



# Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:54 AM JST

PDB ID : 7YVO  
EMDB ID : EMD-34134  
Title : Omicron BA.4/5 SARS-CoV-2 S in complex with TH027/132 Fab  
Authors : Guo, Y.; Zhang, G.; Liang, J.; Liu, F.; Rao, Z.  
Deposited on : 2022-08-19  
Resolution : 3.30 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

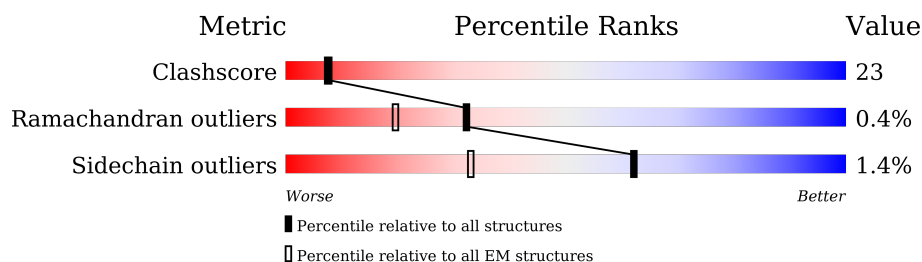
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1288	
1	B	1288	
1	C	1288	
2	H	109	
2	J	109	
3	I	118	
3	K	118	
4	L	110	

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Mol	Chain	Length	Quality of chain
4	N	110	<div><div></div><div>80%</div><div>44%</div><div>55%</div><div>.</div></div>
5	M	123	<div><div></div><div>91%</div><div>50%</div><div>49%</div><div>.</div></div>
5	O	123	<div><div></div><div>85%</div><div>44%</div><div>54%</div><div>..</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30285 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0
			7725	4965	1284	1441	35		
1	B	987	Total	C	N	O	S	0	0
			7413	4772	1227	1381	33		
1	C	1024	Total	C	N	O	S	0	0
			7719	4959	1284	1441	35		

There are 354 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	658	SER	ASN	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	658	SER	ASN	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	658	SER	ASN	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called TH132 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	109	Total	C	N	O	S	0	0
			818	510	138	167	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	109	Total	C	N	O	S	0	0
			818	510	138	167	3		

- Molecule 3 is a protein called TH132 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	118	Total	C	N	O	S	0	0
			865	545	146	169	5		
3	K	118	Total	C	N	O	S	0	0
			865	545	146	169	5		

- Molecule 4 is a protein called TH27 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	110	Total	C	N	O	S	0	0
			816	505	143	166	2		
4	N	110	Total	C	N	O	S	0	0
			816	505	143	166	2		

- Molecule 5 is a protein called TH27 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	122	Total	C	N	O	S	0	0
			956	612	162	178	4		
5	O	122	Total	C	N	O	S	0	0
			956	612	162	178	4		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

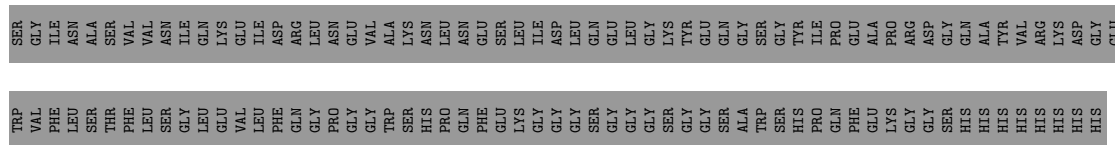
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	







Chain B:  53% 23% • 23%

[illegible]

- Molecule 1: Spike glycoprotein

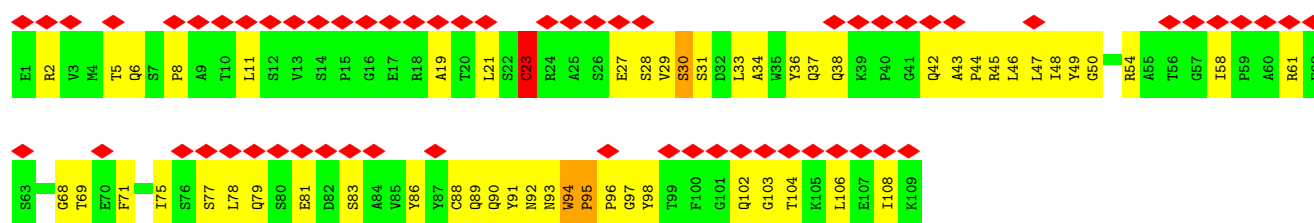


LEU	V1128	L977	K811	T676	Q564	M487	Y423	F347	A243	F168	D80
ILE	V1129	M978	R815	GLN	F565	C488	K424		K243	E169	
ASP		D979		THR		Y489	L425	V350	L244	E170	P82
LEU	T1132	L980	R815	LYS	1569	F490	P426			V171	
GLN	V1133	L981	D820	SER	D574	P491	G431	A352	L249	S172	D88
GLU	N1134	R982	L821	HIS	L821	L492	C432	K353	Q173	Q173	
LEU		R983	L822	GLY		Q493	Y433	N354	F174	F175	Y91
GLY	D1139	L984		SER	P579	S494	C433	K355	S255	S256	
LYS			L828	ALA			L434	K356	C257	L176	N99
TYR	D1146	A989	ASP	SER	E583	F497	A435	K357		MET	
GLU			ASP	SER	1584	P498	Y436	I358	A262	ASP	R102
GLN		I983	ALA	VAL		P499	N437	S359	A263	LEU	
GLY			GLY	ALA		T500	S438	N360	GLU	GLY	I105
SER		R1000	PHE	ALA	C590	Y501	K439	K361	A264	GLY	F106
GLY	L1001	L1002	ILE	PERO	S591	G502	K440	V362	P272	LYS	G107
TYR	L1003	L1004	GLN		V595	L441	L441	A363	R273	GLN	T108
ILE	ASP	Q1002	GLN	M697		H505	D442	D364		GLY	
PRO	L1004	L1005	TYR	S698	1598	G506	S443		N280	ASN	K113
GLU	TYR	Q1005	GLY	L699		P507	K444	V367	E281	PHE	I114
ALA	PHE	T1006	ASP	VAL	T602	Y508	Y445		K187		
PRO	LYS	Y1007	LYS	ALA	N603	R509	G446	N370	N188	ARG	
ASN	ARG	V1008	GLY	PERO	G502	V510	G447	F371	L189	THR	L117
HIS	THR	E1017	GLY	P715	N616	V511	N448	A372	R190	GLN	L118
THR		I1018	ASP		C617		Y449	P373	E191		I119
GLN	SER	R1019	ILE	T720	T618	S514	N450		N196		V126
ALA	PHO	L1019	ALA	E725	V620	F515	Y451	F376	I197	V127	A27
VAL	VAL	ASP	ARG	L726	PRO	E516	R452	A377	D198	I128	
ARG	ASP	ASP	ASP	L727	VAL	L517	Y453	C379	G199	K129	
LYS	LEU	K1028	LEU		ALA	A520	L455		Y200	V130	
ASP	GLY		ILE	S735	ILE	P521	F456	S383	F201	C131	S31
GLY		V1040	CYS		HIS	A522	R457		K202		
GLY	ASP	D1041	GLN	E738	ALA	T523	K458	K386	I203	F133	V36
TRP	SER	L1041	GLN	T739	ASP	V524	S459	N388	Y204	Q134	Y37
VAL	GLY	L1049	LYS		GLN	C525	N460	D389	S205	F135	
PHE	ILE		F855	T742	LEU	G526	L461		K206		K41
LEU	ASN	G1059	ASN	C743	THR	P527	R462	L390	H207	F140	L54
LEU	SER		L858		PHO	K528	P463	C391	T208	D141	
THR		E1072	T859	L752	THR	K529	F464	F392	P209	D142	
PHE	VAL	L1072	V860	L753	TRP	S530	T393	N394	ASN	VAL	F58
LEU	VAL	T1077	L861	L754	ARG	T531	R466	V395	LEU	TYR	F59
SER	ASN	A1078		Q755	VAL	N532	D467	Y396	GLY	TRR	S80
GLY	ILE		D867	Y756	TYR	L533	S468	A397	ARG	HIS	N61
LEU	GLN	E1092	E868	G757	SER	V534	S469	R328	LYS	LYS	
GLU	LYS			S758	THR			D398		ASN	W64
VAL	GLY	S1097	W886		GLY	C538	T470	S399	F329	ASN	F65
LEU	ILE	N1098		T761	SER	V539	E471	F400	P330	ASN	H66
PHE	ASP		T896	Q762	N641	N540	I472	V401	N331	A222	H66
GLN	ARG	W1102				N541	Y473	T332	L223	L223	A67
F1103	LEU	F1103	Y904	L767	C649	N542	Q474	R403	T333	TRP	I68
PRO	ASN	V1104	R905			N543	A475	G404	N334	MET	H69
GLY	GLY			E773	N657	N544	F543	N405	L335	V227	V770
GLY	VAL	I1115	Y917		S658	G545			C336	D228	SER
TRP	ALA			V781	S659	G545	K478		P337	L229	GLY
LEU	GLY					L546	P479	G416		P230	THR
SER	LYS	D1118	T934				C480	N417	E340	I231	
HIS	ASN	N1119		N801	C662	S555	N481	N418	V341	G232	GLY
PRO	LEU		L959		D663		G482	A419	F342	I233	THR
GLN	ASN	N1125	L806			L560	V483	D420	N165		LYS
PHE	THR	C1126	L962		C671			Y421	T345	F238	ARG
THR	SER			S510		G562	K483	Y422		C239	THR

LYS  
GLY  
GLY  
GLY  
SER  
GLY  
GLY  
GLY  
SER  
SER  
GLY  
GLY  
GLY  
ALA  
TRP  
SER  
HIS  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS  
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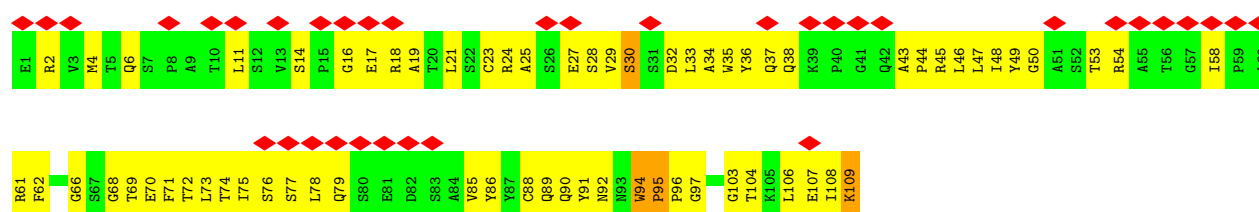
• Molecule 2: TH132 Fab light chain

Chain H: 




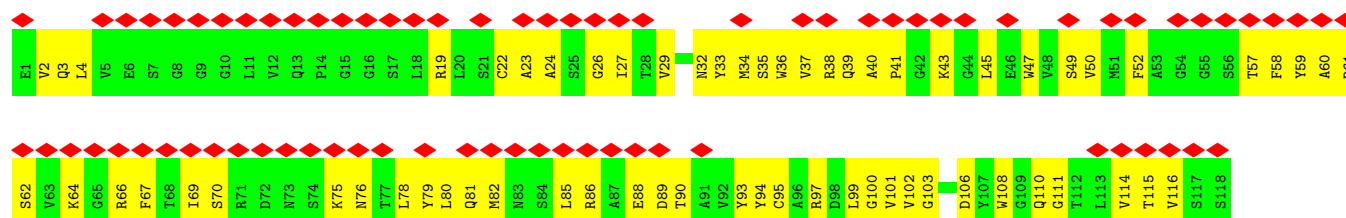
• Molecule 2: TH132 Fab light chain

Chain J: 



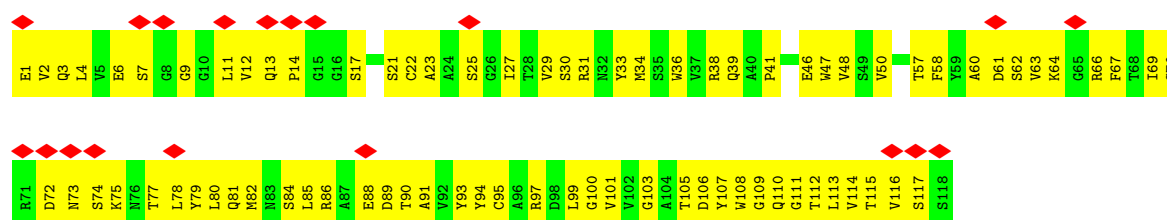
• Molecule 3: TH132 Fab heavy chain

Chain I: 



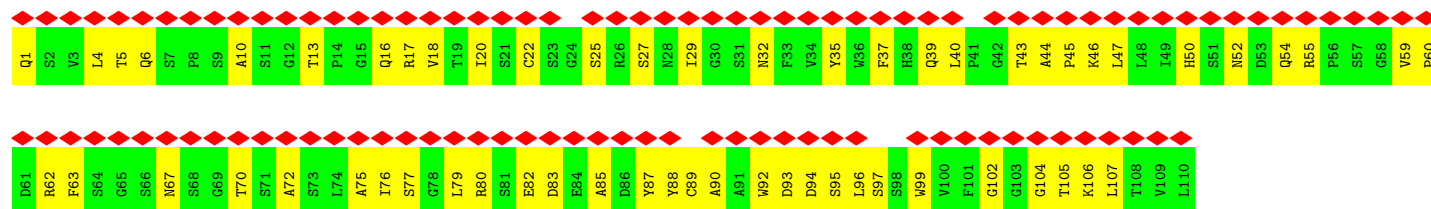
• Molecule 3: TH132 Fab heavy chain

Chain K: 

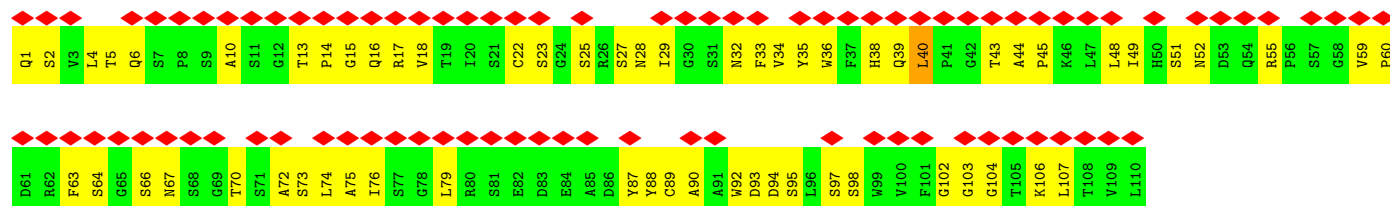
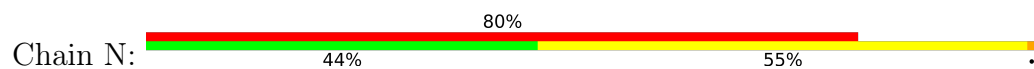


