LEU:N	2.44	0.51
1:A:419:ASN:ND2	1:A:451:ARG:O	2.43	0.51
1:C:74:THR:OG1	1:C:76:ARG:NH1	2.43	0.51
1:A:434:ASN:HA	1:A:505:TYR:HD1	1.76	0.51
1:E:372:PHE:HB2	1:E:433:TRP:HA	1.92	0.51
1:A:159:ASN:N	1:A:159:ASN:OD1	2.43	0.51
1:A:332:LEU:HA	1:A:359:VAL:HB	1.93	0.51
1:E:348:TYR:OH	1:E:449:LEU:HB3	2.11	0.51
1:E:449:LEU:HD23	1:E:489:LEU:HB3	1.91	0.51
2:G:39:GLN:NE2	2:G:43:LYS:O	2.42	0.51
3:L:4:LEU:O	3:L:100:GLY:HA2	2.11	0.51
2:G:47:TRP:HZ2	2:G:50:ILE:HG12	1.75	0.51
4:Y:1:NAG:O7	4:Y:2:NAG:O6	2.25	0.51
1:C:325:ARG:HH12	1:C:529:ASN:HA	1.75	0.51
1:C:444:GLY:HA3	1:C:495:ARG:HG3	1.92	0.51
1:C:989:GLN:HE21	1:C:992:ARG:NH2	2.07	0.51
1:A:277:ASN:OD1	1:A:281:THR:N	2.44	0.51
1:A:812:ARG:HD2	1:A:816:GLU:HB3	1.92	0.51
2:B:6:GLN:NE2	2:B:112:THR:OG1	2.44	0.51
1:E:56:LEU:N	1:E:267:LEU:HG	2.25	0.51
1:C:350:TRP:CE2	1:C:463:ARG:HB2	2.45	0.51
1:A:315:PHE:HZ	1:A:612:VAL:HG21	1.76	0.51
1:A:969:ALA:HA	1:A:992:ARG:HH21	1.75	0.51
3:D:24:ARG:NH1	3:D:71:ASP:OD1	2.44	0.51
1:E:592:VAL:HG11	1:E:630:TRP:HZ3	1.75	0.51
2:G:2:VAL:HG22	2:G:27:PHE:HB3	1.92	0.51
1:C:723:ILE:HD13	1:C:941:ALA:HB3	1.93	0.51
1:A:419:ASN:OD1	1:A:451:ARG:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TRP:O	2:B:99:GLY:N	2.44	0.51
1:E:400:ARG:NH2	1:E:492:TYR:O	2.38	0.51
1:A:445:ASN:ND2	1:A:492:TYR:OH	2.44	0.50
1:E:844:ARG:HA	1:E:848:CYS:HB2	1.92	0.50
1:C:415:ILE:HG13	1:C:419:ASN:ND2	2.26	0.50
1:C:853:LYS:HE3	1:C:963:LEU:HD13	1.93	0.50
1:C:140:ASP:HB2	1:C:144:ASN:HD22	1.77	0.50
1:C:1073:THR:OG1	1:C:1094:SER:HB3	2.11	0.50
2:H:30:THR:HG23	2:H:52:TYR:HE1	1.76	0.50
2:H:64:PHE:HA	2:H:67:GLN:HB2	1.93	0.50
1:A:118:VAL:HG23	1:A:120:ASN:H	1.75	0.50
1:A:376:CYS:HA	1:A:429:CYS:HA	1.92	0.50
1:A:407:ILE:HD13	1:A:415:ILE:HG13	1.93	0.50
1:C:1112:ILE:HG22	1:C:1134:VAL:HG13	1.93	0.50
2:H:51:ILE:HB	2:H:58:THR:HG23	1.93	0.50
3:L:39:GLN:NE2	3:L:40:LYS:O	2.45	0.50
3:L:48:LEU:HD22	3:L:87:TYR:HD2	1.76	0.50
1:A:463:ARG:HH11	1:A:465:ILE:HD11	1.77	0.50
1:A:730:LYS:HD2	1:A:768:ALA:HB1	1.93	0.50
1:A:904:ASN:ND2	1:A:910:GLN:HE21	2.10	0.50
1:E:900:ALA:HB2	1:E:913:LEU:HD22	1.93	0.50
1:C:407:ILE:HA	1:C:416:ALA:HB2	1.92	0.50
1:C:433:TRP:O	1:C:506:ARG:N	2.45	0.50
1:A:325:ARG:HA	1:A:325:ARG:HE	1.75	0.50
1:A:659:CYS:HB2	1:A:694:MET:SD	2.51	0.50
1:E:140:ASP:HA	1:E:242:HIS:HA	1.92	0.50
1:C:139:LEU:HD22	1:C:151:GLU:HG3	1.93	0.50
1:C:910:GLN:NE2	1:A:1087:PRO:O	2.43	0.50
2:H:34:ILE:HD13	2:H:98:ARG:HB3	1.92	0.50
2:H:39:GLN:O	2:H:93:MET:N	2.37	0.50
1:E:200:SER:HB3	1:E:223:LEU:HD23	1.94	0.50
1:C:241:LEU:HB3	1:C:255:TRP:CD1	2.46	0.50
3:L:24:ARG:HH12	3:L:70:THR:HG23	1.76	0.50
2:B:7:SER:N	2:B:21:SER:O	2.44	0.50
1:E:132:GLN:HB3	1:E:156:SER:HB2	1.93	0.50
1:E:850:GLN:HE21	1:E:855:LEU:HD22	1.76	0.50
1:E:871:THR:HG21	1:E:1052:SER:HB3	1.92	0.50
2:G:6:GLN:NE2	2:G:94:TYR:O	2.44	0.50
1:C:799:PHE:HB3	1:C:803:LEU:HD23	1.93	0.50
1:C:397:PHE:CZ	1:C:509:VAL:HG23	2.47	0.50
3:L:25:ALA:O	3:L:70:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:GLN:HG2	1:E:271:THR:HB	1.94	0.50
1:E:1025:LYS:NZ	1:E:1039:PHE:O	2.44	0.50
1:C:317:VAL:HG13	1:C:587:CYS:HB3	1.93	0.49
2:H:21:SER:HA	2:H:79:ALA:O	2.12	0.49
3:L:39:GLN:HG2	3:L:45:PRO:HG3	1.94	0.49
1:A:449:LEU:HB3	1:A:489:LEU:HB3	1.93	0.49
1:E:960:VAL:HA	1:E:963:LEU:HD23	1.94	0.49
3:F:36:TRP:O	3:F:48:LEU:N	2.32	0.49
2:G:52:TYR:HB3	2:G:57:ASP:HB3	1.93	0.49
1:C:81:VAL:HG21	1:C:234:ARG:CZ	2.41	0.49
1:C:413:GLY:O	1:C:417:ASP:N	2.36	0.49
1:C:914:TYR:HB3	1:A:1126:VAL:HG13	1.94	0.49
2:H:43:LYS:HG2	2:H:44:GLY:H	1.76	0.49
2:H:47:TRP:HZ2	2:H:50:ILE:HG23	1.77	0.49
1:A:1036:ARG:HD2	1:E:1036:ARG:HD2	1.94	0.49
1:E:140:ASP:HB2	1:E:149:GLU:HG2	1.94	0.49
1:A:1094:SER:HB3	1:A:1099:TRP:HA	1.94	0.49
2:B:24:GLY:HA3	2:B:29:PHE:CZ	2.47	0.49
1:E:437:LYS:HG3	2:G:52:TYR:CE1	2.47	0.49
1:C:738:TYR:HA	1:C:853:LYS:HD3	1.94	0.49
1:A:288:CYS:HA	1:A:294:SER:HB3	1.93	0.49
1:A:444:GLY:HA3	1:A:495:ARG:HD3	1.94	0.49
1:E:472:ALA:HB3	1:E:484:ASN:HB3	1.94	0.49
2:G:69:THR:OG1	2:G:82:GLN:HB3	2.12	0.49
1:C:709:ILE:O	1:C:1072:PHE:N	2.44	0.49
1:A:819:LEU:HD21	1:A:935:LEU:HD13	1.93	0.49
2:G:41:PRO:HD3	2:G:92:ALA:HA	1.95	0.49
1:C:853:LYS:HG2	1:C:963:LEU:HD11	1.95	0.49
1:C:324:VAL:H	1:C:528:THR:HB	1.78	0.49
1:C:419:ASN:OD1	1:C:451:ARG:N	2.46	0.49
1:E:183:ASN:N	1:E:183:ASN:OD1	2.46	0.49
3:F:8:PRO:HD2	3:F:11:LEU:HD11	1.94	0.49
1:C:347:VAL:HG12	1:C:419:ASN:HB3	1.94	0.49
1:C:398:VAL:HA	1:C:506:ARG:HH12	1.77	0.49
1:A:109:ASP:OD1	1:A:111:LYS:HG2	2.13	0.49
1:E:102:TRP:H	1:E:117:ILE:HB	1.77	0.49
1:C:118:VAL:HG23	1:C:139:LEU:HD11	1.93	0.49
3:L:35:ALA:N	3:L:90:GLN:O	2.46	0.49
3:L:38:GLN:OE1	3:L:40:LYS:HD2	2.13	0.49
1:A:68:ILE:HG13	1:A:259:ALA:HA	1.94	0.49
1:C:325:ARG:HE	1:C:577:GLN:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:ASP:O	1:A:995:THR:HG23	2.13	0.49
1:E:831:ILE:HG23	1:E:833:GLN:H	1.78	0.49
2:G:2:VAL:HB	2:G:107:ILE:HG13	1.95	0.49
1:C:64:TRP:NE1	1:C:66:HIS:HB2	2.27	0.48
1:C:423:PRO:HD3	1:C:460:PRO:HB2	1.93	0.48
3:L:48:LEU:O	3:L:49:ILE:HG13	2.13	0.48
1:A:98:ILE:HD13	1:A:260:ALA:HB2	1.95	0.48
1:A:275:LYS:HD2	1:A:303:PHE:CZ	2.48	0.48
1:A:432:ALA:HB2	1:A:507:VAL:HG22	1.94	0.48
1:A:767:ILE:HD11	1:A:1009:LEU:HG	1.95	0.48
1:E:350:TRP:HZ3	1:E:397:PHE:CG	2.31	0.48
1:C:850:GLN:NE2	1:C:956:LEU:HB3	2.27	0.48
2:H:6:GLN:HG3	2:H:22:CYS:HB2	1.95	0.48
3:L:38:GLN:HB2	3:L:48:LEU:HB2	1.94	0.48
1:A:482:GLY:N	1:A:485:CYS:O	2.35	0.48
1:E:182:LYS:HB2	1:E:208:ARG:HD2	1.94	0.48
1:C:278:GLU:OE1	1:C:278:GLU:N	2.45	0.48
3:L:27:GLN:N	3:L:27:GLN:OE1	2.46	0.48
1:A:188:VAL:HG23	1:A:220:LEU:HD22	1.95	0.48
1:A:459:LYS:HE3	1:A:462:GLU:HB2	1.94	0.48
2:B:6:GLN:HB2	2:B:110:GLN:H	1.78	0.48
1:E:452:LEU:HB2	1:E:490:ARG:HB2	1.95	0.48
1:C:293:LEU:HB2	1:C:605:VAL:HG11	1.95	0.48
1:C:658:GLU:OE1	1:C:659:CYS:N	2.47	0.48
1:C:849:ALA:HA	1:A:567:ALA:HB2	1.95	0.48
2:B:61:SER:O	2:B:65:GLN:N	2.46	0.48
1:C:49:HIS:NE2	1:C:51:THR:OG1	2.45	0.48
1:C:1137:PRO:O	1:C:1141:GLU:HG2	2.12	0.48
3:L:50:TYR:HD1	3:L:56:ALA:HA	1.77	0.48
1:A:480:VAL:HG22	1:A:481:ALA:N	2.28	0.48
1:E:273:LEU:HD22	1:E:301:LYS:HZ3	1.78	0.48
1:E:1090:GLY:H	1:E:1104:ARG:HE	1.59	0.48
1:C:384:LEU:HD11	1:C:512:PHE:HE2	1.78	0.48
1:A:64:TRP:HB2	1:A:263:TYR:HD2	1.78	0.48
1:A:132:GLN:HG3	1:A:156:SER:OG	2.12	0.48
1:A:339:PHE:HE2	1:A:431:ILE:HG21	1.79	0.48
1:A:355:ILE:HG23	1:A:358:CYS:SG	2.53	0.48
2:B:105:PHE:HB2	2:B:108:TRP:NE1	2.29	0.48
1:C:448:TYR:O	1:C:492:TYR:HB3	2.14	0.48
2:H:38:ARG:HD2	2:H:83:TRP:CZ2	2.48	0.48
2:H:47:TRP:CZ2	2:H:50:ILE:HG23	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ASN:ND2	1:A:504:PRO:HD2	2.28	0.48
2:B:24:GLY:HA3	2:B:29:PHE:HZ	1.77	0.48
2:B:58:THR:HG21	2:B:70:ILE:HB	1.95	0.48
3:D:2:ILE:HG12	3:D:27:GLN:HB2	1.96	0.48
1:E:320:THR:OG1	1:E:321:GLU:OE1	2.26	0.48
3:F:2:ILE:H	3:F:2:ILE:HD12	1.79	0.48
1:C:910:GLN:HE21	1:A:1086:PHE:HB3	1.79	0.48
1:E:468:GLU:O	1:E:488:PRO:HD3	2.14	0.48
2:G:9:ALA:HA	2:G:112:THR:HG23	1.96	0.48
1:C:393:TYR:HD2	1:C:511:SER:HB3	1.79	0.48
1:A:352:ARG:HB2	1:A:393:TYR:CE1	2.45	0.48
1:E:990:ILE:O	1:E:994:ILE:HG12	2.14	0.48
1:C:98:ILE:HG22	1:C:239:LEU:HD11	1.95	0.48
1:C:696:LEU:HD11	1:E:866:MET:HB2	1.96	0.48
1:C:806:PRO:O	1:C:811:LYS:NZ	2.47	0.48
2:B:29:PHE:HB3	2:B:53:PRO:CB	2.43	0.48
3:D:1:GLU:HG3	3:D:96:PRO:HB2	1.96	0.48
1:E:1139:GLN:HB3	1:E:1140:PRO:HD3	1.95	0.48
2:H:12:LYS:O	2:H:117:SER:N	2.47	0.47
2:H:70:ILE:HG12	2:H:81:LEU:HD21	1.96	0.47
1:E:572:ALA:HB1	1:E:581:ILE:HD11	1.96	0.47
1:C:427:THR:HG21	1:C:514:LEU:HD21	1.95	0.47
3:L:39:GLN:HA	3:L:45:PRO:HB3	1.96	0.47
1:A:1089:GLU:O	1:A:1104:ARG:NH1	2.47	0.47
1:E:131:PHE:CD1	1:E:155:TYR:HB2	2.49	0.47
1:E:414:ASN:OD1	1:E:415:ILE:N	2.47	0.47
1:C:451:ARG:HH22	1:C:467:THR:HA	1.79	0.47
1:C:556:PHE:HB2	1:C:581:ILE:HD11	1.97	0.47
3:L:36:TRP:HB3	3:L:48:LEU:HB3	1.96	0.47
1:A:43:PHE:HE1	1:A:280:GLY:HA3	1.79	0.47
1:A:79:ASN:ND2	1:A:239:LEU:HD22	2.30	0.47
1:A:81:VAL:HG21	1:A:234:ARG:HH11	1.79	0.47
3:D:38:GLN:N	3:D:46:ARG:O	2.41	0.47
1:E:389:PHE:HB3	1:E:512:PHE:HB2	1.96	0.47
1:E:899:MET:HB3	1:E:913:LEU:HD11	1.96	0.47
1:C:451:ARG:NH2	1:C:466:SER:O	2.46	0.47
1:A:777:GLU:O	1:A:781:GLN:NE2	2.47	0.47
1:E:33:THR:O	1:E:33:THR:OG1	2.33	0.47
1:E:273:LEU:HG	1:E:298:CYS:SG	2.54	0.47
1:E:1126:VAL:HG13	1:E:1129:ILE:HB	1.96	0.47
1:C:400:ARG:HH22	1:C:492:TYR:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:O	3:L:98:THR:OG1	2.27	0.47
1:A:487:PHE:O	1:A:490:ARG:NH2	2.43	0.47
1:C:20:THR:OG1	1:C:21:ARG:N	2.47	0.47
1:C:57:PRO:HA	1:C:270:ARG:NH2	2.30	0.47
1:C:94:GLU:OE1	1:C:94:GLU:N	2.48	0.47
1:C:404:VAL:HG13	1:C:405:ARG:HH11	1.79	0.47
1:C:707:ASN:ND2	1:C:1073:THR:HB	2.28	0.47
1:A:833:GLN:HG3	1:E:613:ASN:HD22	1.79	0.47
1:E:449:LEU:HG	1:E:491:SER:HA	1.95	0.47
1:E:458:LEU:HD12	1:E:458:LEU:H	1.78	0.47
2:G:39:GLN:N	2:G:93:MET:O	2.35	0.47
1:C:318:GLN:H	1:C:625:GLN:HG2	1.80	0.47
1:C:631:ARG:HE	1:C:633:TYR:HA	1.80	0.47
1:C:726:VAL:HG23	1:C:1056:GLY:HA2	1.97	0.47
1:C:1028:GLU:OE2	1:A:1036:ARG:NH1	2.48	0.47
2:B:68:VAL:HA	2:B:84:SER:HB3	1.97	0.47
1:E:534:LYS:HE2	1:E:534:LYS:HB3	1.80	0.47
1:E:799:PHE:CD1	1:E:802:ILE:HD11	2.48	0.47
2:G:72:ALA:HA	2:G:79:ALA:HA	1.96	0.47
1:C:169:PRO:O	1:C:171:LEU:N	2.47	0.47
1:C:324:VAL:HG22	1:C:526:LYS:HD3	1.96	0.47
1:C:326:PHE:HB3	1:C:577:GLN:OE1	2.15	0.47
1:C:589:PHE:HZ	1:E:851:LYS:HG2	1.80	0.47
3:L:37:TYR:HA	3:L:48:LEU:H	1.80	0.47
1:A:325:ARG:HB2	1:A:540:PHE:HA	1.96	0.47
1:E:173:ASP:HB3	1:E:185:ARG:HE	1.78	0.47
2:G:36:TRP:CD2	2:G:81:LEU:HD12	2.49	0.47
1:C:173:ASP:HB2	1:C:185:ARG:HH21	1.79	0.47
1:C:277:ASN:OD1	1:C:280:GLY:N	2.48	0.47
3:L:38:GLN:HB2	3:L:48:LEU:HD13	1.97	0.47
3:L:63:PHE:CD1	3:L:76:ILE:HD13	2.50	0.47
1:A:64:TRP:HB2	1:A:263:TYR:CD2	2.50	0.47
1:A:333:CYS:HB3	1:A:335:PHE:CD1	2.51	0.47
1:E:275:LYS:HB2	1:E:303:PHE:CE1	2.50	0.47
3:F:18:ARG:HH12	3:F:20:THR:HG1	1.56	0.47
1:C:600:ASN:OD1	1:C:601:THR:N	2.49	0.46
3:L:37:TYR:HE1	3:L:47:LEU:HD12	1.80	0.46
1:A:377:TYR:HB2	1:A:426:PHE:HD2	1.80	0.46
1:E:344:PHE:HB3	1:E:506:ARG:NH1	2.30	0.46
3:F:35:ALA:HB2	3:F:92:TYR:HD2	1.79	0.46
3:F:66:SER:OG	3:F:73:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG22	1:A:234:ARG:HD2	1.97	0.46
1:A:371:PHE:CD1	1:A:433:TRP:HB3	2.51	0.46
3:D:35:ALA:N	3:D:90:GLN:O	2.49	0.46
3:D:55:ARG:NH1	3:D:61:ASP:HA	2.29	0.46
1:E:326:PHE:H	1:E:527:SER:HB2	1.80	0.46
2:G:91:THR:HG23	2:G:115:THR:HA	1.98	0.46
1:C:350:TRP:O	1:C:463:ARG:NE	2.38	0.46
1:C:418:TYR:HA	1:C:454:ARG:NH2	2.30	0.46
1:A:307:LYS:HD3	1:A:660:ASP:OD1	2.16	0.46
1:A:600:ASN:HB3	5:A:1301:NAG:H2	1.96	0.46
1:A:716:THR:HG23	1:A:1065:VAL:HB	1.96	0.46
1:E:107:THR:HG1	1:E:112:THR:HG1	1.58	0.46
1:E:348:TYR:CZ	1:E:489:LEU:HG	2.50	0.46
1:E:371:PHE:CE2	1:E:374:PHE:HB2	2.50	0.46
1:E:471:GLN:OE1	1:E:477:CYS:N	2.44	0.46
3:L:61:ASP:OD1	3:L:62:ARG:N	2.48	0.46
1:A:66:HIS:CD2	1:A:68:ILE:HB	2.50	0.46
1:A:404:VAL:O	1:A:407:ILE:HG22	2.16	0.46
1:A:1025:LYS:NZ	1:A:1039:PHE:O	2.32	0.46
1:E:243:ARG:HG2	1:E:244:SER:N	2.30	0.46
1:E:379:VAL:HG22	1:E:380:SER:H	1.80	0.46
2:G:7:SER:O	2:G:112:THR:OG1	2.27	0.46
1:A:434:ASN:HA	1:A:505:TYR:CD1	2.50	0.46
1:A:470:TYR:N	1:A:486:TYR:O	2.45	0.46
1:A:735:CYS:SG	1:A:736:THR:N	2.88	0.46
3:D:2:ILE:HG23	3:D:27:GLN:H	1.81	0.46
1:E:181:PHE:HA	1:E:208:ARG:HH12	1.79	0.46
1:E:350:TRP:HD1	1:E:463:ARG:HG3	1.80	0.46
1:E:448:TYR:HB3	1:E:492:TYR:HD2	1.80	0.46
1:E:557:LEU:H	1:E:560:GLN:HE21	1.64	0.46
1:E:597:PRO:HB3	1:E:671:TYR:HB2	1.98	0.46
1:E:753:TYR:OH	1:E:991:ASP:OD1	2.31	0.46
3:F:36:TRP:CE2	3:F:74:LEU:HB2	2.50	0.46
1:C:785:ILE:HD11	1:A:696:LEU:HB3	1.97	0.46
2:H:105:PHE:HB2	2:H:108:TRP:NE1	2.29	0.46
3:D:34:LEU:HG	3:D:91:GLN:HA	1.97	0.46
1:E:48:LEU:O	1:E:301:LYS:NZ	2.43	0.46
1:E:403:GLU:HG3	1:E:406:GLN:HG3	1.95	0.46
1:C:67:VAL:HB	1:C:75:LYS:HD2	1.97	0.46
1:C:195:TYR:O	1:C:197:LYS:NZ	2.49	0.46
1:A:213:LEU:O	1:A:215:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:HB2	2:B:110:GLN:N	2.30	0.46
1:E:1135:TYR:HE1	1:E:1140:PRO:HG2	1.80	0.46
1:C:469:ILE:HD13	1:C:480:VAL:HA	1.97	0.46
1:A:37:TYR:OH	1:A:190:LYS:NZ	2.38	0.46
1:E:98:ILE:HD13	1:E:260:ALA:HB2	1.97	0.46
1:E:270:ARG:HB3	1:E:272:PHE:HE1	1.80	0.46
1:E:316:ARG:O	1:E:318:GLN:NE2	2.49	0.46
1:E:350:TRP:CD1	1:E:463:ARG:HG3	2.51	0.46
1:E:705:SER:OG	1:E:706:ASN:N	2.49	0.46
2:G:15:GLY:N	2:G:86:LEU:O	2.42	0.46
2:G:93:MET:SD	2:G:94:TYR:N	2.89	0.46
1:C:415:ILE:O	1:C:419:ASN:N	2.48	0.46
1:A:403:GLU:OE1	1:A:415:ILE:HG12	2.15	0.46
1:A:660:ASP:HB3	1:A:670:SER:HB2	1.98	0.46
1:E:348:TYR:HE1	1:E:451:ARG:HB2	1.80	0.46
1:E:454:ARG:NE	1:E:456:SER:O	2.48	0.46
1:E:469:ILE:HA	1:E:487:PHE:HA	1.98	0.46
1:E:785:ILE:HG23	1:E:873:ALA:HB2	1.98	0.46
1:E:1080:HIS:CD2	1:E:1134:VAL:H	2.34	0.46
1:C:399:ILE:HG22	1:C:401:GLY:N	2.31	0.45
1:C:696:LEU:HD21	1:E:866:MET:HB2	1.97	0.45
1:E:707:ASN:OD1	1:E:707:ASN:N	2.48	0.45
2:H:98:ARG:NE	2:H:106:ASP:HB3	2.31	0.45
3:L:25:ALA:HB3	3:L:70:THR:HA	1.98	0.45
1:A:418:TYR:HA	1:A:454:ARG:NH2	2.31	0.45
1:E:422:LEU:HD23	1:E:426:PHE:CZ	2.51	0.45
1:E:625:GLN:OE1	1:E:626:LEU:N	2.50	0.45
1:C:68:ILE:HG23	1:C:76:ARG:HG2	1.98	0.45
1:C:140:ASP:HB2	1:C:144:ASN:ND2	2.31	0.45
1:C:480:VAL:HG13	1:C:481:ALA:N	2.32	0.45
1:C:737:MET:HA	1:C:740:CYS:O	2.15	0.45
3:L:33:TYR:HB3	3:L:51:GLY:HA2	1.98	0.45
1:A:42:VAL:HB	1:A:44:ARG:HH21	1.82	0.45
1:A:123:ASN:HD22	1:A:125:VAL:CG2	2.29	0.45
1:A:307:LYS:NZ	1:A:597:PRO:HA	2.32	0.45
1:A:866:MET:HA	1:A:869:GLN:HB2	1.98	0.45
1:E:243:ARG:HG2	1:E:244:SER:H	1.81	0.45
1:E:314:ASN:HA	1:E:591:GLY:HA2	1.98	0.45
1:E:392:VAL:HG21	1:E:521:VAL:HB	1.98	0.45
1:E:823:VAL:HG23	1:E:946:GLN:HG2	1.99	0.45
1:C:83:PRO:HA	1:C:234:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ASN:H	1:C:520:THR:HG1	1.63	0.45
1:C:431:ILE:HB	1:C:508:VAL:HG13	1.97	0.45
1:A:341:ALA:HB3	1:A:344:PHE:CE1	2.52	0.45
2:B:36:TRP:CG	2:B:81:LEU:HD12	2.52	0.45
2:B:69:THR:OG1	2:B:82:GLN:HB2	2.17	0.45
3:D:48:LEU:HD12	3:D:59:ILE:HD12	1.98	0.45
1:E:142:LYS:HE2	1:E:142:LYS:HB3	1.75	0.45
1:E:363:SER:HA	1:E:366:TYR:CD2	2.51	0.45
1:C:510:LEU:HD23	1:C:510:LEU:HA	1.86	0.45
1:A:859:PRO:HG3	1:E:644:ALA:HA	1.99	0.45
1:C:61:ASN:OD1	5:C:1302:NAG:H4	2.16	0.45
1:C:397:PHE:HZ	1:C:509:VAL:HG23	1.80	0.45
1:C:480:VAL:HG22	1:C:481:ALA:H	1.81	0.45
1:C:730:LYS:NZ	1:C:858:LEU:O	2.39	0.45
2:H:40:MET:CE	2:H:43:LYS:HB3	2.47	0.45
2:B:34:ILE:HG12	2:B:53:PRO:HG3	1.98	0.45
1:E:712:PRO:HA	1:E:1069:GLU:HA	1.99	0.45
2:G:51:ILE:O	2:G:53:PRO:HD3	2.16	0.45
1:C:383:LYS:HA	1:C:383:LYS:HD2	1.85	0.45
1:C:660:ASP:HB3	1:C:670:SER:HB2	1.99	0.45
2:H:108:TRP:NE1	3:L:45:PRO:O	2.50	0.45
1:A:31:SER:O	1:A:34:ARG:HG2	2.17	0.45
1:A:81:VAL:HG22	1:A:234:ARG:HB3	1.98	0.45
1:A:436:ASN:HD22	1:A:503:GLN:HG3	1.82	0.45
2:B:16:GLU:N	2:B:16:GLU:OE2	2.49	0.45
2:B:45:LEU:HD12	2:B:45:LEU:H	1.81	0.45
1:C:770:GLU:OE1	1:C:1016:ARG:NE	2.50	0.45
1:A:368:LEU:HD23	1:A:368:LEU:HA	1.84	0.45
1:A:550:THR:O	1:A:583:ASP:N	2.49	0.45
1:A:947:ASP:HB3	1:A:951:HIS:CE1	2.52	0.45
3:D:40:LYS:HD3	3:D:40:LYS:HA	1.64	0.45
1:E:673:THR:OG1	1:E:687:GLN:NE2	2.50	0.45
1:C:459:LYS:O	1:C:462:GLU:HB3	2.17	0.45
1:C:530:LEU:HD23	1:C:530:LEU:H	1.81	0.45
1:C:738:TYR:HD1	1:C:739:ILE:HD13	1.81	0.45
2:H:27:PHE:HD2	2:H:32:TYR:HB2	1.82	0.45
3:L:34:LEU:HA	3:L:92:TYR:H	1.81	0.45
3:L:47:LEU:HD21	3:L:50:TYR:HB3	1.97	0.45
1:A:311:GLN:NE2	1:A:313:SER:O	2.47	0.45
1:E:151:GLU:O	1:E:154:VAL:HG22	2.17	0.45
1:C:64:TRP:HE1	1:C:66:HIS:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:THR:HG23	1:C:343:ARG:HG2	1.99	0.45
1:C:801:GLN:HB3	1:C:815:ILE:HD11	1.99	0.45
1:A:33:THR:HA	1:A:58:PHE:CD1	2.52	0.45
1:A:557:LEU:O	1:A:574:ARG:NH2	2.50	0.45
2:B:15:GLY:N	2:B:86:LEU:O	2.48	0.45
1:E:32:PHE:H	1:E:59:PHE:HA	1.82	0.45
1:E:78:ASP:OD1	1:E:78:ASP:N	2.50	0.45
1:E:88:VAL:HG23	1:E:264:VAL:HG23	1.99	0.45
1:E:314:ASN:O	1:E:626:LEU:HD23	2.16	0.45
1:E:439:ASP:C	1:E:445:ASN:HD22	2.20	0.45
1:E:736:THR:OG1	1:E:737:MET:N	2.49	0.45
3:F:39:GLN:HA	3:F:45:PRO:HA	1.99	0.45
1:C:188:VAL:HB	1:C:199:TYR:HB2	1.99	0.44
1:C:534:LYS:HB3	1:C:534:LYS:HE2	1.62	0.44
1:C:1071:ASN:HB3	4:O:1:NAG:HN2	1.82	0.44
1:A:124:VAL:HG23	1:A:126:ILE:HG12	1.99	0.44
2:B:12:LYS:HE2	2:B:18:LEU:HB2	1.99	0.44
1:E:345:ALA:HB1	1:E:349:ALA:HB3	1.98	0.44
1:E:399:ILE:HD12	1:E:399:ILE:HA	1.91	0.44
2:G:6:GLN:HG2	2:G:112:THR:OG1	2.17	0.44
1:A:336:ASP:O	1:A:340:ASN:N	2.35	0.44
1:E:374:PHE:CE2	1:E:381:PRO:HB3	2.53	0.44
1:E:850:GLN:NE2	1:E:855:LEU:HD22	2.32	0.44
3:L:56:ALA:HB3	3:L:59:ILE:HB	1.98	0.44
1:E:285:ALA:HA	1:E:303:PHE:HZ	1.82	0.44
1:E:654:ASN:HB3	5:E:1305:NAG:C7	2.47	0.44
1:C:67:VAL:HG23	1:C:260:ALA:HB3	1.99	0.44
2:B:40:MET:HG3	2:B:43:LYS:HB2	2.00	0.44
1:C:383:LYS:NZ	1:C:386:ASP:HB2	2.33	0.44
1:A:970:ILE:HG12	1:A:989:GLN:HG2	2.00	0.44
1:A:989:GLN:NE2	1:A:992:ARG:HH22	2.16	0.44
3:D:89:CYS:H	3:D:100:GLY:HA3	1.83	0.44
1:E:406:GLN:HB3	1:E:413:GLY:HA3	1.99	0.44
1:C:560:GLN:O	1:C:574:ARG:NH1	2.51	0.44
2:H:81:LEU:HD22	2:H:83:TRP:CE3	2.52	0.44
1:A:415:ILE:HG22	1:A:419:ASN:ND2	2.31	0.44
1:A:959:LEU:HD12	1:A:959:LEU:HA	1.86	0.44
1:A:977:ILE:HG23	1:A:981:LEU:HD13	1.99	0.44
2:B:105:PHE:H	3:D:47:LEU:HD12	1.83	0.44
1:E:75:LYS:HD2	1:E:77:PHE:HE2	1.82	0.44
2:G:35:GLY:HA3	2:G:50:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:86:LEU:HD13	2:G:116:VAL:HG13	1.98	0.44
1:C:183:ASN:HB3	1:C:185:ARG:NE	2.32	0.44
3:L:48:LEU:HD21	3:L:74:LEU:HD22	1.99	0.44
1:A:57:PRO:HD3	1:A:268:GLN:HG2	1.99	0.44
1:A:124:VAL:HG12	1:A:170:PHE:N	2.33	0.44
1:A:275:LYS:O	1:A:282:ILE:HD12	2.18	0.44
1:A:982:ASP:HB2	1:A:985:GLU:OE1	2.16	0.44
1:E:110:SER:O	1:E:130:GLU:HB3	2.18	0.44
1:C:822:LYS:NZ	1:C:935:LEU:O	2.50	0.44
1:C:957:ASN:O	1:C:961:LYS:HG3	2.18	0.44
1:A:415:ILE:O	1:A:419:ASN:N	2.50	0.44
1:A:799:PHE:CD1	1:A:802:ILE:HD11	2.53	0.44
5:A:1308:NAG:O4	5:A:1309:NAG:O3	2.30	0.44
3:D:16:GLY:HA2	3:D:78:ARG:HG2	2.00	0.44
1:E:185:ARG:HB3	1:E:187:PHE:CE1	2.52	0.44
1:E:352:ARG:HH21	1:E:463:ARG:HG2	1.83	0.44
4:I:1:NAG:H61	4:I:2:NAG:HN2	1.83	0.44
1:C:914:TYR:CZ	1:A:1076:PRO:HB3	2.53	0.44
1:A:140:ASP:OD1	1:A:242:HIS:ND1	2.50	0.44
1:A:326:PHE:CD1	1:A:327:PRO:HD2	2.53	0.44
1:A:345:ALA:HB1	1:A:349:ALA:O	2.18	0.44
1:A:662:PRO:HA	1:A:668:CYS:SG	2.58	0.44
2:B:19:LYS:N	2:B:19:LYS:HD3	2.33	0.44
3:D:24:ARG:HH12	3:D:71:ASP:HA	1.83	0.44
1:E:125:VAL:HG12	1:E:127:LYS:HG2	1.99	0.44
2:G:48:MET:HA	2:G:64:PHE:HD2	1.82	0.44
1:C:48:LEU:HD21	1:C:303:PHE:HD1	1.82	0.43
1:C:104:PHE:HB2	1:C:115:LEU:HB3	1.99	0.43
1:C:445:ASN:ND2	2:H:101:TYR:OH	2.51	0.43
1:A:270:ARG:HD3	1:A:270:ARG:HA	1.88	0.43
1:E:67:VAL:O	1:E:68:ILE:HD13	2.18	0.43
1:C:761:LYS:HE2	1:C:761:LYS:HB2	1.85	0.43
1:C:900:ALA:HB2	1:C:913:LEU:HD22	2.00	0.43
3:L:37:TYR:HB2	3:L:88:TYR:HB2	2.00	0.43
1:A:115:LEU:HD13	1:A:128:VAL:HG22	1.99	0.43
1:A:316:ARG:HG3	1:A:589:PHE:HB3	2.00	0.43
1:A:325:ARG:HA	1:A:325:ARG:NE	2.33	0.43
1:A:673:THR:HA	1:A:687:GLN:HA	2.00	0.43
2:B:70:ILE:HG23	2:B:81:LEU:HG	2.00	0.43
1:E:83:PRO:HA	1:E:234:ARG:HA	2.01	0.43
1:E:102:TRP:HB3	1:E:235:PHE:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:LEU:HB2	1:E:234:ARG:HH21	1.83	0.43
1:E:197:LYS:HD2	1:E:197:LYS:HA	1.76	0.43
2:G:71:SER:O	2:G:80:TYR:N	2.51	0.43
1:C:438:LEU:HD12	1:C:438:LEU:H	1.82	0.43
3:L:11:LEU:N	3:L:104:LYS:O	2.52	0.43
3:L:34:LEU:HD11	3:L:89:CYS:HB2	1.99	0.43
3:L:80:GLU:HB2	3:L:82:GLU:HG2	2.00	0.43
1:A:745:GLU:HB2	1:A:978:PHE:CZ	2.53	0.43
1:A:959:LEU:HD21	1:A:1001:LEU:HD23	2.00	0.43
3:D:34:LEU:HA	3:D:92:TYR:H	1.83	0.43
1:E:495:ARG:CZ	1:E:496:PRO:HD2	2.48	0.43
1:C:132:GLN:HB3	1:C:156:SER:HB2	2.00	0.43
1:C:883:TRP:HH2	1:C:901:TYR:HB3	1.83	0.43
1:A:401:GLY:HA3	1:A:505:TYR:CD2	2.54	0.43
1:A:966:LYS:HB3	1:A:966:LYS:HE2	1.78	0.43
1:E:414:ASN:O	1:E:418:TYR:N	2.52	0.43
1:E:831:ILE:HD12	1:E:831:ILE:HA	1.90	0.43
2:H:6:GLN:HA	2:H:22:CYS:HA	2.00	0.43
1:A:830:PHE:O	1:A:832:LYS:NZ	2.51	0.43
1:E:544:LYS:HD2	1:E:544:LYS:HA	1.85	0.43
1:E:805:ASP:OD2	1:E:807:SER:OG	2.28	0.43
3:F:68:SER:N	3:F:71:ASP:O	2.51	0.43
3:F:90:GLN:HE21	3:F:98:THR:C	2.22	0.43
2:G:68:VAL:HG12	2:G:83:TRP:HA	1.99	0.43
3:L:24:ARG:HA	3:L:24:ARG:HH11	1.83	0.43
3:L:35:ALA:N	3:L:92:TYR:HB2	2.33	0.43
1:A:53:ASP:OD1	1:A:54:LEU:N	2.52	0.43
1:A:201:LYS:HD2	1:A:202:HIS:H	1.84	0.43
1:A:325:ARG:NH2	1:A:529:ASN:HA	2.34	0.43
1:A:600:ASN:OD1	1:A:600:ASN:N	2.51	0.43
1:A:989:GLN:HE21	1:A:992:ARG:HH22	1.64	0.43
1:E:127:LYS:HA	1:E:127:LYS:HD3	1.77	0.43
1:C:532:LYS:HZ3	1:C:550:THR:HA	1.83	0.43
1:C:993:LEU:HD23	1:C:993:LEU:HA	1.81	0.43
3:L:20:THR:HA	3:L:74:LEU:O	2.19	0.43
1:A:168:GLN:HE22	1:A:172:MET:HB3	1.84	0.43
1:E:350:TRP:CZ2	1:E:419:ASN:HB3	2.53	0.43
1:E:393:TYR:O	1:E:511:SER:N	2.38	0.43
1:C:79:ASN:N	1:C:80:PRO:HD3	2.34	0.43
1:C:86:ASP:N	1:C:86:ASP:OD1	2.48	0.43
1:C:127:LYS:HZ3	1:C:164:GLU:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ASN:HB3	1:C:316:ARG:NH2	2.34	0.43
1:C:453:PHE:H	1:C:488:PRO:HA	1.84	0.43
1:C:759:GLN:HG3	1:C:762:ARG:HH12	1.84	0.43
1:C:945:LEU:HD21	1:C:1056:GLY:HA3	2.00	0.43
1:C:945:LEU:HD23	1:C:945:LEU:HA	1.92	0.43
3:L:66:SER:HB2	3:L:73:THR:O	2.19	0.43
1:A:94:GLU:HG3	1:A:185:ARG:NH1	2.34	0.43
1:A:833:GLN:OE1	1:E:613:ASN:ND2	2.52	0.43
2:B:2:VAL:HG11	2:B:98:ARG:CZ	2.47	0.43
1:E:28:TYR:HE1	1:E:63:THR:HG22	1.82	0.43
1:E:100:ARG:HD2	1:E:119:ASN:HB3	2.01	0.43
1:E:124:VAL:HG22	1:E:167:SER:H	1.84	0.43
1:E:556:PHE:O	1:E:574:ARG:NH2	2.52	0.43
1:E:956:LEU:HD23	1:E:956:LEU:HA	1.89	0.43
1:C:124:VAL:HG12	1:C:169:PRO:HA	2.01	0.43
1:C:127:LYS:HG3	1:C:129:CYS:SG	2.59	0.43
1:C:745:GLU:O	1:C:749:LEU:HD12	2.19	0.43
3:L:11:LEU:HD12	3:L:11:LEU:O	2.18	0.43
1:A:195:TYR:CE1	1:A:227:PRO:HA	2.53	0.43
1:E:300:LEU:HD23	1:E:305:VAL:HG22	2.01	0.43
1:E:300:LEU:HG	1:E:302:SER:HB3	2.01	0.43
1:E:324:VAL:O	1:E:528:THR:N	2.52	0.43
3:F:5:THR:HB	3:F:24:ARG:HB2	2.01	0.43
3:F:39:GLN:NE2	3:F:40:LYS:O	2.51	0.43
4:Z:1:NAG:H4	4:Z:2:NAG:H2	1.35	0.43
2:H:81:LEU:HD22	2:H:83:TRP:HE3	1.82	0.43
1:A:32:PHE:HA	1:A:59:PHE:CD1	2.54	0.43
1:A:210:PRO:O	1:A:263:TYR:OH	2.29	0.43
1:A:557:LEU:HB2	1:A:560:GLN:HG2	2.01	0.43
1:E:350:TRP:HZ2	1:E:419:ASN:HB3	1.84	0.43
1:E:673:THR:HA	1:E:687:GLN:HA	2.00	0.43
2:H:58:THR:HB	2:H:60:TYR:HE1	1.84	0.42
2:H:95:TYR:HB3	2:H:108:TRP:HE3	1.84	0.42
1:A:362:TYR:CE2	1:A:384:LEU:HG	2.54	0.42
1:A:454:ARG:HH22	1:A:458:LEU:HD22	1.84	0.42
3:D:13:LEU:HD12	3:D:14:SER:O	2.18	0.42
1:E:81:VAL:HG22	1:E:234:ARG:HB3	2.00	0.42
2:G:61:SER:O	2:G:65:GLN:N	2.52	0.42
1:C:92:SER:OG	1:C:185:ARG:HB2	2.19	0.42
3:L:55:ARG:NH2	3:L:60:PRO:O	2.52	0.42
1:A:437:LYS:HG3	2:B:33:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:PRO:HG3	1:E:268:GLN:NE2	2.33	0.42
1:E:138:PHE:HA	1:E:239:LEU:O	2.19	0.42
1:E:183:ASN:HD22	1:E:185:ARG:NH2	2.18	0.42
1:E:557:LEU:HB2	1:E:560:GLN:HG3	2.01	0.42
1:E:770:GLU:OE2	1:E:771:GLN:NE2	2.53	0.42
1:C:989:GLN:HG3	1:C:992:ARG:HH21	1.85	0.42
2:H:60:TYR:HB2	2:H:65:GLN:HA	1.99	0.42
3:L:6:GLN:OE1	3:L:101:GLN:N	2.53	0.42
1:A:344:PHE:CD2	1:A:396:SER:HB3	2.54	0.42
1:A:377:TYR:HB3	1:A:426:PHE:HB3	2.01	0.42
1:A:534:LYS:HE2	1:A:534:LYS:HB3	1.66	0.42
3:D:39:GLN:HB2	3:D:45:PRO:HB3	2.01	0.42
3:D:52:ALA:HB1	3:D:72:PHE:CE1	2.53	0.42
1:C:99:ILE:HG12	1:C:239:LEU:HD13	2.01	0.42
1:C:124:VAL:HG22	1:C:167:SER:N	2.35	0.42
1:C:384:LEU:HD11	1:C:512:PHE:CE2	2.54	0.42
1:A:384:LEU:HD13	1:A:512:PHE:CE2	2.54	0.42
1:A:740:CYS:HB3	1:A:746:CYS:HB3	1.75	0.42
3:D:4:LEU:HD11	3:D:91:GLN:HG2	2.00	0.42
1:E:740:CYS:HB3	1:E:746:CYS:HB3	1.94	0.42
1:C:392:VAL:HG13	1:C:512:PHE:HD1	1.85	0.42
3:L:51:GLY:O	3:L:53:SER:N	2.53	0.42
1:A:561:GLN:NE2	1:A:574:ARG:HD2	2.34	0.42
1:A:1112:ILE:HG22	1:A:1134:VAL:HG13	2.00	0.42
3:D:29:VAL:HG22	3:D:32:SER:H	1.84	0.42
3:F:34:LEU:HD21	3:F:89:CYS:HB2	2.01	0.42
1:C:832:LYS:HA	1:C:832:LYS:HD2	1.78	0.42
1:A:436:ASN:HA	1:A:504:PRO:HB2	2.02	0.42
1:A:1027:SER:OG	1:E:1038:ASP:HB2	2.19	0.42
1:A:1071:ASN:HD21	4:U:1:NAG:H62	1.84	0.42
1:E:132:GLN:O	1:E:156:SER:N	2.42	0.42
1:E:323:ILE:N	1:E:537:ASN:O	2.40	0.42
1:E:659:CYS:HB2	1:E:694:MET:CE	2.49	0.42
1:C:946:GLN:HG3	1:C:950:ASN:HD21	1.83	0.42
1:C:969:ALA:HA	1:C:992:ARG:CZ	2.50	0.42
1:A:88:VAL:HG21	1:A:235:PHE:CZ	2.54	0.42
1:A:956:LEU:HD23	1:A:956:LEU:HA	1.88	0.42
1:A:971:SER:H	1:A:977:ILE:HD11	1.85	0.42
1:A:1088:ARG:NH2	1:A:1114:THR:O	2.52	0.42
2:B:34:ILE:HG22	2:B:98:ARG:HG2	2.02	0.42
1:E:87:GLY:HA3	1:E:190:LYS:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:PHE:HA	1:E:157:SER:O	2.20	0.42
1:E:938:THR:N	1:E:939:PRO:HD2	2.34	0.42
1:E:1094:SER:HB2	1:E:1099:TRP:CD2	2.54	0.42
1:C:401:GLY:HA3	1:C:505:TYR:HE2	1.85	0.42
1:C:559:PHE:CE2	1:C:560:GLN:HG3	2.55	0.42
1:C:770:GLU:OE2	1:C:771:GLN:NE2	2.52	0.42
1:A:314:ASN:HA	1:A:591:GLY:HA2	2.00	0.42
1:A:427:THR:O	1:A:511:SER:HA	2.19	0.42
2:B:41:PRO:HD3	2:B:92:ALA:HA	2.02	0.42
1:E:77:PHE:HB2	1:E:239:LEU:HD21	2.01	0.42
1:E:709:ILE:O	1:E:1072:PHE:N	2.52	0.42
1:E:959:LEU:HD12	1:E:959:LEU:HA	1.85	0.42
1:E:1022:ALA:O	1:E:1026:MET:N	2.50	0.42
2:G:88:ALA:HA	2:G:116:VAL:HB	2.01	0.42
4:V:2:NAG:O7	4:V:2:NAG:O4	2.21	0.42
1:C:241:LEU:HB3	1:C:255:TRP:HD1	1.85	0.42
1:C:446:TYR:HD2	1:C:495:ARG:HH21	1.67	0.42
1:C:562:PHE:HB2	1:C:564:ARG:NH1	2.27	0.42
2:H:19:LYS:HD3	2:H:80:TYR:HB3	2.02	0.42
1:A:325:ARG:HD2	1:A:575:ASP:OD2	2.20	0.42
1:A:354:ARG:HH22	1:A:356:SER:HB2	1.85	0.42
1:C:770:GLU:OE1	1:C:1016:ARG:HB2	2.20	0.42
1:A:914:TYR:CZ	1:E:1076:PRO:HB3	2.55	0.42
2:B:96:CYS:O	2:B:109:GLY:N	2.53	0.42
1:C:1144:SER:O	1:C:1144:SER:OG	2.26	0.41
1:A:871:THR:HG21	1:A:1052:SER:HB2	2.01	0.41
1:E:57:PRO:HG3	1:E:268:GLN:HE22	1.84	0.41
1:E:183:ASN:HA	1:E:204:PRO:HA	2.02	0.41
1:E:325:ARG:NH1	1:E:577:GLN:HE21	2.18	0.41
1:E:413:GLY:O	1:E:417:ASP:N	2.43	0.41
1:C:268:GLN:OE1	1:C:268:GLN:N	2.53	0.41
1:C:437:LYS:HE3	2:H:33:TRP:CG	2.55	0.41
1:C:490:ARG:HD3	1:C:490:ARG:HA	1.61	0.41
1:C:951:HIS:HB3	1:C:1011:ARG:CZ	2.50	0.41
3:L:6:GLN:NE2	3:L:88:TYR:HA	2.35	0.41
1:A:342:THR:HG23	1:A:343:ARG:HG2	2.00	0.41
1:A:1072:PHE:HB3	1:A:1093:VAL:HG23	2.01	0.41
1:E:388:CYS:HB3	1:E:519:ALA:CB	2.49	0.41
1:E:732:SER:HB3	1:E:858:LEU:HD11	2.00	0.41
3:F:79:LEU:HD11	3:F:84:PHE:HB3	2.03	0.41
1:C:190:LYS:HG3	1:C:197:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HE3	1:A:131:PHE:HZ	1.85	0.41
1:A:324:VAL:HG13	1:A:526:LYS:HA	2.00	0.41
1:A:1135:TYR:HE1	1:A:1140:PRO:HG2	1.85	0.41
2:B:4:LEU:HD11	2:B:98:ARG:HG2	2.02	0.41
1:C:140:ASP:HB3	1:C:142:LYS:O	2.20	0.41
1:C:325:ARG:NH1	1:C:529:ASN:HA	2.35	0.41
1:A:41:LYS:HZ1	1:E:561:GLN:HG2	1.85	0.41
1:A:480:VAL:CG2	1:A:481:ALA:H	2.33	0.41
1:A:709:ILE:O	1:A:1072:PHE:N	2.52	0.41
1:A:1001:LEU:HD23	1:A:1001:LEU:HA	1.85	0.41
2:B:46:GLU:N	2:B:46:GLU:OE1	2.53	0.41
2:B:102:GLU:HB2	3:D:92:TYR:CZ	2.56	0.41
1:E:278:GLU:H	1:E:278:GLU:HG3	1.69	0.41
1:E:324:VAL:HB	1:E:528:THR:HG23	2.03	0.41
1:E:730:LYS:NZ	1:E:860:PRO:HA	2.36	0.41
1:C:28:TYR:CG	5:C:1302:NAG:H82	2.56	0.41
1:C:132:GLN:O	1:C:156:SER:N	2.43	0.41
1:C:980:ARG:H	1:C:980:ARG:HG3	1.70	0.41
1:A:348:TYR:CG	1:A:489:LEU:HD21	2.56	0.41
2:B:60:TYR:HB2	2:B:65:GLN:HG3	2.02	0.41
1:E:87:GLY:HA3	1:E:190:LYS:NZ	2.36	0.41
1:E:864:ASP:OD1	1:E:864:ASP:N	2.53	0.41
3:F:10:THR:HG23	3:F:104:LYS:HG3	2.02	0.41
3:F:45:PRO:HG2	2:G:45:LEU:HD21	2.01	0.41
2:G:20:ILE:HG23	2:G:81:LEU:HB3	2.02	0.41
1:C:450:TYR:CE2	1:C:452:LEU:HD21	2.56	0.41
1:C:609:TYR:CZ	1:C:621:ILE:HD11	2.55	0.41
1:A:296:THR:HG22	1:A:312:THR:HG21	2.03	0.41
1:A:344:PHE:HB2	1:A:506:ARG:NE	2.33	0.41
1:A:439:ASP:HB3	1:A:494:PHE:HD2	1.85	0.41
1:A:494:PHE:HD1	1:A:494:PHE:HA	1.74	0.41
2:B:38:ARG:HB3	2:B:48:MET:SD	2.60	0.41
1:E:95:LYS:HB2	1:E:182:LYS:HZ2	1.86	0.41
1:C:43:PHE:CE2	1:A:554:LYS:HD3	2.55	0.41
1:C:307:LYS:HG3	1:C:661:ILE:HD11	2.02	0.41
1:C:323:ILE:HG21	1:C:530:LEU:HA	2.01	0.41
1:C:401:GLY:HA3	1:C:505:TYR:CE2	2.56	0.41
1:C:418:TYR:O	1:C:451:ARG:HD2	2.20	0.41
1:C:990:ILE:O	1:C:994:ILE:HG13	2.20	0.41
2:H:6:GLN:OE1	2:H:96:CYS:N	2.53	0.41
1:A:958:THR:HA	1:A:961:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:36:TRP:CE3	3:D:74:LEU:HD22	2.55	0.41
1:E:452:LEU:N	1:E:488:PRO:O	2.49	0.41
1:E:577:GLN:H	1:E:577:GLN:HG2	1.65	0.41
3:F:99:PHE:HB2	2:G:45:LEU:O	2.21	0.41
1:C:56:LEU:HD22	1:C:89:TYR:CD2	2.55	0.41
1:C:127:LYS:HD2	1:C:127:LYS:HA	1.67	0.41
1:C:242:HIS:CG	1:C:243:ARG:H	2.38	0.41
1:A:142:LYS:HB2	1:A:242:HIS:HD2	1.85	0.41
1:A:376:CYS:HB2	1:A:379:VAL:O	2.20	0.41
2:B:64:PHE:HA	2:B:67:GLN:HB2	2.02	0.41
3:D:104:LYS:HE3	3:D:104:LYS:HB3	1.88	0.41
1:E:123:ASN:HD22	1:E:125:VAL:CG2	2.33	0.41
1:E:593:SER:HB2	1:E:610:GLN:HE22	1.86	0.41
1:E:943:GLY:O	1:E:947:ASP:N	2.50	0.41
1:C:454:ARG:HG3	1:C:468:GLU:HB2	2.03	0.41
2:H:4:LEU:HD23	2:H:96:CYS:SG	2.61	0.41
2:H:98:ARG:HB2	2:H:106:ASP:CB	2.50	0.41
3:L:87:TYR:O	3:L:102:GLY:HA2	2.19	0.41
1:A:413:GLY:O	1:A:417:ASP:N	2.43	0.41
1:A:419:ASN:ND2	1:A:450:TYR:HB2	2.36	0.41
2:B:29:PHE:HB3	2:B:53:PRO:HG2	2.03	0.41
3:D:35:ALA:HB2	3:D:92:TYR:HD1	1.86	0.41
1:E:235:PHE:CZ	1:E:237:THR:HG22	2.56	0.41
1:E:378:GLY:O	1:E:379:VAL:HG12	2.21	0.41
1:E:395:ASP:HB3	1:E:509:VAL:HG12	2.02	0.41
1:E:471:GLN:HE22	1:E:477:CYS:HB2	1.85	0.41
1:E:723:ILE:HB	1:E:944:LYS:HZ1	1.86	0.41
1:E:947:ASP:HB3	1:E:951:HIS:CE1	2.55	0.41
1:E:982:ASP:HA	1:E:983:PRO:HD3	1.93	0.41
3:F:52:ALA:HB1	3:F:72:PHE:HE2	1.86	0.41
1:C:123:ASN:OD1	1:C:123:ASN:N	2.54	0.41
1:C:418:TYR:HB3	1:C:451:ARG:HG2	2.01	0.41
1:C:441:LYS:HE2	1:C:496:PRO:HD2	2.03	0.41
1:E:93:ILE:HG13	1:E:93:ILE:O	2.21	0.41
1:E:555:LYS:HB2	1:E:555:LYS:HE2	1.80	0.41
3:F:39:GLN:HE22	3:F:42:GLY:H	1.69	0.41
1:C:433:TRP:HZ3	1:C:508:VAL:HG12	1.85	0.40
1:C:597:PRO:HB3	1:C:671:TYR:HB2	2.02	0.40
2:H:29:PHE:CZ	2:H:77:SER:HA	2.57	0.40
2:H:69:THR:O	2:H:81:LEU:HD23	2.21	0.40
3:L:59:ILE:HG13	3:L:60:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:86:VAL:HA	3:L:103:THR:O	2.20	0.40
1:A:793:TYR:HB3	4:Y:1:NAG:O3	2.21	0.40
1:A:1021:LEU:O	1:A:1025:LYS:HG3	2.21	0.40
1:A:1080:HIS:CG	1:A:1134:VAL:H	2.39	0.40
1:E:549:LEU:HD11	1:E:584:ILE:HG13	2.03	0.40
1:C:34:ARG:HA	1:C:34:ARG:HD3	1.87	0.40
1:C:119:ASN:ND2	1:C:169:PRO:HB2	2.31	0.40
1:C:228:ILE:HD12	1:C:228:ILE:H	1.87	0.40
1:C:557:LEU:H	1:C:560:GLN:NE2	2.19	0.40
3:L:67:GLY:HA3	3:L:72:PHE:HA	2.03	0.40
1:A:95:LYS:HB2	1:A:182:LYS:HG2	2.04	0.40
1:A:270:ARG:NH1	1:A:287:ASP:OD2	2.54	0.40
2:B:35:GLY:H	2:B:98:ARG:HA	1.86	0.40
1:E:268:GLN:OE1	1:E:268:GLN:N	2.54	0.40
1:E:428:GLY:HA2	1:E:512:PHE:CZ	2.56	0.40
1:E:743:SER:HG	1:E:978:PHE:HE2	1.68	0.40
3:F:51:GLY:H	3:F:92:TYR:HE2	1.65	0.40
1:C:314:ASN:HA	1:C:591:GLY:HA2	2.03	0.40
1:C:454:ARG:HH22	1:C:458:LEU:HD22	1.86	0.40
1:C:459:LYS:N	1:C:462:GLU:OE2	2.48	0.40
1:C:707:ASN:O	1:C:1073:THR:HA	2.21	0.40
1:C:724:LEU:HD11	1:C:1025:LYS:HD2	2.04	0.40
1:C:1081:ASP:HB2	1:C:1083:LYS:NZ	2.36	0.40
1:A:43:PHE:CE1	1:A:280:GLY:HA3	2.56	0.40
1:A:110:SER:HB2	1:A:132:GLN:HA	2.03	0.40
1:A:324:VAL:HG22	1:A:526:LYS:HD3	2.04	0.40
1:E:735:CYS:SG	1:E:736:THR:N	2.94	0.40
5:E:1305:NAG:O7	5:E:1305:NAG:O4	2.30	0.40
1:C:173:ASP:HB2	1:C:185:ARG:NH2	2.36	0.40
1:C:575:ASP:HB3	1:C:578:THR:O	2.21	0.40
1:C:883:TRP:CH2	1:C:901:TYR:HB3	2.56	0.40
2:H:13:LYS:HA	2:H:14:PRO:HD3	1.98	0.40
2:H:40:MET:SD	2:H:43:LYS:HD3	2.60	0.40
1:A:135:ASN:OD1	1:A:136:ASP:N	2.55	0.40
1:A:197:LYS:HB2	1:A:197:LYS:HE2	1.88	0.40
1:A:335:PHE:HE2	1:A:365:LEU:HD21	1.86	0.40
1:A:788:THR:HG22	1:A:876:ALA:HB2	2.03	0.40
1:A:874:LEU:HD23	1:A:874:LEU:HA	1.78	0.40
3:D:38:GLN:HB2	3:D:48:LEU:HB2	2.03	0.40
1:E:474:ASN:OD1	1:E:475:LYS:N	2.54	0.40
1:E:495:ARG:HH21	1:E:497:THR:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:909:THR:HG22	1:E:911:ASN:H	1.86	0.40
1:E:945:LEU:HD21	1:E:1056:GLY:HA3	2.02	0.40
2:G:16:GLU:H	2:G:86:LEU:HB2	1.87	0.40
1:C:163:PHE:CD2	1:C:228:ILE:HD11	2.56	0.40
1:C:188:VAL:HG23	1:C:220:LEU:HD22	2.04	0.40
1:C:451:ARG:HE	1:C:464:ASP:CG	2.24	0.40
1:C:698:ALA:O	1:E:785:ILE:N	2.55	0.40
1:C:822:LYS:HA	1:C:822:LYS:HD2	1.82	0.40
1:A:233:THR:OG1	5:A:1307:NAG:O7	2.30	0.40
1:E:142:LYS:HD3	1:E:245:TYR:HE1	1.87	0.40
1:E:347:VAL:HG21	1:E:450:TYR:HA	2.04	0.40
1:E:893:ILE:HG13	1:E:894:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1062/1285 (83%)	1034 (97%)	27 (2%)	1 (0%)	51	84
1	C	1063/1285 (83%)	1024 (96%)	38 (4%)	1 (0%)	51	84
1	E	1056/1285 (82%)	1026 (97%)	28 (3%)	2 (0%)	47	81
2	B	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
2	G	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	H	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
3	D	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17	56
3	F	107/109 (98%)	101 (94%)	5 (5%)	1 (1%)	17	56
3	L	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17	56
All	All	3850/4536 (85%)	3718 (97%)	125 (3%)	7 (0%)	50	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	96	PRO
1	A	480	VAL
3	D	96	PRO
1	E	370	PRO
1	E	379	VAL
3	F	96	PRO
1	C	480	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	943/1116 (84%)	906 (96%)	37 (4%)	32	64
1	C	948/1116 (85%)	912 (96%)	36 (4%)	33	65
1	E	938/1116 (84%)	908 (97%)	30 (3%)	39	69
2	B	98/98 (100%)	94 (96%)	4 (4%)	30	63
2	G	98/98 (100%)	91 (93%)	7 (7%)	14	46
2	H	98/98 (100%)	93 (95%)	5 (5%)	24	57
3	D	90/90 (100%)	86 (96%)	4 (4%)	28	62
3	F	90/90 (100%)	86 (96%)	4 (4%)	28	62
3	L	90/90 (100%)	86 (96%)	4 (4%)	28	62
All	All	3393/3912 (87%)	3262 (96%)	131 (4%)	36	64