• Molecule 4: TH27 Fab light chain

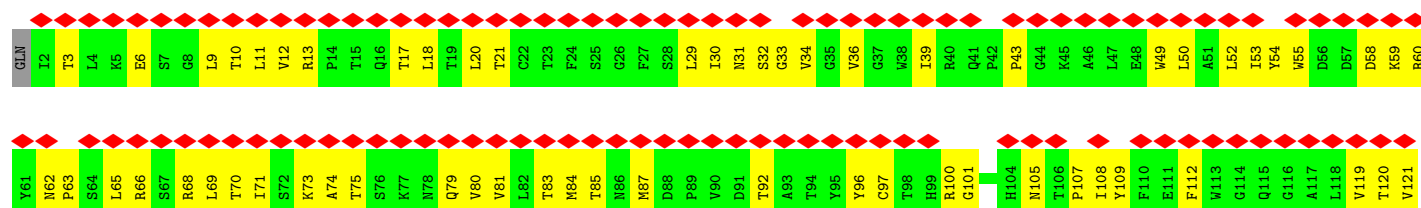
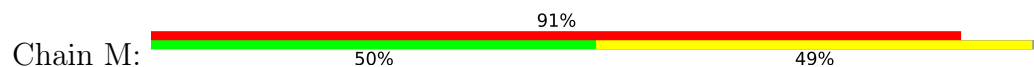
Chain L: 



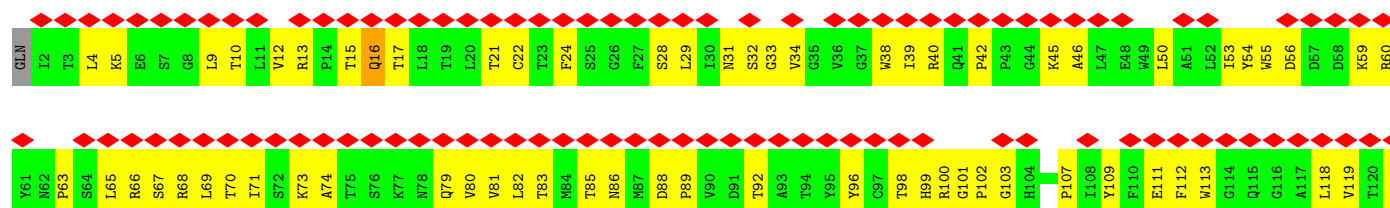
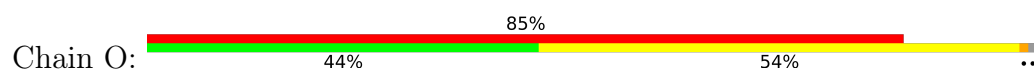
• Molecule 4: TH27 Fab light chain



• Molecule 5: TH27 Fab heavy chain



• Molecule 5: TH27 Fab heavy chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.651	Depositor
Minimum map value	-0.756	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.14	Depositor
Map size ( $\text{\AA}$ )	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.03	3/7912 (0.0%)	0.78	7/10810 (0.1%)
1	B	1.03	2/7589 (0.0%)	0.80	7/10370 (0.1%)
1	C	1.06	9/7905 (0.1%)	0.80	7/10801 (0.1%)
2	H	0.43	0/837	0.77	1/1140 (0.1%)
2	J	0.45	0/837	0.77	1/1140 (0.1%)
3	I	0.36	0/881	0.68	0/1196
3	K	0.43	0/881	0.68	0/1196
4	L	0.33	0/836	0.62	0/1138
4	N	0.35	0/836	0.68	1/1138 (0.1%)
5	M	0.36	0/981	0.65	0/1340
5	O	0.34	0/981	0.63	0/1340
All	All	0.93	14/30476 (0.0%)	0.77	24/41609 (0.1%)

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
2	H	0	1
2	J	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	649	CYS	CB-SG	-9.97	1.65	1.82
1	C	617	CYS	CB-SG	-9.05	1.66	1.82
1	C	886	TRP	CB-CG	-9.01	1.34	1.50
1	A	617	CYS	CB-SG	-7.83	1.69	1.82
1	B	424	LYS	C-N	7.29	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	743	CYS	CB-SG	-5.90	1.72	1.81
1	C	291	CYS	CB-SG	-5.88	1.72	1.81
1	C	505	HIS	C-N	-5.60	1.21	1.34
1	C	671	CYS	CB-SG	-5.40	1.73	1.81
1	B	223	LEU	C-N	-5.35	1.21	1.34
1	C	781	VAL	CB-CG1	-5.18	1.42	1.52
1	A	671	CYS	CB-SG	-5.11	1.73	1.81
1	C	743	CYS	CB-SG	-5.05	1.73	1.81
1	C	917	TYR	CD1-CE1	-5.02	1.31	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	CYS	CA-CB-SG	9.05	130.29	114.00
1	A	538	CYS	CA-CB-SG	8.17	128.70	114.00
1	A	590	CYS	CA-CB-SG	7.74	127.93	114.00
4	N	40	LEU	CB-CG-CD2	7.62	123.95	111.00
1	C	538	CYS	CA-CB-SG	7.47	127.44	114.00
1	C	590	CYS	CA-CB-SG	7.23	127.01	114.00
1	A	519	HIS	C-N-CA	-6.65	105.07	121.70
1	B	760	CYS	CA-CB-SG	6.22	125.19	114.00
1	B	590	CYS	CA-CB-SG	6.08	124.95	114.00
1	C	649	CYS	CA-CB-SG	5.75	124.34	114.00
1	B	521	PRO	N-CA-C	-5.72	97.22	112.10
1	B	560	LEU	CA-CB-CG	-5.63	102.35	115.30
1	C	886	TRP	CB-CA-C	-5.58	99.25	110.40
2	H	23	CYS	CA-CB-SG	5.52	123.94	114.00
1	A	878	LEU	CA-CB-CG	-5.51	102.64	115.30
1	C	328	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	492	LEU	CA-CB-CG	5.39	127.70	115.30
2	J	23	CYS	CA-CB-SG	5.36	123.64	114.00
1	B	276	LEU	CA-CB-CG	-5.35	102.99	115.30
1	C	326	ILE	C-N-CA	5.26	134.84	121.70
1	A	546	LEU	CA-CB-CG	-5.14	103.48	115.30
1	C	767	LEU	CA-CB-CG	-5.06	103.65	115.30
1	A	878	LEU	CB-CG-CD2	-5.03	102.46	111.00
1	A	552	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	H	95	PRO	Peptide
2	J	95	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7725	0	7317	278	0
1	B	7413	0	7008	256	0
1	C	7719	0	7310	345	0
2	H	818	0	777	69	0
2	J	818	0	777	65	0
3	I	865	0	833	68	0
3	K	865	0	833	79	0
4	L	816	0	772	52	0
4	N	816	0	772	53	0
5	M	956	0	950	71	0
5	O	956	0	950	74	0
6	A	168	0	156	21	0
6	B	168	0	156	25	0
6	C	182	0	169	22	0
All	All	30285	0	28780	1338	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 23.