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	66	HIS
1	C	78	ASP
1	C	127	LYS
1	C	138	PHE
1	C	140	ASP
1	C	235	PHE

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Mol	Chain	Res	Type
1	C	263	TYR
1	C	284	ASP
1	C	315	PHE
1	C	318	GLN
1	C	322	SER
1	C	325	ARG
1	C	332	LEU
1	C	375	LYS
1	C	393	TYR
1	C	450	TYR
1	C	459	LYS
1	C	464	ASP
1	C	470	TYR
1	C	491	SER
1	C	495	ARG
1	C	496	PRO
1	C	506	ARG
1	C	511	SER
1	C	537	ASN
1	C	555	LYS
1	C	562	PHE
1	C	643	ARG
1	C	672	GLN
1	C	735	CYS
1	C	752	GLN
1	C	753	TYR
1	C	870	TYR
1	C	937	SER
1	C	1040	CYS
1	C	1098	HIS
2	H	22	CYS
2	H	40	MET
2	H	52	TYR
2	H	105	PHE
2	H	113	MET
3	L	18	ARG
3	L	33	TYR
3	L	38	GLN
3	L	68	SER
1	A	34	ARG
1	A	45	SER
1	A	75	LYS

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Mol	Chain	Res	Type
1	A	97	ASN
1	A	111	LYS
1	A	123	ASN
1	A	141	HIS
1	A	153	ARG
1	A	172	MET
1	A	173	ASP
1	A	208	ARG
1	A	236	GLN
1	A	288	CYS
1	A	316	ARG
1	A	325	ARG
1	A	348	TYR
1	A	352	ARG
1	A	402	ASP
1	A	405	ARG
1	A	412	THR
1	A	459	LYS
1	A	470	TYR
1	A	475	LYS
1	A	492	TYR
1	A	498	TYR
1	A	555	LYS
1	A	582	LEU
1	A	589	PHE
1	A	600	ASN
1	A	735	CYS
1	A	753	TYR
1	A	756	PHE
1	A	918	LYS
1	A	954	GLN
1	A	1016	ARG
1	A	1095	ASN
1	A	1124	ASP
2	B	33	TRP
2	B	52	TYR
2	B	59	ARG
2	B	105	PHE
3	D	23	CYS
3	D	24	ARG
3	D	38	GLN
3	D	78	ARG