All (1338) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.36	1.08
1:C:329:PHE:H	1:C:531:THR:HG23	1.24	1.02
1:A:489:TYR:HE2	3:I:99:LEU:HD13	1.27	0.99
1:A:334:ASN:HB3	1:A:362:VAL:HG12	1.45	0.98
1:C:353:TRP:O	1:C:466:ARG:NH2	1.98	0.95
1:A:379:CYS:HA	1:A:432:CYS:HB3	1.49	0.92
2:J:28:SER:O	2:J:92:ASN:ND2	2.06	0.89
1:A:456:PHE:HB2	1:A:491:PRO:HA	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.56	0.87
1:B:709:ASN:HD21	6:B:1311:NAG:H2	1.38	0.87
4:N:1:GLN:O	4:N:28:ASN:ND2	2.07	0.87
1:C:327:VAL:HB	1:C:531:THR:HA	1.57	0.85
2:H:91:TYR:HE2	3:I:101:VAL:HA	1.41	0.85
5:M:29:LEU:HD13	5:M:73:LYS:HD2	1.59	0.84
1:C:351:TYR:HB3	1:C:422:ASN:HD22	1.42	0.84
3:K:97:ARG:HG2	3:K:107:TYR:HB2	1.60	0.84
3:K:12:VAL:HG21	3:K:85:LEU:HD12	1.60	0.84
2:J:6:GLN:HE21	2:J:104:THR:HG23	1.41	0.83
5:M:18:LEU:HD21	5:M:20:LEU:HG	1.59	0.83
1:B:330:PRO:HD3	1:B:579:PRO:HB2	1.59	0.83
2:H:47:LEU:HA	2:H:58:ILE:HG13	1.59	0.83
1:B:70:VAL:HG21	1:B:255:SER:HA	1.60	0.83
2:J:47:LEU:HA	2:J:58:ILE:HG13	1.63	0.81
2:J:85:VAL:HA	2:J:104:THR:O	1.81	0.81
1:A:1074:ASN:ND2	6:A:1307:NAG:O7	2.12	0.81
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.60	0.81
1:C:335:LEU:HD23	1:C:336:CYS:H	1.46	0.81
1:C:328:ARG:HH22	1:C:544:ASN:N	1.80	0.80
4:N:5:THR:OG1	4:N:23:SER:OG	1.99	0.80
1:A:489:TYR:CE2	3:I:99:LEU:HD13	2.15	0.80
1:A:709:ASN:HD21	6:A:1311:NAG:H2	1.47	0.80
1:C:353:TRP:HZ3	1:C:355:ARG:HD3	1.45	0.80
4:N:55:ARG:NH2	4:N:60:PRO:O	2.15	0.80
2:H:96:PRO:HB3	3:I:50:VAL:HG11	1.64	0.79
1:B:1134:ASN:ND2	6:B:1308:NAG:O7	2.14	0.79
1:C:68:ILE:HG13	1:C:69:HIS:H	1.48	0.79
2:J:2:ARG:O	2:J:90:GLN:NE2	2.16	0.79
3:K:82:MET:HB3	3:K:85:LEU:HD21	1.65	0.79
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.48	0.79
1:A:365:TYR:HD2	1:A:388:ASN:HA	1.47	0.78
1:C:379:CYS:HA	1:C:432:CYS:CB	2.13	0.78
5:M:68:ARG:HH11	5:M:69:LEU:HD21	1.49	0.78
1:A:440:LYS:HE3	5:M:105:ASN:HA	1.65	0.78
1:C:81:ASN:O	1:C:239:GLN:NE2	2.17	0.78
5:M:53:ILE:HG22	5:M:59:LYS:HD2	1.64	0.78
1:A:396:TYR:O	1:A:513:LEU:HA	1.84	0.77
1:C:165:ASN:ND2	6:C:1312:NAG:O6	2.17	0.77
4:L:93:ASP:O	4:L:97:SER:N	2.16	0.77
1:C:738:CYS:SG	1:C:739:THR:N	2.58	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:NH2	1:C:545:GLY:H	1.83	0.76
3:K:90:THR:HA	3:K:114:VAL:O	1.86	0.76
3:K:90:THR:HG22	3:K:115:THR:HA	1.65	0.76
1:C:480:CYS:HB2	1:C:483:VAL:HG23	1.67	0.76
1:C:657:ASN:ND2	6:C:1303:NAG:O7	2.18	0.76
1:C:446:GLY:O	1:C:498:ARG:NH1	2.19	0.76
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.68	0.76
1:B:68:ILE:HG13	1:B:69:HIS:H	1.50	0.75
1:C:383:SER:H	1:C:386:LYS:NZ	1.84	0.75
3:I:19:ARG:HG3	3:I:81:GLN:HE21	1.52	0.75
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.66	0.75
1:C:354:ASN:ND2	1:C:399:SER:O	2.20	0.75
1:C:450:ASN:ND2	5:O:56:ASP:OD2	2.20	0.75
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.20	0.74
1:A:440:LYS:HB2	1:A:441:LEU:HD12	1.70	0.74
1:C:1134:ASN:ND2	6:C:1306:NAG:O7	2.20	0.74
1:A:546:LEU:HD22	1:A:565:PHE:HE1	1.51	0.73
1:B:379:CYS:CA	1:B:432:CYS:HB3	2.10	0.73
1:B:328:ARG:NH2	1:B:531:THR:O	2.20	0.73
5:O:13:ARG:NE	5:O:122:SER:O	2.17	0.73
3:K:4:LEU:HD23	3:K:95:CYS:HB3	1.68	0.73
3:K:38:ARG:NH2	3:K:89:ASP:OD1	2.21	0.73
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.70	0.72
5:O:22:CYS:HB3	5:O:80:VAL:HG22	1.71	0.72
3:K:17:SER:OG	3:K:81:GLN:NE2	2.23	0.72
2:H:21:LEU:HD21	2:H:106:LEU:HD11	1.70	0.72
5:M:69:LEU:HD23	5:M:84:MET:HG3	1.72	0.72
5:O:99:HIS:HD2	5:O:112:PHE:HD2	1.37	0.72
5:M:36:VAL:HG11	5:M:80:VAL:HG21	1.72	0.72
1:A:81:ASN:ND2	1:A:265:TYR:OH	2.17	0.72
1:C:401:VAL:HG12	1:C:509:ARG:HG2	1.72	0.71
3:K:93:TYR:O	3:K:111:GLY:HA2	1.91	0.71
1:B:30:ASN:HA	1:B:61:ASN:HA	1.73	0.71
2:H:42:GLN:OE1	2:H:43:ALA:N	2.24	0.71
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.72	0.71
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.73	0.71
1:A:131:CYS:HA	1:A:166:CYS:HA	1.73	0.71
1:B:363:ALA:N	1:B:525:CYS:O	2.22	0.71
5:M:33:GLY:O	5:M:100:ARG:NH2	2.23	0.71
5:M:79:GLN:HE22	5:M:81:VAL:HG13	1.56	0.70
1:C:329:PHE:N	1:C:531:THR:HG23	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:37:VAL:HG23	3:I:94:TYR:HB2	1.73	0.70
5:M:17:THR:HG22	5:M:85:THR:HA	1.72	0.70
1:A:327:VAL:HG23	1:A:542:ASN:HB3	1.72	0.70
1:C:282:ASN:ND2	6:C:1313:NAG:HN2	1.89	0.70
1:A:657:ASN:HD21	6:A:1305:NAG:H2	1.55	0.70
5:M:101:GLY:O	5:M:108:ILE:N	2.24	0.70
1:A:31:SER:N	1:A:60:SER:O	2.17	0.69
2:J:86:TYR:O	2:J:103:GLY:HA2	1.91	0.69
4:N:32:ASN:HD22	4:N:92:TRP:H	1.38	0.69
5:O:98:THR:HG22	5:O:113:TRP:HA	1.73	0.69
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.57	0.69
1:C:446:GLY:O	1:C:449:TYR:OH	2.09	0.69
1:C:439:ASN:HA	1:C:507:PRO:HG2	1.73	0.69
1:B:134:GLN:O	1:B:162:SER:N	2.24	0.69
1:A:424:LYS:HE3	1:A:463:PRO:HG3	1.73	0.68
2:H:21:LEU:HD11	2:H:106:LEU:HD21	1.76	0.68
3:I:50:VAL:O	3:I:57:THR:OG1	2.08	0.68
5:O:70:THR:HG23	5:O:83:THR:HB	1.74	0.68
1:C:383:SER:H	1:C:386:LYS:HZ3	1.40	0.68
5:O:29:LEU:HD12	5:O:34:VAL:HG13	1.75	0.68
1:A:1098:ASN:ND2	6:A:1309:NAG:O7	2.27	0.68
1:C:353:TRP:NE1	1:C:466:ARG:HB2	2.08	0.68
1:C:353:TRP:CE2	1:C:466:ARG:HB2	2.29	0.68
5:O:21:THR:HG23	5:O:79:GLN:OE1	1.94	0.68
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.59	0.67
1:B:140:PHE:HB2	1:B:249:LEU:HD11	1.77	0.67
1:B:386:LYS:HE2	1:C:982:SER:O	1.94	0.67
3:I:67:PHE:HB3	3:I:80:LEU:HD21	1.74	0.67
1:A:30:ASN:HA	1:A:61:ASN:HA	1.75	0.67
3:K:38:ARG:NE	3:K:46:GLU:OE2	2.28	0.67
1:A:282:ASN:HB2	6:A:1303:NAG:H82	1.75	0.67
1:B:81:ASN:O	1:B:239:GLN:NE2	2.26	0.67
1:C:117:LEU:HD21	1:C:119:ILE:HG23	1.76	0.67
1:A:1054:GLN:HB2	1:A:1061:VAL:HG23	1.76	0.66
3:I:34:MET:O	3:I:50:VAL:HA	1.95	0.66
3:K:72:ASP:OD1	3:K:74:SER:OG	2.13	0.66
1:B:282:ASN:ND2	6:B:1303:NAG:O7	2.28	0.66
1:B:438:SER:O	1:B:507:PRO:HG2	1.95	0.66
2:H:94:TRP:CD1	2:H:95:PRO:HD3	2.30	0.66
5:O:68:ARG:NH1	5:O:86:ASN:O	2.28	0.66
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HG22	1:C:128:ILE:HG23	1.78	0.66
1:A:603:ASN:OD1	6:A:1306:NAG:H2	1.96	0.66
1:B:350:VAL:HA	1:B:400:PHE:HB2	1.78	0.66
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.31	0.65
1:A:726:ILE:HG13	1:A:1061:VAL:HG12	1.76	0.65
1:C:441:LEU:HD23	5:O:32:SER:HB3	1.77	0.65
2:J:96:PRO:HG3	3:K:58:PHE:CG	2.31	0.65
1:C:280:ASN:OD1	1:C:284:THR:N	2.19	0.65
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.30	0.65
1:C:329:PHE:H	1:C:531:THR:CG2	2.07	0.65
3:I:59:TYR:HD1	3:I:64:LYS:HZ3	1.43	0.65
3:K:66:ARG:NH2	3:K:84:SER:O	2.30	0.65
1:A:336:CYS:HB2	1:A:337:PRO:HD2	1.78	0.65
1:B:453:TYR:HB3	1:B:495:TYR:CZ	2.30	0.65
4:L:40:LEU:HD12	4:L:85:ALA:HB2	1.77	0.65
1:A:917:TYR:HB3	1:C:1129:VAL:HG23	1.79	0.65
1:C:544:ASN:HD21	1:C:579:PRO:HG3	1.62	0.65
5:M:34:VAL:O	5:M:55:TRP:HB3	1.96	0.65
1:C:560:LEU:N	1:C:563:GLN:OE1	2.28	0.65
5:O:101:GLY:N	5:O:111:GLU:OE2	2.29	0.65
1:C:326:ILE:O	1:C:328:ARG:N	2.26	0.65
1:C:357:ARG:HG3	1:C:396:TYR:HE1	1.61	0.65
3:K:6:GLU:OE1	3:K:110:GLN:N	2.30	0.65
4:N:6:GLN:HE21	4:N:102:GLY:HA3	1.61	0.65
1:A:486:VAL:HG13	1:A:487:ASN:H	1.62	0.65
1:C:440:LYS:NZ	5:O:102:PRO:HB2	2.12	0.64
1:C:616:ASN:OD1	1:C:618:THR:N	2.27	0.64
5:O:92:THR:HG22	5:O:121:VAL:H	1.62	0.64
1:C:327:VAL:CB	1:C:531:THR:HA	2.27	0.64
4:L:10:ALA:HB2	4:L:20:ILE:HD11	1.78	0.64
1:C:336:CYS:HB2	1:C:337:PRO:HD2	1.80	0.64
1:A:68:ILE:HG12	1:A:69:HIS:ND1	2.13	0.64
1:C:328:ARG:HH12	1:C:544:ASN:HA	1.61	0.64
5:M:100:ARG:O	5:M:100:ARG:HG3	1.96	0.64
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.63	0.64
1:A:379:CYS:HA	1:A:432:CYS:CB	2.24	0.64
1:C:452:ARG:HA	1:C:493:GLN:O	1.97	0.64
4:N:33:PHE:HB3	4:N:51:SER:HA	1.80	0.64
1:B:709:ASN:ND2	6:B:1311:NAG:H2	2.10	0.64
1:C:1092:GLU:OE2	1:C:1092:GLU:N	2.31	0.64
4:L:4:LEU:HD21	4:L:29:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ASP:OD1	1:C:390:LEU:N	2.31	0.64
1:C:448:ASN:OD1	1:C:450:ASN:ND2	2.31	0.64
1:C:170:TYR:HE1	1:C:172:SER:HG	1.44	0.63
1:C:328:ARG:NH2	1:C:542:ASN:O	2.32	0.63
3:K:13:GLN:HG2	3:K:14:PRO:HD2	1.81	0.63
5:M:10:THR:HA	5:M:119:VAL:HG22	1.80	0.63
1:B:657:ASN:ND2	6:B:1304:NAG:H2	2.13	0.63
3:K:95:CYS:O	3:K:109:GLY:N	2.31	0.63
4:L:35:TYR:HB2	4:L:90:ALA:HB3	1.80	0.63
1:A:438:SER:HB2	1:A:509:ARG:HG3	1.79	0.63
5:M:65:LEU:HD22	5:M:68:ARG:HH12	1.64	0.63
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.34	0.63
1:A:861:LEU:HD22	1:A:861:LEU:H	1.62	0.63
3:K:36:TRP:HE1	3:K:78:LEU:HG	1.64	0.63
5:M:30:ILE:HG23	5:M:75:THR:HG21	1.81	0.63
4:N:18:VAL:HG13	4:N:79:LEU:HD11	1.80	0.63
5:M:54:TYR:HD2	5:M:58:ASP:HB3	1.63	0.63
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.34	0.63
1:A:663:ASP:N	1:A:663:ASP:OD1	2.31	0.62
3:I:2:VAL:HG12	3:I:26:GLY:HA3	1.80	0.62
1:A:330:PRO:HA	1:A:579:PRO:O	1.98	0.62
1:A:457:ARG:HG2	1:A:458:LYS:H	1.65	0.62
1:B:353:TRP:NE1	1:B:423:TYR:HD2	1.97	0.62