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Mol	Chain	Res	Type
1	E	30	ASN
1	E	76	ARG
1	E	77	PHE
1	E	79	ASN
1	E	123	ASN
1	E	208	ARG
1	E	241	LEU
1	E	288	CYS
1	E	352	ARG
1	E	405	ARG
1	E	420	TYR
1	E	426	PHE
1	E	446	TYR
1	E	453	PHE
1	E	458	LEU
1	E	463	ARG
1	E	475	LYS
1	E	490	ARG
1	E	498	TYR
1	E	502	HIS
1	E	541	ASN
1	E	556	PHE
1	E	568	ASP
1	E	593	SER
1	E	631	ARG
1	E	699	GLU
1	E	735	CYS
1	E	901	TYR
1	E	1034	SER
1	E	1040	CYS
3	F	13	LEU
3	F	24	ARG
3	F	68	SER
3	F	91	GLN
2	G	1	GLU
2	G	48	MET
2	G	52	TYR
2	G	61	SER
2	G	83	TRP
2	G	85	SER
2	G	105	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56)

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	97	ASN
1	C	119	ASN
1	C	484	ASN
1	C	502	HIS
1	C	560	GLN
1	C	561	GLN
1	C	610	GLN
1	C	638	ASN
1	C	700	ASN
1	C	850	GLN
1	C	916	ASN
1	C	946	GLN
1	C	950	ASN
1	C	989	GLN
1	C	1008	GLN
1	C	1033	GLN
1	C	1055	HIS
1	C	1098	HIS
1	C	1103	GLN
1	A	183	ASN
1	A	357	ASN
1	A	434	ASN
1	A	436	ASN
1	A	445	ASN
1	A	457	ASN
1	A	484	ASN
1	A	560	GLN
1	A	561	GLN
1	A	610	GLN
1	A	638	ASN
1	A	910	GLN
1	A	916	ASN
1	A	989	GLN
1	A	1055	HIS
1	A	1105	ASN
3	D	6	GLN
1	E	141	HIS
1	E	318	GLN
1	E	367	ASN
1	E	385	ASN
1	E	391	ASN
1	E	434	ASN

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Mol	Chain	Res	Type
1	E	484	ASN
1	E	503	GLN
1	E	560	GLN
1	E	577	GLN
1	E	638	ASN
1	E	687	GLN
1	E	850	GLN
1	E	917	GLN
1	E	951	HIS
1	E	1002	GLN
1	E	1008	GLN
1	E	1080	HIS
1	E	1085	HIS
3	F	90	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

40 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	$\# Z > 2$
4	NAG	I	1	4,1	14,14,15	1.14	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	I	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	J	1	4,1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	J	2	4	14,14,15	0.42	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	K	1	4,1	14,14,15	0.50	0	17,19,21	0.42	0
4	NAG	K	2	4	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	M	1	4,1	14,14,15	0.58	0	17,19,21	1.23	1 (5%)
4	NAG	M	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	N	1	4,1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	N	2	4	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	O	1	4,1	14,14,15	0.40	0	17,19,21	0.60	0
4	NAG	O	2	4	14,14,15	0.31	0	17,19,21	0.50	0
4	NAG	P	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	0.82	1 (5%)
4	NAG	P	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.81	0
4	NAG	Q	1	4,1	14,14,15	1.12	1 (7%)	17,19,21	1.43	1 (5%)
4	NAG	Q	2	4	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	R	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	0.60	0
4	NAG	R	2	4	14,14,15	0.39	0	17,19,21	0.51	0
4	NAG	S	1	4,1	14,14,15	0.89	1 (7%)	17,19,21	1.30	1 (5%)
4	NAG	S	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	T	1	4,1	14,14,15	0.66	0	17,19,21	0.48	0
4	NAG	T	2	4	14,14,15	0.34	0	17,19,21	0.45	0
4	NAG	U	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.34	1 (5%)
4	NAG	U	2	4	14,14,15	0.26	0	17,19,21	0.51	0
4	NAG	V	1	4,1	14,14,15	0.43	0	17,19,21	0.37	0
4	NAG	V	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.80	0
4	NAG	W	1	4,1	14,14,15	0.40	0	17,19,21	0.39	0
4	NAG	W	2	4	14,14,15	0.37	0	17,19,21	0.36	0
4	NAG	X	1	4,1	14,14,15	0.47	0	17,19,21	0.63	0
4	NAG	X	2	4	14,14,15	0.21	0	17,19,21	0.36	0
4	NAG	Y	1	4,1	14,14,15	1.36	1 (7%)	17,19,21	1.35	3 (17%)
4	NAG	Y	2	4	14,14,15	0.86	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	Z	1	4,1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	Z	2	4	14,14,15	0.39	0	17,19,21	0.36	0
4	NAG	a	1	4,1	14,14,15	0.34	0	17,19,21	0.43	0
4	NAG	a	2	4	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	b	1	4,1	14,14,15	0.87	1 (7%)	17,19,21	1.32	1 (5%)
4	NAG	b	2	4	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	c	1	4,1	14,14,15	0.25	0	17,19,21	0.57	0
4	NAG	c	2	4	14,14,15	0.23	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	4/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	W	2	4	-	4/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	1/6/23/26	0/1/1/1

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	1	NAG	O5-C1	-4.88	1.35	1.43
4	I	1	NAG	O5-C1	-4.01	1.37	1.43
4	Q	1	NAG	O5-C1	3.95	1.50	1.43
4	U	1	NAG	O5-C1	3.53	1.49	1.43
4	S	1	NAG	O5-C1	3.21	1.48	1.43
4	b	1	NAG	O5-C1	3.16	1.48	1.43
4	R	1	NAG	O5-C1	-2.86	1.39	1.43
4	Y	2	NAG	O5-C1	2.80	1.48	1.43
4	P	1	NAG	C1-C2	2.76	1.56	1.52
4	P	2	NAG	O5-C1	-2.31	1.40	1.43
4	V	2	NAG	O5-C1	-2.30	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	1	NAG	C1-O5-C5	5.59	119.76	112.19
4	b	1	NAG	C1-O5-C5	5.23	119.28	112.19
4	U	1	NAG	C1-O5-C5	5.21	119.25	112.19
4	S	1	NAG	C1-O5-C5	5.16	119.18	112.19
4	M	1	NAG	C1-O5-C5	4.74	118.61	112.19
4	Y	2	NAG	C1-O5-C5	3.67	117.16	112.19
4	Y	1	NAG	C4-C3-C2	3.18	115.68	111.02
4	Y	1	NAG	C3-C4-C5	2.86	115.33	110.24
4	Y	1	NAG	C1-O5-C5	-2.61	108.66	112.19
4	I	1	NAG	C3-C4-C5	2.45	114.60	110.24
4	P	1	NAG	C4-C3-C2	2.10	114.09	111.02

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	V	1	NAG	C4-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
4	W	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6

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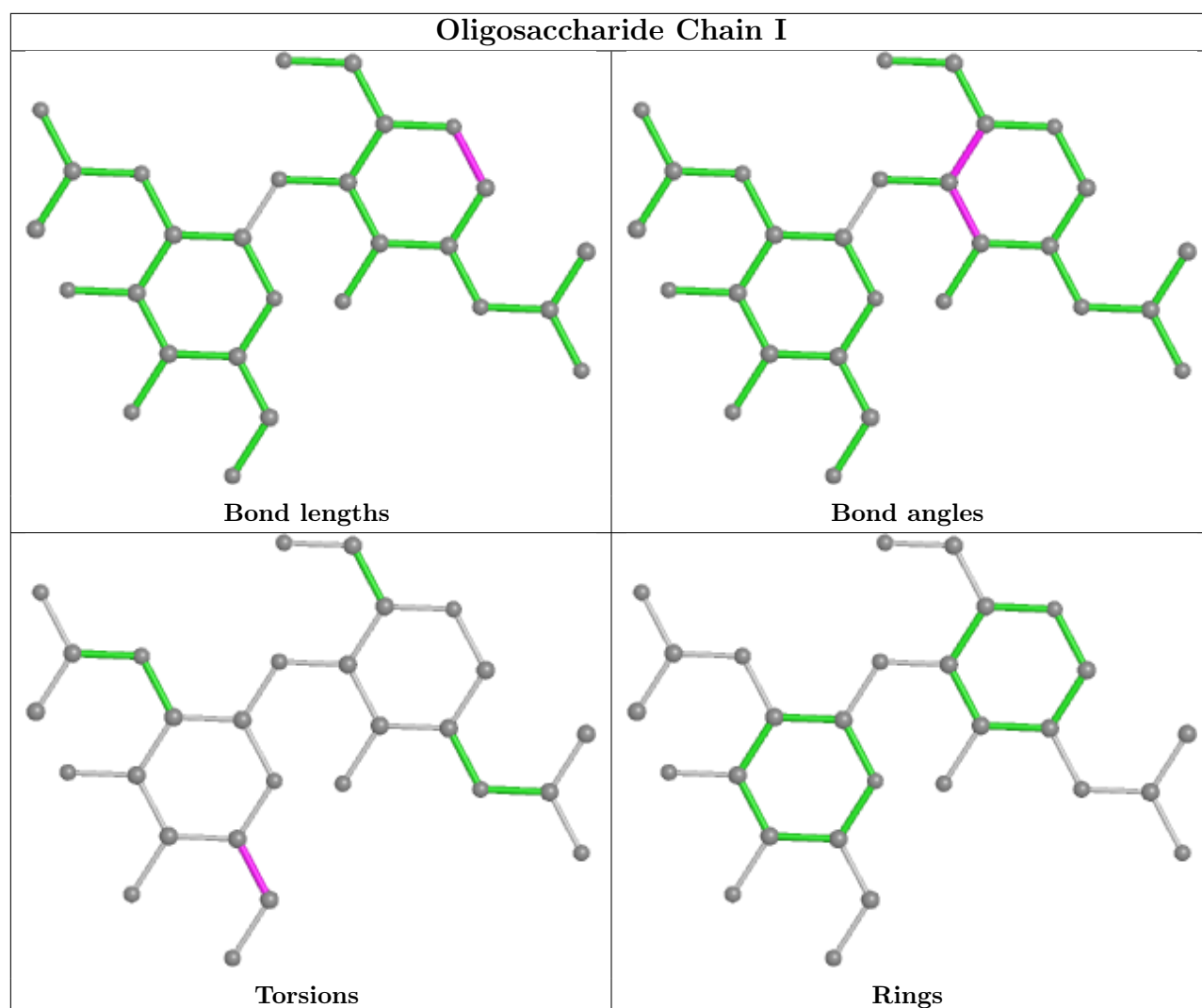
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	C1-C2-N2-C7
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C1-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	c	1	NAG	C3-C2-N2-C7
4	V	2	NAG	C1-C2-N2-C7
4	b	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	P	2	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	C3-C2-N2-C7

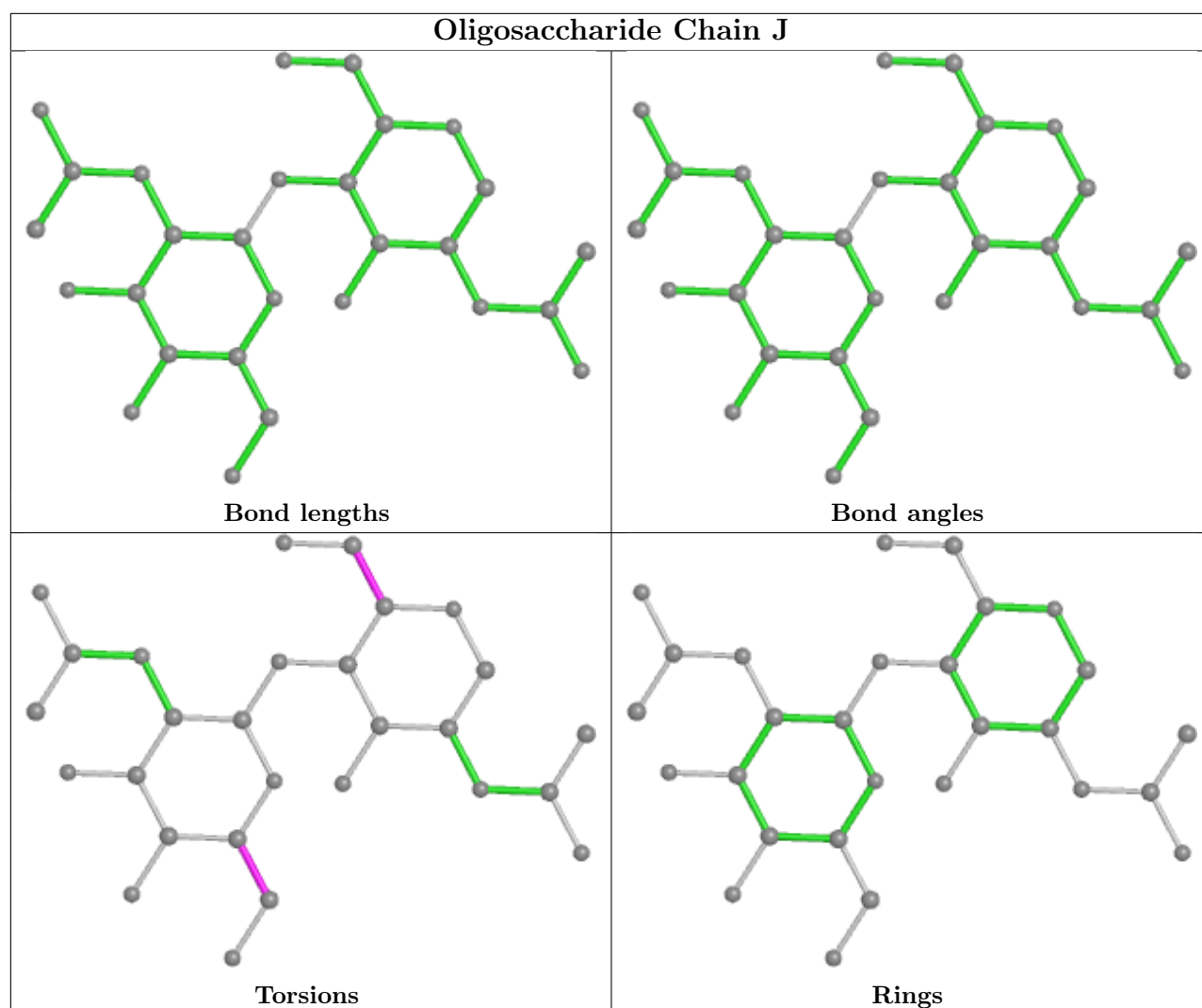
There are no ring outliers.

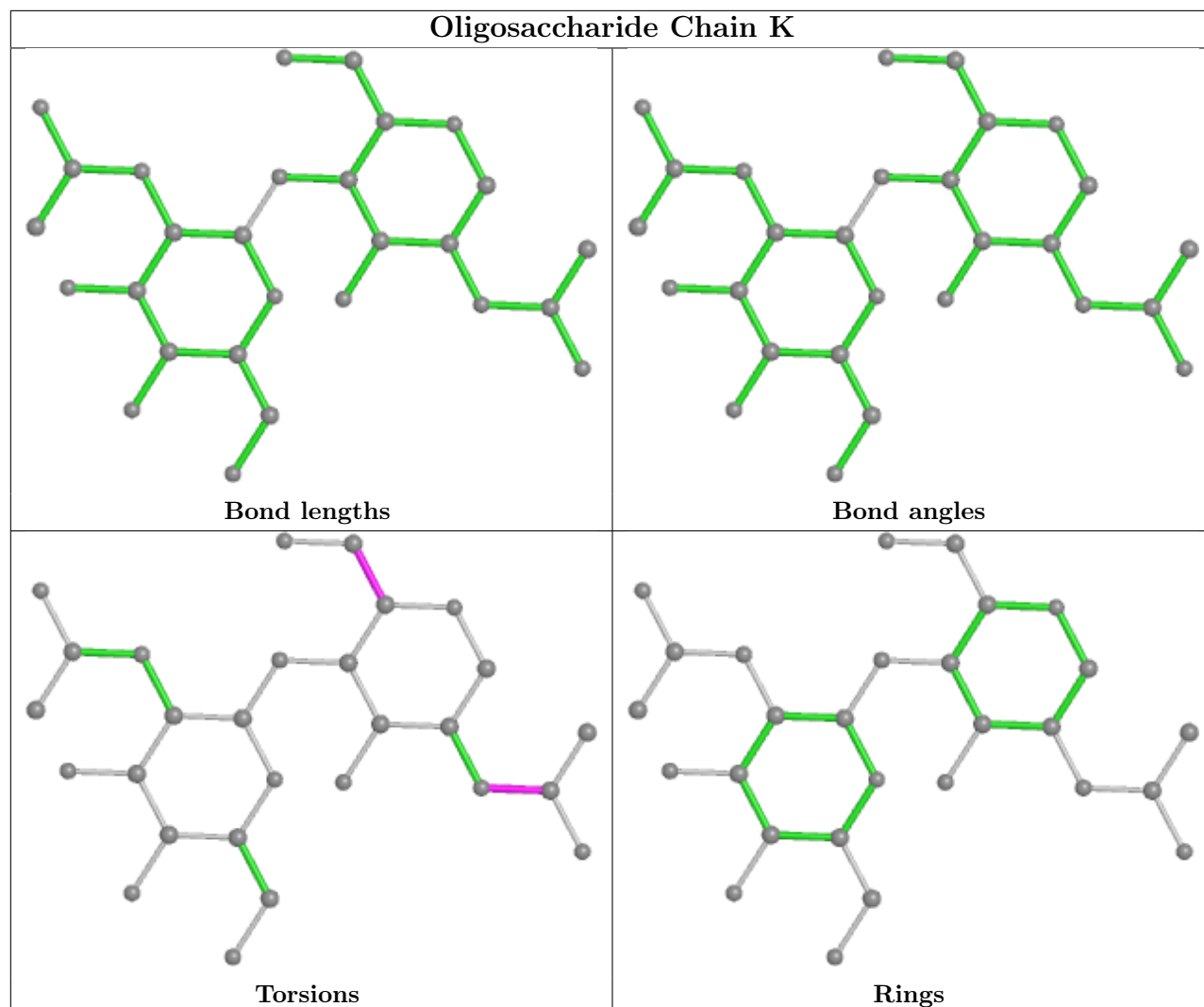
10 monomers are involved in 9 short contacts:

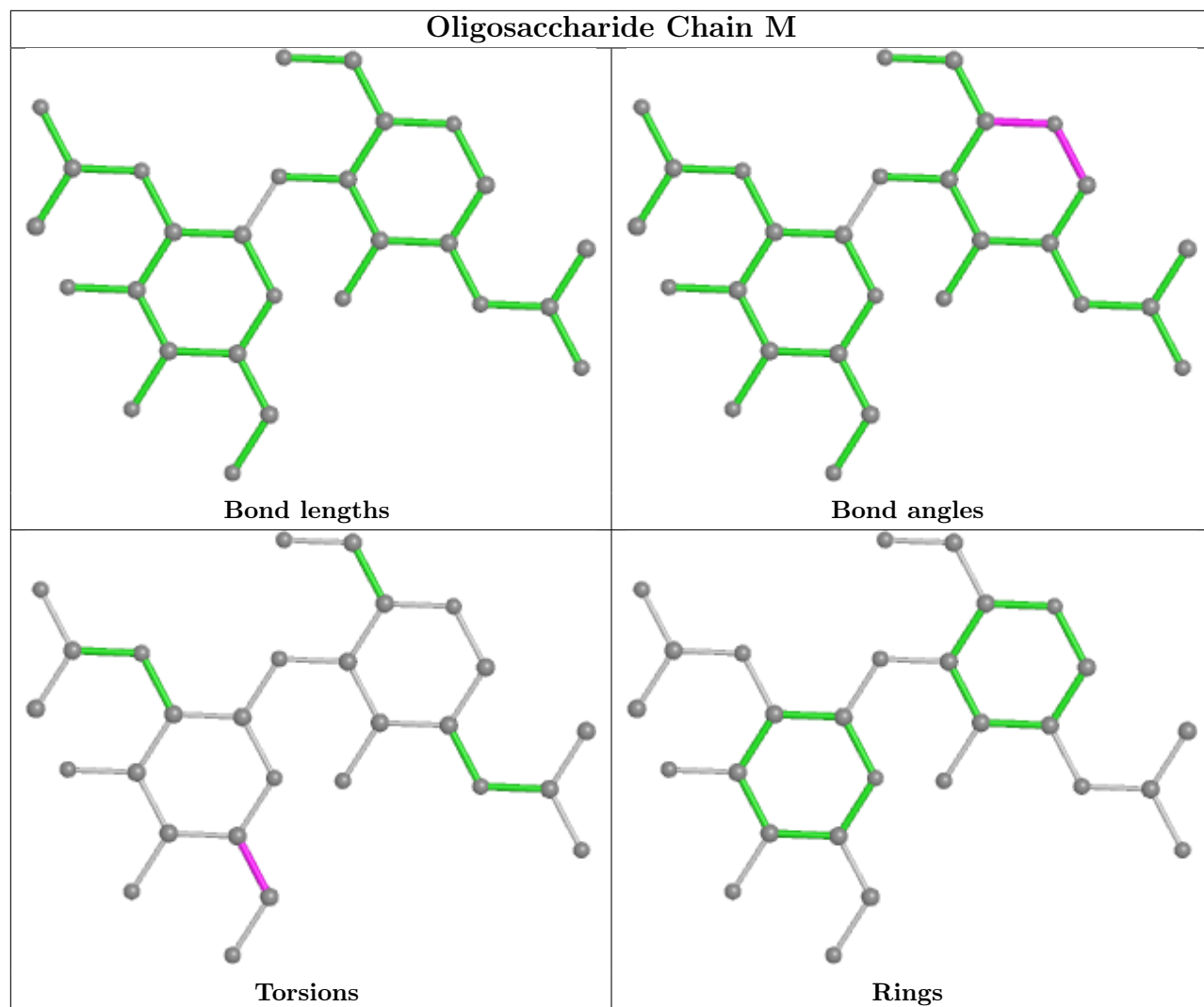
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	1	NAG	2	0
4	R	2	NAG	1	0
4	Y	2	NAG	2	0
4	V	2	NAG	1	0
4	Z	1	NAG	1	0
4	I	1	NAG	1	0
4	Z	2	NAG	1	0
4	U	1	NAG	1	0
4	I	2	NAG	1	0
4	O	1	NAG	1	0

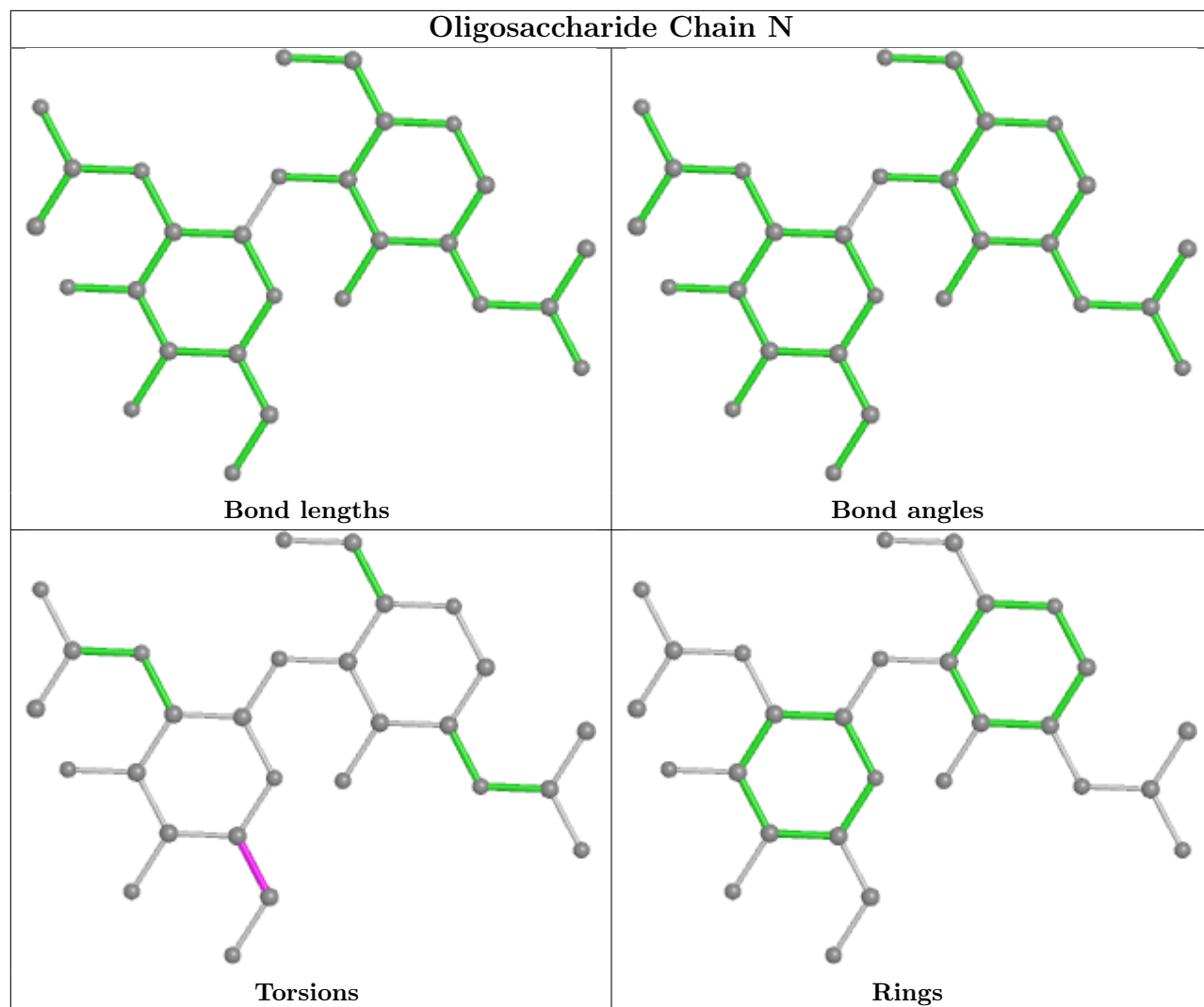
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