2:H:94:TRP:CG	2:H:95:PRO:HD3	2.34	0.62
5:M:92:THR:HG23	5:M:120:THR:HA	1.81	0.62
4:N:1:GLN:HA	4:N:25:SER:HB2	1.80	0.62
1:A:234:ASN:ND2	6:A:1301:NAG:O6	2.33	0.62
1:A:657:ASN:ND2	6:A:1305:NAG:O7	2.32	0.62
1:B:578:ASP:HB2	1:B:582:LEU:N	2.14	0.62
1:C:367:VAL:O	1:C:370:ASN:ND2	2.33	0.62
1:C:383:SER:OG	1:C:386:LYS:HG2	1.99	0.62
1:B:353:TRP:HE1	1:B:423:TYR:HB2	1.64	0.62
1:B:196:ASN:ND2	1:B:201:PHE:HB2	2.14	0.62
1:B:392:PHE:HB2	1:B:524:VAL:HG23	1.81	0.62
2:H:42:GLN:CD	2:H:43:ALA:H	2.03	0.62
4:N:93:ASP:O	4:N:97:SER:N	2.32	0.62
1:C:487:ASN:HA	1:C:489:TYR:CE2	2.35	0.62
2:H:96:PRO:HG3	3:I:58:PHE:CG	2.35	0.62
4:N:38:HIS:HB2	4:N:48:LEU:HD11	1.82	0.62
1:A:68:ILE:HG23	1:A:69:HIS:H	1.65	0.61
1:B:1092:GLU:OE2	1:B:1093:GLY:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ALA:HB1	1:C:373:PRO:HD2	1.82	0.61
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.35	0.61
1:B:732:THR:OG1	1:B:955:ASN:OD1	2.16	0.61
2:J:94:TRP:O	2:J:97:GLY:N	2.33	0.61
1:C:419:ALA:HA	1:C:423:TYR:O	2.00	0.61
3:I:59:TYR:O	3:I:64:LYS:HE2	2.01	0.61
1:B:34:ARG:NH2	1:B:219:GLY:O	2.33	0.61
2:J:94:TRP:CG	2:J:95:PRO:HD3	2.35	0.61
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.83	0.61
1:C:486:VAL:HG13	1:C:487:ASN:H	1.66	0.61
2:J:34:ALA:HA	2:J:49:TYR:HA	1.80	0.61
4:L:6:GLN:HE22	4:L:88:TYR:HA	1.66	0.61
1:B:394:ASN:ND2	1:C:200:TYR:OH	2.34	0.61
1:C:663:ASP:OD1	1:C:663:ASP:N	2.31	0.61
1:C:142:ASP:HA	1:C:157:PHE:O	2.01	0.61
1:B:663:ASP:OD1	1:B:663:ASP:N	2.33	0.61
1:C:396:TYR:HB2	1:C:514:SER:OG	2.00	0.61
4:N:13:THR:H	4:N:79:LEU:HD13	1.65	0.61
4:N:87:TYR:O	4:N:104:GLY:HA2	2.01	0.61
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.36	0.60
6:B:1311:NAG:O4	6:C:1301:NAG:H5	2.00	0.60
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.36	0.60
2:H:44:PRO:HG2	3:I:45:LEU:HD11	1.83	0.60
2:J:94:TRP:CD1	2:J:95:PRO:HD3	2.36	0.60
4:L:79:LEU:HD21	4:L:107:LEU:HD11	1.83	0.60
1:A:34:ARG:NH2	1:A:219:GLY:O	2.35	0.60
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.36	0.60
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.34	0.60
1:B:108:THR:OG1	1:B:234:ASN:O	2.19	0.60
1:B:419:ALA:HA	1:B:423:TYR:O	2.01	0.60
1:A:140:PHE:HB2	1:A:249:LEU:HD11	1.83	0.60
1:C:106:PHE:HD1	1:C:238:PHE:HB2	1.66	0.60
2:H:34:ALA:HA	2:H:49:TYR:HA	1.82	0.60
3:I:4:LEU:HA	3:I:23:ALA:O	2.00	0.60
1:C:91:TYR:OH	1:C:191:GLU:OE2	2.12	0.60
1:C:328:ARG:HH22	1:C:545:GLY:H	1.49	0.60
1:C:461:LEU:HD23	1:C:461:LEU:H	1.65	0.60
6:C:1302:NAG:C1	6:C:1309:NAG:H4	2.31	0.60
3:I:99:LEU:HB2	3:I:103:GLY:O	2.01	0.60
4:N:22:CYS:HB3	4:N:72:ALA:HB3	1.83	0.60
1:A:354:ASN:ND2	1:A:399:SER:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:THR:OG1	1:B:394:ASN:N	2.35	0.60
1:B:712:ILE:HG13	1:B:1077:THR:HG21	1.83	0.60
1:A:327:VAL:HG12	1:A:531:THR:HG23	1.84	0.60
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.35	0.60
1:C:189:LEU:HB3	1:C:208:THR:HG23	1.84	0.60
1:A:327:VAL:N	1:A:531:THR:OG1	2.33	0.59
1:C:403:ARG:HD3	1:C:505:HIS:HA	1.83	0.59
1:B:327:VAL:HG12	1:B:542:ASN:HB3	1.84	0.59
1:B:616:ASN:OD1	1:B:617:CYS:N	2.35	0.59
1:C:457:ARG:HG2	1:C:458:LYS:H	1.67	0.59
1:B:351:TYR:HD2	1:B:454:ARG:HG2	1.67	0.59
2:J:18:ARG:HA	2:J:75:ILE:O	2.02	0.59
1:A:417:ASN:O	1:A:421:TYR:HB2	2.02	0.59
1:B:384:PRO:O	1:B:387:LEU:HB3	2.03	0.59
3:K:6:GLU:HB3	3:K:112:THR:HG23	1.83	0.59
5:M:70:THR:HG23	5:M:83:THR:HB	1.84	0.59
1:B:331:ASN:HD21	6:B:1305:NAG:C7	2.15	0.59
1:B:555:SER:OG	1:B:584:ILE:HB	2.02	0.59
6:B:1303:NAG:C7	6:B:1303:NAG:HO3	2.15	0.59
3:K:99:LEU:HB2	3:K:103:GLY:O	2.01	0.59
5:O:100:ARG:O	5:O:100:ARG:HG3	2.02	0.59
1:A:70:VAL:HG13	1:A:80:ASP:HA	1.84	0.59
1:A:441:LEU:HD23	5:M:32:SER:HB3	1.83	0.59
1:C:189:LEU:HB2	1:C:210:ILE:HD11	1.83	0.59
1:C:440:LYS:HZ3	5:O:102:PRO:HB2	1.68	0.59
1:B:36:VAL:HG11	1:B:220:PHE:CZ	2.37	0.58
3:K:34:MET:HB3	3:K:78:LEU:HD22	1.84	0.58
1:A:480:CYS:HB3	1:A:483:VAL:HG23	1.84	0.58
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.38	0.58
2:H:91:TYR:HB3	2:H:98:TYR:CD1	2.38	0.58
1:C:1125:ASN:ND2	1:C:1127:ASP:OD1	2.30	0.58
2:J:61:ARG:O	2:J:75:ILE:HA	2.03	0.58
1:B:377:PHE:C	1:B:378:LYS:HD3	2.23	0.58
1:A:247:SER:HA	1:A:258:TRP:CE2	2.39	0.58
1:B:99:ASN:O	1:B:102:ARG:NE	2.26	0.58
1:C:345:THR:O	5:O:32:SER:HB2	2.03	0.58
3:K:72:ASP:HB2	3:K:79:TYR:HE2	1.68	0.58
5:M:74:ALA:HB3	5:M:79:GLN:HE21	1.69	0.58
1:A:189:LEU:HB2	1:A:210:ILE:HD11	1.84	0.58
1:A:424:LYS:HG3	1:A:463:PRO:HA	1.84	0.58
1:B:578:ASP:HB2	1:B:582:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:SER:OG	1:B:698:SER:HB3	2.03	0.58
1:C:229:LEU:HD13	1:C:231:ILE:HD13	1.85	0.58
1:C:498:ARG:NH2	1:C:501:TYR:OH	2.36	0.58
1:A:372:ALA:HB1	1:A:373:PRO:HD2	1.84	0.58
1:B:365:TYR:HB2	1:B:388:ASN:HD22	1.67	0.58
1:C:81:ASN:OD1	1:C:82:PRO:HD2	2.02	0.58
4:L:13:THR:O	4:L:16:GLN:HG2	2.03	0.58
1:A:616:ASN:ND2	6:A:1310:NAG:O7	2.37	0.58
1:C:459:SER:OG	1:C:460:ASN:N	2.36	0.58
1:A:281:GLU:OE1	1:A:281:GLU:N	2.32	0.58
1:A:461:LEU:HD23	1:A:461:LEU:H	1.69	0.58
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.86	0.58
1:B:351:TYR:HE2	1:B:454:ARG:HH21	1.50	0.58
1:C:335:LEU:CD2	1:C:336:CYS:H	2.17	0.58
5:O:42:PRO:HG2	5:O:45:LYS:HD2	1.86	0.58
1:C:440:LYS:HD2	5:O:103:GLY:C	2.23	0.57
5:M:18:LEU:HB2	5:M:87:MET:SD	2.44	0.57
1:C:141:LEU:HG	1:C:243:ALA:HA	1.85	0.57
4:N:16:GLN:HB3	4:N:79:LEU:HD12	1.84	0.57
5:O:38:TRP:CD1	5:O:82:LEU:HD13	2.40	0.57
5:O:79:GLN:HE22	5:O:81:VAL:HG13	1.70	0.57
1:A:353:TRP:CE2	1:A:466:ARG:HB2	2.39	0.57
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.86	0.57
1:C:329:PHE:CB	1:C:530:SER:HA	2.34	0.57
1:A:393:THR:HG23	1:A:521:PRO:HD2	1.86	0.57
1:C:867:ASP:OD1	1:C:868:GLU:N	2.37	0.57
3:I:40:ALA:HB3	3:I:43:LYS:HD3	1.86	0.57
1:A:167:THR:O	1:C:357:ARG:NH2	2.38	0.57
1:A:431:GLY:HA3	1:A:513:LEU:O	2.05	0.57
1:A:444:LYS:O	1:A:498:ARG:HA	2.04	0.57
1:A:1074:ASN:HD21	6:A:1307:NAG:C7	2.16	0.57
1:C:69:HIS:HB2	1:C:257:GLY:HA3	1.85	0.57
5:M:63:PRO:HA	5:M:66:ARG:HE	1.69	0.57
1:A:314:GLN:CD	1:A:314:GLN:H	2.08	0.57
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.40	0.57
1:B:106:PHE:HD1	1:B:238:PHE:HB2	1.68	0.57
1:C:480:CYS:N	1:C:488:CYS:SG	2.75	0.57
2:J:14:SER:N	2:J:17:GLU:OE2	2.38	0.57
2:J:91:TYR:HE2	3:K:101:VAL:HA	1.69	0.57
4:L:87:TYR:HB2	4:L:105:THR:HG22	1.86	0.57
1:B:337:PRO:O	1:B:340:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:CYS:SG	1:B:522:ALA:HB1	2.44	0.57
3:I:86:ARG:HB2	3:I:88:GLU:OE2	2.05	0.57
4:L:93:ASP:O	4:L:97:SER:CA	2.53	0.57
6:B:1311:NAG:H4	6:C:1301:NAG:C1	2.34	0.57
4:N:28:ASN:OD1	4:N:29:ILE:N	2.36	0.57
1:B:656:VAL:HG22	1:B:658:SER:H	1.69	0.57
1:A:106:PHE:HB3	1:A:235:ILE:HG13	1.87	0.56
1:C:583:GLU:OE2	1:C:584:ILE:N	2.37	0.56
1:A:167:THR:HB	1:C:357:ARG:HH22	1.70	0.56
1:C:226:LEU:HG	1:C:227:VAL:HG22	1.88	0.56
3:I:27:ILE:HD11	3:I:32:ASN:HD21	1.70	0.56
1:A:326:ILE:HD13	1:A:534:VAL:HG12	1.87	0.56
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.40	0.56
1:C:867:ASP:OD1	1:C:867:ASP:N	2.37	0.56
5:O:9:LEU:HD13	5:O:12:VAL:HB	1.85	0.56
1:C:376:ALA:O	1:C:434:ILE:HD12	2.05	0.56
5:O:59:LYS:HZ1	5:O:71:ILE:C	2.09	0.56
1:B:68:ILE:HG13	1:B:69:HIS:N	2.20	0.56
1:B:344:ALA:HB1	1:B:346:ARG:HG2	1.87	0.56
1:C:676:THR:HA	1:C:690:GLN:N	2.21	0.56
1:B:339:ASP:OD1	1:B:339:ASP:N	2.38	0.56
1:B:364:ASP:O	1:B:368:LEU:HG	2.06	0.56
2:H:6:GLN:HE21	2:H:104:THR:HG23	1.71	0.56
1:B:357:ARG:NH2	1:C:230:PRO:O	2.37	0.56
1:C:31:SER:O	1:C:59:PHE:HA	2.06	0.56
1:C:470:THR:HB	1:C:490:PHE:CE1	2.41	0.56
4:N:17:ARG:HD2	4:N:18:VAL:N	2.21	0.56
1:A:616:ASN:OD1	1:A:617:CYS:N	2.38	0.56
1:B:353:TRP:CE2	1:B:423:TYR:CD2	2.94	0.56
1:B:353:TRP:CB	1:B:400:PHE:HB3	2.36	0.56
4:L:62:ARG:HE	4:L:80:ARG:HH11	1.54	0.56
1:C:453:TYR:CE1	1:C:493:GLN:HB2	2.42	0.55
4:N:32:ASN:ND2	4:N:92:TRP:H	2.04	0.55
1:A:356:LYS:O	1:A:396:TYR:HA	2.06	0.55
1:B:826:VAL:HG11	1:B:1057:PRO:HG2	1.88	0.55
1:C:308:VAL:N	1:C:602:THR:OG1	2.33	0.55
1:C:417:ASN:O	1:C:421:TYR:HB2	2.06	0.55
4:L:32:ASN:ND2	4:L:92:TRP:HB3	2.21	0.55
1:A:298:GLU:O	1:A:302:THR:HG23	2.07	0.55
1:A:1140:PRO:O	1:A:1143:PRO:HD2	2.07	0.55
1:B:398:ASP:HB2	1:B:512:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:TRP:O	2:H:97:GLY:N	2.39	0.55
3:K:67:PHE:HB3	3:K:80:LEU:HD21	1.89	0.55
5:M:62:ASN:HB3	5:M:65:LEU:HB2	1.89	0.55
5:O:74:ALA:CB	5:O:79:GLN:HE21	2.20	0.55
5:O:33:GLY:O	5:O:100:ARG:NH2	2.40	0.55
1:B:961:THR:HA	1:B:964:LYS:HD2	1.89	0.55
1:C:141:LEU:HD21	1:C:244:LEU:CB	2.37	0.55
1:C:342:PHE:HZ	1:C:434:ILE:HG21	1.72	0.55
1:C:657:ASN:ND2	6:C:1303:NAG:O3	2.39	0.55
1:C:861:LEU:H	1:C:861:LEU:HD22	1.71	0.55
3:K:1:GLU:O	3:K:25:SER:OG	2.24	0.55
4:L:50:HIS:CE1	4:L:54:GLN:HB3	2.42	0.55
4:N:55:ARG:NH1	4:N:63:PHE:O	2.40	0.55
1:C:546:LEU:HD22	1:C:565:PHE:CE1	2.42	0.55
2:H:6:GLN:OE1	2:H:88:CYS:N	2.40	0.55
2:H:75:ILE:HG21	2:H:78:LEU:HD23	1.89	0.55
2:J:78:LEU:HD13	2:J:106:LEU:HD21	1.87	0.55
1:A:133:PHE:HA	1:A:163:ALA:O	2.07	0.55
1:A:442:ASP:O	1:A:448:ASN:ND2	2.35	0.55
1:A:1134:ASN:HD21	6:A:1308:NAG:C7	2.20	0.55
6:A:1304:NAG:O6	6:A:1311:NAG:O6	2.25	0.55
1:B:383:SER:HB3	1:B:386:LYS:NZ	2.22	0.55
5:M:9:LEU:HD13	5:M:12:VAL:HB	1.88	0.55
1:B:350:VAL:HG22	1:B:418:ILE:HG12	1.89	0.55
2:H:29:VAL:HG11	2:H:33:LEU:HD13	1.89	0.55
1:B:436:TRP:O	1:B:508:TYR:HA	2.07	0.55
1:C:57:PRO:HB3	1:C:273:ARG:NH1	2.22	0.55
3:K:66:ARG:NH2	3:K:84:SER:OG	2.40	0.55
1:A:422:ASN:OD1	1:A:422:ASN:N	2.40	0.54
4:L:6:GLN:HE21	4:L:102:GLY:HA3	1.73	0.54
1:A:353:TRP:HZ3	1:A:355:ARG:HD3	1.72	0.54
1:C:324:GLU:HB3	1:C:539:VAL:HG23	1.88	0.54
1:C:982:SER:OG	1:C:983:ARG:N	2.41	0.54
1:A:324:GLU:HB3	1:A:539:VAL:HG23	1.90	0.54
1:C:403:ARG:CD	1:C:505:HIS:HA	2.36	0.54
5:M:62:ASN:HD22	5:M:65:LEU:HD12	1.71	0.54
1:C:457:ARG:NH2	1:C:459:SER:O	2.39	0.54
2:H:27:GLU:O	2:H:69:THR:HG22	2.07	0.54
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.90	0.54
5:M:39:ILE:HD13	5:M:49:TRP:HA	1.90	0.54
1:C:455:LEU:N	1:C:491:PRO:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:GLN:OE1	2:H:45:ARG:NH1	2.38	0.54
2:J:2:ARG:HA	2:J:27:GLU:OE1	2.08	0.54
5:M:32:SER:HA	5:M:55:TRP:CD1	2.42	0.54
1:A:70:VAL:HG21	1:A:255:SER:HA	1.90	0.54
1:C:979:ASP:OD1	1:C:983:ARG:NE	2.41	0.54
1:A:395:VAL:HG23	1:A:524:VAL:HG11	1.90	0.54
5:M:49:TRP:O	5:M:62:ASN:ND2	2.40	0.54
5:O:28:SER:OG	5:O:31:ASN:ND2	2.41	0.54
1:C:662:CYS:HB2	1:C:697:MET:HG2	1.89	0.54
3:I:47:TRP:HZ2	3:I:50:VAL:HG12	1.73	0.54
4:L:52:ASN:HD22	4:L:67:ASN:HB2	1.72	0.54
1:A:402:ILE:O	1:A:507:PRO:HA	2.08	0.54
1:B:353:TRP:CE2	1:B:423:TYR:HD2	2.26	0.54
1:C:402:ILE:HD11	1:C:510:VAL:HG21	1.90	0.54
1:C:442:ASP:HB2	1:C:507:PRO:CG	2.38	0.54
1:C:444:LYS:O	1:C:498:ARG:HA	2.08	0.54
3:K:47:TRP:HZ2	3:K:50:VAL:HG12	1.72	0.54
5:O:34:VAL:HG23	5:O:99:HIS:HE1	1.73	0.54
1:C:360:ASN:O	1:C:360:ASN:ND2	2.41	0.53
1:C:479:PRO:HG2	1:C:481:ASN:OD1	2.09	0.53
3:K:2:VAL:HA	3:K:25:SER:O	2.08	0.53
4:L:6:GLN:NE2	4:L:89:CYS:H	2.06	0.53
1:A:425:LEU:HD23	1:A:425:LEU:H	1.73	0.53
1:C:113:LYS:HA	6:C:1312:NAG:H81	1.91	0.53
1:C:393:THR:OG1	1:C:520:ALA:HB2	2.08	0.53
1:A:118:LEU:HD21	1:A:120:VAL:HG23	1.90	0.53
1:B:557:LYS:NZ	1:B:586:ASP:OD1	2.41	0.53
4:N:94:ASP:OD1	4:N:95:SER:N	2.41	0.53
1:A:444:LYS:HD3	5:M:54:TYR:CE2	2.44	0.53
1:B:461:LEU:HD21	1:B:465:GLU:O	2.08	0.53
3:I:36:TRP:HD1	3:I:69:ILE:HD12	1.72	0.53
1:B:350:VAL:HG23	1:B:400:PHE:CD1	2.44	0.53
1:B:454:ARG:HD2	1:B:492:LEU:HD12	1.90	0.53
1:C:401:VAL:CG1	1:C:509:ARG:HG2	2.37	0.53
1:C:709:ASN:HD21	6:C:1309:NAG:C1	2.22	0.53
3:I:59:TYR:OH	3:I:69:ILE:N	2.34	0.53
1:C:416:GLY:O	1:C:420:ASP:HB2	2.09	0.53
4:N:35:TYR:HB2	4:N:90:ALA:HB3	1.90	0.53
1:A:712:ILE:HD11	1:B:896:ILE:HG13	1.90	0.53
1:B:107:GLY:H	1:B:235:ILE:HG23	1.73	0.53
2:J:30:SER:HA	2:J:68:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:O	1:A:102:ARG:NE	2.33	0.53
1:B:351:TYR:HD2	1:B:454:ARG:CG	2.21	0.53
3:K:48:VAL:O	3:K:60:ALA:N	2.36	0.53
1:A:438:SER:O	1:A:442:ASP:HB2	2.09	0.53
1:B:34:ARG:NH2	1:B:217:PRO:O	2.42	0.53
1:B:142:ASP:HB2	1:B:243:ALA:CB	2.39	0.53
1:B:1134:ASN:HD21	6:B:1308:NAG:C7	2.21	0.53
4:L:40:LEU:HB3	4:L:43:THR:CG2	2.39	0.53
5:M:68:ARG:NH1	5:M:69:LEU:HD21	2.22	0.53
4:N:45:PRO:HD2	5:O:113:TRP:CZ3	2.43	0.53
5:O:74:ALA:HB3	5:O:79:GLN:HE21	1.72	0.53
6:A:1304:NAG:O5	6:A:1311:NAG:H4	2.09	0.52
1:B:234:ASN:HD21	6:B:1301:NAG:C1	2.22	0.52
2:H:29:VAL:HG22	2:H:92:ASN:HD21	1.74	0.52
1:A:971:GLY:O	1:A:995:ARG:NH2	2.42	0.52
1:B:371:PHE:HB3	1:B:374:PHE:CZ	2.44	0.52
1:C:99:ASN:O	1:C:102:ARG:NE	2.31	0.52
1:C:326:ILE:HG21	1:C:534:VAL:HG12	1.90	0.52
1:C:422:ASN:OD1	1:C:422:ASN:N	2.41	0.52
2:H:42:GLN:NE2	3:I:110:GLN:HA	2.25	0.52
5:O:10:THR:HB	5:O:118:LEU:O	2.09	0.52
1:B:522:ALA:HB3	1:B:544:ASN:OD1	2.10	0.52
1:C:443:SER:O	5:O:107:PRO:HG2	2.10	0.52
1:C:475:ALA:HB1	1:C:486:VAL:HG13	1.91	0.52
2:H:6:GLN:HB2	2:H:102:GLN:NE2	2.24	0.52
1:B:108:THR:HG23	6:B:1301:NAG:H62	1.91	0.52
3:K:106:ASP:O	3:K:108:TRP:HD1	1.93	0.52
1:A:397:ALA:HA	1:A:512:VAL:O	2.09	0.52
1:A:401:VAL:HA	1:A:508:TYR:O	2.09	0.52
2:J:6:GLN:NE2	2:J:104:THR:HG23	2.18	0.52
1:A:134:GLN:O	1:A:162:SER:N	2.30	0.52
1:B:115:GLN:HA	1:B:132:GLU:CB	2.40	0.52
1:B:175:PHE:O	1:B:176:LEU:HD23	2.09	0.52
1:C:231:ILE:CG2	1:C:233:ILE:HG12	2.40	0.52
3:K:41:PRO:HD3	3:K:91:ALA:HA	1.91	0.52
5:M:53:ILE:HD12	5:M:73:LYS:HG2	1.91	0.52
5:O:65:LEU:O	5:O:69:LEU:HD13	2.09	0.52
1:A:374:PHE:CD1	1:A:434:ILE:HD11	2.44	0.52
1:B:295:PRO:O	1:B:299:THR:HG23	2.10	0.52
1:B:353:TRP:HB3	1:B:400:PHE:HB3	1.90	0.52
1:C:449:TYR:OH	1:C:498:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:76:ILE:HG13	4:L:76:ILE:O	2.10	0.52
5:O:65:LEU:HD23	5:O:69:LEU:HD21	1.91	0.52
5:O:74:ALA:HB3	5:O:79:GLN:HG3	1.91	0.52
1:B:729:VAL:HG23	1:B:1059:GLY:HA2	1.92	0.52
1:C:546:LEU:HD22	1:C:565:PHE:HE1	1.74	0.52
1:C:616:ASN:OD1	1:C:617:CYS:N	2.43	0.52
3:K:106:ASP:N	3:K:106:ASP:OD1	2.43	0.52
1:B:676:THR:H	1:B:690:GLN:N	2.08	0.52
2:H:6:GLN:HG2	2:H:23:CYS:CB	2.40	0.52
3:I:59:TYR:HB2	3:I:64:LYS:HD3	1.91	0.52
3:I:66:ARG:NH1	3:I:89:ASP:OD2	2.43	0.52
4:L:62:ARG:HH12	4:L:83:ASP:HB3	1.74	0.52
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.45	0.52
1:C:735:SER:CB	1:C:861:LEU:HD21	2.40	0.52
2:H:86:TYR:CD1	2:H:106:LEU:HD13	2.44	0.52
2:J:6:GLN:OE1	2:J:88:CYS:N	2.40	0.52
2:J:32:ASP:OD2	2:J:92:ASN:HA	2.10	0.52
4:L:87:TYR:O	4:L:104:GLY:HA2	2.10	0.52
5:M:29:LEU:HB3	5:M:73:LYS:NZ	2.25	0.52
1:A:141:LEU:O	1:A:249:LEU:HD13	2.10	0.51
1:A:175:PHE:O	1:A:176:LEU:HD23	2.10	0.51
1:C:330:PRO:HA	1:C:544:ASN:HD21	1.74	0.51
1:C:439:ASN:HB2	1:C:507:PRO:HD2	1.91	0.51
1:C:659:SER:OG	1:C:698:SER:HB3	2.10	0.51
1:B:338:PHE:HD1	1:B:342:PHE:CE1	2.28	0.51
1:B:452:ARG:NH2	1:B:492:LEU:HB3	2.25	0.51
1:B:971:GLY:O	1:B:995:ARG:NH2	2.43	0.51
1:A:338:PHE:CE1	1:A:358:ILE:HG21	2.45	0.51
1:B:583:GLU:OE2	1:B:584:ILE:N	2.42	0.51
1:B:1074:ASN:HD21	6:B:1307:NAG:C7	2.23	0.51
2:H:91:TYR:HB3	2:H:98:TYR:CE1	2.46	0.51
6:B:1305:NAG:O7	6:B:1305:NAG:O3	2.29	0.51
4:N:64:SER:OG	4:N:75:ALA:HB3	2.11	0.51
1:A:31:SER:OG	1:A:60:SER:O	2.26	0.51
1:B:551:VAL:HG12	1:B:588:THR:O	2.09	0.51
2:H:6:GLN:HG2	2:H:23:CYS:HB2	1.91	0.51
2:H:78:LEU:HB3	2:H:108:ILE:HD11	1.93	0.51
3:I:106:ASP:N	3:I:106:ASP:OD1	2.43	0.51
4:L:76:ILE:HD12	4:L:79:LEU:HD21	1.91	0.51
1:A:489:TYR:HD2	3:I:99:LEU:HD22	1.74	0.51
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HA	1:A:210:ILE:HB	1.91	0.51
1:A:351:TYR:CZ	1:A:492:LEU:HD21	2.45	0.51
1:A:376:ALA:HB3	1:A:435:ALA:HB3	1.91	0.51
1:A:443:SER:O	5:M:107:PRO:HG2	2.11	0.51
1:A:982:SER:OG	1:A:983:ARG:N	2.43	0.51
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.92	0.51
1:C:437:ASN:HB2	1:C:508:TYR:CE2	2.46	0.51
3:K:11:LEU:HD11	3:K:117:SER:HA	1.92	0.51
1:A:616:ASN:HD22	6:A:1310:NAG:C7	2.23	0.51
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.92	0.51
4:L:46:LYS:HD2	4:L:47:LEU:N	2.26	0.51
1:B:247:SER:HA	1:B:258:TRP:CZ2	2.46	0.51
1:B:364:ASP:OD1	1:B:364:ASP:N	2.36	0.51
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.46	0.51
1:B:128:ILE:O	1:B:169:GLU:HA	2.11	0.50
4:N:15:GLY:N	4:N:79:LEU:O	2.27	0.50
1:A:444:LYS:HD3	5:M:54:TYR:CZ	2.46	0.50
1:B:99:ASN:HB3	1:B:102:ARG:HH11	1.75	0.50
1:B:578:ASP:OD2	1:B:583:GLU:HB3	2.12	0.50
1:C:31:SER:O	1:C:59:PHE:CA	2.59	0.50
1:C:128:ILE:HD13	1:C:170:TYR:HD1	1.76	0.50
2:J:96:PRO:HB2	3:K:47:TRP:CZ2	2.47	0.50
4:L:1:GLN:HA	4:L:25:SER:HB2	1.94	0.50
1:A:125:ASN:HB2	1:A:172:SER:O	2.12	0.50
2:H:48:ILE:HG12	2:H:54:ARG:HG2	1.93	0.50
3:K:23:ALA:HA	3:K:77:THR:HG22	1.93	0.50
1:C:196:ASN:ND2	1:C:201:PHE:HB2	2.27	0.50
2:J:36:TYR:O	2:J:86:TYR:HA	2.11	0.50
1:A:445:VAL:HG23	5:M:109:TYR:CZ	2.47	0.50
1:A:456:PHE:HE1	3:I:33:TYR:CD2	2.28	0.50
1:B:457:ARG:HH21	1:B:491:PRO:HB3	1.77	0.50
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.92	0.50
3:I:75:LYS:NZ	3:I:79:TYR:OH	2.24	0.50
4:L:17:ARG:HD3	4:L:18:VAL:N	2.26	0.50
4:N:6:GLN:HB2	4:N:104:GLY:H	1.75	0.50
1:A:376:ALA:O	1:A:434:ILE:HA	2.12	0.50
1:A:395:VAL:HG22	1:A:515:PHE:CD1	2.47	0.50
1:C:228:ASP:O	1:C:229:LEU:C	2.50	0.50
6:C:1310:NAG:O7	6:C:1310:NAG:O3	2.28	0.50
2:J:38:GLN:HB3	2:J:85:VAL:HG13	1.93	0.50
1:A:583:GLU:OE2	1:A:584:ILE:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PHE:HB2	1:C:249:LEU:HD11	1.94	0.50
1:C:502:GLY:O	1:C:506:GLN:HG3	2.11	0.50
1:A:347:PHE:CE2	1:A:399:SER:HB3	2.46	0.50
1:A:367:VAL:O	1:A:370:ASN:ND2	2.45	0.50
1:A:424:LYS:O	1:A:463:PRO:HA	2.11	0.50
1:A:826:VAL:HG23	1:A:949:GLN:OE1	2.12	0.50
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.45	0.50
1:B:281:GLU:OE1	1:B:281:GLU:N	2.32	0.50
1:B:905:ARG:NH2	1:B:1049:LEU:O	2.45	0.50
1:C:30:ASN:HA	1:C:61:ASN:HA	1.93	0.50