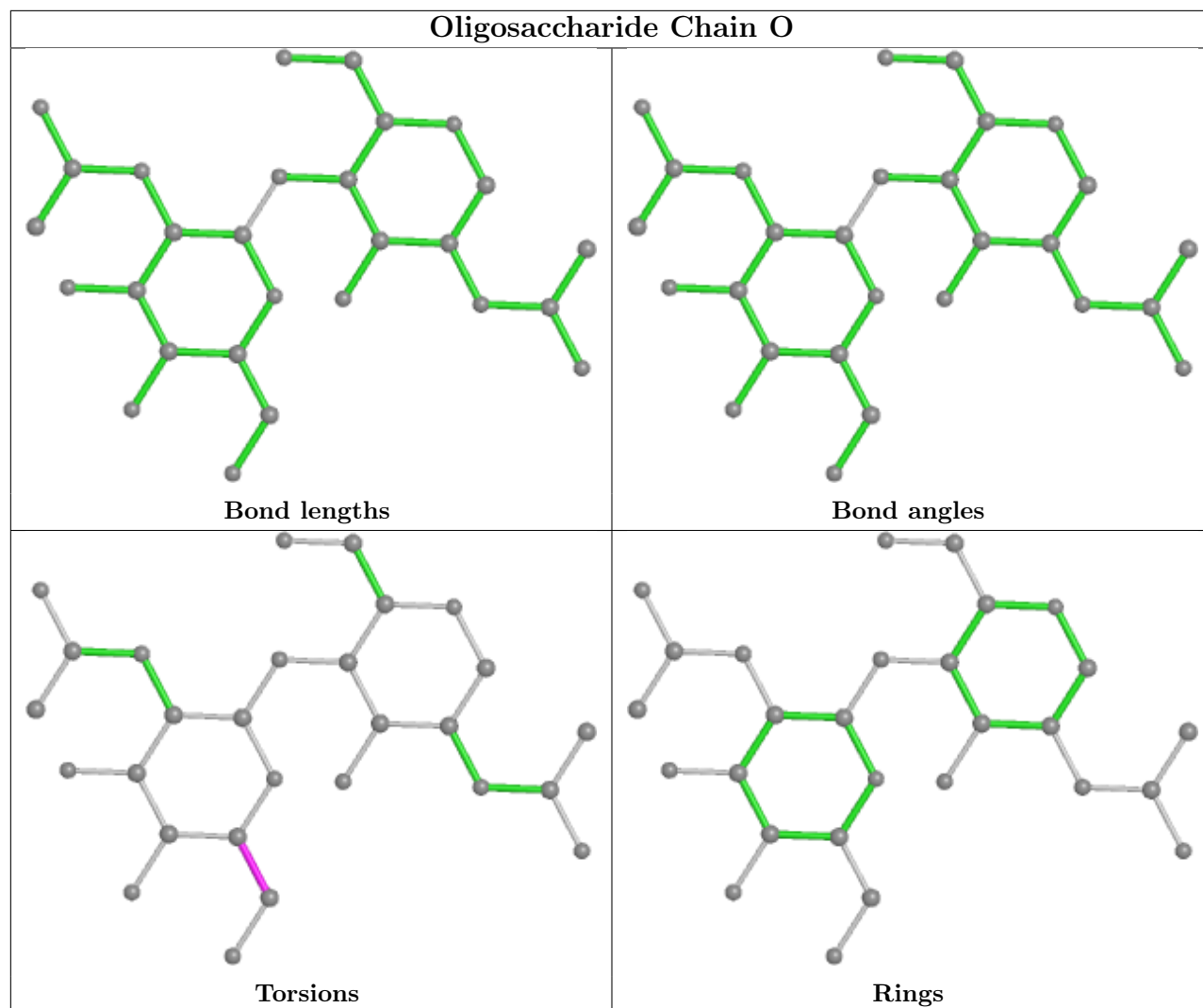


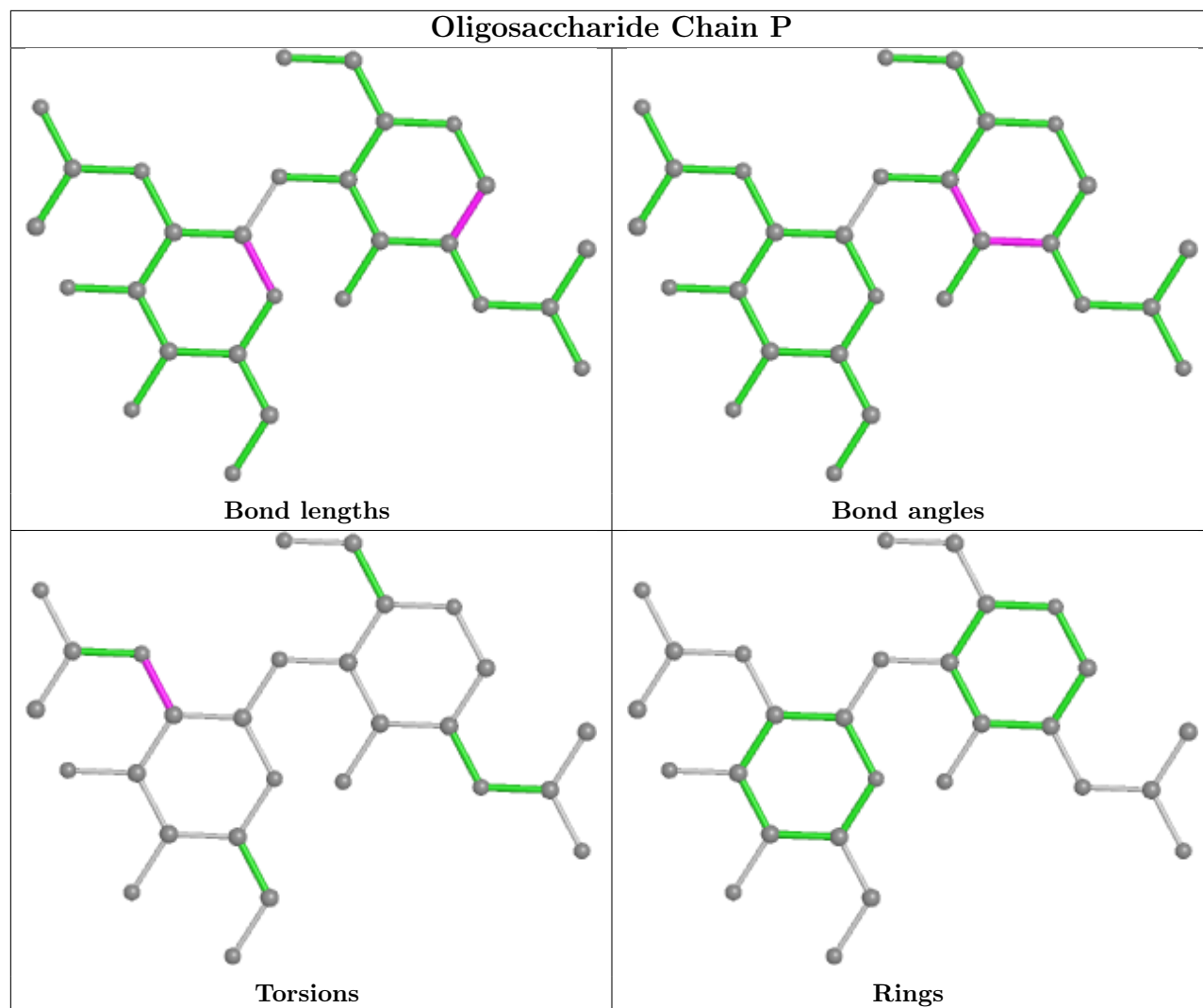


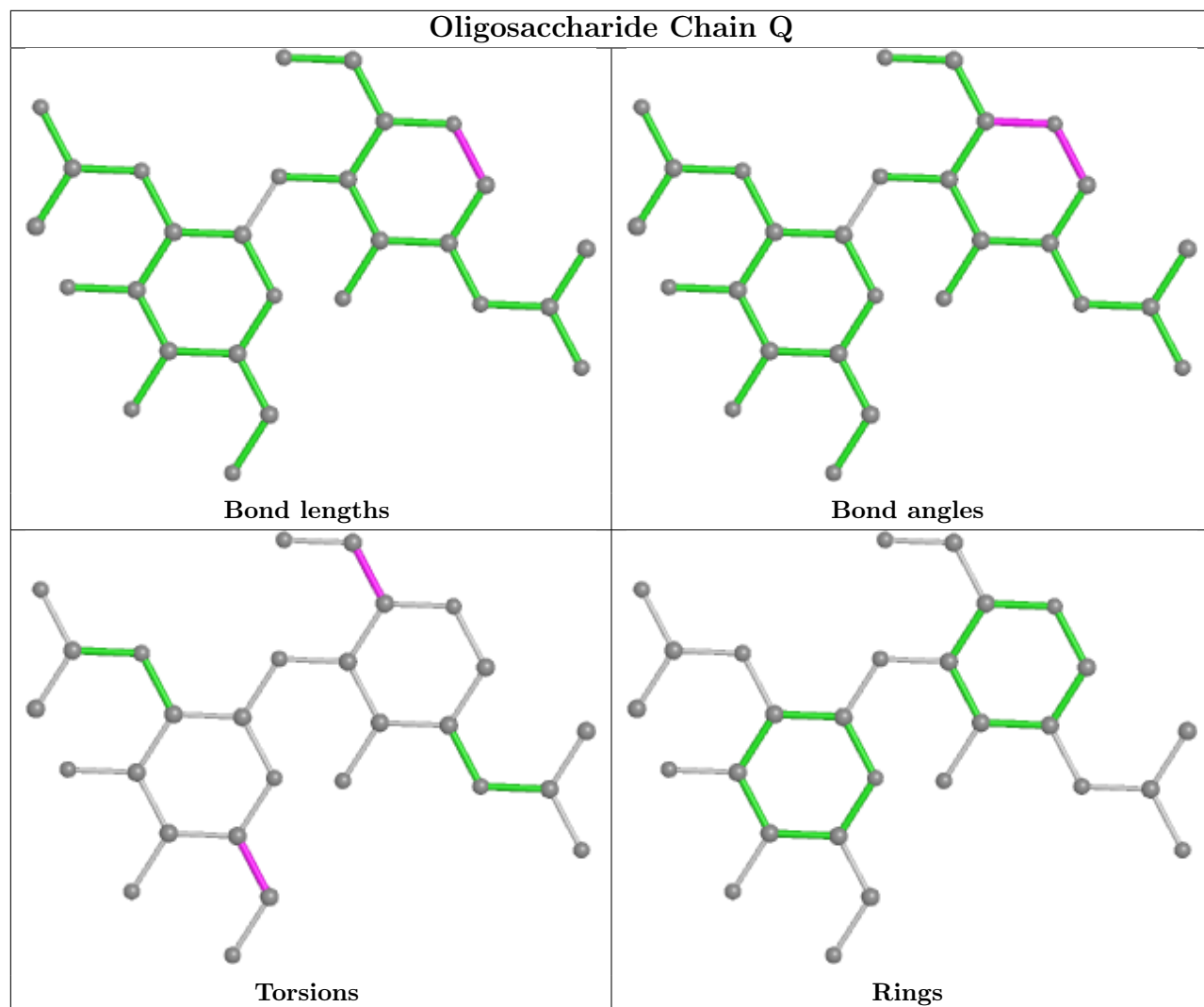


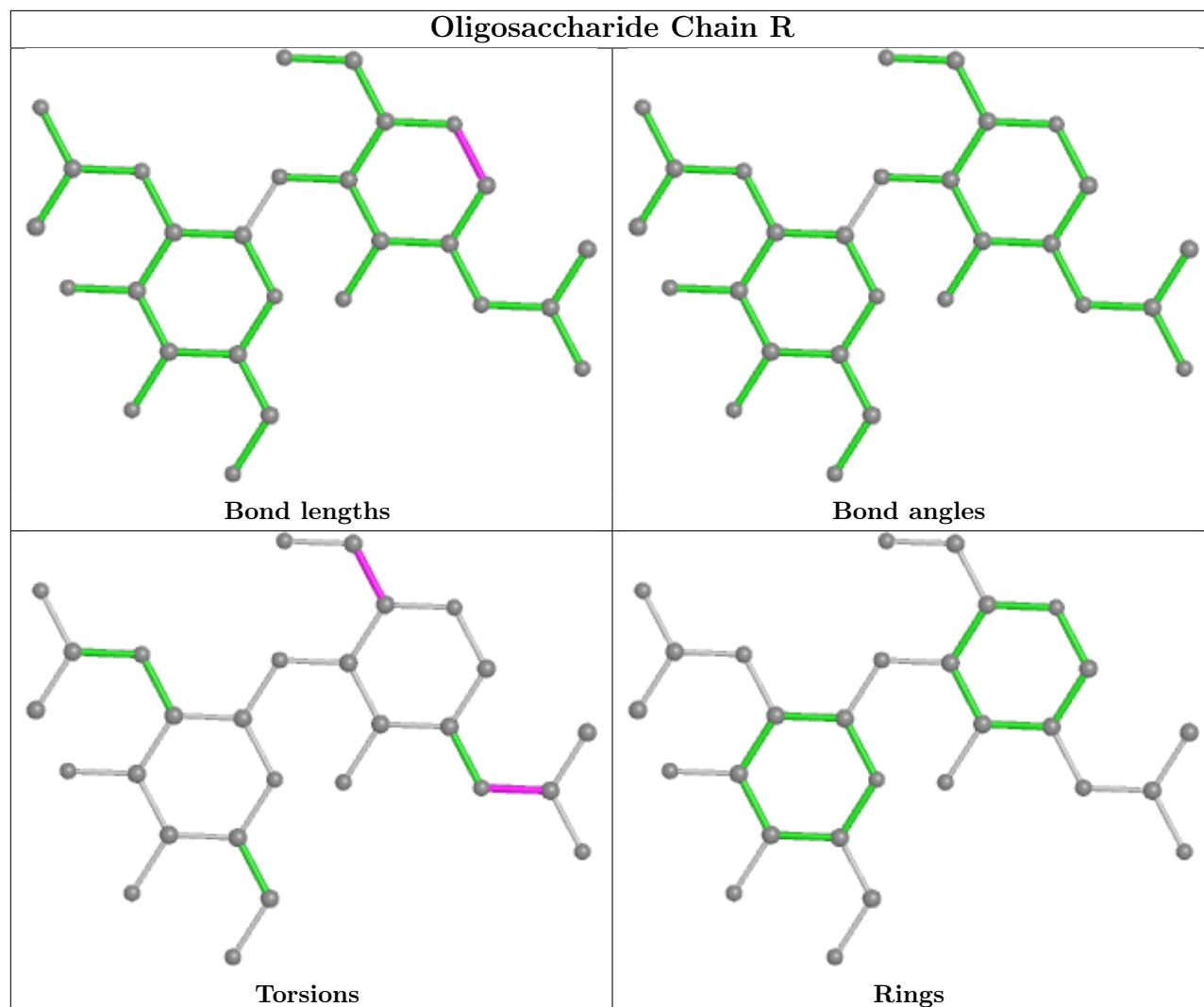












Oligosaccharide Chain S

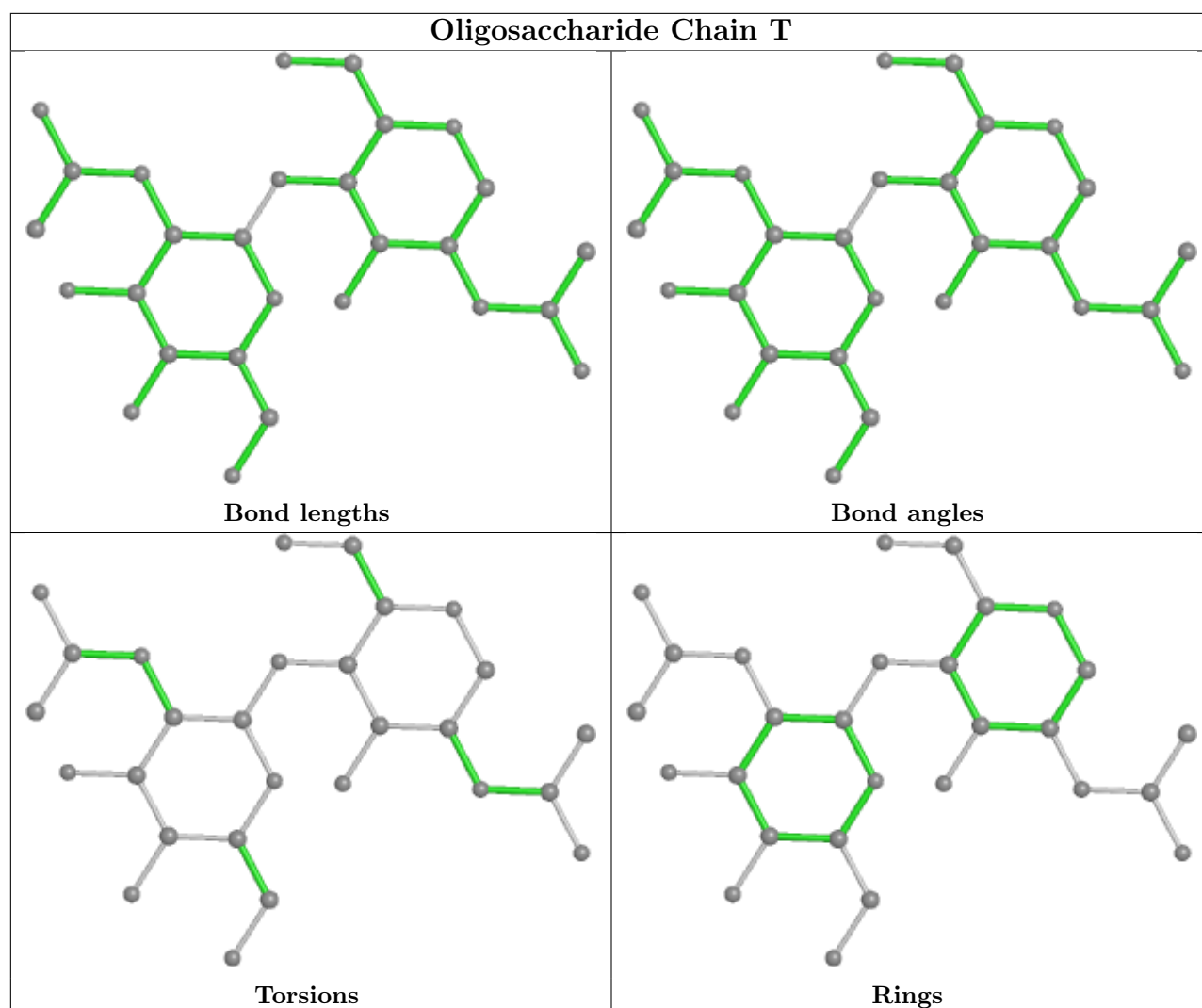
The figure displays four panels illustrating different structural parameters of Oligosaccharide Chain S, which is a branched chain of six pyranose rings. The panels are arranged in a 2x2 grid. Each panel shows the same molecular structure with different parameters highlighted in green. The top-left panel highlights bond lengths, the top-right panel highlights bond angles, the bottom-left panel highlights torsions, and the bottom-right panel highlights rings. The labels for each panel are: Bond lengths, Bond angles, Torsions, and Rings.

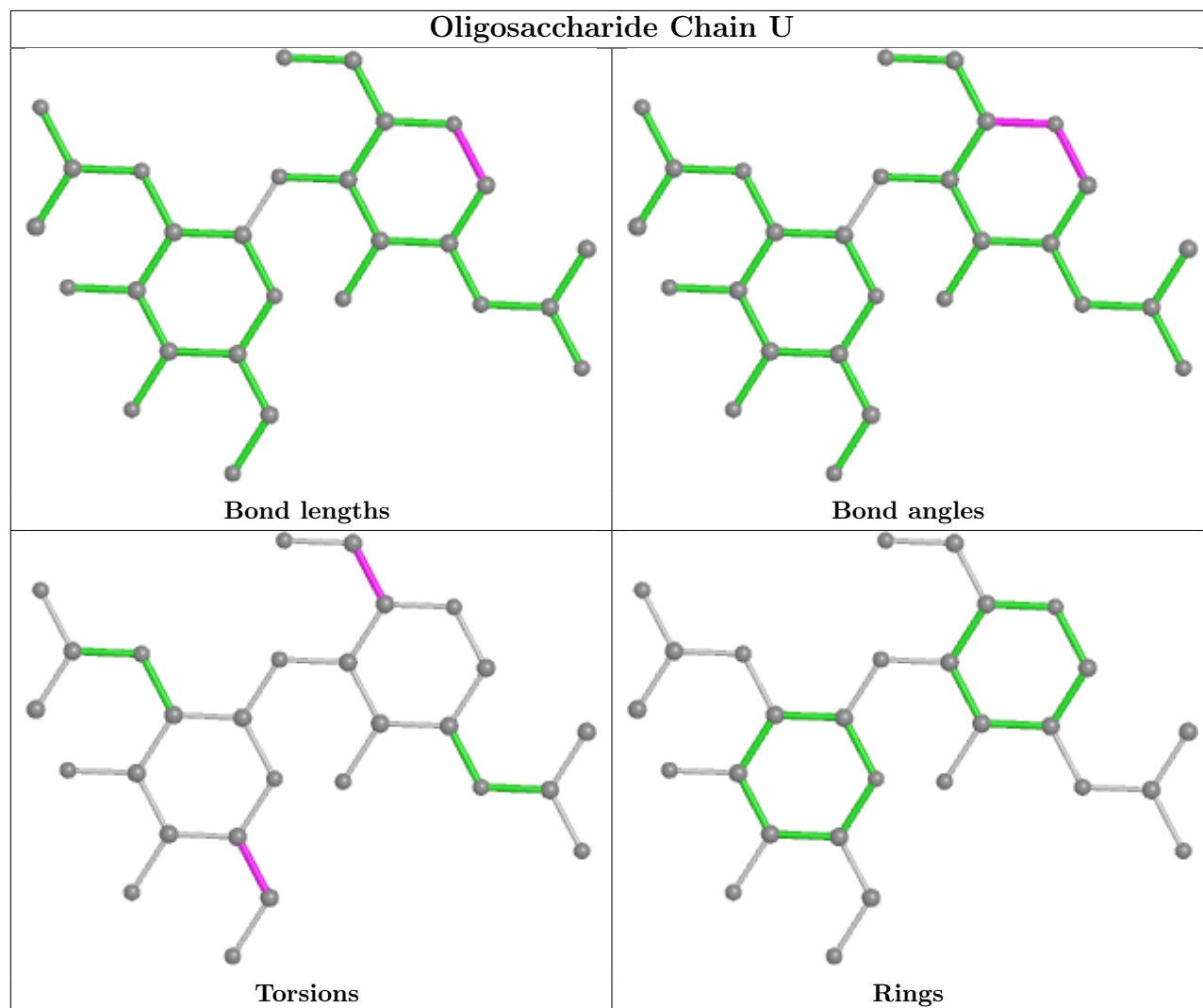
Bond lengths

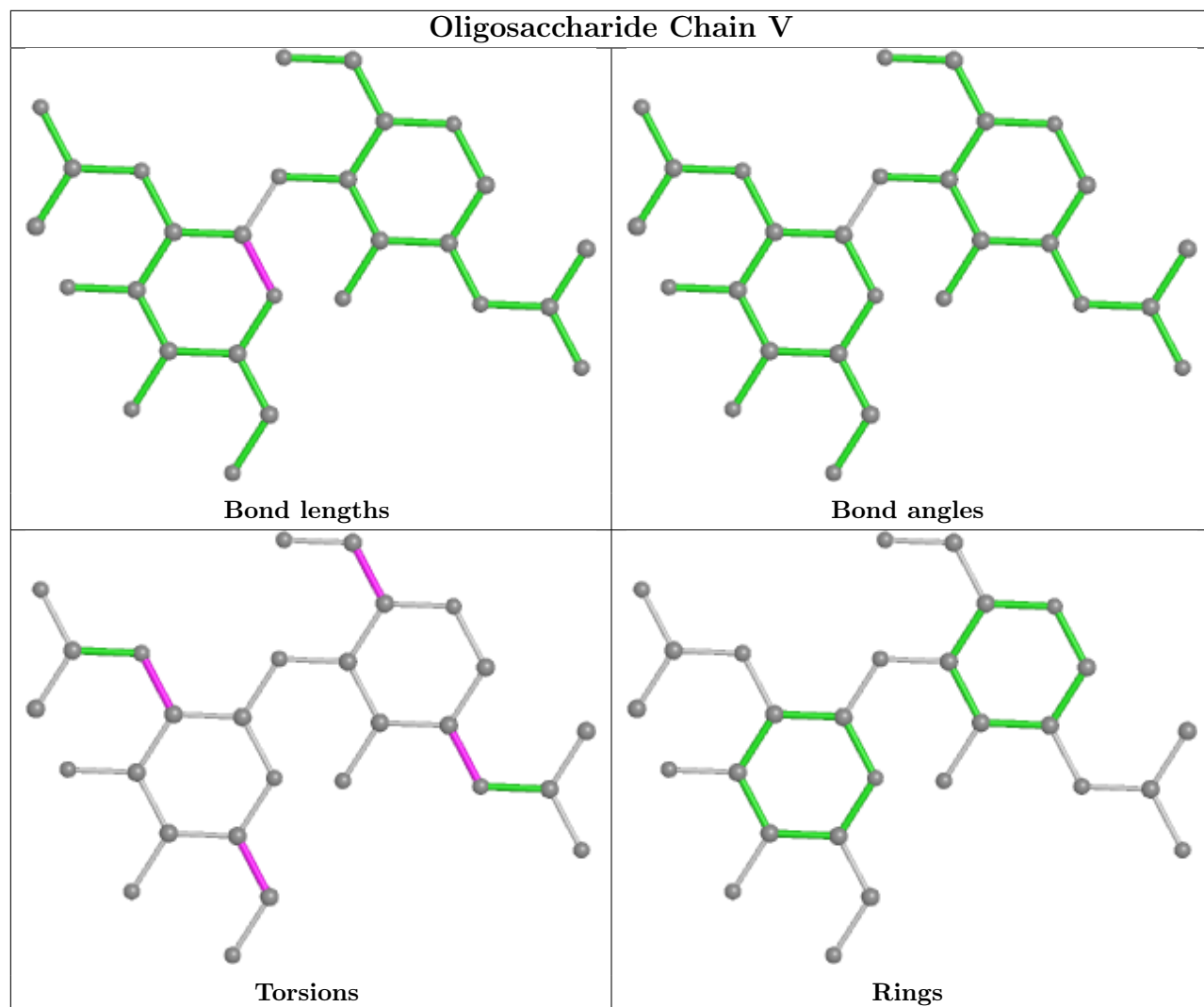
Bond angles

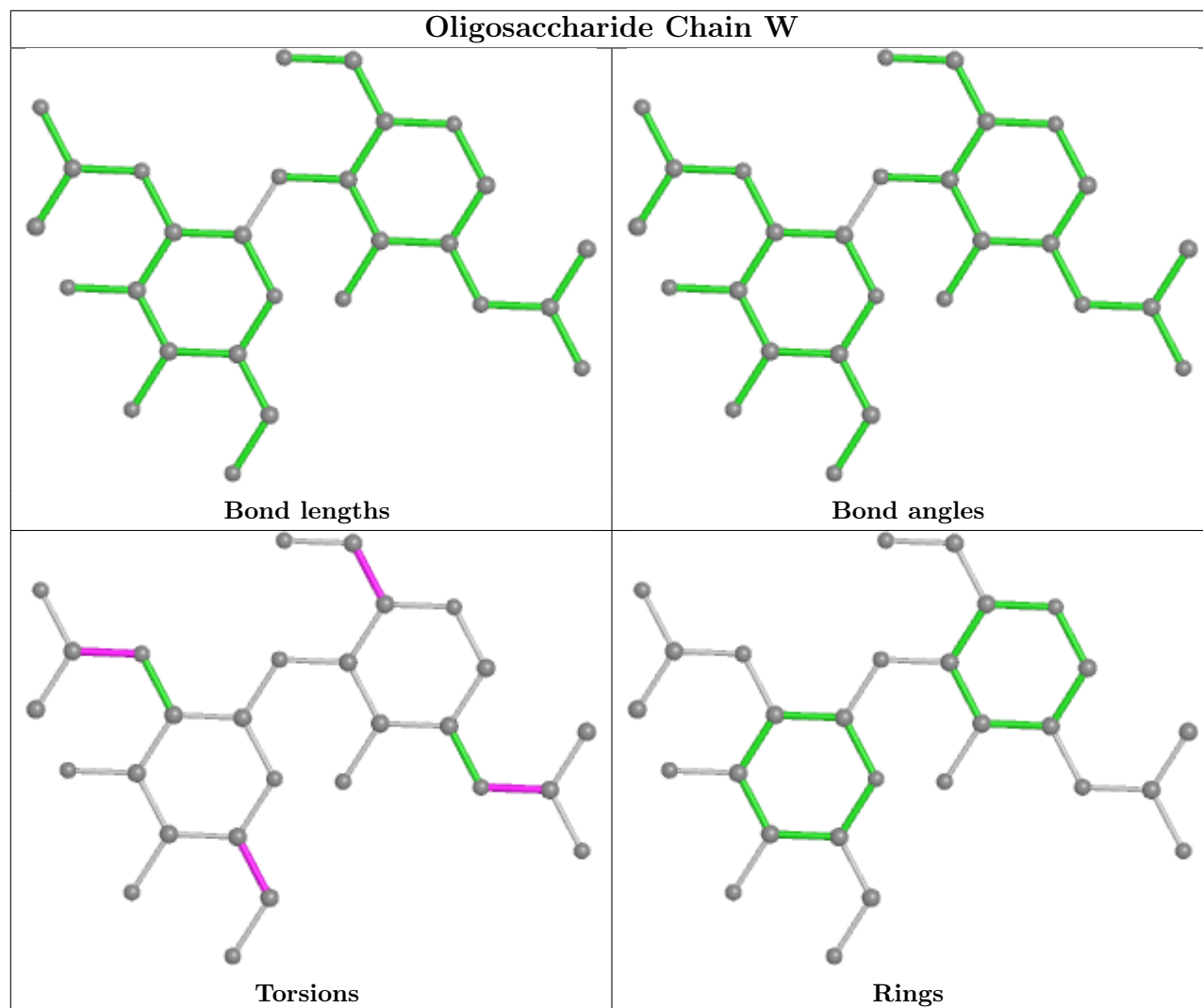
Torsions

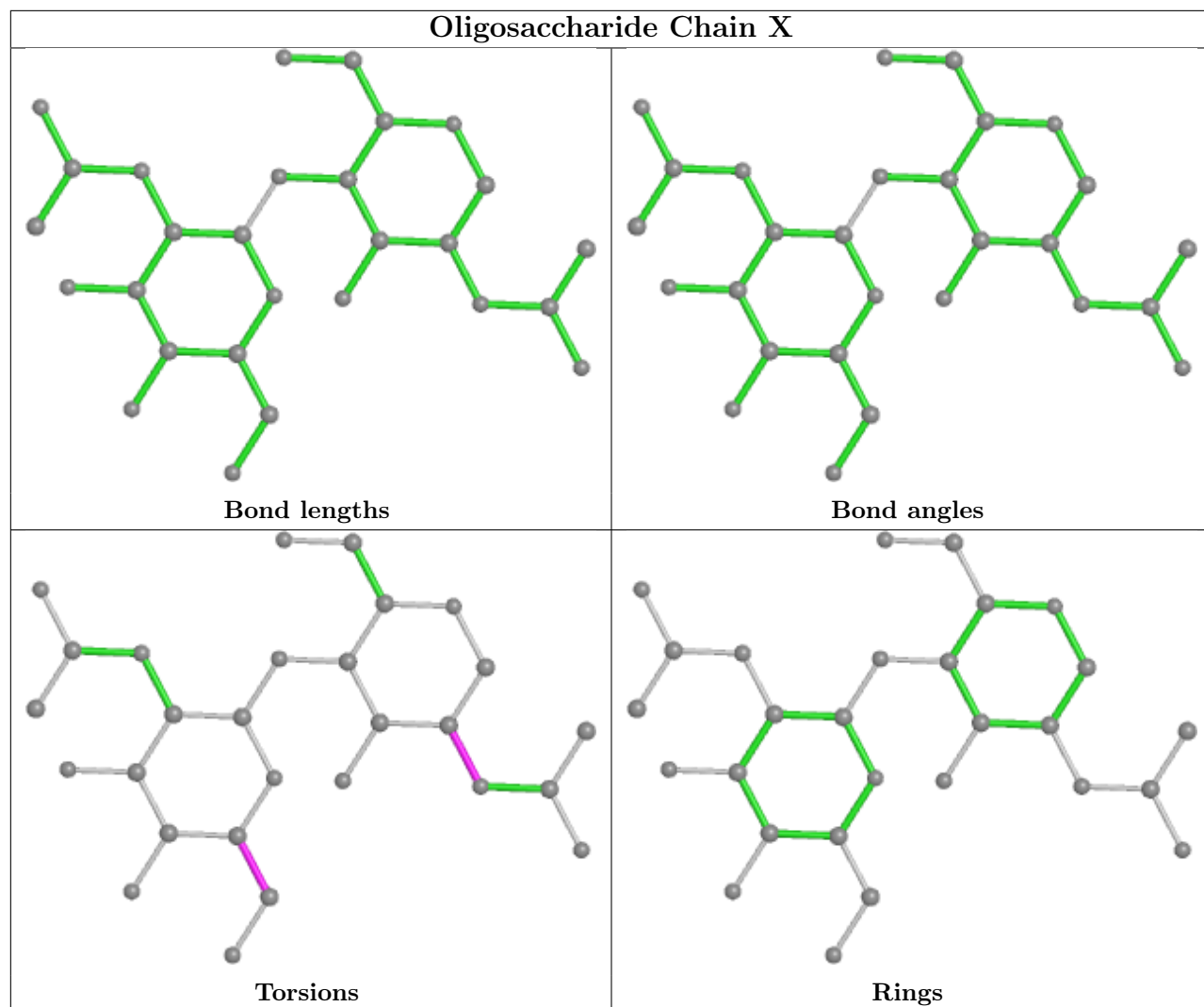
Rings

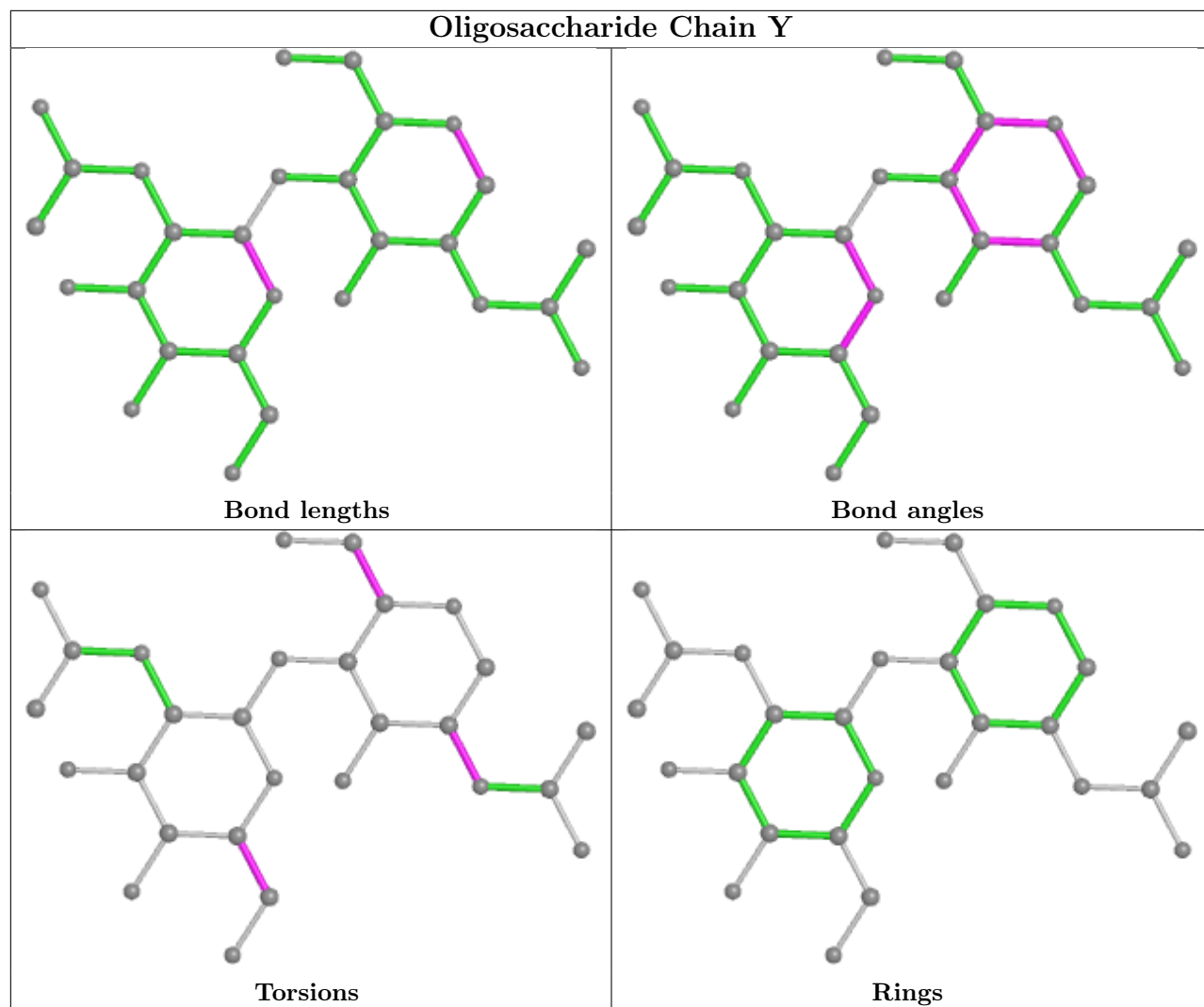


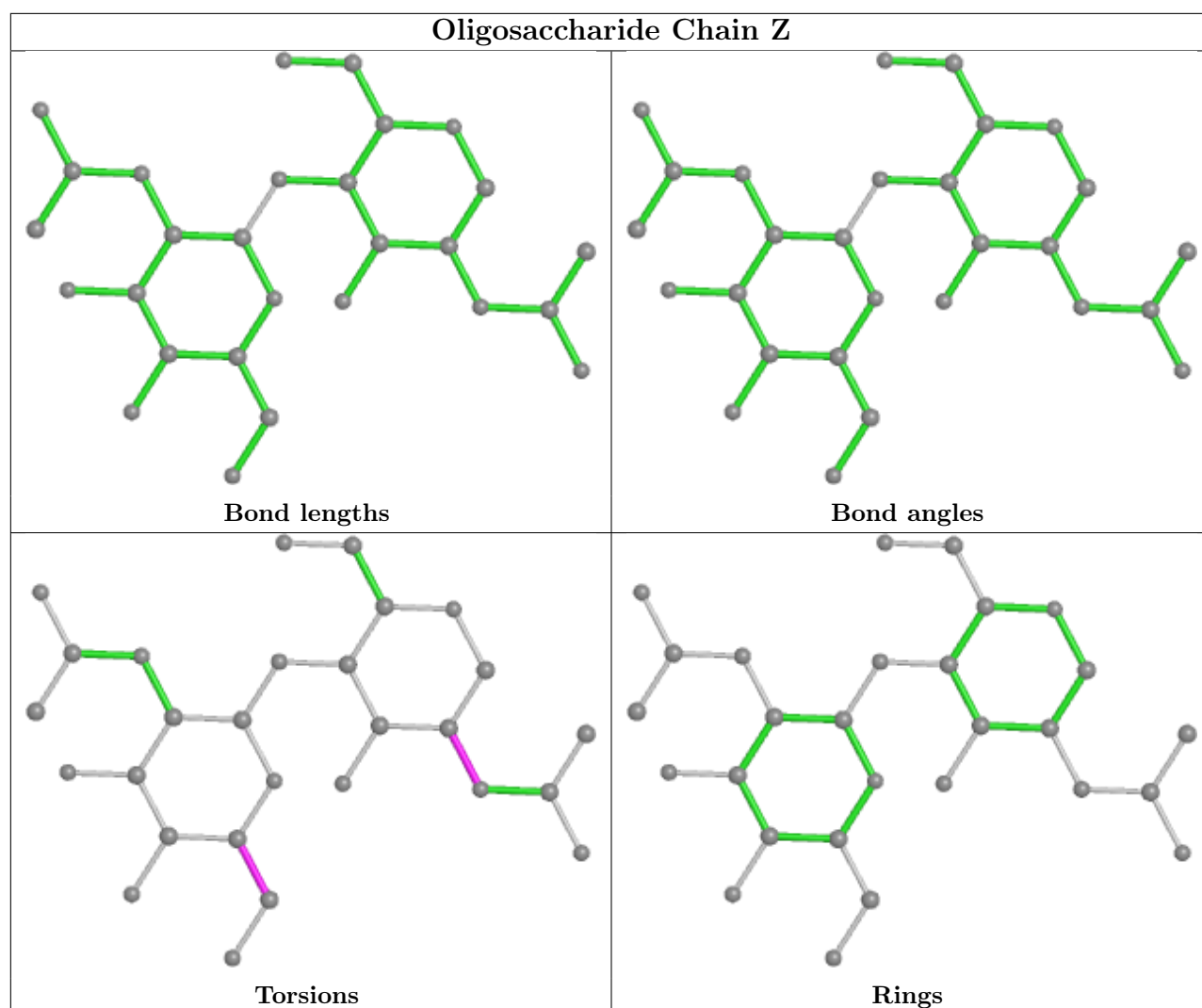


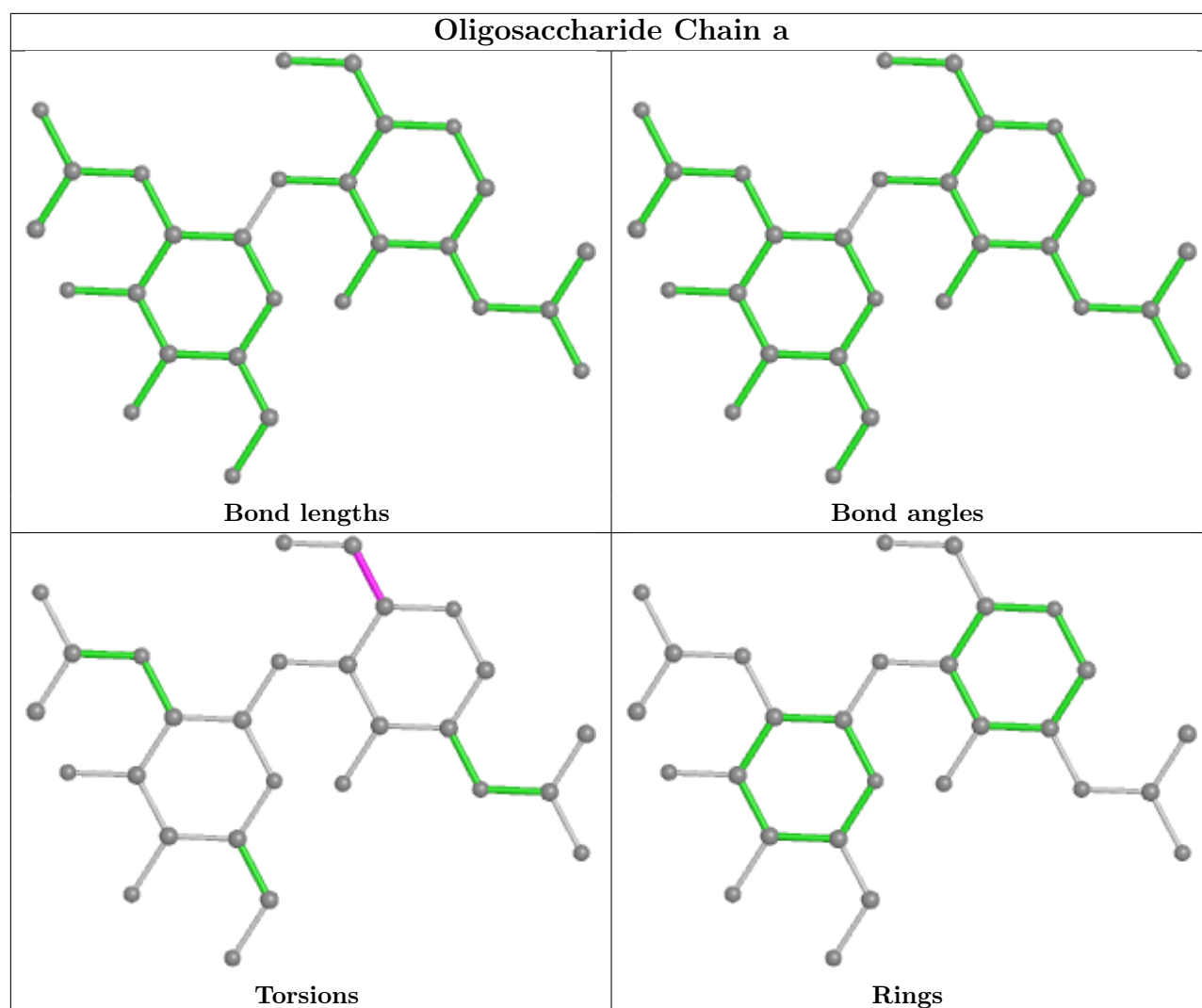


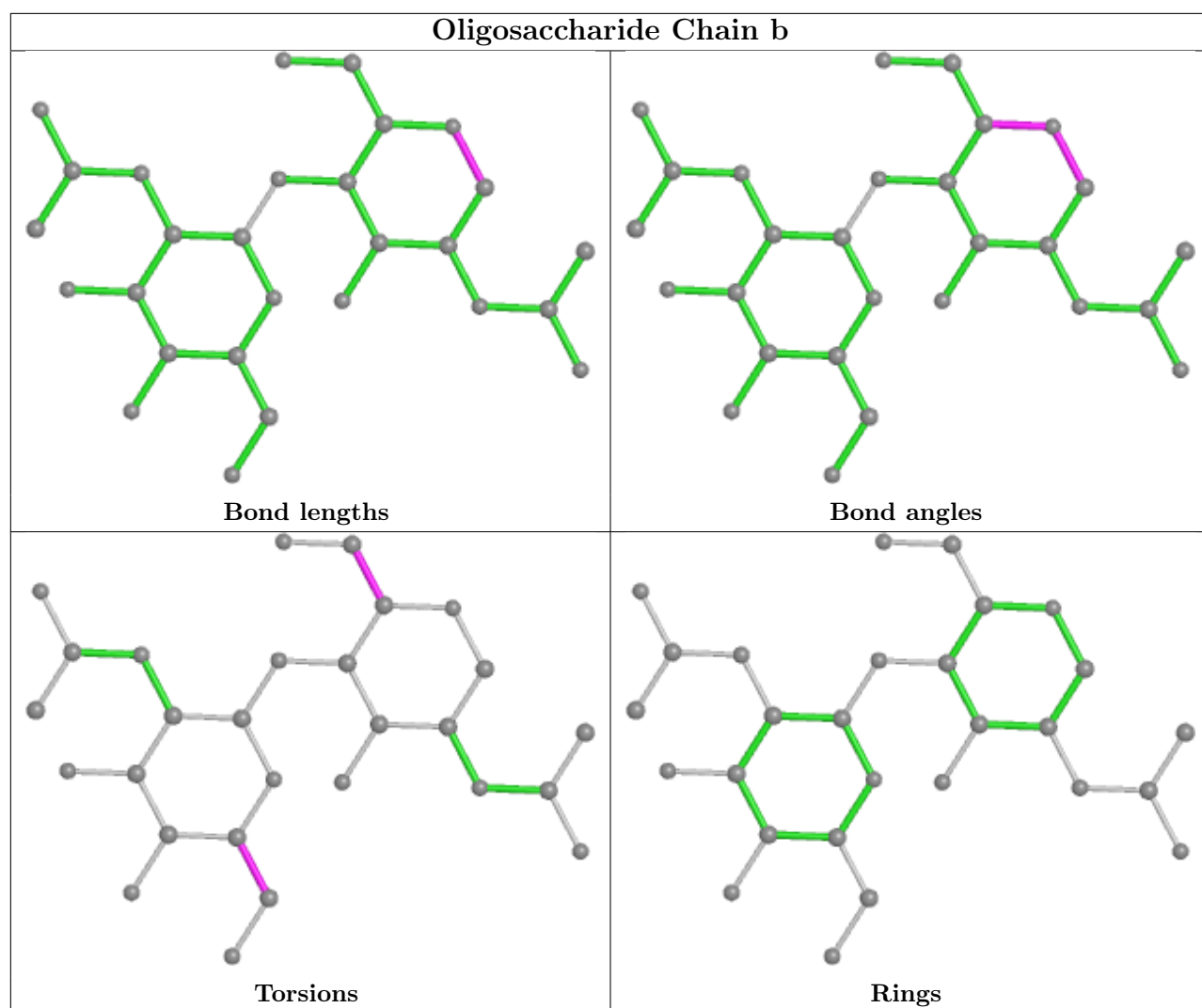


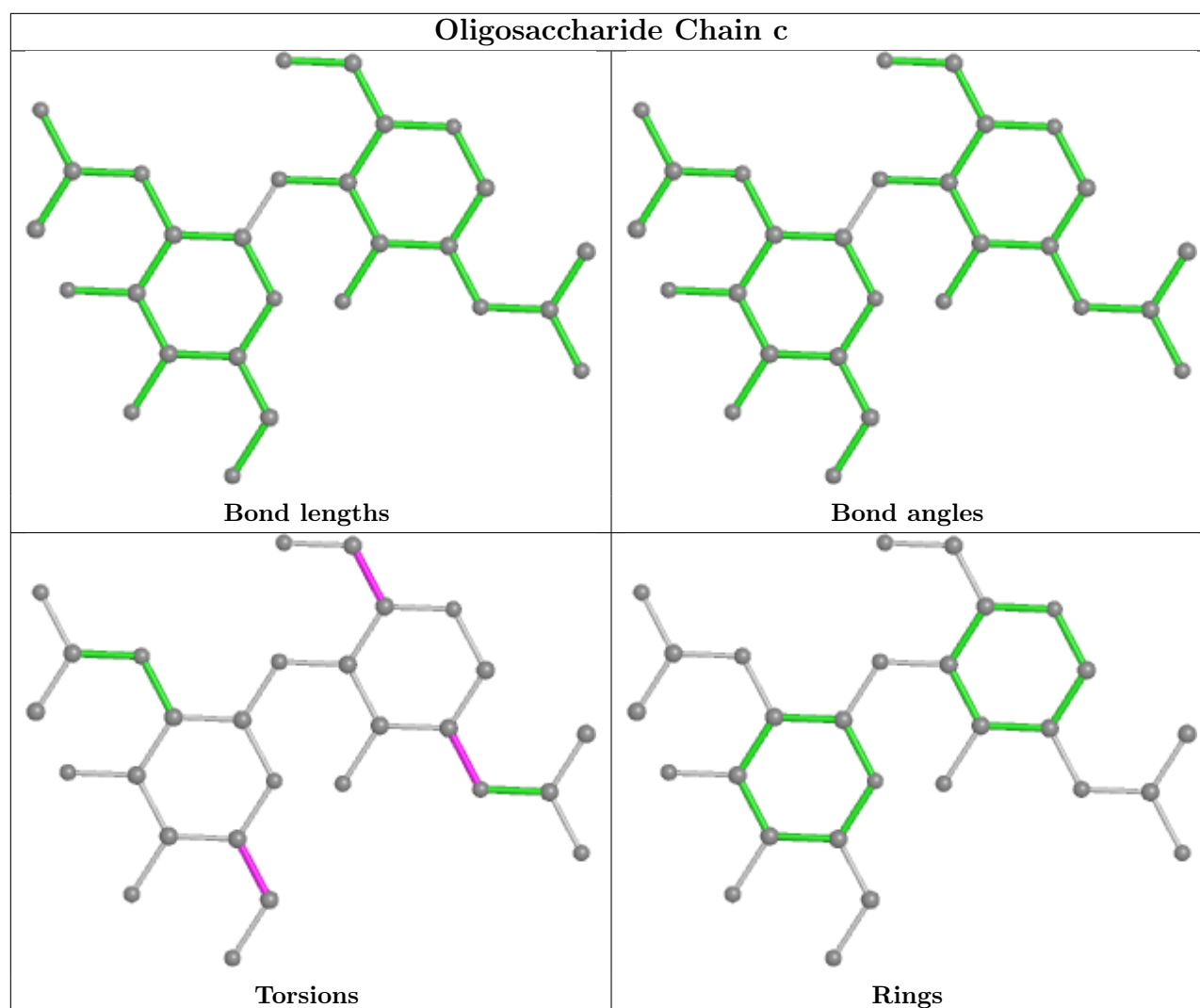












5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
5	NAG	C	1304	1	14,14,15	0.70	1 (7%)	17,19,21	0.75	0
5	NAG	A	1306	-	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	C	1305	-	14,14,15	0.20	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1301	1	14,14,15	0.25	0	17,19,21	0.38	0
5	NAG	E	1309	1	14,14,15	0.43	0	17,19,21	0.41	0
5	NAG	A	1301	1	14,14,15	0.37	0	17,19,21	0.37	0
5	NAG	E	1305	1	14,14,15	0.75	1 (7%)	17,19,21	0.83	0
5	NAG	E	1303	1	14,14,15	0.58	1 (7%)	17,19,21	0.50	0
5	NAG	A	1309	1	14,14,15	0.48	0	17,19,21	0.64	0
5	NAG	E	1302	1	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.38	0
5	NAG	A	1307	1	14,14,15	0.45	0	17,19,21	0.64	1 (5%)
5	NAG	C	1301	1	14,14,15	0.46	0	17,19,21	0.43	0
5	NAG	E	1304	1	14,14,15	0.49	0	17,19,21	0.54	0
5	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	A	1302	1	14,14,15	1.30	1 (7%)	17,19,21	1.40	1 (5%)
5	NAG	E	1306	1	14,14,15	0.98	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	E	1308	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	C	1302	1	14,14,15	1.30	2 (14%)	17,19,21	1.34	1 (5%)
5	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	E	1307	1	14,14,15	0.27	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
5	NAG	E	1301	1	-	3/6/23/26	0/1/1/1
5	NAG	E	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1305	1	-	1/6/23/26	0/1/1/1
5	NAG	E	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	E	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1304	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1308	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	4/6/23/26	0/1/1/1
5	NAG	E	1307	1	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1302	NAG	O5-C1	4.49	1.50	1.43
5	C	1302	NAG	O5-C1	4.34	1.50	1.43
5	E	1306	NAG	O5-C1	3.46	1.49	1.43
5	E	1305	NAG	O5-C1	-2.45	1.39	1.43
5	C	1304	NAG	O5-C1	-2.43	1.39	1.43
5	C	1302	NAG	C1-C2	2.13	1.55	1.52
5	E	1303	NAG	O5-C1	-2.02	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1302	NAG	C1-O5-C5	5.56	119.73	112.19
5	C	1302	NAG	C1-O5-C5	5.30	119.38	112.19
5	E	1306	NAG	C1-O5-C5	4.96	118.91	112.19
5	A	1307	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	1305	NAG	O5-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	E	1308	NAG	O5-C5-C6-O6
5	E	1309	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	E	1303	NAG	O5-C5-C6-O6
5	E	1306	NAG	C4-C5-C6-O6
5	A	1307	NAG	C1-C2-N2-C7
5	C	1303	NAG	C4-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	E	1308	NAG	C4-C5-C6-O6
5	C	1302	NAG	C8-C7-N2-C2
5	C	1302	NAG	O7-C7-N2-C2
5	A	1308	NAG	C8-C7-N2-C2
5	A	1308	NAG	O7-C7-N2-C2
5	E	1301	NAG	C8-C7-N2-C2
5	E	1301	NAG	O7-C7-N2-C2
5	E	1302	NAG	C8-C7-N2-C2
5	E	1302	NAG	O7-C7-N2-C2
5	E	1304	NAG	C8-C7-N2-C2
5	E	1304	NAG	O7-C7-N2-C2
5	E	1304	NAG	O5-C5-C6-O6
5	E	1304	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	E	1303	NAG	C4-C5-C6-O6
5	E	1309	NAG	C4-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	E	1306	NAG	O5-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	E	1302	NAG	O5-C5-C6-O6
5	E	1309	NAG	C1-C2-N2-C7
5	A	1305	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	E	1301	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	E	1305	NAG	C1-C2-N2-C7
5	A	1304	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	A	1307	NAG	C3-C2-N2-C7
5	A	1309	NAG	C3-C2-N2-C7
5	E	1307	NAG	C3-C2-N2-C7
5	E	1308	NAG	C3-C2-N2-C7
5	C	1304	NAG	C3-C2-N2-C7
5	E	1309	NAG	C3-C2-N2-C7
5	E	1302	NAG	C4-C5-C6-O6
5	C	1304	NAG	C1-C2-N2-C7

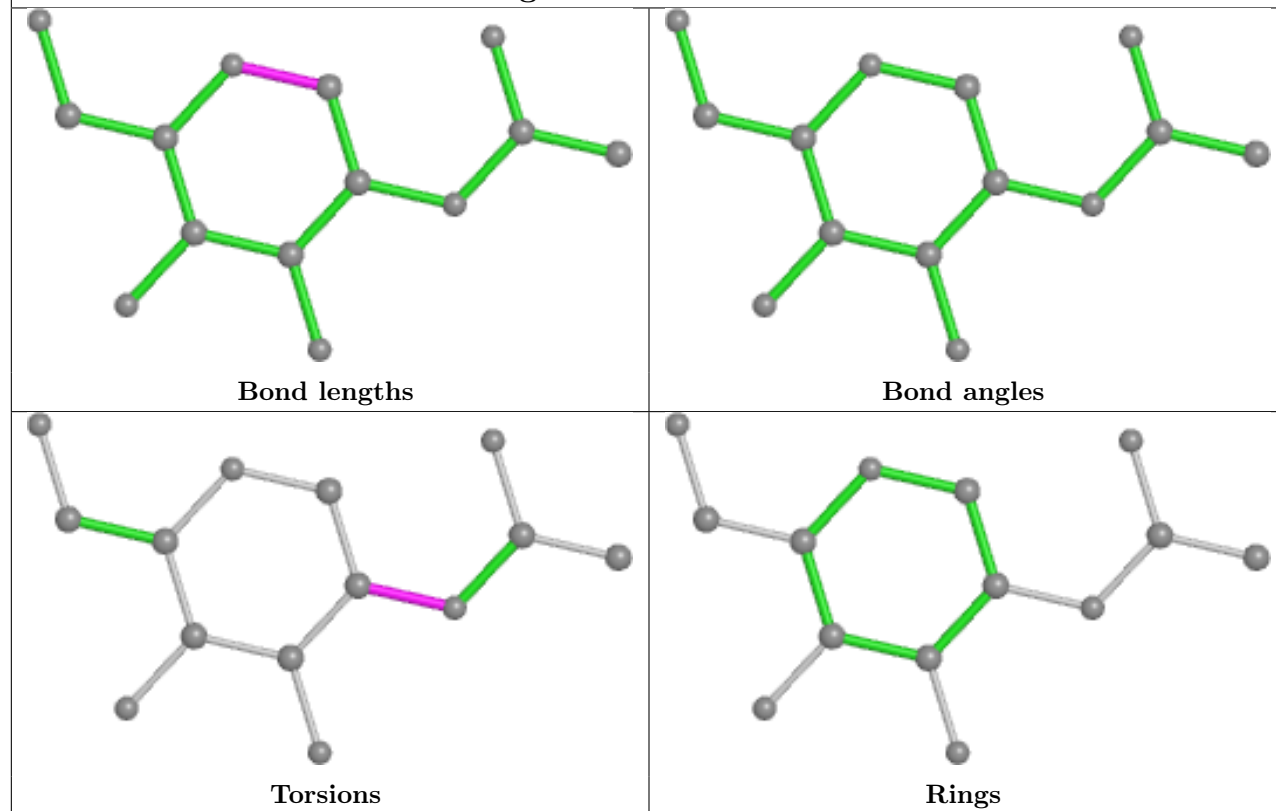
There are no ring outliers.

7 monomers are involved in 9 short contacts:

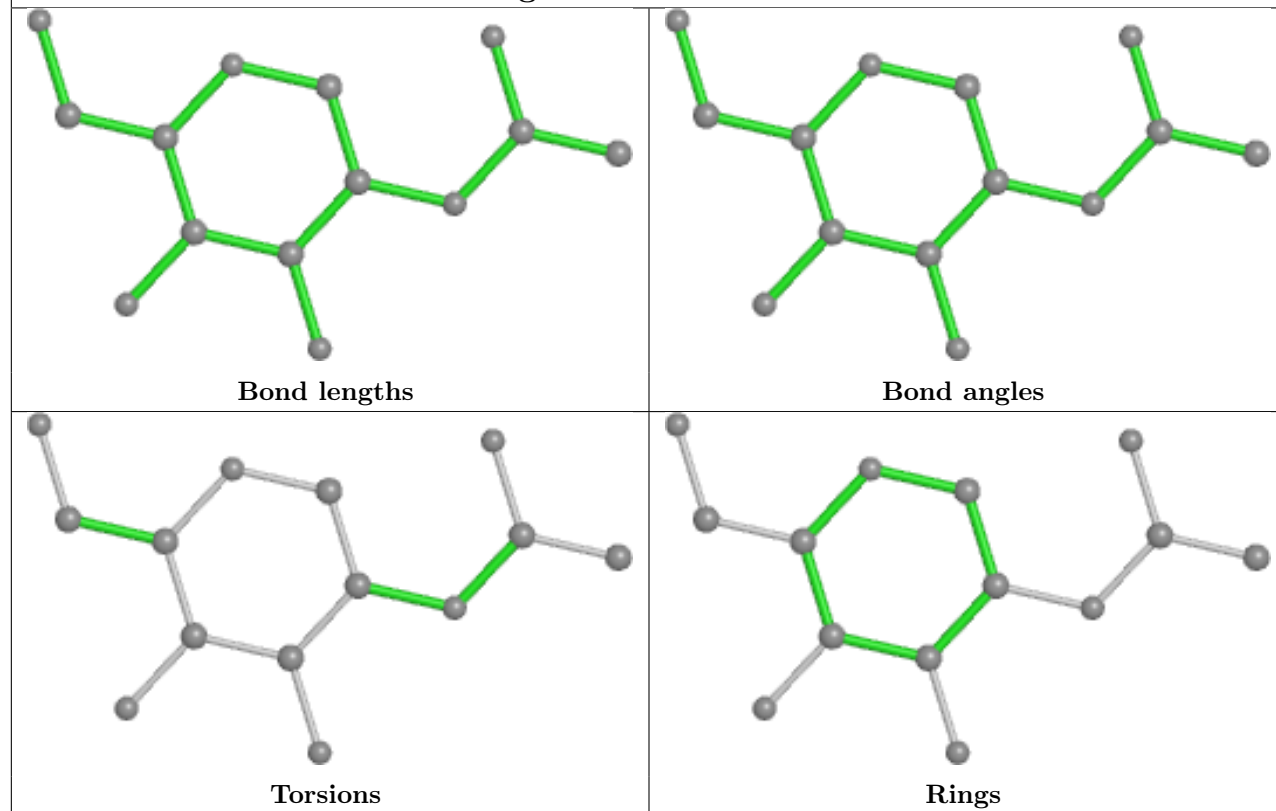
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1301	NAG	1	0
5	E	1305	NAG	2	0
5	A	1309	NAG	2	0
5	E	1302	NAG	1	0
5	A	1307	NAG	1	0
5	C	1302	NAG	2	0
5	A	1308	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