1:C:444:LYS:HE3	1:C:448:ASN:ND2	2.27	0.50
1:C:1139:ASP:OD1	1:C:1139:ASP:N	2.42	0.50
1:A:405:ASN:N	1:A:504:GLY:O	2.45	0.50
1:C:391:CYS:SG	1:C:522:ALA:HB1	2.51	0.50
1:C:815:ARG:NH2	1:C:820:ASP:OD1	2.45	0.50
4:N:6:GLN:HE22	4:N:88:TYR:HA	1.75	0.50
1:A:365:TYR:CD2	1:A:388:ASN:HA	2.37	0.49
1:A:437:ASN:HB2	1:A:508:TYR:CZ	2.46	0.49
2:H:30:SER:HA	2:H:68:GLY:H	1.77	0.49
2:H:38:GLN:HA	2:H:44:PRO:HA	1.94	0.49
3:I:36:TRP:HE1	3:I:78:LEU:HG	1.77	0.49
3:I:70:SER:O	3:I:78:LEU:HD12	2.12	0.49
3:K:13:GLN:NE2	3:K:14:PRO:O	2.45	0.49
4:L:5:THR:O	4:L:22:CYS:HA	2.12	0.49
5:M:53:ILE:CG2	5:M:59:LYS:HD2	2.40	0.49
1:A:353:TRP:O	1:A:466:ARG:NH2	2.44	0.49
1:A:435:ALA:CB	1:A:510:VAL:HG12	2.42	0.49
1:B:326:ILE:HD13	1:B:534:VAL:HG22	1.93	0.49
1:B:519:HIS:CE1	1:C:41:LYS:HD2	2.47	0.49
1:B:792:PRO:O	1:B:795:LYS:NZ	2.31	0.49
1:C:118:LEU:HD11	1:C:135:PHE:CE1	2.48	0.49
1:C:376:ALA:HB3	1:C:435:ALA:HB3	1.94	0.49
3:I:41:PRO:O	3:I:43:LYS:HD2	2.13	0.49
2:J:34:ALA:O	2:J:88:CYS:HA	2.12	0.49
4:L:1:GLN:NE2	4:L:27:SER:OG	2.40	0.49
4:N:10:ALA:HB3	4:N:107:LEU:HA	1.93	0.49
1:B:190:ARG:HH21	1:B:207:HIS:CD2	2.30	0.49
1:C:320:VAL:HG22	1:C:591:SER:O	2.13	0.49
1:C:442:ASP:HB2	1:C:507:PRO:HG3	1.93	0.49
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.78	0.49
2:J:77:SER:O	2:J:79:GLN:NE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:93:ASP:O	4:L:97:SER:HA	2.12	0.49
1:A:345:THR:OG1	5:M:31:ASN:HA	2.13	0.49
1:A:399:SER:HA	1:A:510:VAL:O	2.13	0.49
1:A:431:GLY:HA2	1:A:515:PHE:CE2	2.47	0.49
1:B:112:SER:O	6:B:1302:NAG:H2	2.12	0.49
1:B:776:LYS:O	1:B:780:GLU:HG3	2.13	0.49
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.95	0.49
2:J:29:VAL:HA	2:J:92:ASN:HD21	1.76	0.49
1:A:334:ASN:ND2	1:A:361:CYS:HA	2.27	0.49
1:C:168:PHE:CG	1:C:231:ILE:HD11	2.48	0.49
1:C:438:SER:HB3	1:C:509:ARG:HG3	1.93	0.49
1:C:905:ARG:NH2	1:C:1049:LEU:O	2.45	0.49
3:I:35:SER:HA	3:I:49:SER:O	2.13	0.49
3:I:36:TRP:CD1	3:I:69:ILE:HD12	2.47	0.49
1:A:198:ASP:OD1	1:A:200:TYR:HB2	2.13	0.49
1:B:443:SER:HA	1:B:497:PHE:HB3	1.93	0.49
1:C:356:LYS:O	1:C:396:TYR:HA	2.13	0.49
1:C:452:ARG:HA	1:C:494:SER:HA	1.93	0.49
2:H:19:ALA:HB2	2:H:78:LEU:HD11	1.93	0.49
2:H:30:SER:OG	2:H:31:SER:N	2.45	0.49
1:A:105:ILE:HG13	1:A:241:LEU:HD21	1.95	0.49
1:A:318:PHE:CZ	1:A:615:VAL:HG11	2.44	0.49
1:B:234:ASN:ND2	6:B:1301:NAG:O7	2.45	0.49
1:C:88:ASP:N	1:C:88:ASP:OD1	2.43	0.49
1:C:326:ILE:HD11	1:C:541:PHE:HB3	1.94	0.49
1:C:327:VAL:HB	1:C:531:THR:CA	2.37	0.49
1:C:353:TRP:NE1	1:C:423:TYR:HD1	2.11	0.49
2:H:31:SER:O	2:H:50:GLY:HA2	2.13	0.49
4:L:4:LEU:HD13	4:L:89:CYS:HB3	1.95	0.49
1:A:92:PHE:HE1	1:A:94:SER:OG	1.96	0.49
1:A:366:SER:HA	1:A:369:TYR:CE2	2.48	0.49
1:A:801:ASN:HD21	6:A:1312:NAG:C2	2.26	0.49
1:C:205:SER:OG	1:C:206:LYS:N	2.43	0.49
1:C:326:ILE:CG1	1:C:541:PHE:HA	2.43	0.49
1:C:616:ASN:OD1	1:C:616:ASN:C	2.50	0.49
2:H:36:TYR:O	2:H:86:TYR:HA	2.13	0.49
3:K:38:ARG:HD2	3:K:93:TYR:CZ	2.48	0.49
3:K:70:SER:O	3:K:78:LEU:HD12	2.13	0.49
5:M:54:TYR:CD2	5:M:58:ASP:HB3	2.45	0.49
5:O:40:ARG:HB3	5:O:50:LEU:HD11	1.94	0.49
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASN:N	1:A:497:PHE:O	2.41	0.49
1:B:126:VAL:O	1:B:171:VAL:HA	2.13	0.49
1:B:419:ALA:O	1:B:424:LYS:HA	2.13	0.49
3:I:60:ALA:O	3:I:64:LYS:HG2	2.13	0.49
1:A:92:PHE:CE1	1:A:94:SER:OG	2.66	0.48
1:A:419:ALA:HA	1:A:423:TYR:O	2.13	0.48
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.94	0.48
3:K:7:SER:OG	3:K:21:SER:HB3	2.13	0.48
5:M:11:LEU:HA	5:M:120:THR:O	2.13	0.48
1:A:748:GLU:O	1:A:752:LEU:HG	2.13	0.48
1:B:142:ASP:HB2	1:B:243:ALA:HB1	1.94	0.48
1:B:332:ILE:O	1:B:333:THR:O	2.31	0.48
1:C:444:LYS:HD3	5:O:54:TYR:CD2	2.48	0.48
3:I:106:ASP:O	3:I:108:TRP:HD1	1.96	0.48
1:A:578:ASP:OD1	1:A:585:LEU:HD23	2.13	0.48
1:B:403:ARG:CB	1:B:505:HIS:HA	2.44	0.48
1:B:519:HIS:O	1:B:521:PRO:HD3	2.13	0.48
1:B:738:CYS:SG	1:B:739:THR:N	2.86	0.48
6:B:1309:NAG:O7	6:B:1309:NAG:O3	2.28	0.48
1:C:312:ILE:HD12	1:C:598:ILE:HD11	1.95	0.48
4:L:17:ARG:HH21	4:L:77:SER:HB2	1.78	0.48
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.48
1:B:142:ASP:O	1:B:244:LEU:N	2.47	0.48
1:C:99:ASN:HB3	1:C:102:ARG:HH11	1.78	0.48
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.49	0.48
4:L:39:GLN:HG3	4:L:45:PRO:HG3	1.94	0.48
1:C:421:TYR:HE2	3:K:33:TYR:OH	1.96	0.48
1:C:444:LYS:HD3	5:O:54:TYR:CE2	2.49	0.48
3:I:79:TYR:HB3	3:I:81:GLN:HE22	1.78	0.48
1:A:455:LEU:HB3	1:A:493:GLN:OE1	2.13	0.48
1:B:200:TYR:HA	1:B:229:LEU:O	2.14	0.48
1:B:383:SER:HB3	1:B:386:LYS:HZ3	1.79	0.48
1:C:326:ILE:HD11	1:C:541:PHE:CB	2.44	0.48
1:C:403:ARG:HD2	1:C:405:ASN:OD1	2.12	0.48
1:C:421:TYR:CD1	1:C:457:ARG:HB3	2.48	0.48
1:A:141:LEU:HD21	1:A:244:LEU:CB	2.44	0.48
1:A:826:VAL:HG11	1:A:1057:PRO:HG2	1.96	0.48
1:B:513:LEU:HB3	1:B:515:PHE:CE1	2.49	0.48
1:B:1125:ASN:ND2	1:B:1127:ASP:OD1	2.43	0.48
1:C:31:SER:O	1:C:59:PHE:N	2.47	0.48
1:C:70:VAL:HG11	1:C:255:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:78:LEU:HD23	3:I:95:CYS:SG	2.54	0.48
3:K:11:LEU:HA	3:K:115:THR:O	2.14	0.48
4:L:96:LEU:O	5:M:63:PRO:HG2	2.14	0.48
1:A:452:ARG:HB3	1:A:492:LEU:HG	1.96	0.48
1:B:503:VAL:HA	1:B:506:GLN:HE21	1.79	0.48
1:B:1141:LEU:HD23	1:B:1141:LEU:O	2.14	0.48
3:K:94:TYR:HD1	3:K:109:GLY:O	1.96	0.48
1:A:357:ARG:HH11	1:A:359:SER:CB	2.27	0.48
1:A:704:SER:O	1:A:704:SER:OG	2.30	0.48
1:B:131:CYS:HB3	1:B:166:CYS:CA	2.44	0.48
1:B:712:ILE:HD11	1:C:896:ILE:HG13	1.96	0.48
1:C:340:GLU:OE2	1:C:340:GLU:N	2.46	0.48
2:J:36:TYR:HA	2:J:45:ARG:O	2.13	0.48
1:A:351:TYR:CE2	1:A:492:LEU:HD21	2.48	0.48
1:A:489:TYR:CE1	3:I:102:VAL:HG22	2.49	0.48
1:A:616:ASN:OD1	1:A:616:ASN:C	2.52	0.48
1:B:390:LEU:HD11	1:C:983:ARG:HB3	1.95	0.48
1:C:417:ASN:ND2	3:K:33:TYR:OH	2.47	0.48
1:A:346:ARG:NH2	5:M:32:SER:OG	2.47	0.47
1:A:396:TYR:HB2	1:A:514:SER:OG	2.14	0.47
1:A:402:ILE:HA	1:A:495:TYR:HE2	1.78	0.47
2:H:29:VAL:N	2:H:68:GLY:O	2.42	0.47
3:I:38:ARG:NH2	3:I:67:PHE:HE2	2.12	0.47
4:L:44:ALA:HB2	5:M:96:TYR:CE1	2.48	0.47
5:M:55:TRP:H	5:M:55:TRP:HE3	1.62	0.47
1:A:497:PHE:CG	1:A:507:PRO:HD3	2.49	0.47
1:B:374:PHE:HA	1:B:436:TRP:NE1	2.28	0.47
1:C:231:ILE:H	1:C:231:ILE:HD12	1.79	0.47
1:A:309:GLU:OE1	1:A:309:GLU:N	2.47	0.47
1:B:810:SER:OG	1:B:811:LYS:N	2.47	0.47
2:H:29:VAL:CG1	2:H:33:LEU:HD13	2.44	0.47
2:H:96:PRO:HG3	3:I:58:PHE:CB	2.44	0.47
1:A:1098:ASN:HD21	6:A:1309:NAG:C1	2.28	0.47
1:B:171:VAL:O	1:B:172:SER:OG	2.32	0.47
1:B:374:PHE:N	1:B:374:PHE:CD1	2.80	0.47
2:J:96:PRO:HB3	3:K:50:VAL:HG11	1.95	0.47
4:L:55:ARG:HB2	4:L:59:VAL:CG2	2.45	0.47
1:A:231:ILE:HG22	1:A:233:ILE:HG22	1.97	0.47
1:A:234:ASN:ND2	6:A:1301:NAG:O5	2.47	0.47
1:A:363:ALA:HB2	1:A:524:VAL:HG23	1.96	0.47
6:A:1312:NAG:O7	6:A:1312:NAG:O3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:GLN:HB2	2:H:102:GLN:HE21	1.79	0.47
2:J:44:PRO:HD2	3:K:108:TRP:CZ3	2.50	0.47
4:N:6:GLN:NE2	4:N:89:CYS:H	2.12	0.47
1:C:328:ARG:HD2	1:C:542:ASN:HB3	1.97	0.47
1:C:1077:THR:OG1	1:C:1078:ALA:N	2.47	0.47
3:K:12:VAL:O	3:K:116:VAL:HA	2.14	0.47
3:K:62:SER:O	3:K:86:ARG:NH1	2.48	0.47
1:A:379:CYS:CA	1:A:432:CYS:HB3	2.32	0.47
1:A:659:SER:HB3	1:A:698:SER:HB3	1.96	0.47
6:B:1311:NAG:C4	6:C:1301:NAG:H5	2.44	0.47
1:C:454:ARG:HG3	1:C:491:PRO:HB2	1.96	0.47
1:A:409:GLN:OE1	1:A:418:ILE:HG12	2.15	0.47
1:C:130:VAL:O	1:C:130:VAL:HG13	2.14	0.47
4:L:94:ASP:OD1	4:L:95:SER:N	2.48	0.47
4:N:13:THR:HG23	4:N:14:PRO:HD2	1.97	0.47
1:A:314:GLN:O	1:A:314:GLN:HG2	2.15	0.47
1:A:364:ASP:O	1:A:367:VAL:HG22	2.14	0.47
1:B:503:VAL:HG23	1:B:506:GLN:HE21	1.80	0.47
1:C:70:VAL:HG21	1:C:255:SER:HA	1.97	0.47
1:C:126:VAL:HG22	1:C:173:GLN:O	2.15	0.47
1:C:350:VAL:HG21	1:C:418:ILE:HB	1.95	0.47
4:L:50:HIS:CE1	5:M:108:ILE:HD12	2.50	0.47
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.61	0.47
1:A:398:ASP:O	1:A:511:VAL:HA	2.15	0.47
1:B:282:ASN:ND2	6:B:1303:NAG:H2	2.30	0.47
6:B:1312:NAG:O7	6:B:1312:NAG:O3	2.32	0.47
1:C:326:ILE:HG12	1:C:540:ASN:O	2.14	0.47
1:C:617:CYS:C	1:C:619:GLU:N	2.68	0.47
5:M:49:TRP:HE1	5:M:52:LEU:HG	1.80	0.47
5:M:65:LEU:HD22	5:M:68:ARG:HH22	1.79	0.47
1:B:517:LEU:HD22	1:C:983:ARG:NH2	2.29	0.46
1:C:175:PHE:O	1:C:176:LEU:HD23	2.15	0.46
1:C:455:LEU:HB3	1:C:493:GLN:OE1	2.15	0.46
1:C:532:ASN:OD1	1:C:533:LEU:N	2.48	0.46
1:C:754:LEU:HA	1:C:754:LEU:HD13	1.61	0.46
4:N:27:SER:HB2	4:N:94:ASP:OD1	2.14	0.46
1:B:616:ASN:OD1	1:B:616:ASN:C	2.54	0.46
1:C:54:LEU:HD23	1:C:272:PRO:HA	1.97	0.46
1:C:358:ILE:N	1:C:395:VAL:O	2.48	0.46
1:C:361:CYS:SG	1:C:524:VAL:HG23	2.55	0.46
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ASN:HB2	1:A:508:TYR:CE2	2.49	0.46
1:B:452:ARG:HE	1:B:492:LEU:HD23	1.80	0.46
1:B:764:LYS:O	1:B:768:THR:HG23	2.15	0.46
1:C:1002:GLN:O	1:C:1006:THR:HG23	2.15	0.46
1:C:342:PHE:CZ	1:C:434:ILE:HG21	2.50	0.46
2:J:2:ARG:CB	2:J:27:GLU:HB2	2.46	0.46
4:N:44:ALA:HB2	5:O:96:TYR:CE1	2.50	0.46
1:A:353:TRP:CZ2	1:A:466:ARG:HB2	2.51	0.46
1:B:242:LEU:N	1:B:242:LEU:HD22	2.31	0.46
1:C:388:ASN:O	1:C:527:PRO:HD3	2.16	0.46
1:C:657:ASN:HD21	6:C:1303:NAG:H2	1.80	0.46
1:C:1118:ASP:OD1	1:C:1119:ASN:N	2.48	0.46
2:J:43:ALA:HB2	3:K:94:TYR:CE1	2.50	0.46
1:A:426:PRO:N	1:A:463:PRO:HB3	2.30	0.46
1:A:456:PHE:HE2	1:A:489:TYR:CB	2.29	0.46
6:A:1304:NAG:HO6	6:A:1311:NAG:HO6	1.49	0.46
1:B:720:ILE:HG21	1:B:720:ILE:HD13	1.65	0.46
2:H:43:ALA:HB2	3:I:94:TYR:CE1	2.50	0.46
2:J:24:ARG:HE	2:J:24:ARG:HB2	1.34	0.46
5:O:100:ARG:HB2	5:O:109:TYR:HA	1.97	0.46
1:A:330:PRO:HD3	1:A:579:PRO:HB2	1.97	0.46
1:A:738:CYS:HB3	1:A:760:CYS:HB2	1.63	0.46
1:B:70:VAL:HG21	1:B:255:SER:CA	2.39	0.46
1:C:203:ILE:HB	1:C:227:VAL:HG23	1.98	0.46
1:C:1098:ASN:HD21	6:C:1307:NAG:C7	2.29	0.46
2:H:42:GLN:HE21	3:I:110:GLN:HA	1.81	0.46
3:I:82:MET:HB3	3:I:85:LEU:HD11	1.97	0.46
1:A:359:SER:OG	1:A:394:ASN:HA	2.16	0.46
1:A:581:THR:HG23	1:A:583:GLU:H	1.81	0.46
1:A:616:ASN:OD1	1:A:618:THR:N	2.43	0.46
1:B:62:VAL:HB	1:B:267:VAL:O	2.16	0.46
1:B:312:ILE:HD12	1:B:598:ILE:HD11	1.98	0.46
1:B:365:TYR:CD1	1:B:368:LEU:HD12	2.51	0.46
1:B:377:PHE:CB	1:B:434:ILE:HG22	2.45	0.46
2:J:11:LEU:HD23	2:J:106:LEU:HD12	1.98	0.46
2:J:34:ALA:HB1	2:J:46:LEU:HD13	1.97	0.46
5:M:12:VAL:O	5:M:121:VAL:HG13	2.15	0.46
4:N:4:LEU:O	4:N:102:GLY:HA2	2.15	0.46
5:O:100:ARG:NH1	5:O:107:PRO:HB3	2.31	0.46
1:A:532:ASN:OD1	1:A:533:LEU:N	2.49	0.46
1:C:461:LEU:HD23	1:C:461:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ASP:OD1	1:C:467:ASP:N	2.49	0.46
1:C:555:SER:HB2	1:C:584:ILE:HB	1.98	0.46
2:H:61:ARG:HH22	2:H:79:GLN:H	1.63	0.46
2:J:47:LEU:HD13	2:J:62:PHE:CE1	2.51	0.46
1:A:316:SER:O	1:A:595:VAL:HG12	2.16	0.46
1:A:347:PHE:HD2	1:A:400:PHE:N	2.13	0.46
1:B:364:ASP:O	1:B:367:VAL:HG12	2.15	0.46
1:C:327:VAL:HG12	1:C:529:LYS:O	2.16	0.46
1:C:364:ASP:O	1:C:367:VAL:HG22	2.16	0.46
1:C:725:GLU:OE1	1:C:1028:LYS:NZ	2.47	0.46
1:C:1000:ARG:O	1:C:1003:SER:OG	2.27	0.46
2:J:66:GLY:HA3	2:J:71:PHE:HA	1.97	0.46
3:K:6:GLU:OE2	3:K:95:CYS:HB2	2.16	0.46
3:K:86:ARG:HE	3:K:88:GLU:CD	2.19	0.46
1:A:361:CYS:O	1:A:524:VAL:HA	2.16	0.45
1:A:986:PRO:O	1:A:990:GLU:HG2	2.16	0.45
1:B:247:SER:HA	1:B:258:TRP:CE2	2.52	0.45
1:B:658:SER:OG	1:B:660:TYR:CZ	2.65	0.45
1:C:105:ILE:HG22	1:C:118:LEU:HG	1.96	0.45
1:C:490:PHE:CD1	1:C:491:PRO:HD2	2.51	0.45
1:C:735:SER:HB2	1:C:861:LEU:HD21	1.98	0.45
1:A:70:VAL:HA	1:A:80:ASP:HA	1.98	0.45
1:A:1129:VAL:HG13	1:A:1132:ILE:HB	1.98	0.45
1:B:536:ASN:HA	1:B:551:VAL:HG23	1.96	0.45
1:C:119:ILE:HG13	1:C:119:ILE:O	2.17	0.45
1:C:327:VAL:CG2	1:C:531:THR:HA	2.46	0.45
1:C:761:THR:OG1	1:C:762:GLN:N	2.49	0.45
3:I:39:GLN:HB2	3:I:45:LEU:HD23	1.98	0.45
3:I:40:ALA:CB	3:I:43:LYS:HD3	2.45	0.45
5:O:4:LEU:HD23	5:O:24:PHE:HB3	1.98	0.45
5:O:15:THR:O	5:O:15:THR:HG22	2.15	0.45
5:O:32:SER:HA	5:O:55:TRP:CD1	2.51	0.45
3:I:4:LEU:HD23	3:I:22:CYS:SG	2.56	0.45
2:J:38:GLN:HA	2:J:44:PRO:HA	1.98	0.45
4:N:40:LEU:HB3	4:N:43:THR:CG2	2.47	0.45
1:A:64:TRP:CD1	1:A:65:PHE:N	2.84	0.45
1:B:31:SER:N	1:B:60:SER:O	2.32	0.45
1:B:357:ARG:HH22	1:C:230:PRO:C	2.19	0.45
1:B:461:LEU:HD21	1:B:465:GLU:C	2.37	0.45
1:B:754:LEU:HD13	1:B:754:LEU:HA	1.72	0.45
1:B:1129:VAL:HG23	1:B:1132:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:67:PHE:CD1	3:K:82:MET:HA	2.51	0.45
5:O:13:ARG:NE	5:O:123:SER:HA	2.32	0.45
1:A:357:ARG:NE	1:A:359:SER:OG	2.39	0.45
1:A:1031:GLU:HA	1:C:1040:VAL:CG1	2.46	0.45
1:B:585:LEU:HD23	1:B:585:LEU:HA	1.75	0.45
1:C:336:CYS:HB2	1:C:337:PRO:CD	2.46	0.45
1:C:517:LEU:HD23	1:C:517:LEU:HA	1.72	0.45
1:C:603:ASN:ND2	6:C:1304:NAG:H2	2.31	0.45
1:C:981:LEU:HD23	1:C:981:LEU:HA	1.66	0.45
2:J:48:ILE:HG12	2:J:54:ARG:HA	1.98	0.45
2:J:94:TRP:CE2	3:K:100:GLY:HA3	2.51	0.45
5:M:12:VAL:HG12	5:M:121:VAL:HG22	1.99	0.45
4:N:2:SER:HA	4:N:93:ASP:OD2	2.16	0.45
4:N:34:VAL:HB	4:N:52:ASN:ND2	2.31	0.45
1:A:486:VAL:HG13	1:A:487:ASN:N	2.32	0.45
1:B:357:ARG:HH12	1:C:232:GLY:N	2.15	0.45
1:B:391:CYS:CA	1:B:525:CYS:HB3	2.39	0.45
1:B:616:ASN:HD22	6:B:1310:NAG:C7	2.30	0.45
1:C:316:SER:O	1:C:595:VAL:HG12	2.16	0.45
3:I:47:TRP:HZ2	3:I:50:VAL:CG1	2.29	0.45
4:L:37:PHE:CE2	4:L:47:LEU:HD13	2.52	0.45
5:M:6:GLU:OE1	5:M:97:CYS:N	2.35	0.45
1:A:57:PRO:HB3	1:A:273:ARG:NH1	2.32	0.45
1:A:441:LEU:HB3	5:M:32:SER:OG	2.16	0.45
1:A:773:GLU:OE1	1:A:1019:ARG:HD3	2.17	0.45
1:B:350:VAL:CG2	1:B:418:ILE:HG12	2.47	0.45
1:B:377:PHE:HB3	1:B:434:ILE:HG22	1.98	0.45
1:C:440:LYS:HD2	5:O:103:GLY:O	2.15	0.45
1:C:861:LEU:HD13	1:C:861:LEU:N	2.32	0.45
4:N:4:LEU:HD13	4:N:89:CYS:HB3	1.98	0.45
5:O:17:THR:OG1	5:O:85:THR:HG22	2.15	0.45
5:O:53:ILE:HD12	5:O:59:LYS:HD3	1.98	0.45
1:A:335:LEU:HD13	1:A:335:LEU:HA	1.67	0.45
1:C:326:ILE:HG12	1:C:541:PHE:HA	1.99	0.45
1:C:421:TYR:CE1	1:C:457:ARG:HB3	2.52	0.45
1:C:470:THR:HB	1:C:490:PHE:CZ	2.52	0.45
2:H:2:ARG:CB	2:H:90:GLN:HE22	2.30	0.45
4:N:6:GLN:HG3	4:N:103:GLY:H	1.82	0.45
5:O:39:ILE:HD13	5:O:113:TRP:CH2	2.52	0.45
5:O:53:ILE:HG21	5:O:73:LYS:CE	2.47	0.45
1:A:118:LEU:C	1:A:118:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:PHE:O	1:B:491:PRO:HA	2.16	0.45
1:C:473:TYR:OH	3:K:31:ARG:O	2.13	0.45
5:M:70:THR:CG2	5:M:83:THR:HB	2.46	0.45
4:N:39:GLN:HG3	4:N:45:PRO:HG3	1.98	0.45
1:A:393:THR:HB	1:A:516:GLU:CB	2.47	0.45
1:B:423:TYR:HD1	1:B:465:GLU:O	2.00	0.45
1:B:424:LYS:O	1:B:463:PRO:HA	2.17	0.45
1:B:826:VAL:HG23	1:B:949:GLN:OE1	2.17	0.45
1:B:1097:SER:HB2	1:B:1102:TRP:CE2	2.51	0.45
1:A:456:PHE:HE2	1:A:489:TYR:HB3	1.82	0.44
1:A:490:PHE:CG	1:A:491:PRO:HD2	2.52	0.44
1:B:424:LYS:O	1:B:464:PHE:N	2.45	0.44
1:B:861:LEU:H	1:B:861:LEU:HG	1.46	0.44
1:C:351:TYR:CE1	1:C:492:LEU:HD21	2.52	0.44
2:H:11:LEU:HD21	2:H:106:LEU:HG	1.99	0.44
4:L:70:THR:HG22	4:L:70:THR:O	2.17	0.44
4:N:107:LEU:HD23	4:N:107:LEU:O	2.17	0.44
1:A:826:VAL:CG1	1:A:1057:PRO:HG2	2.47	0.44
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.47	0.44
1:C:440:LYS:HA	5:O:107:PRO:HD3	1.99	0.44
4:L:18:VAL:HB	4:L:76:ILE:HD11	2.00	0.44
4:L:29:ILE:HD11	4:L:72:ALA:HB2	1.98	0.44
4:N:5:THR:O	4:N:22:CYS:HA	2.17	0.44
5:O:92:THR:HA	5:O:119:VAL:O	2.17	0.44
1:B:334:ASN:OD1	1:B:334:ASN:O	2.35	0.44
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.98	0.44
1:B:821:LEU:HA	1:B:821:LEU:HD12	1.76	0.44
1:C:456:PHE:HE1	3:K:33:TYR:HD2	1.63	0.44
2:H:36:TYR:HE2	2:H:89:GLN:HB3	1.82	0.44
3:K:27:ILE:HD13	3:K:97:ARG:HD2	1.99	0.44
3:K:30:SER:HB3	3:K:73:ASN:CB	2.47	0.44
6:A:1305:NAG:O7	6:A:1305:NAG:O3	2.30	0.44
1:B:393:THR:HG23	1:B:516:GLU:O	2.18	0.44
1:B:806:LEU:HA	1:B:806:LEU:HD23	1.85	0.44
1:C:398:ASP:O	1:C:511:VAL:HA	2.16	0.44
1:C:405:ASN:OD1	1:C:405:ASN:N	2.51	0.44
1:C:657:ASN:HD21	6:C:1303:NAG:C2	2.31	0.44
3:I:38:ARG:HD2	3:I:93:TYR:CZ	2.52	0.44
2:J:33:LEU:HB3	2:J:50:GLY:O	2.17	0.44
1:A:240:THR:HG22	1:A:241:LEU:N	2.33	0.44
1:A:348:ALA:HB2	1:A:354:ASN:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:CYS:N	1:A:523:THR:O	2.42	0.44
1:B:196:ASN:HB2	1:B:201:PHE:HD1	1.81	0.44
1:B:439:ASN:HA	1:B:507:PRO:HD2	2.00	0.44
2:J:33:LEU:HA	2:J:89:GLN:O	2.17	0.44
1:C:68:ILE:HG13	1:C:69:HIS:N	2.23	0.44
3:K:63:VAL:HB	3:K:67:PHE:CD2	2.53	0.44
1:A:129:LYS:HB3	1:A:131:CYS:SG	2.58	0.44
1:A:322:PRO:HA	1:A:538:CYS:O	2.17	0.44
1:B:99:ASN:HB3	1:B:102:ARG:NH1	2.32	0.44
1:B:142:ASP:HA	1:B:157:PHE:O	2.17	0.44
1:C:468:ILE:O	1:C:470:THR:HG23	2.17	0.44
3:K:29:VAL:HG21	3:K:77:THR:C	2.37	0.44
5:M:71:ILE:HD12	5:M:81:VAL:O	2.18	0.44
5:O:66:ARG:HA	5:O:66:ARG:HD2	1.73	0.44
1:A:88:ASP:N	1:A:88:ASP:OD1	2.49	0.44
1:A:200:TYR:CD2	1:A:230:PRO:HA	2.53	0.44
1:A:616:ASN:ND2	6:A:1310:NAG:C7	2.81	0.44
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.00	0.44
1:A:754:LEU:HD13	1:A:754:LEU:HA	1.65	0.44
1:B:662:CYS:HB2	1:B:697:MET:HG2	2.00	0.44
1:C:334:ASN:O	1:C:362:VAL:HB	2.17	0.44
1:C:345:THR:OG1	5:O:31:ASN:HA	2.17	0.44
2:H:34:ALA:HB1	2:H:46:LEU:HD13	1.99	0.44
3:I:66:ARG:HH12	3:I:89:ASP:CG	2.22	0.44
2:J:19:ALA:O	2:J:74:THR:HA	2.18	0.44
4:L:40:LEU:HB3	4:L:43:THR:HG21	1.99	0.44
4:N:6:GLN:HE21	4:N:102:GLY:CA	2.29	0.44
1:B:402:ILE:HD12	1:B:402:ILE:HA	1.71	0.44
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.73	0.44
4:L:22:CYS:HB3	4:L:72:ALA:HB3	2.00	0.44
1:A:54:LEU:HD23	1:A:272:PRO:HA	2.00	0.43
1:A:204:TYR:CD2	1:A:225:PRO:HA	2.53	0.43
1:A:761:THR:OG1	1:A:762:GLN:N	2.51	0.43
1:B:546:LEU:HD13	1:B:546:LEU:HA	1.84	0.43
1:B:560:LEU:N	1:B:563:GLN:OE1	2.41	0.43
1:C:431:GLY:HA2	1:C:515:PHE:CE2	2.53	0.43
1:C:439:ASN:O	5:O:107:PRO:HD3	2.18	0.43
1:C:603:ASN:CG	6:C:1304:NAG:H2	2.38	0.43
1:C:616:ASN:ND2	6:C:1308:NAG:C7	2.81	0.43
3:K:97:ARG:NH2	3:K:99:LEU:HD21	2.32	0.43
5:M:43:PRO:HD3	5:M:92:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:TRP:O	1:A:887:THR:C	2.56	0.43
1:A:1001:LEU:HD12	1:A:1001:LEU:HA	1.73	0.43