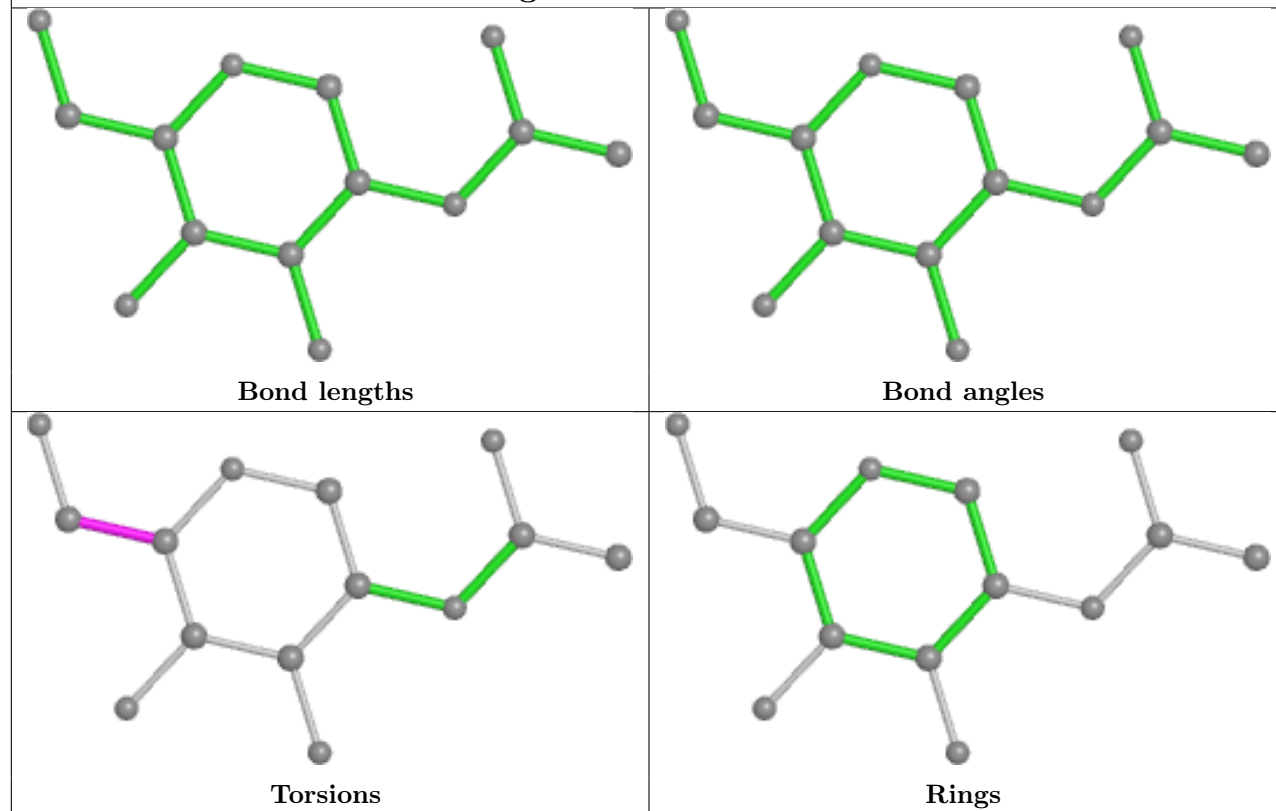
Ligand NAG C 1304



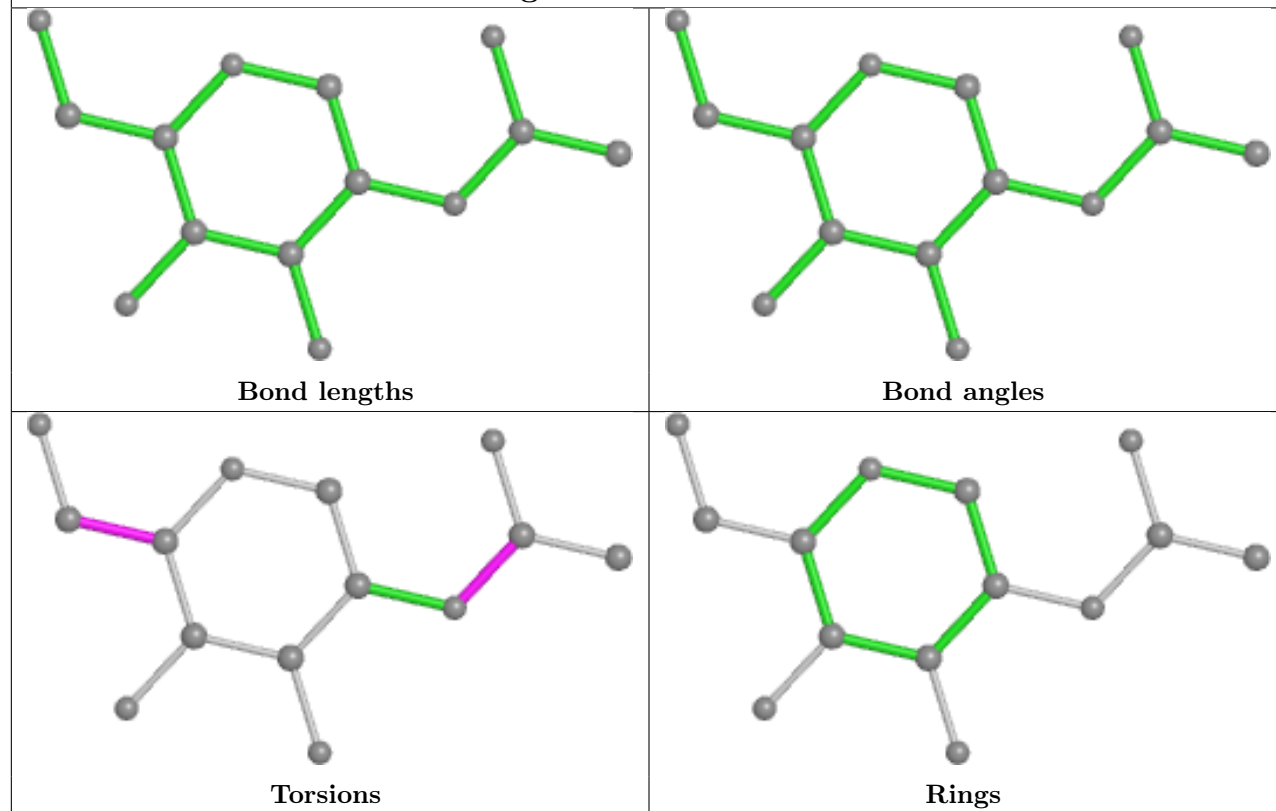
Ligand NAG A 1306

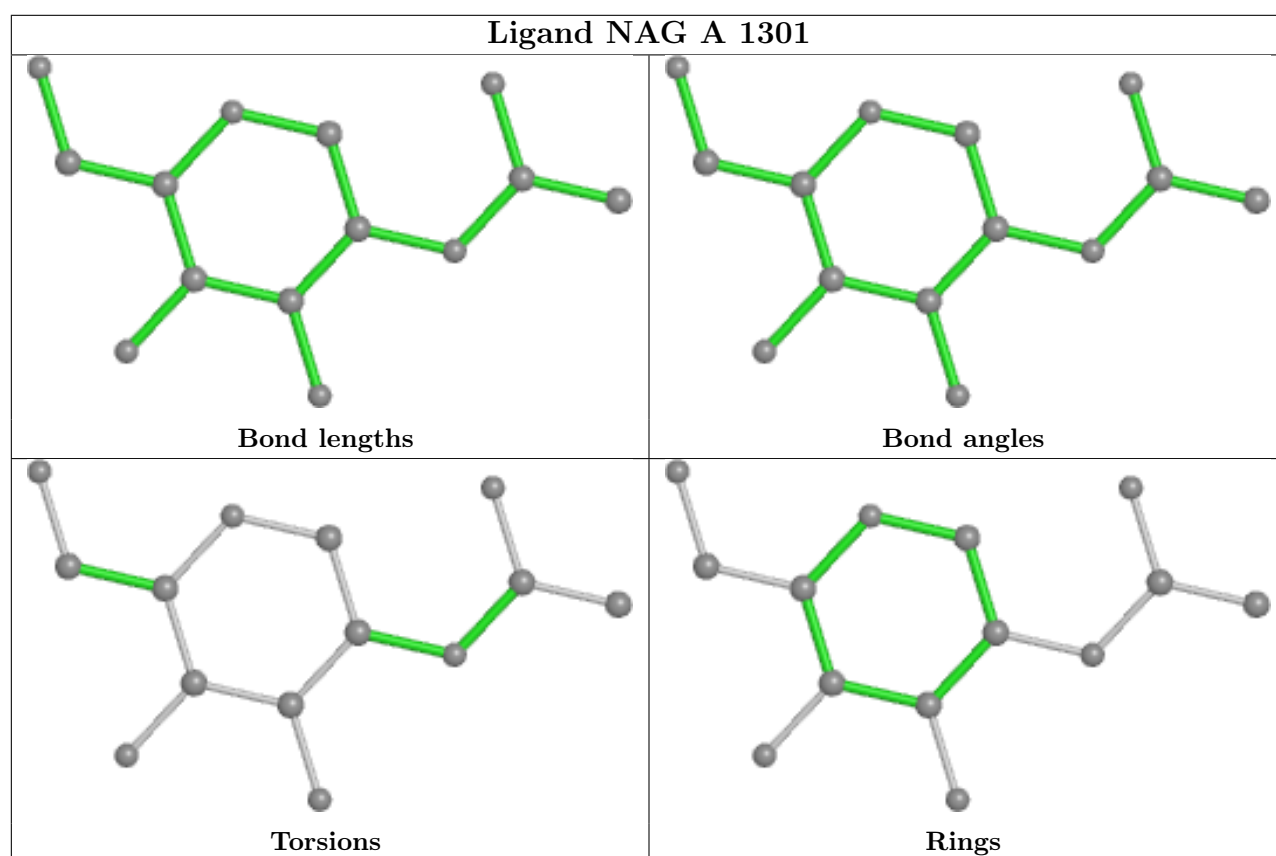
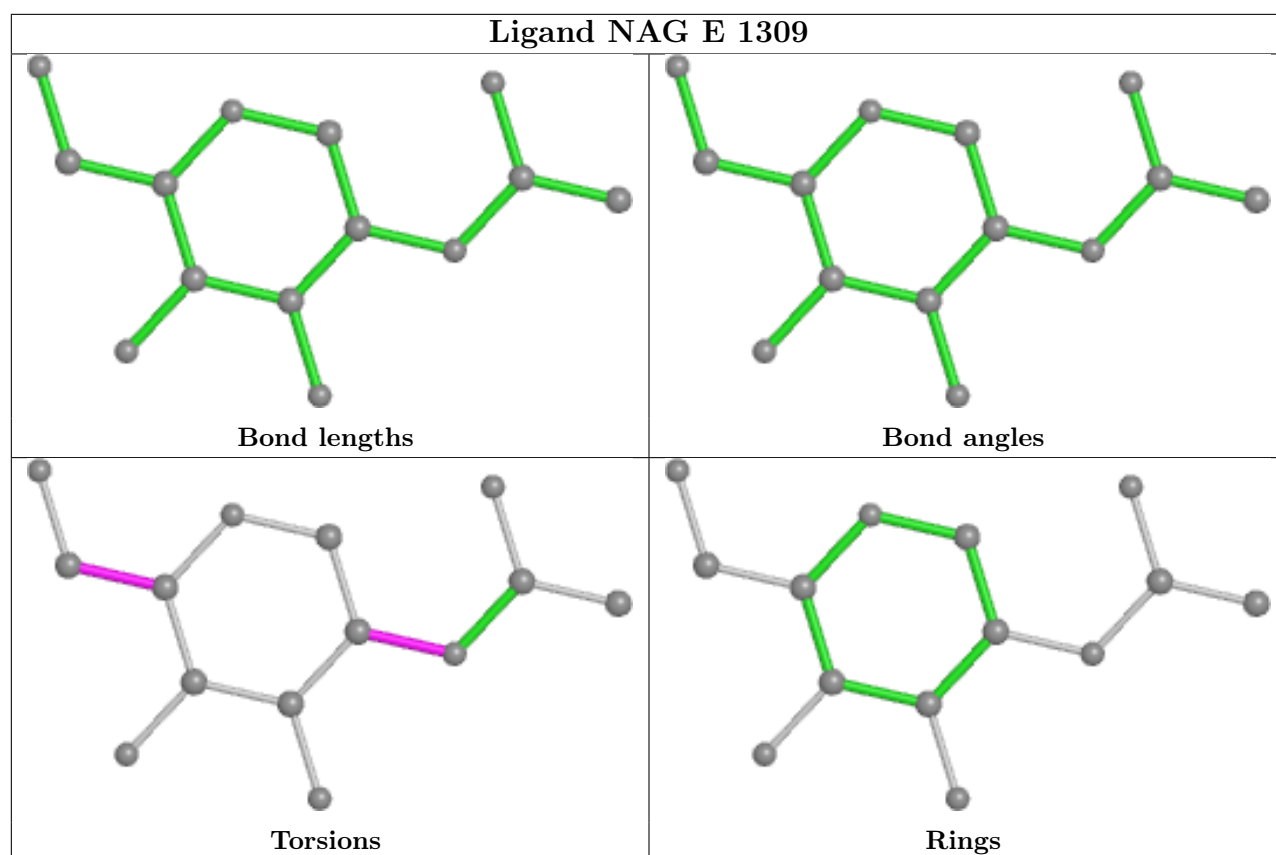


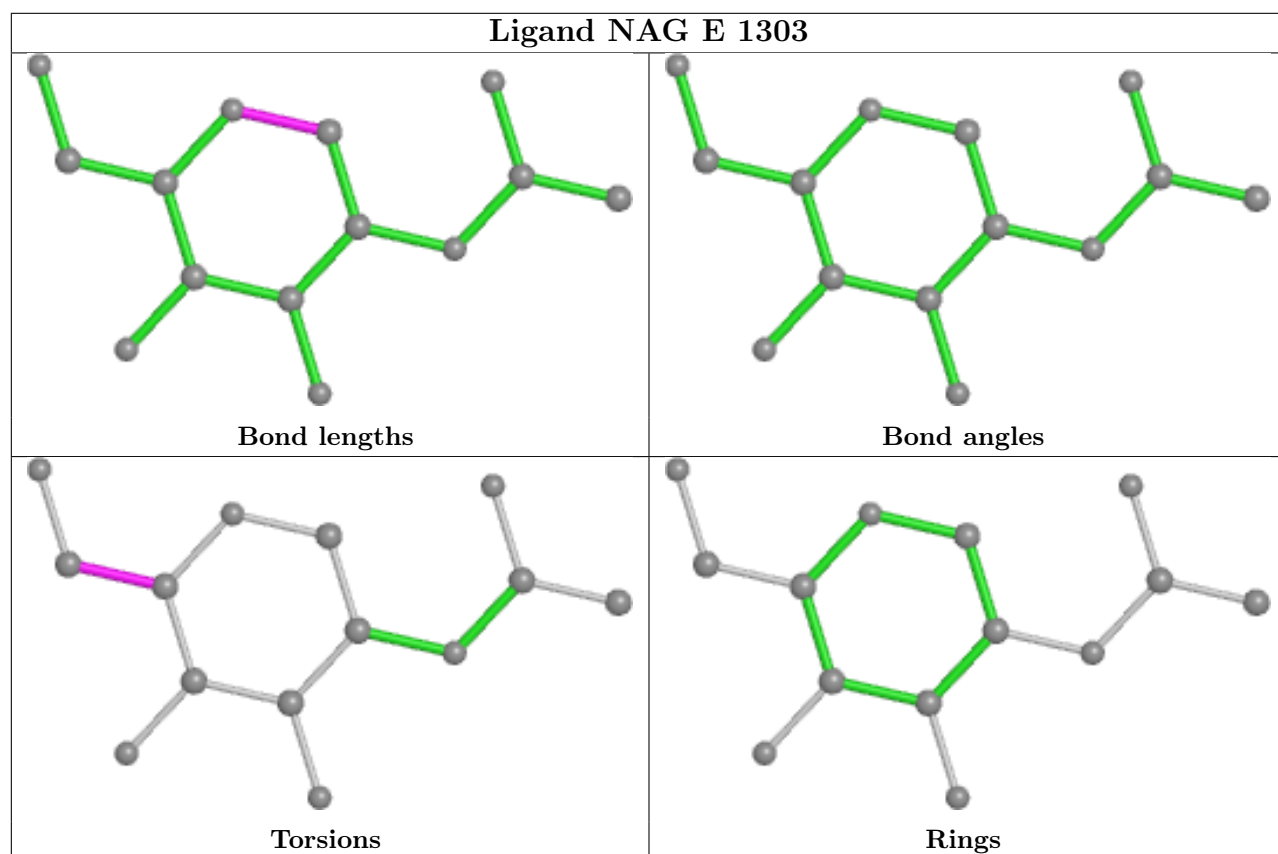
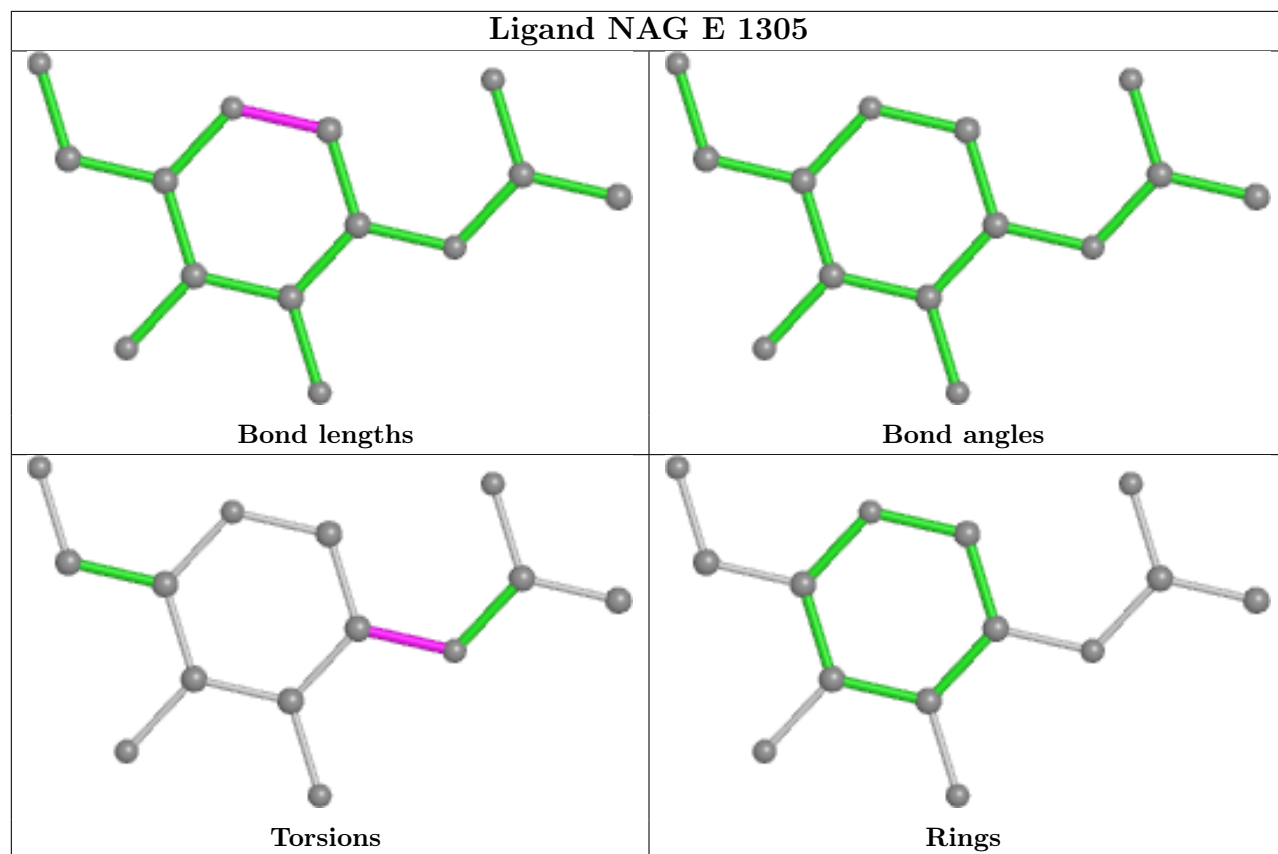
Ligand NAG C 1305



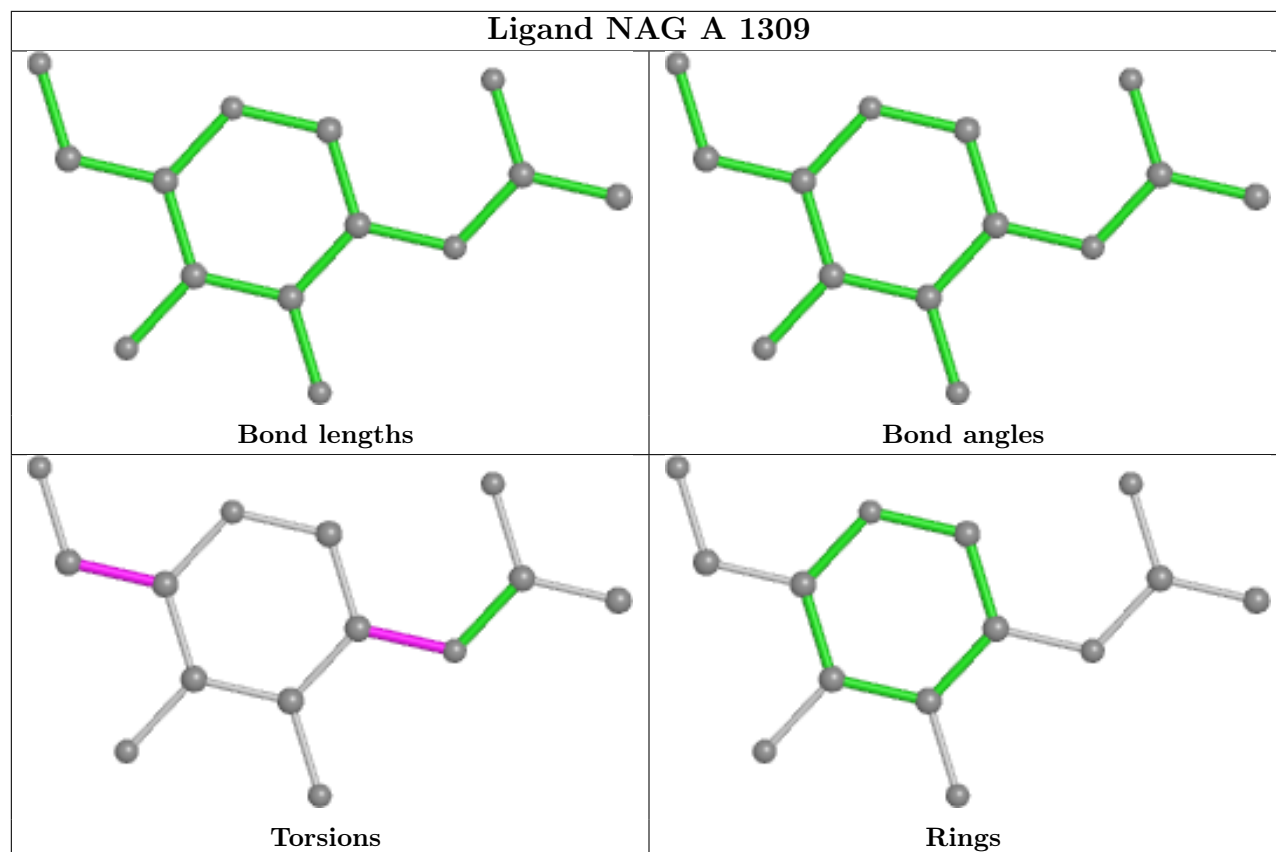
Ligand NAG E 1301



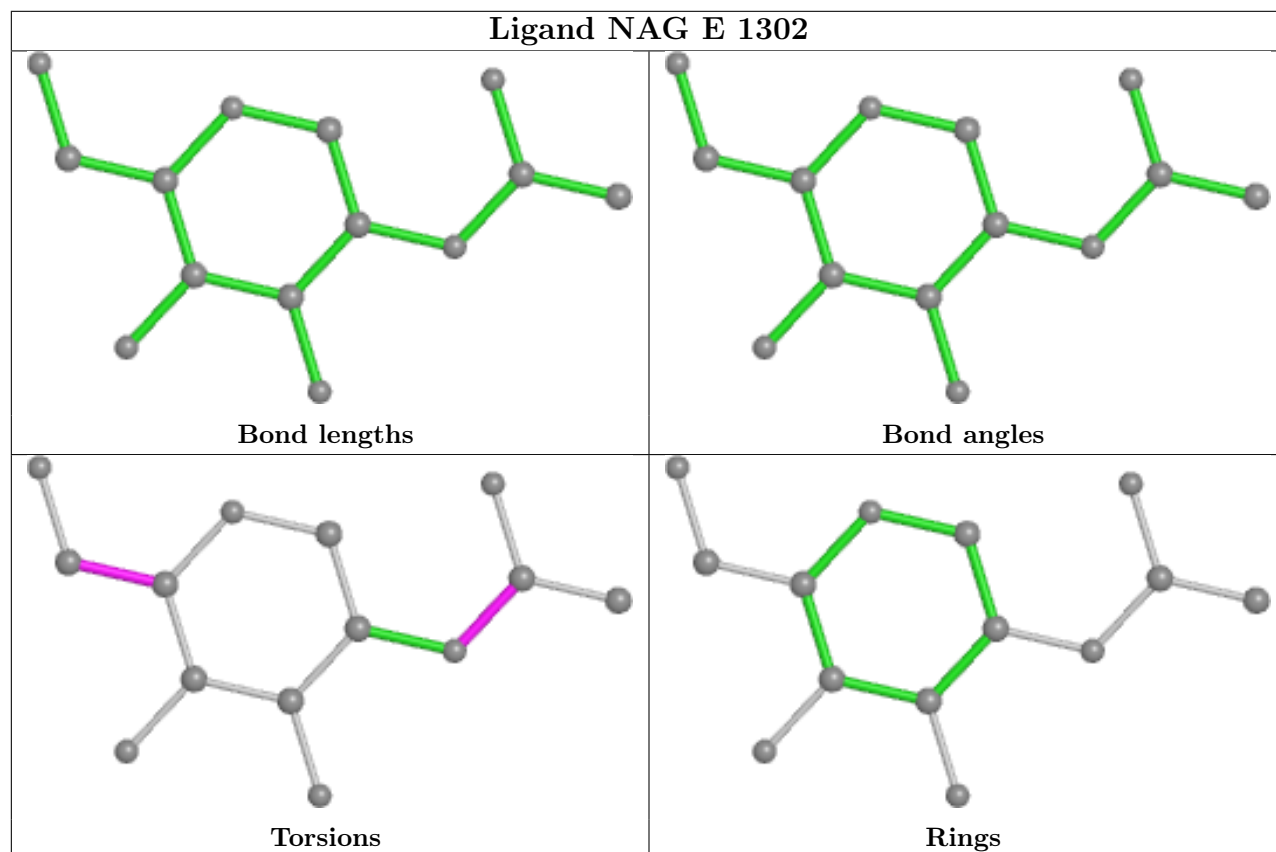




Ligand NAG A 1309



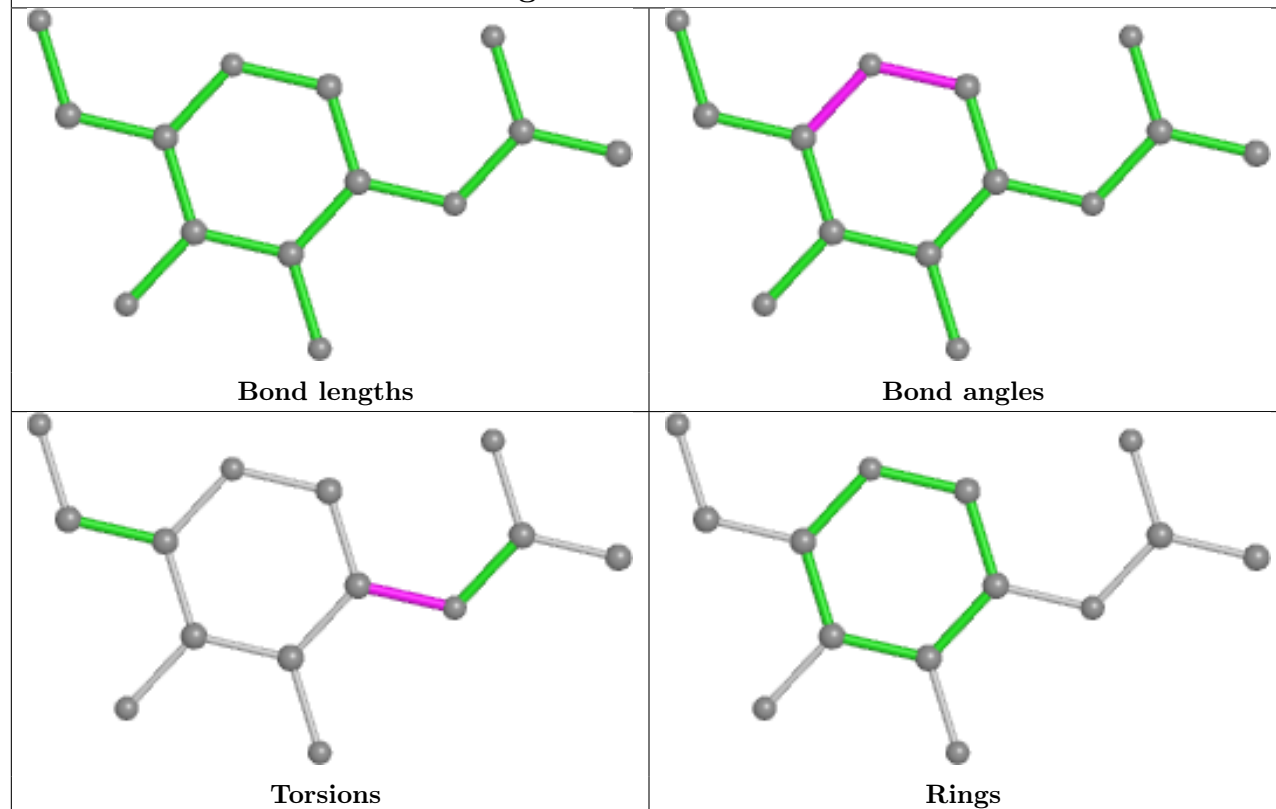
Ligand NAG E 1302



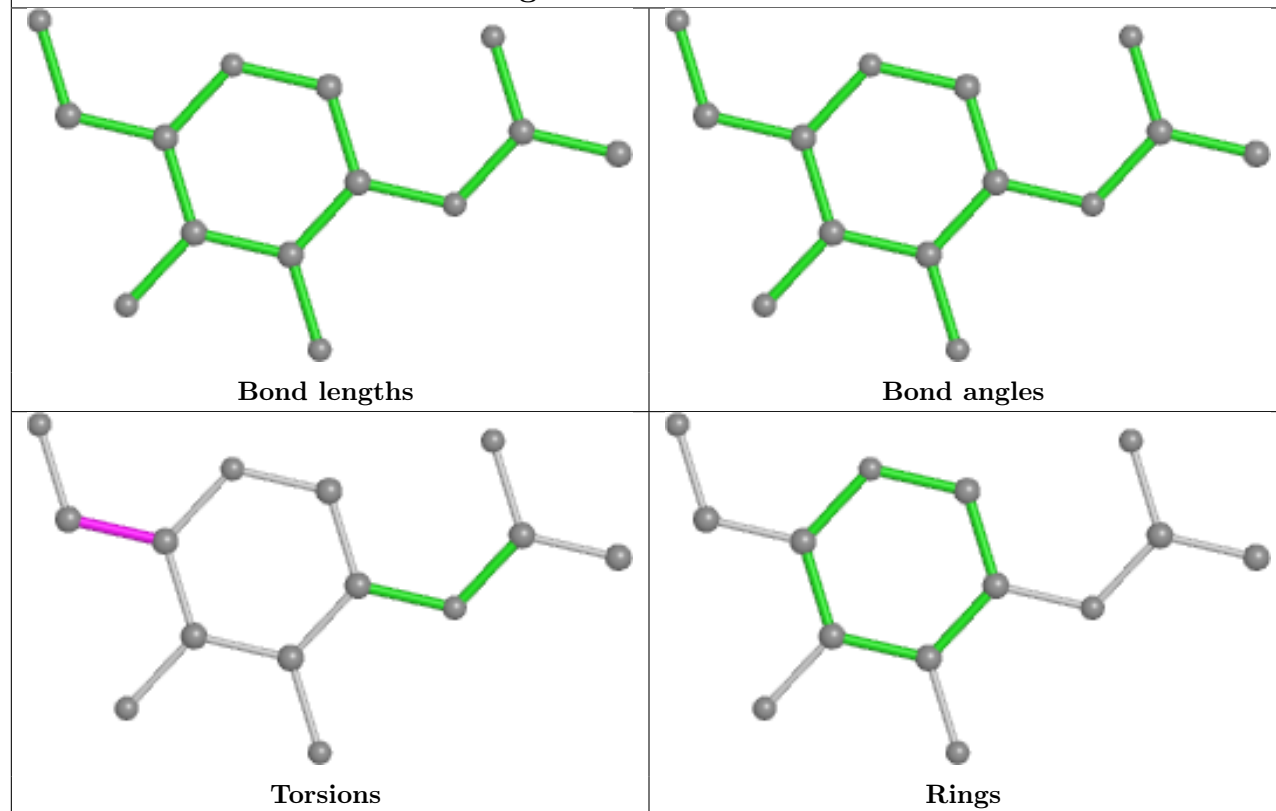
Ligand NAG A 1305



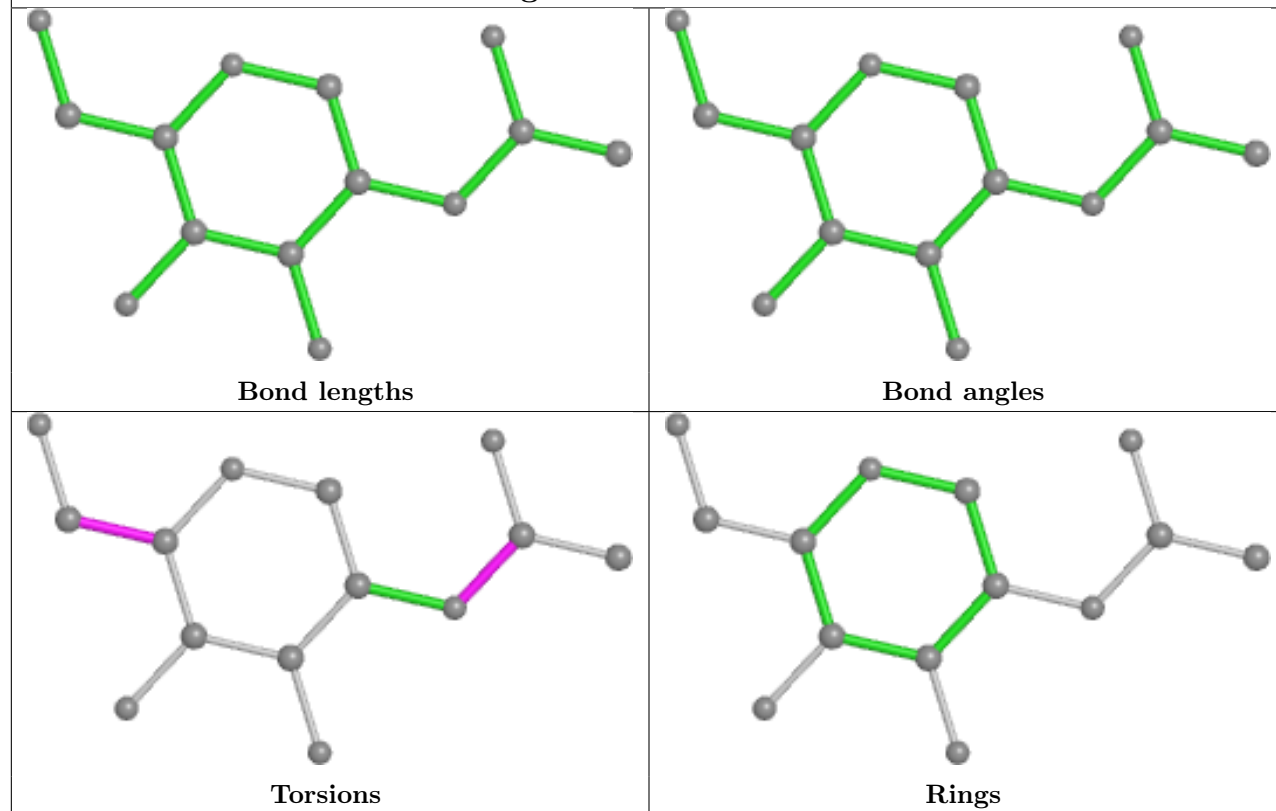
Ligand NAG A 1307



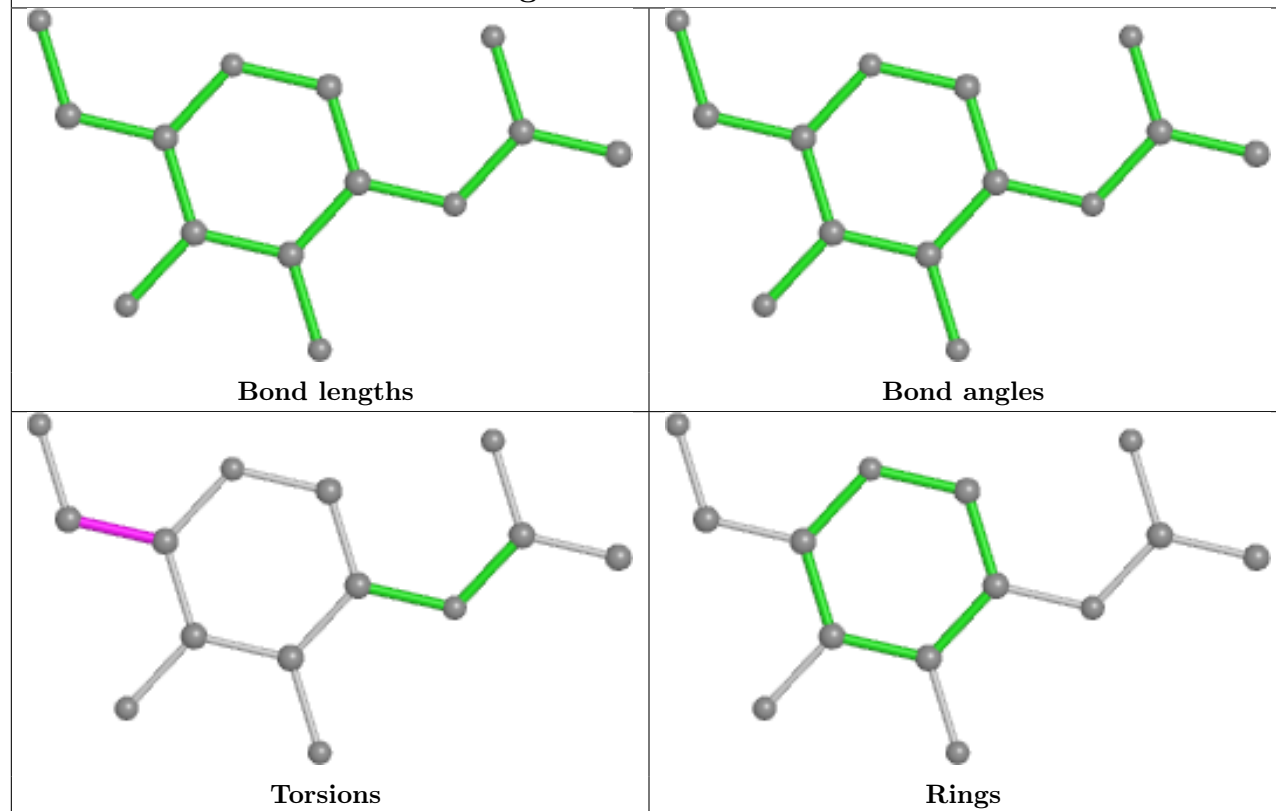
Ligand NAG C 1301



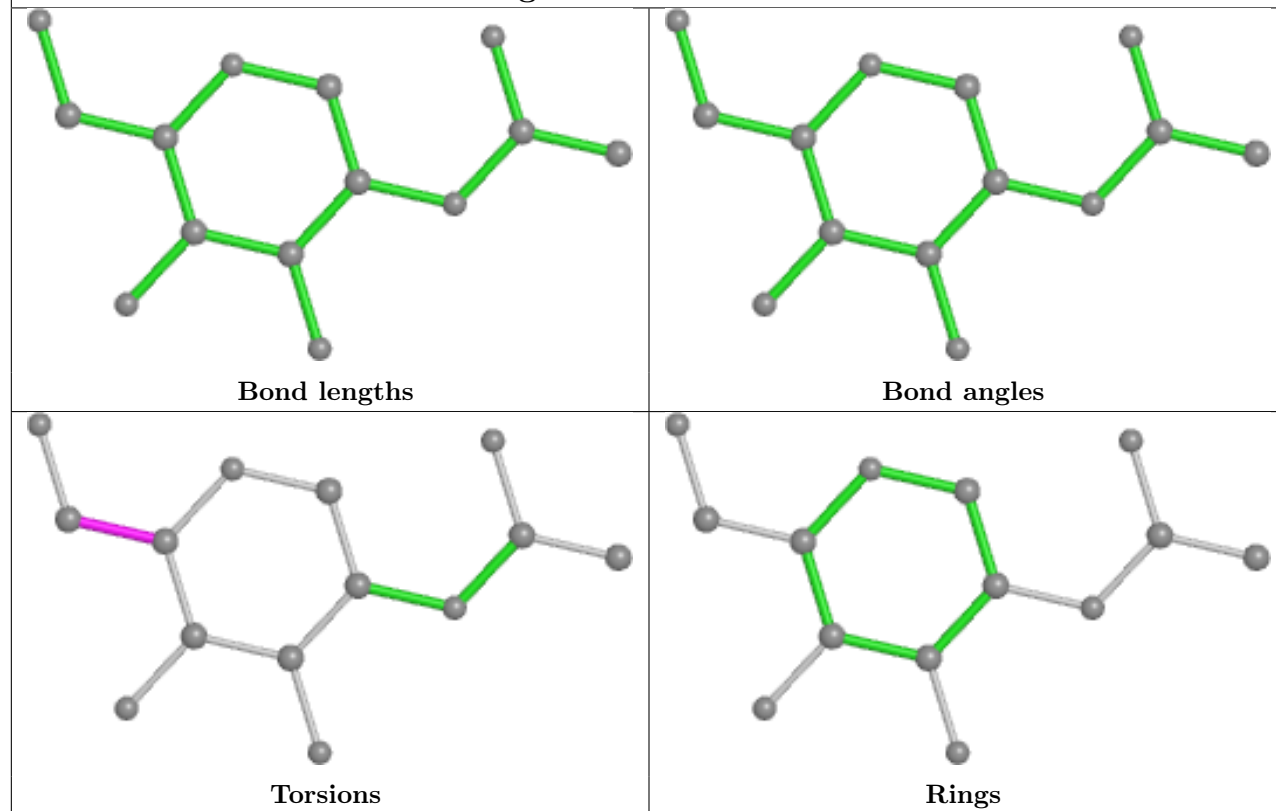
Ligand NAG E 1304



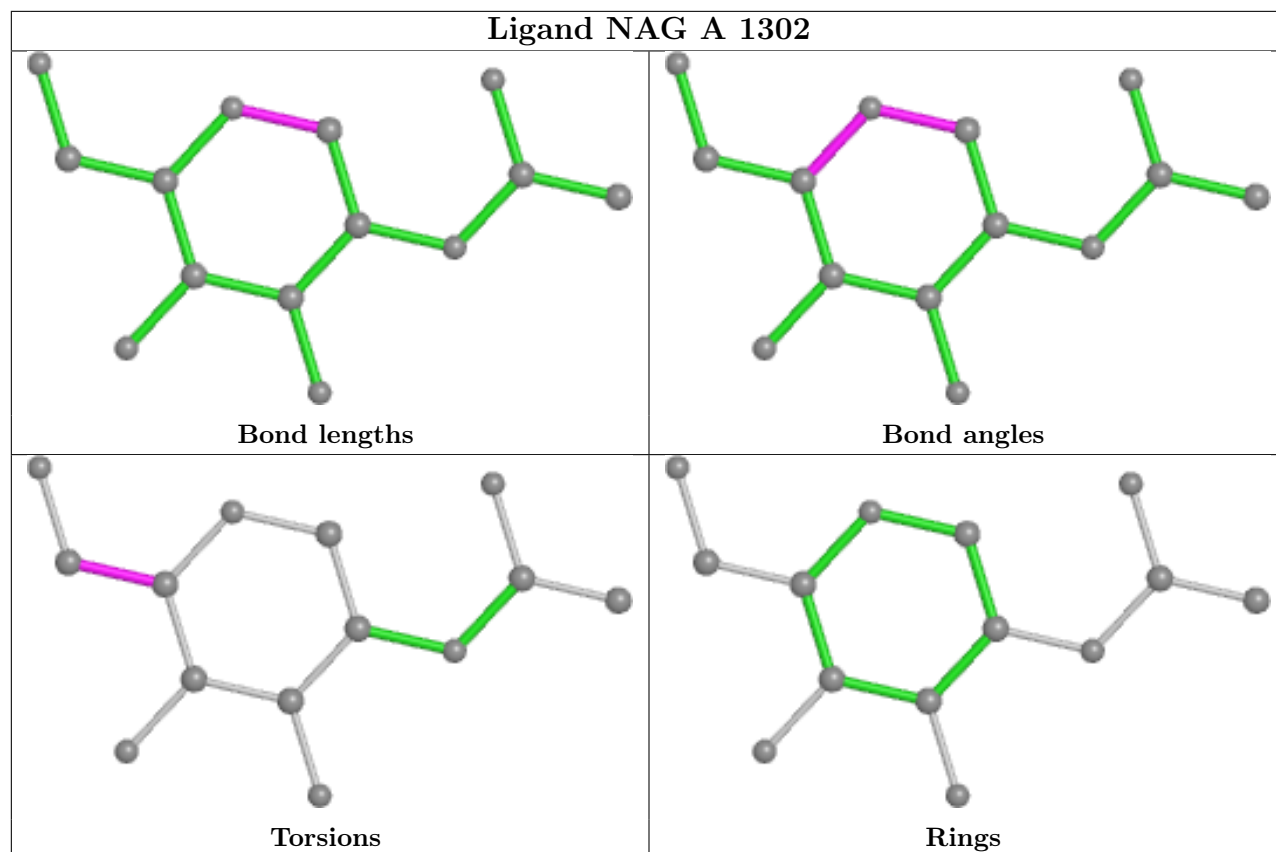
Ligand NAG C 1303



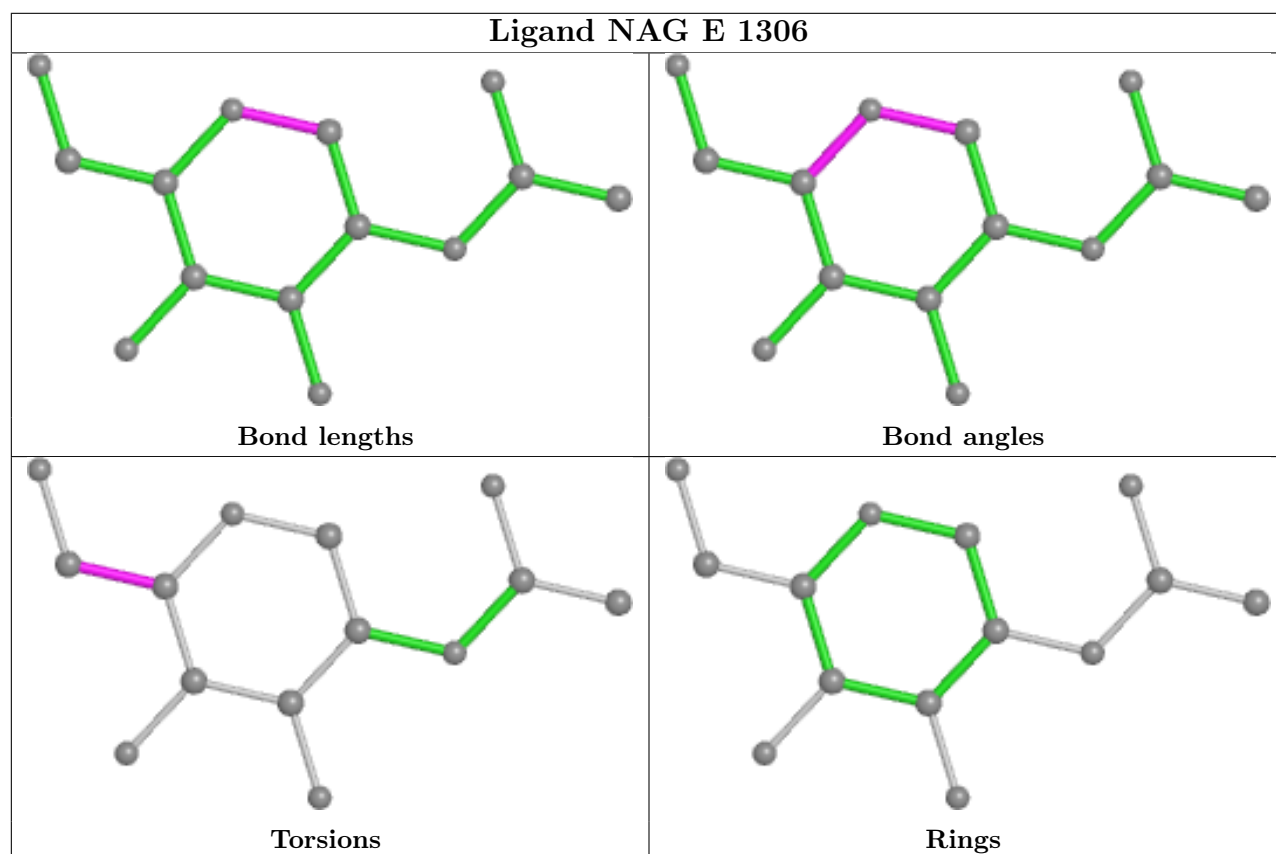
Ligand NAG A 1303

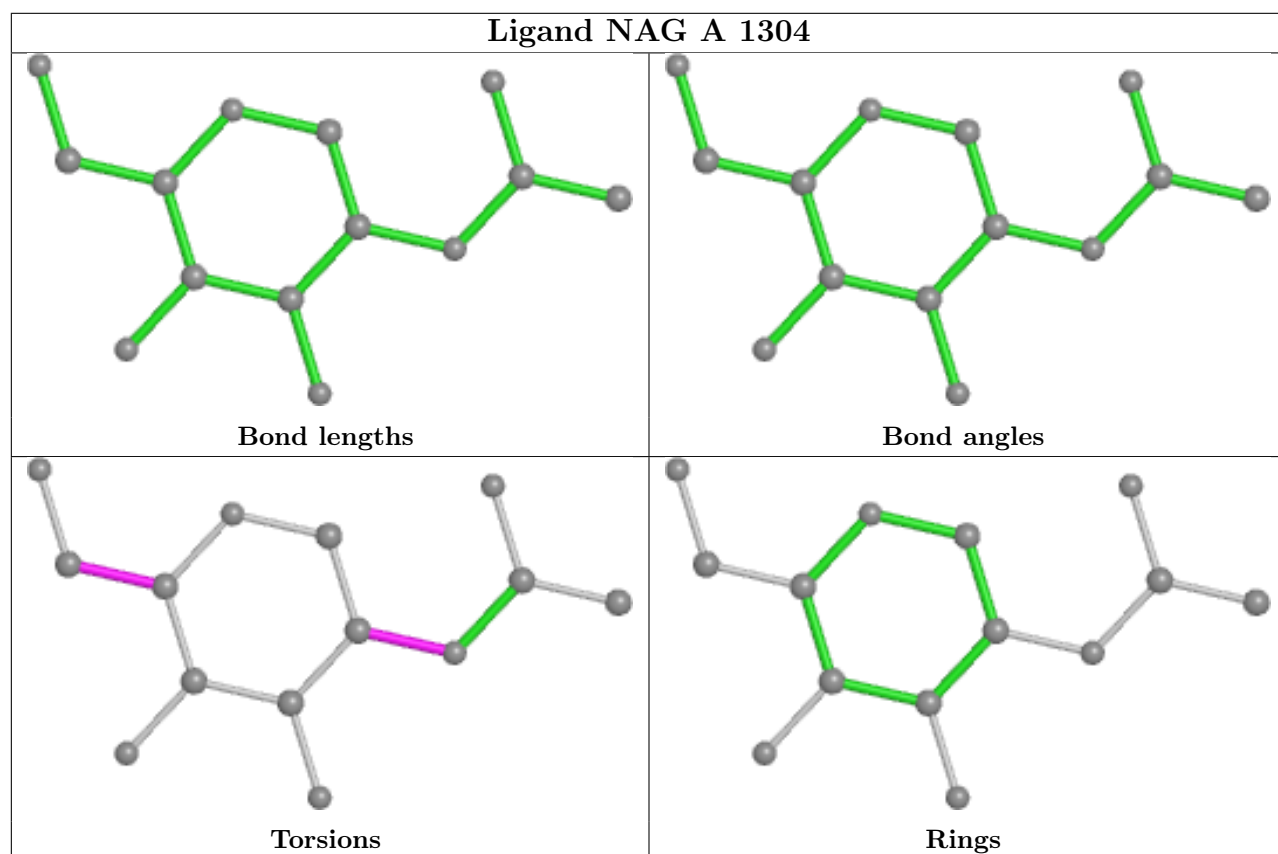
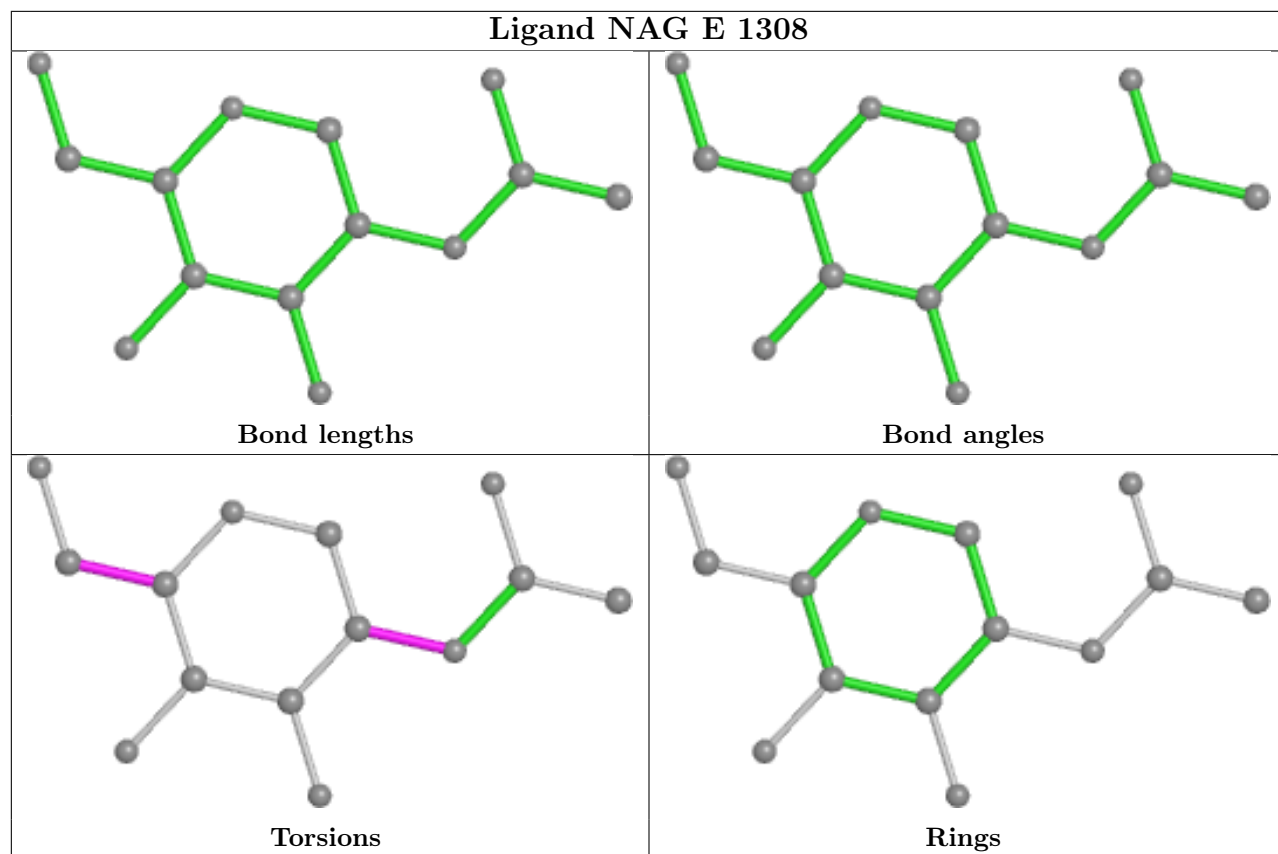


Ligand NAG A 1302

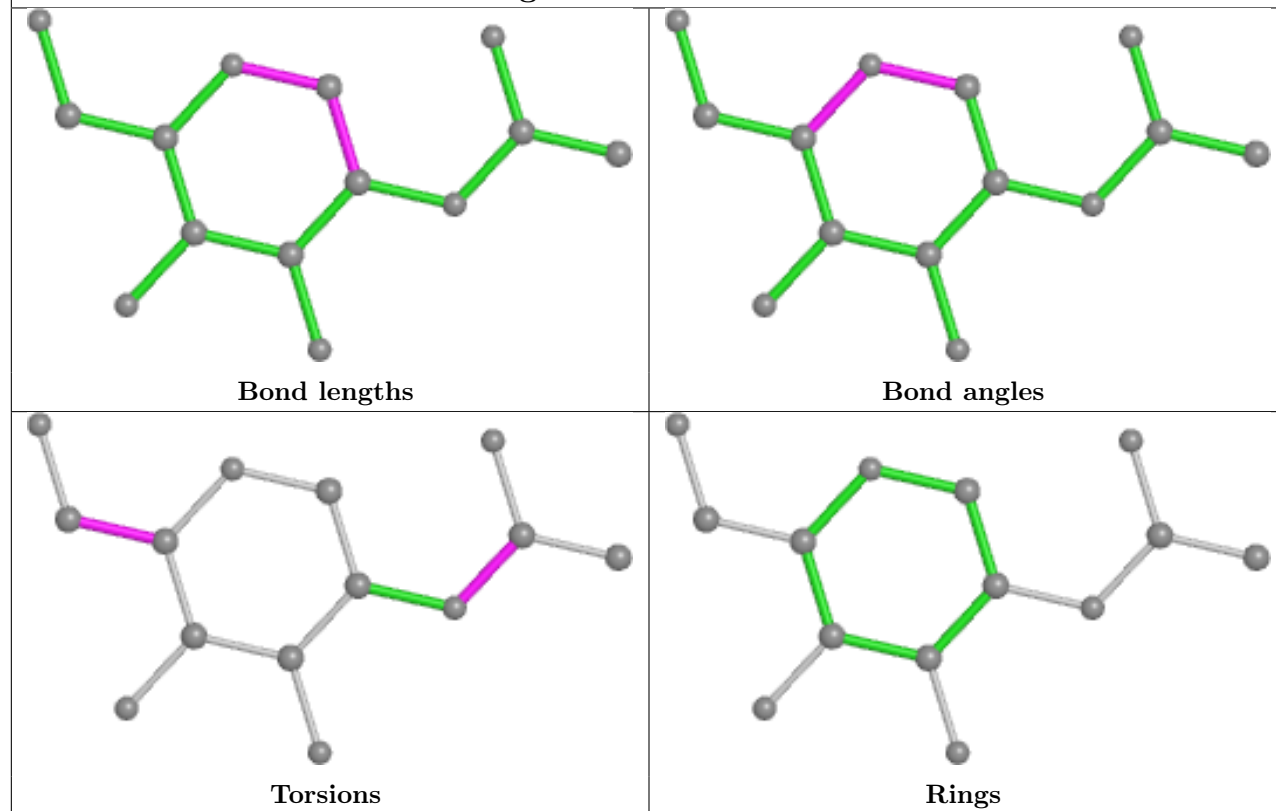


Ligand NAG E 1306

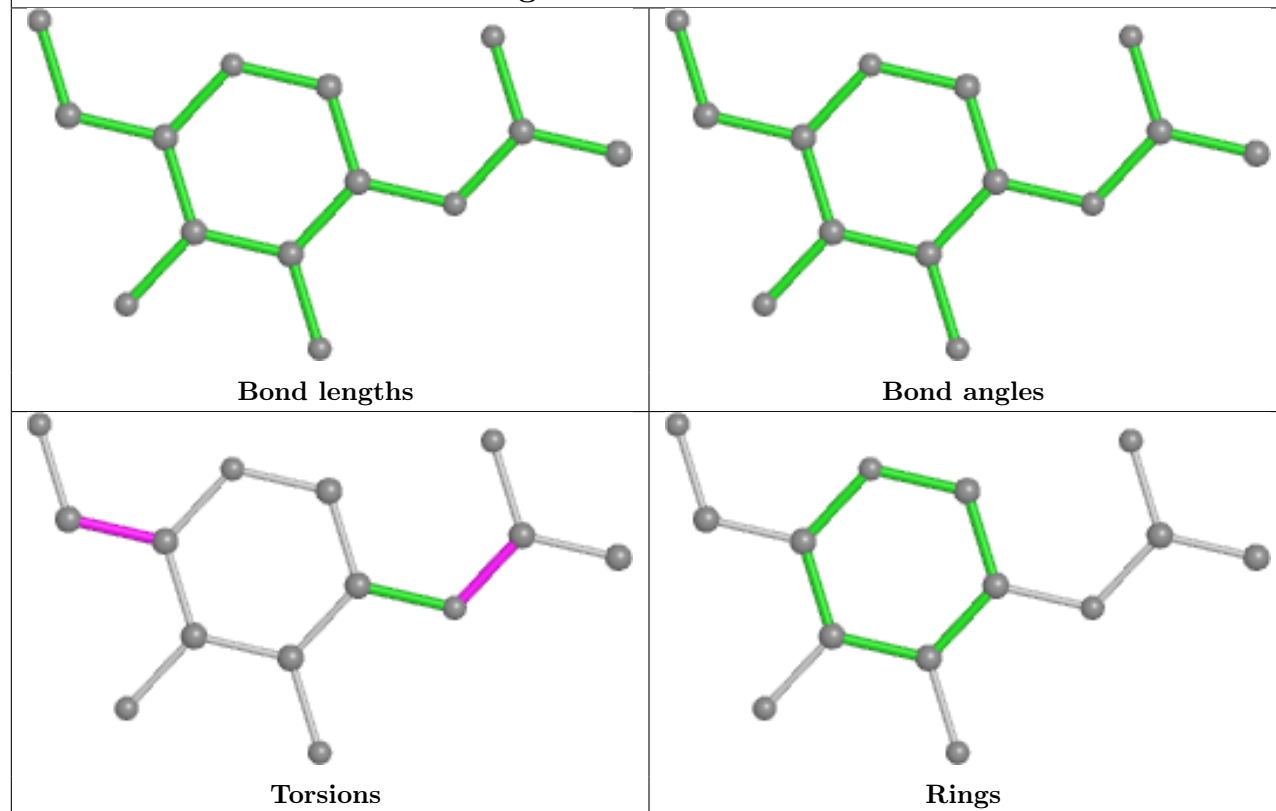


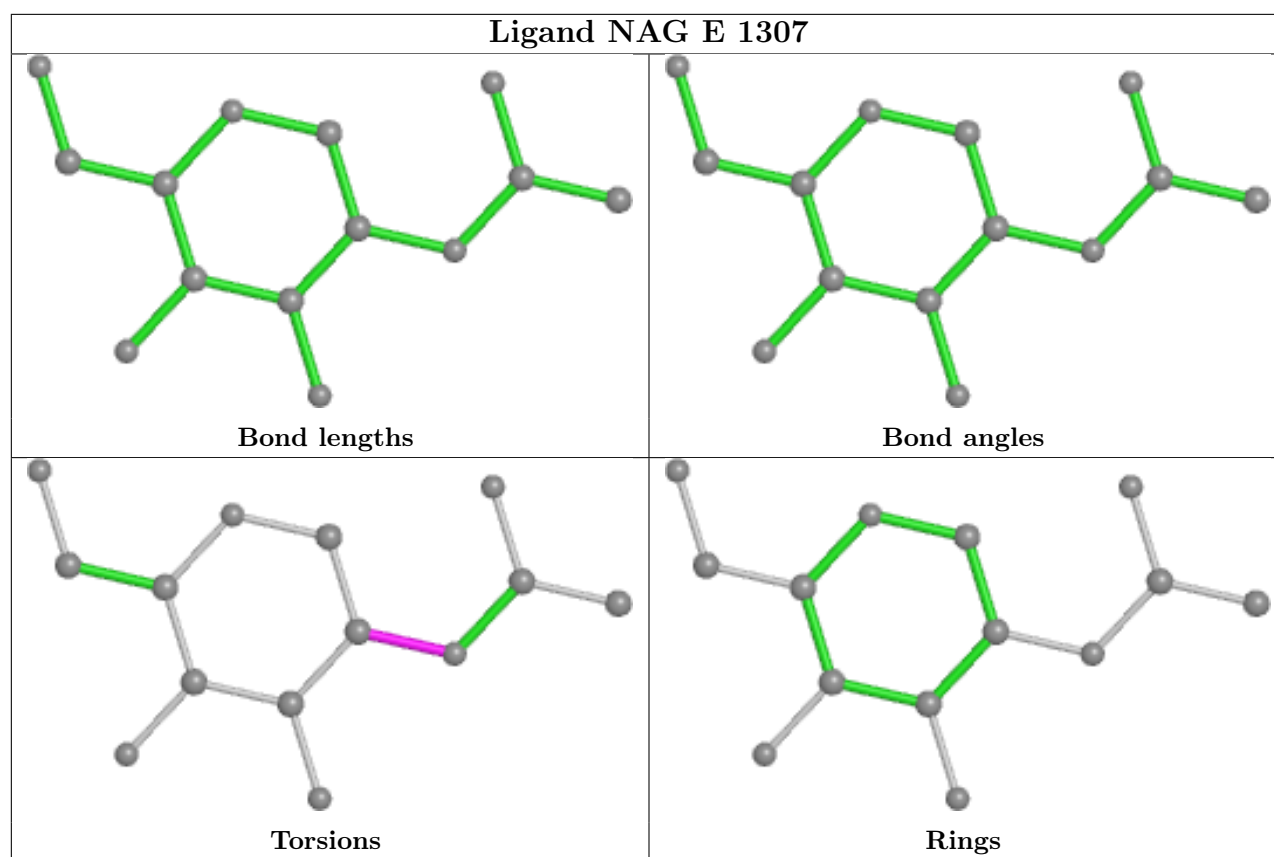


Ligand NAG C 1302



Ligand NAG A 1308





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

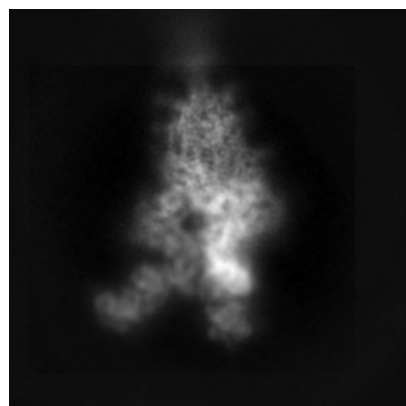
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27799. These allow visual inspection of the internal detail of the map and identification of artifacts.

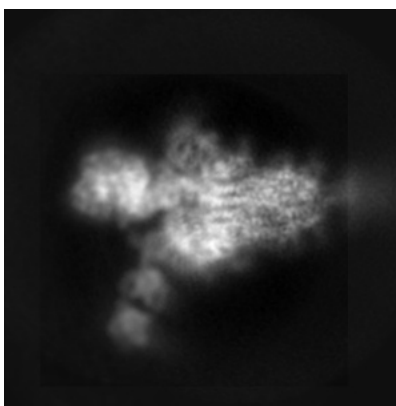
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

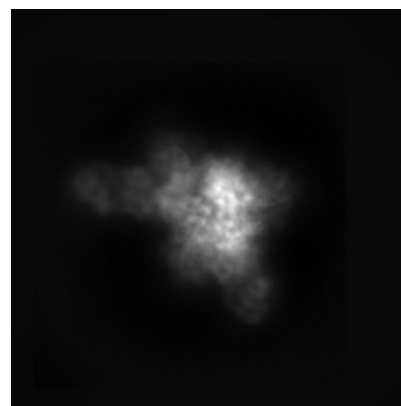
6.1.1 Primary map



X

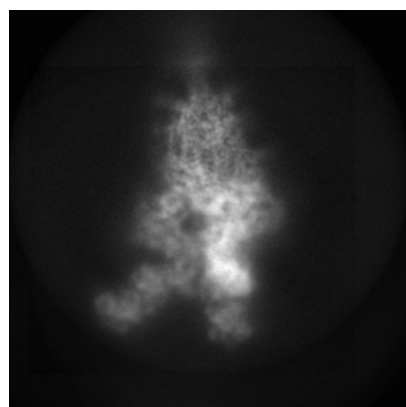


Y

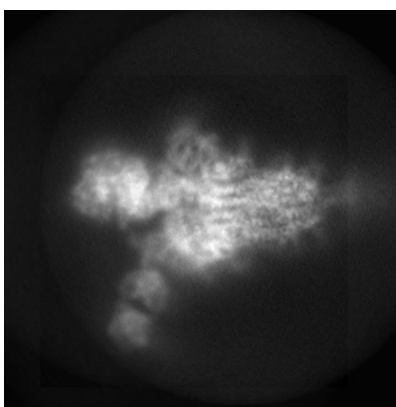


Z

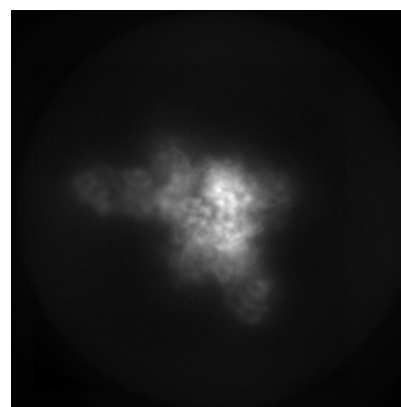
6.1.2 Raw map



X



Y

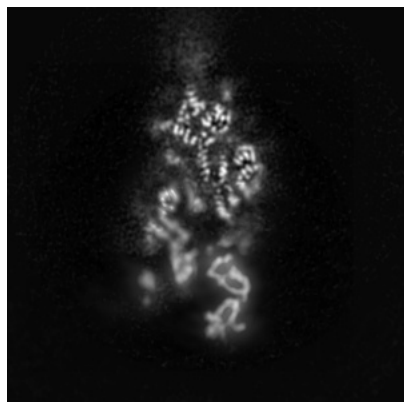


Z

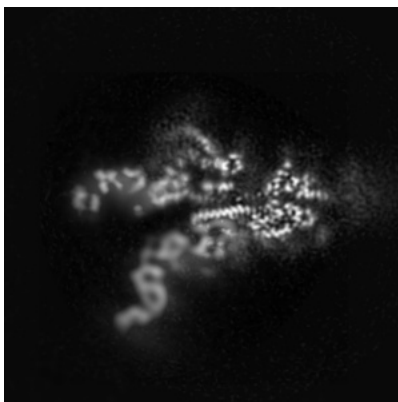
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

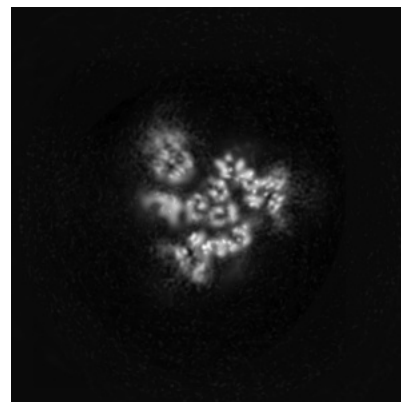
6.2.1 Primary map



X Index: 160

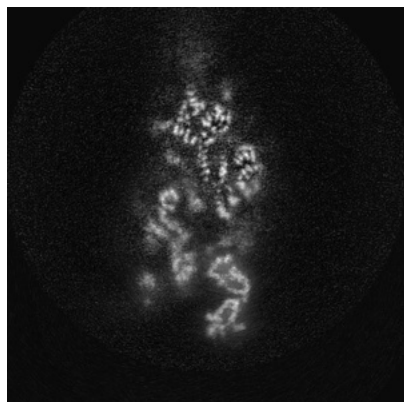


Y Index: 160

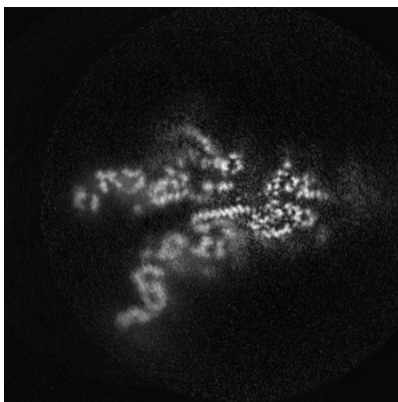


Z Index: 160

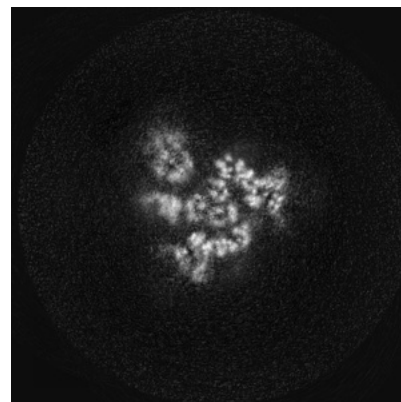
6.2.2 Raw map



X Index: 160



Y Index: 160

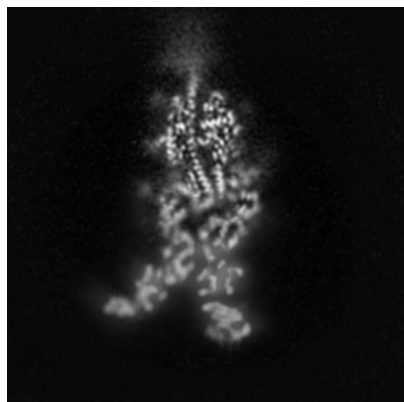


Z Index: 160

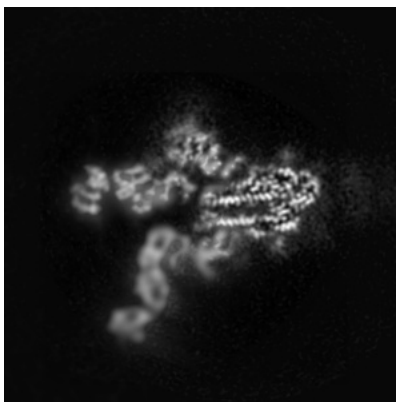
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

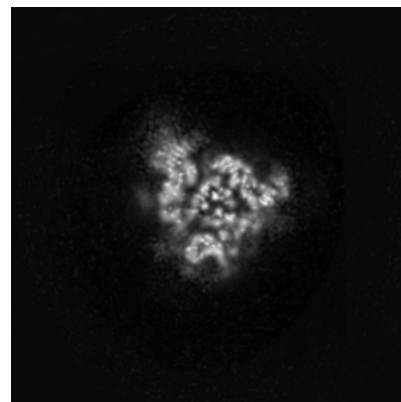
6.3.1 Primary map



X Index: 175

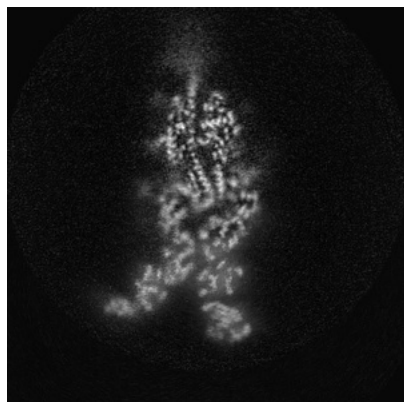


Y Index: 166

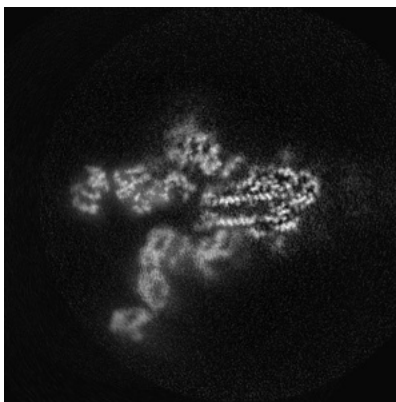


Z Index: 168

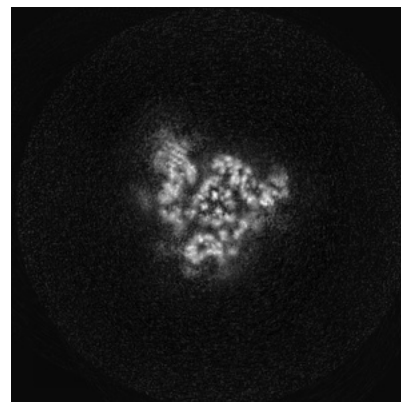
6.3.2 Raw map



X Index: 175



Y Index: 166

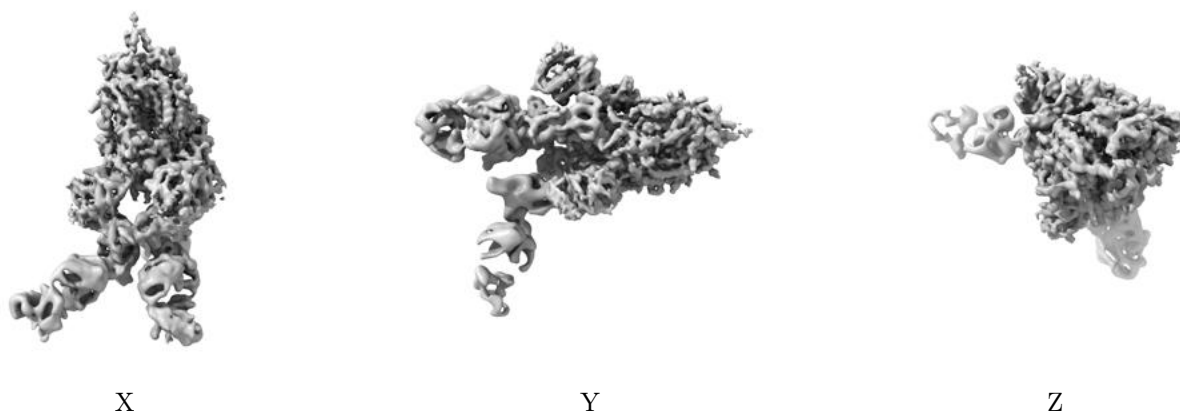


Z Index: 167

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

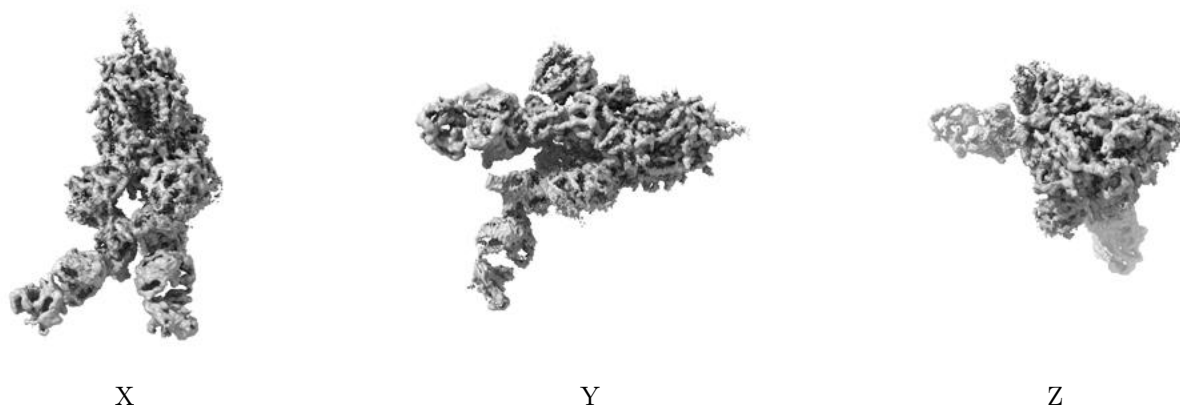
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

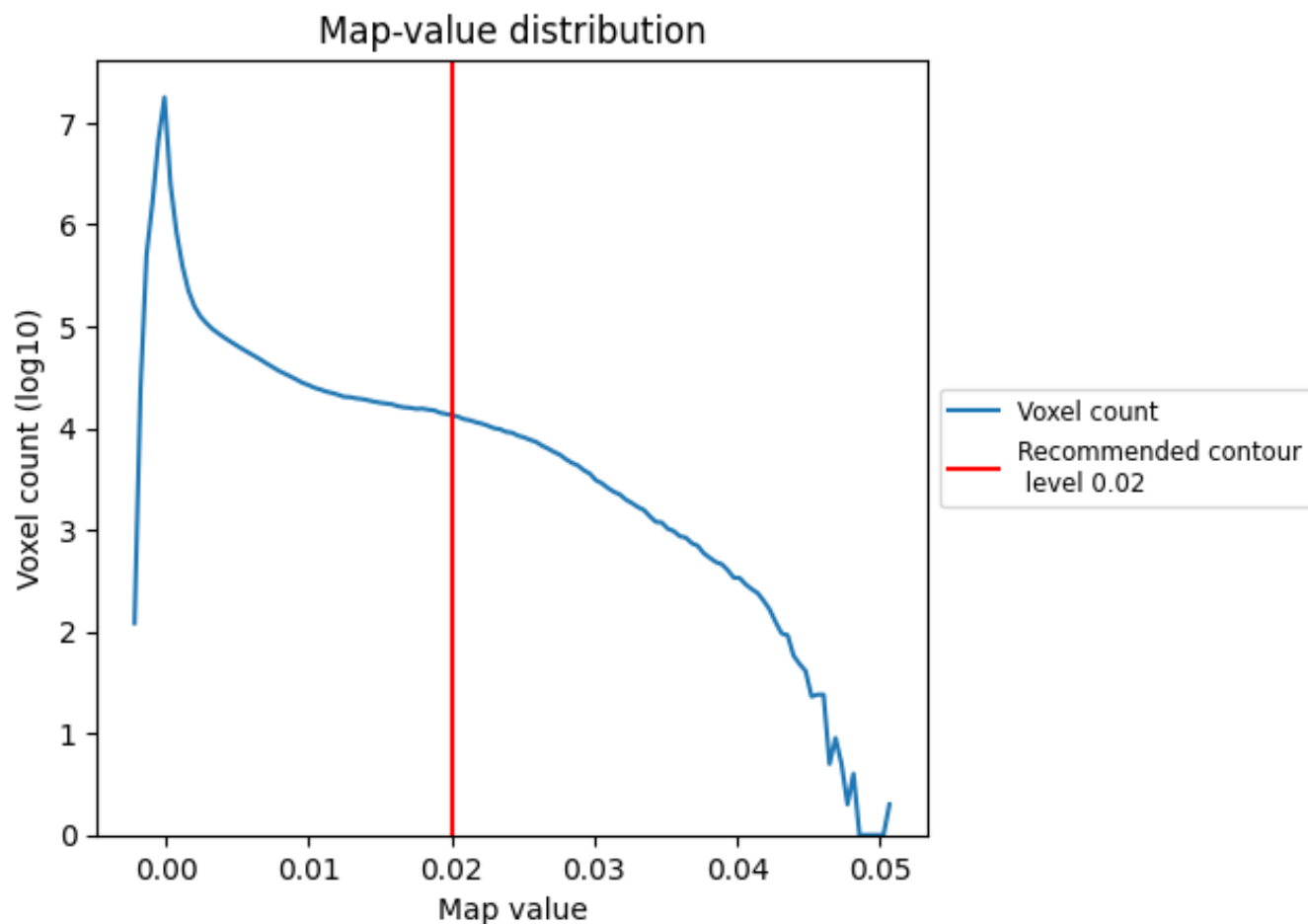
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

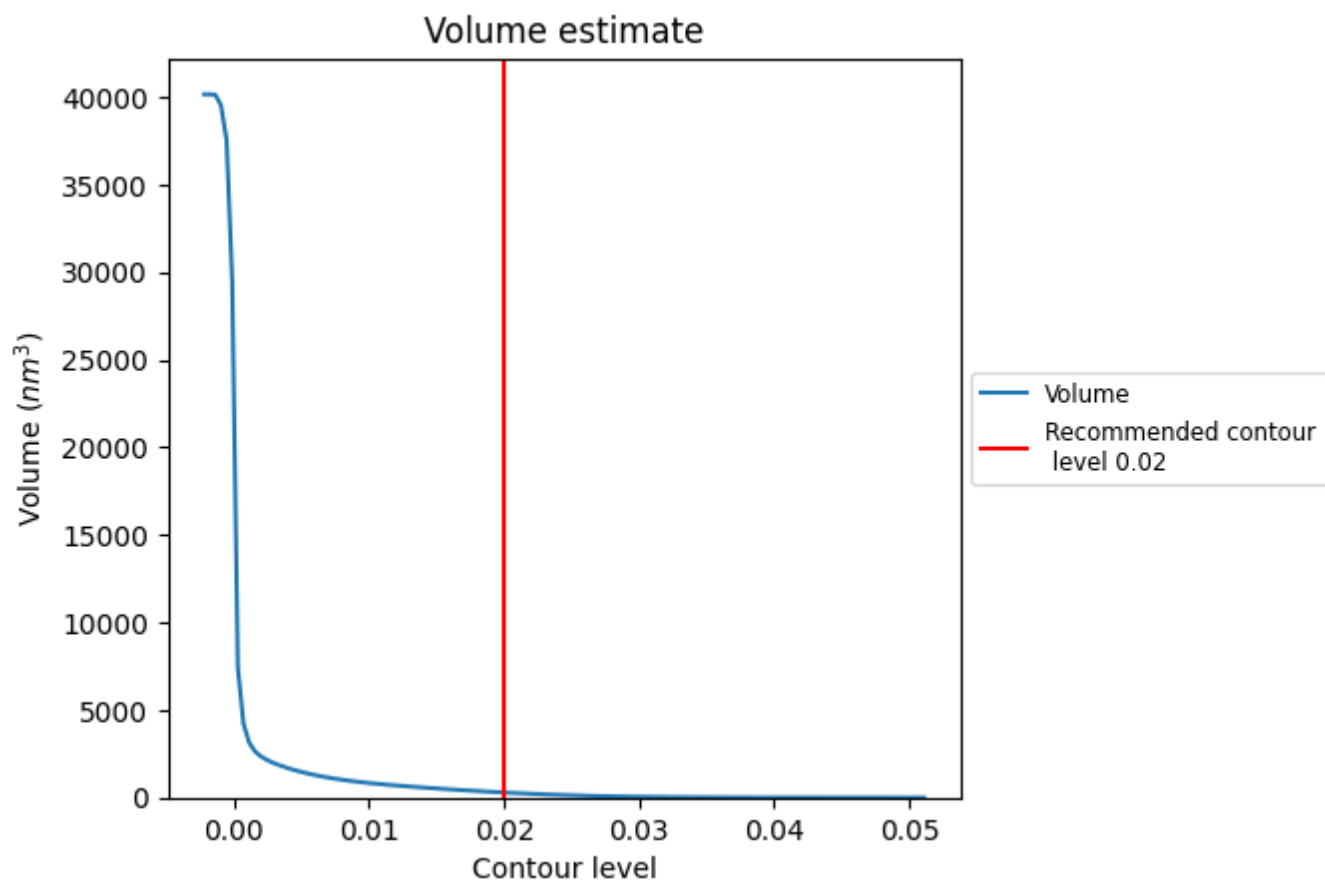
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

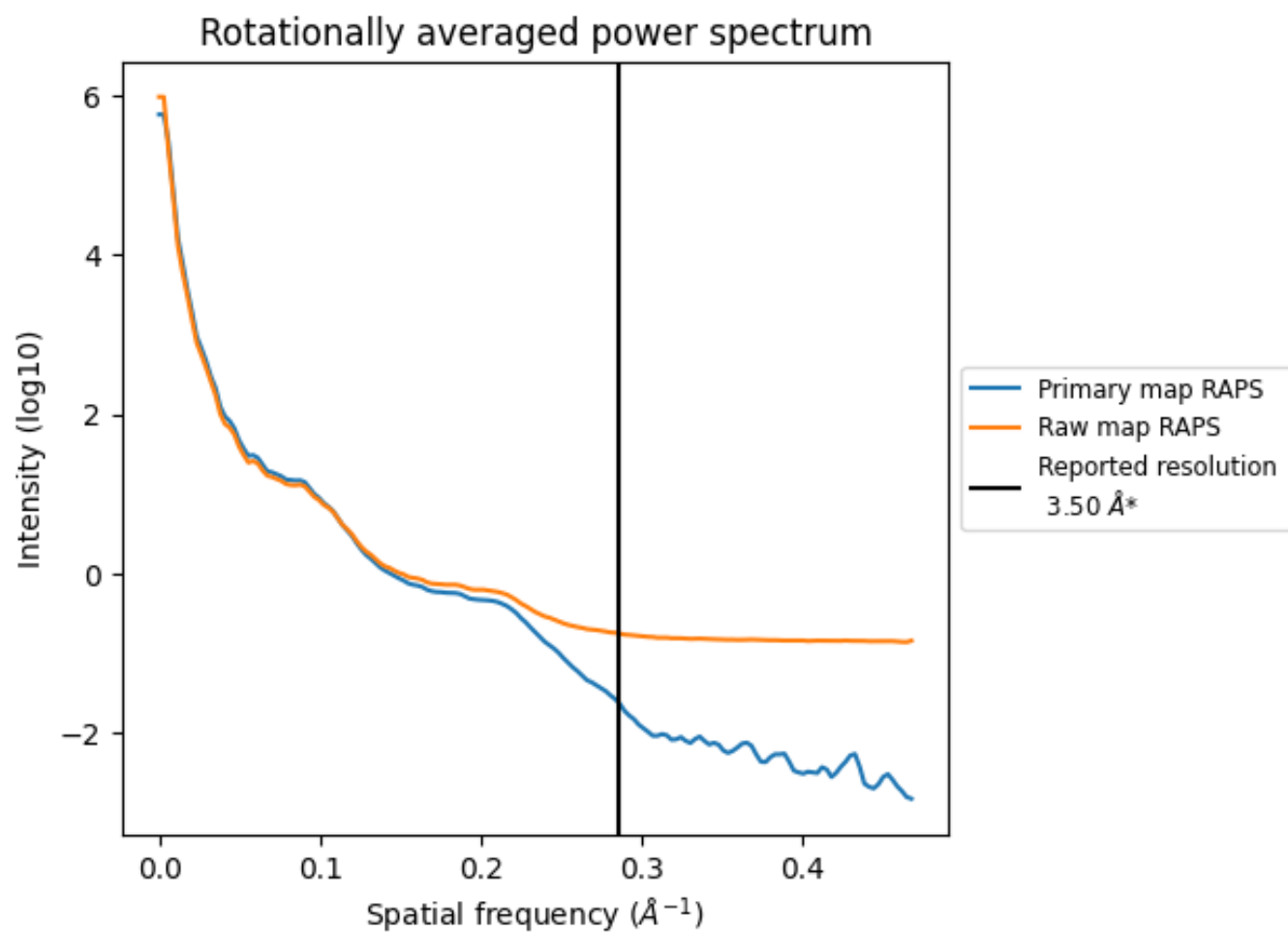
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm³; this corresponds to an approximate mass of 259 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

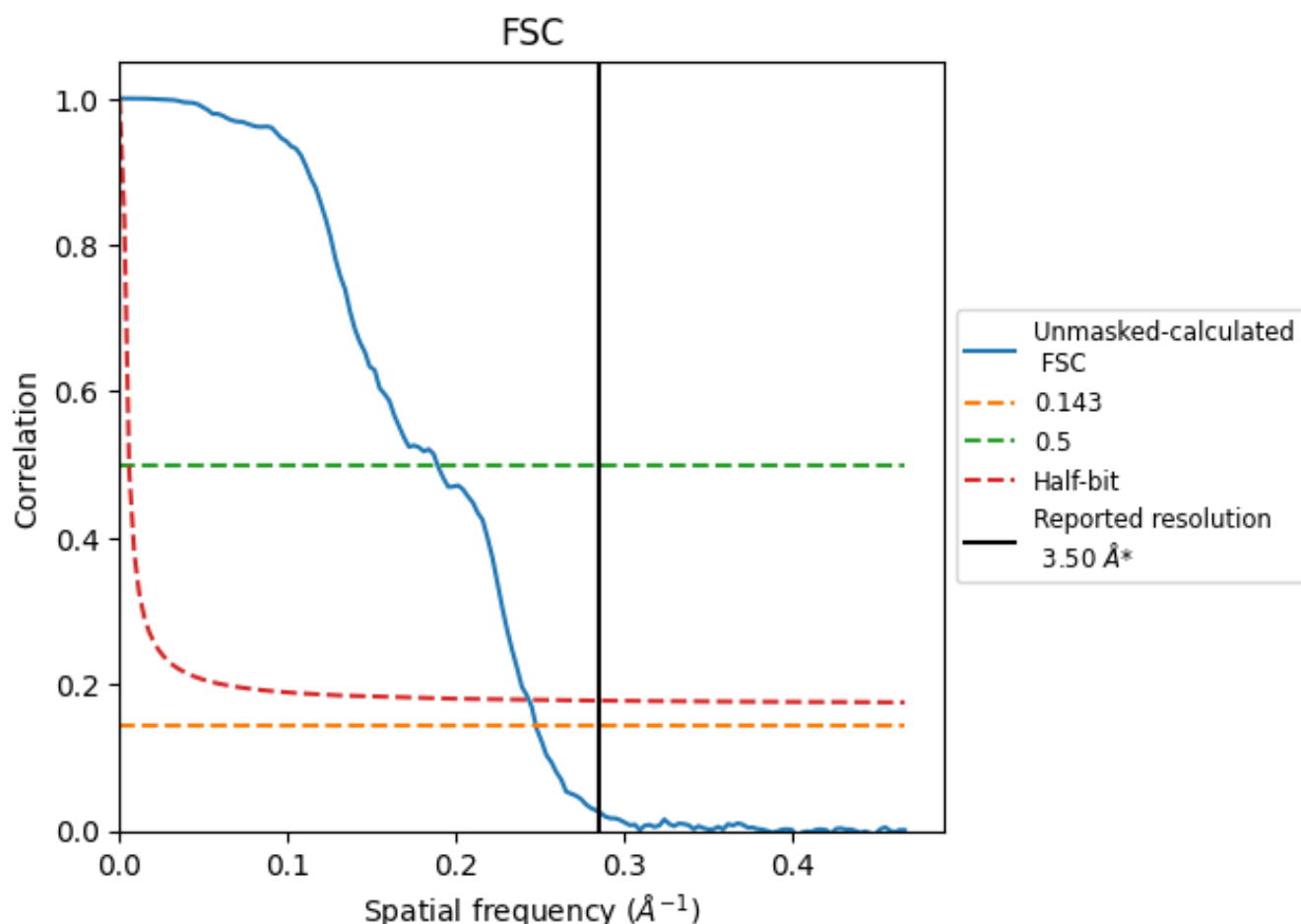


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

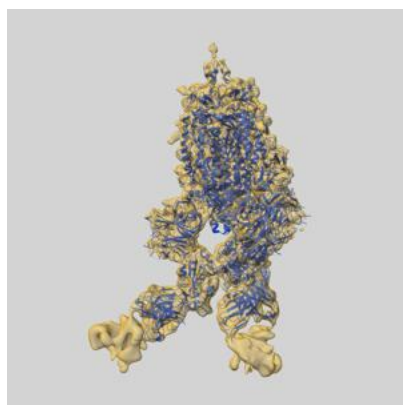
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	5.29	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 3.5 by more than 10 %

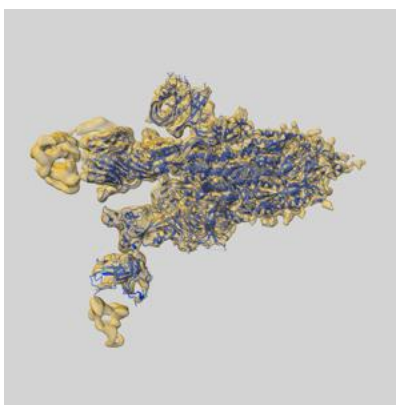
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27799 and PDB model 8DZI. Per-residue inclusion information can be found in section [3](#) on page [17](#).

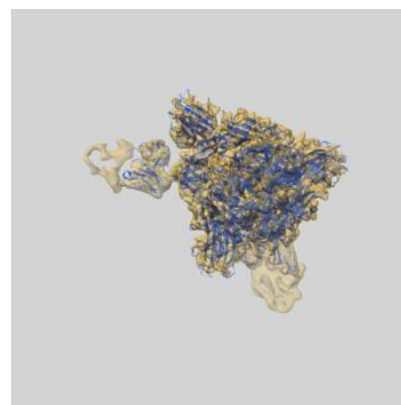
9.1 Map-model overlay [i](#)



X



Y



Z

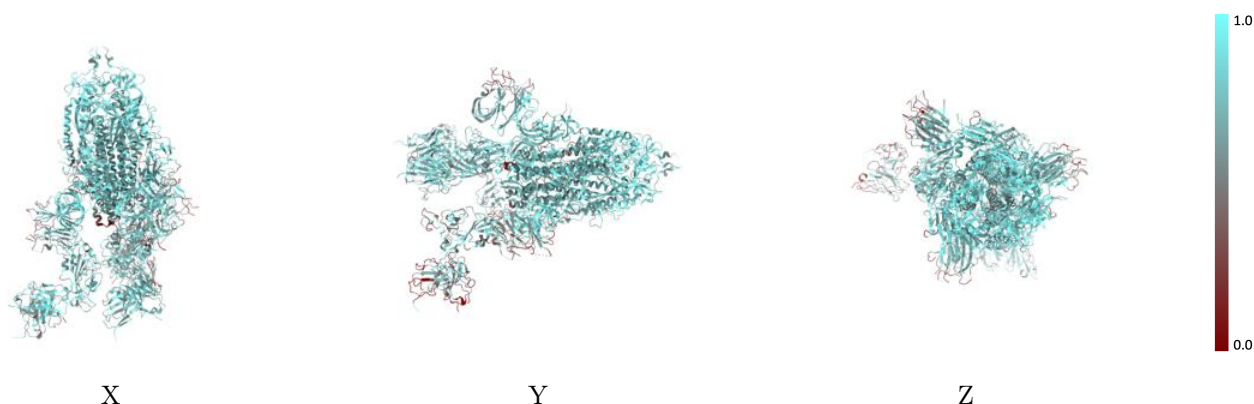
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



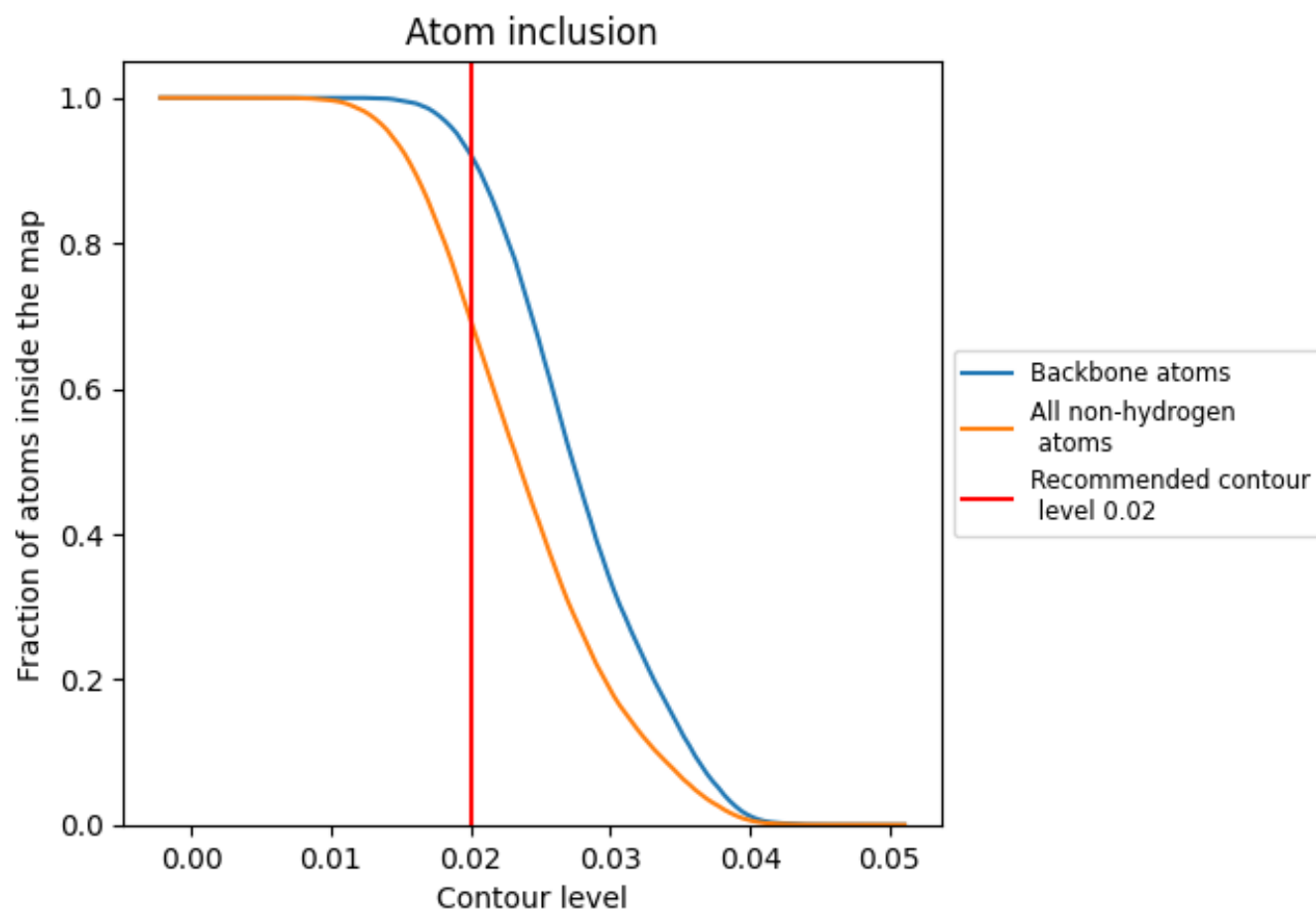
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6949	 0.3180
A	 0.7308	 0.3460
B	 0.6868	 0.2050
C	 0.7023	 0.3260
D	 0.6721	 0.2320
E	 0.7189	 0.3440
F	 0.7032	 0.2480
G	 0.7327	 0.2470
H	 0.4519	 0.1620
I	 0.4643	 0.3810
J	 0.4286	 0.4120
K	 0.2857	 0.3200
L	 0.4401	 0.1810
M	 0.5714	 0.4280
N	 0.6071	 0.4020
O	 0.2143	 0.3250
P	 0.2857	 0.2980
Q	 0.6071	 0.3640
R	 0.2500	 0.2710
S	 0.5714	 0.4420
T	 0.5714	 0.4370
U	 0.1786	 0.2740
V	 0.3571	 0.3550
W	 0.1071	 0.2930
X	 0.1071	 0.3380
Y	 0.3214	 0.2640
Z	 0.4286	 0.3950
a	 0.6071	 0.4370
b	 0.6429	 0.4070
c	 0.5714	 0.4340