1:B:453:TYR:O	1:B:492:LEU:HD12	2.18	0.43
1:B:560:LEU:HD23	1:B:560:LEU:HA	1.70	0.43
1:B:581:THR:HB	6:B:1305:NAG:O6	2.18	0.43
1:B:1145:LEU:HA	1:C:1146:ASP:OD2	2.18	0.43
1:C:36:VAL:HG23	1:C:222:ALA:HA	2.00	0.43
1:C:309:GLU:OE1	1:C:309:GLU:N	2.49	0.43
1:C:424:LYS:HB3	1:C:461:LEU:HG	2.00	0.43
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.00	0.43
3:K:12:VAL:CG2	3:K:85:LEU:HD12	2.41	0.43
1:A:31:SER:O	1:A:59:PHE:N	2.51	0.43
1:A:130:VAL:CG1	1:A:168:PHE:HB3	2.49	0.43
1:A:364:ASP:OD1	1:A:367:VAL:HG13	2.17	0.43
1:B:457:ARG:HD2	1:B:457:ARG:HA	1.85	0.43
2:H:44:PRO:HD2	3:I:108:TRP:CZ3	2.53	0.43
3:I:19:ARG:HE	3:I:81:GLN:NE2	2.15	0.43
5:O:34:VAL:O	5:O:55:TRP:HB3	2.17	0.43
1:A:327:VAL:HG12	1:A:531:THR:CG2	2.47	0.43
1:A:584:ILE:C	1:A:585:LEU:HD22	2.38	0.43
1:B:81:ASN:OD1	1:B:82:PRO:HD2	2.19	0.43
1:C:326:ILE:HG21	1:C:326:ILE:HD13	1.79	0.43
1:C:345:THR:HG23	1:C:346:ARG:N	2.33	0.43
1:C:452:ARG:HE	1:C:490:PHE:HE2	1.65	0.43
5:O:53:ILE:HD12	5:O:59:LYS:CE	2.48	0.43
5:O:66:ARG:HH21	5:O:67:SER:H	1.67	0.43
1:A:471:GLU:H	1:A:471:GLU:HG3	1.68	0.43
1:A:487:ASN:HA	1:A:489:TYR:CE2	2.53	0.43
1:B:353:TRP:NE1	1:B:423:TYR:CD2	2.83	0.43
1:B:559:PHE:CD2	1:B:584:ILE:HD12	2.54	0.43
1:B:580:GLN:C	6:B:1305:NAG:H5	2.39	0.43
1:B:801:ASN:ND2	6:B:1312:NAG:N2	2.63	0.43
1:C:70:VAL:HG22	1:C:80:ASP:CB	2.49	0.43
1:C:128:ILE:HD13	1:C:170:TYR:CD1	2.54	0.43
3:K:75:LYS:HE3	3:K:77:THR:OG1	2.17	0.43
1:A:229:LEU:N	1:A:229:LEU:HD12	2.33	0.43
1:A:389:ASP:N	1:A:389:ASP:OD1	2.44	0.43
1:B:360:ASN:H	1:B:523:THR:CB	2.32	0.43
1:C:709:ASN:ND2	6:C:1309:NAG:O5	2.46	0.43
3:I:29:VAL:HG23	3:I:34:MET:HG3	2.01	0.43
1:A:44:ARG:O	1:A:283:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ALA:HB2	1:A:510:VAL:HG12	2.00	0.43
1:A:727:LEU:O	1:A:1059:GLY:HA3	2.18	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.64	0.43
1:B:962:LEU:HD12	1:B:962:LEU:HA	1.77	0.43
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.54	0.43
1:C:351:TYR:HB3	1:C:422:ASN:ND2	2.21	0.43
1:C:403:ARG:HD3	1:C:505:HIS:CG	2.53	0.43
3:I:33:TYR:CE1	3:I:52:PHE:CD1	3.07	0.43
5:O:59:LYS:NZ	5:O:71:ILE:HG23	2.32	0.43
1:A:325:SER:OG	1:A:540:ASN:HB2	2.18	0.43
1:C:99:ASN:HB3	1:C:102:ARG:NH1	2.33	0.43
1:C:418:ILE:HA	1:C:422:ASN:OD1	2.19	0.43
1:C:773:GLU:OE2	1:C:1019:ARG:HD3	2.18	0.43
1:C:886:TRP:HH2	1:C:904:TYR:HB3	1.83	0.43
4:L:4:LEU:HD23	4:L:4:LEU:HA	1.89	0.43
5:O:53:ILE:HG21	5:O:73:LYS:HE2	2.01	0.43
1:A:42:VAL:HG22	1:C:565:PHE:HB2	2.01	0.43
1:A:196:ASN:ND2	1:A:201:PHE:HB2	2.34	0.43
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.83	0.43
1:C:448:ASN:N	1:C:497:PHE:O	2.50	0.43
2:H:93:ASN:OD1	2:H:93:ASN:N	2.51	0.43
4:L:99:TRP:HB2	5:M:49:TRP:CB	2.49	0.43
5:M:53:ILE:HD13	5:M:71:ILE:HG13	2.00	0.43
1:A:403:ARG:HG3	1:A:497:PHE:HE1	1.84	0.43
1:B:335:LEU:HA	1:B:335:LEU:HD23	1.82	0.43
1:B:353:TRP:HB2	1:B:400:PHE:HB3	2.00	0.43
1:B:1024:LEU:O	1:B:1027:THR:OG1	2.35	0.43
1:C:131:CYS:HB3	1:C:166:CYS:CA	2.49	0.43
1:C:298:GLU:O	1:C:302:THR:HG23	2.19	0.43
1:C:516:GLU:O	1:C:517:LEU:HD23	2.19	0.43
2:H:29:VAL:HG12	2:H:29:VAL:O	2.19	0.43
5:M:54:TYR:HE2	5:M:60:ARG:HE	1.64	0.43
4:N:52:ASN:ND2	4:N:67:ASN:HB2	2.34	0.43
4:N:98:SER:HB3	5:O:63:PRO:HD2	2.01	0.43
5:O:4:LEU:O	5:O:5:LYS:HD2	2.19	0.43
1:A:518:LEU:HD23	1:A:518:LEU:H	1.84	0.42
1:C:328:ARG:HA	1:C:542:ASN:O	2.20	0.42
1:C:762:GLN:H	1:C:762:GLN:HG3	1.54	0.42
1:C:801:ASN:ND2	6:C:1310:NAG:N2	2.60	0.42
6:C:1307:NAG:O7	6:C:1307:NAG:O3	2.32	0.42
2:H:2:ARG:O	2:H:90:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:18:VAL:CG1	4:N:79:LEU:HD11	2.47	0.42
1:A:387:LEU:HD11	1:A:515:PHE:CE2	2.53	0.42
1:A:760:CYS:HA	1:A:763:LEU:HG	2.00	0.42
1:C:353:TRP:CZ2	1:C:466:ARG:HB2	2.55	0.42
1:C:359:SER:OG	1:C:394:ASN:HA	2.18	0.42
1:C:403:ARG:HG3	1:C:497:PHE:HE1	1.84	0.42
1:C:544:ASN:OD1	1:C:579:PRO:HB3	2.19	0.42
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.85	0.42
1:C:822:LEU:HA	1:C:822:LEU:HD23	1.83	0.42
1:C:1005:GLN:O	1:C:1008:VAL:HG12	2.19	0.42
3:K:39:GLN:O	3:K:91:ALA:HB1	2.19	0.42
3:K:60:ALA:O	3:K:64:LYS:HB2	2.19	0.42
5:M:74:ALA:CB	5:M:79:GLN:HE21	2.31	0.42
5:O:68:ARG:NH1	5:O:88:ASP:OD1	2.52	0.42
5:O:70:THR:CG2	5:O:83:THR:HB	2.45	0.42
1:A:118:LEU:CD2	1:A:120:VAL:HG23	2.50	0.42
1:B:341:VAL:HG13	1:B:342:PHE:HD1	1.82	0.42
1:B:375:PHE:HB2	1:B:436:TRP:HA	2.02	0.42
1:C:231:ILE:HG23	1:C:233:ILE:HG23	2.00	0.42
1:C:435:ALA:CB	1:C:510:VAL:HG22	2.49	0.42
1:C:962:LEU:HA	1:C:962:LEU:HD12	1.74	0.42
2:H:77:SER:O	2:H:77:SER:OG	2.37	0.42
3:I:3:GLN:O	3:I:24:ALA:HA	2.20	0.42
3:I:115:THR:HG22	3:I:116:VAL:N	2.34	0.42
3:K:14:PRO:HA	3:K:85:LEU:O	2.19	0.42
3:K:36:TRP:HE1	3:K:78:LEU:CG	2.32	0.42
3:K:57:THR:OG1	3:K:69:ILE:HG21	2.19	0.42
4:L:17:ARG:NH1	4:L:75:ALA:HB1	2.34	0.42
5:M:63:PRO:O	5:M:66:ARG:HG2	2.18	0.42
1:B:347:PHE:O	1:B:401:VAL:HG12	2.20	0.42
1:B:815:ARG:NH2	1:B:820:ASP:OD1	2.52	0.42
3:I:90:THR:HA	3:I:114:VAL:O	2.19	0.42
2:J:27:GLU:O	2:J:69:THR:HG22	2.19	0.42
2:J:43:ALA:HB2	3:K:94:TYR:CD1	2.53	0.42
5:M:79:GLN:NE2	5:M:81:VAL:HG13	2.29	0.42
1:A:124:THR:HG23	1:A:125:ASN:OD1	2.19	0.42
1:A:650:LEU:HA	1:A:650:LEU:HD12	1.82	0.42
1:A:1129:VAL:HG23	1:B:917:TYR:HB3	2.02	0.42
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.83	0.42
1:C:197:ILE:HG13	1:C:198:ASP:N	2.33	0.42
1:C:444:LYS:HZ1	5:O:56:ASP:CG	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ILE:H	1:C:569:ILE:HD12	1.84	0.42
2:H:33:LEU:O	2:H:91:TYR:HE1	2.02	0.42
2:H:81:GLU:OE1	2:H:81:GLU:N	2.52	0.42
2:H:91:TYR:CE2	3:I:101:VAL:HA	2.33	0.42
2:J:107:GLU:N	2:J:107:GLU:OE2	2.52	0.42
3:K:22:CYS:O	3:K:77:THR:HB	2.20	0.42
5:M:54:TYR:HD1	5:M:100:ARG:NH2	2.17	0.42
5:O:28:SER:O	5:O:34:VAL:HG11	2.20	0.42
5:O:45:LYS:HG2	5:O:46:ALA:H	1.84	0.42
1:A:70:VAL:HA	1:A:80:ASP:CA	2.49	0.42
1:B:398:ASP:HB2	1:B:512:VAL:CG2	2.49	0.42
1:B:605:SER:OG	1:B:606:ASN:N	2.52	0.42
1:C:133:PHE:HA	1:C:163:ALA:O	2.19	0.42
1:C:426:PRO:HG3	1:C:463:PRO:CB	2.50	0.42
1:C:727:LEU:O	1:C:1059:GLY:HA3	2.19	0.42
1:C:752:LEU:HD12	1:C:752:LEU:HA	1.85	0.42
1:C:934:ILE:HD13	1:C:934:ILE:HA	1.86	0.42
1:C:989:ALA:O	1:C:993:ILE:HG12	2.19	0.42
2:J:4:MET:SD	2:J:25:ALA:HB2	2.60	0.42
1:A:345:THR:HG23	1:A:346:ARG:N	2.35	0.42
1:A:805:ILE:HG21	1:A:805:ILE:HD13	1.81	0.42
1:C:350:VAL:HG13	1:C:422:ASN:ND2	2.35	0.42
2:J:33:LEU:N	2:J:91:TYR:CE1	2.88	0.42
4:L:35:TYR:OH	5:M:109:TYR:HB2	2.19	0.42
5:O:99:HIS:HD2	5:O:112:PHE:CD2	2.26	0.42
1:A:416:GLY:O	1:A:420:ASP:HB2	2.20	0.42
1:B:117:LEU:HD21	1:B:119:ILE:HG13	2.00	0.42
1:B:1054:GLN:HA	1:B:1054:GLN:NE2	2.35	0.42
1:C:603:ASN:OD1	6:C:1304:NAG:H2	2.20	0.42
1:C:720:ILE:HD13	1:C:720:ILE:HG21	1.70	0.42
2:J:33:LEU:O	2:J:91:TYR:HE1	2.03	0.42
3:K:3:GLN:O	3:K:4:LEU:HD12	2.20	0.42
4:L:80:ARG:NE	4:L:82:GLU:OE2	2.53	0.42
5:O:12:VAL:HG22	5:O:16:GLN:HB3	2.02	0.42
1:A:405:ASN:N	1:A:405:ASN:OD1	2.44	0.42
1:B:133:PHE:HA	1:B:163:ALA:O	2.20	0.42
1:B:200:TYR:HB3	1:B:228:ASP:OD1	2.20	0.42
1:B:437:ASN:ND2	1:B:508:TYR:OH	2.53	0.42
1:B:865:LEU:HD23	1:B:865:LEU:HA	1.80	0.42
1:C:378:LYS:O	1:C:432:CYS:HB2	2.20	0.42
1:C:544:ASN:ND2	1:C:579:PRO:HG3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.55	0.42
4:N:87:TYR:CE1	4:N:107:LEU:HD13	2.55	0.42
5:O:99:HIS:CD2	5:O:112:PHE:HD2	2.27	0.42
1:A:81:ASN:OD1	1:A:82:PRO:HD2	2.20	0.42
1:A:140:PHE:CE1	1:A:159:VAL:HA	2.55	0.42
1:A:340:GLU:OE2	1:A:340:GLU:N	2.53	0.42
1:A:347:PHE:CD1	1:A:509:ARG:HD3	2.55	0.42
1:C:64:TRP:CD1	1:C:65:PHE:N	2.87	0.42
1:C:272:PRO:C	1:C:273:ARG:HG2	2.39	0.42
1:C:392:PHE:CD2	1:C:515:PHE:HB3	2.55	0.42
1:C:453:TYR:O	1:C:492:LEU:HA	2.19	0.42
1:C:1129:VAL:HG13	1:C:1132:ILE:HB	2.02	0.42
3:K:9:GLY:CA	3:K:113:LEU:O	2.68	0.42
4:L:16:GLN:HE21	4:L:18:VAL:CG2	2.33	0.42
4:L:44:ALA:HB2	5:M:96:TYR:CD1	2.54	0.42
4:N:64:SER:O	4:N:74:LEU:HD12	2.19	0.42
5:O:54:TYR:HE2	5:O:60:ARG:HE	1.68	0.42
1:A:341:VAL:HG21	1:A:397:ALA:HB1	2.01	0.41
1:A:1049:LEU:HD23	1:A:1049:LEU:HA	1.73	0.41
1:B:226:LEU:HA	1:B:226:LEU:HD12	1.88	0.41
1:B:308:VAL:N	1:B:602:THR:OG1	2.45	0.41
1:C:353:TRP:CZ3	1:C:355:ARG:HD3	2.37	0.41
2:J:36:TYR:OH	3:K:105:THR:HB	2.20	0.41
1:B:131:CYS:HA	1:B:166:CYS:HA	2.01	0.41
1:B:315:THR:HG23	1:B:316:SER:N	2.36	0.41
1:C:335:LEU:CG	1:C:336:CYS:H	2.32	0.41
2:J:108:ILE:C	2:J:109:LYS:HG3	2.40	0.41
4:L:60:PRO:HG2	4:L:80:ARG:HH12	1.85	0.41
4:L:106:LYS:HA	4:L:106:LYS:HD3	1.85	0.41
5:M:21:THR:HG23	5:M:79:GLN:OE1	2.20	0.41
1:A:190:ARG:HH21	1:A:207:HIS:CD2	2.39	0.41
1:A:231:ILE:HG22	1:A:233:ILE:H	1.85	0.41
1:A:351:TYR:CD2	1:A:492:LEU:HD11	2.55	0.41
1:B:805:ILE:HD13	1:B:805:ILE:HG21	1.80	0.41
1:B:822:LEU:HD23	1:B:822:LEU:HA	1.85	0.41
2:J:29:VAL:HG11	2:J:33:LEU:HD13	2.02	0.41
2:J:62:PHE:HB3	2:J:73:LEU:HD11	2.02	0.41
5:M:3:THR:HA	5:M:112:PHE:CE2	2.55	0.41
4:N:66:SER:OG	4:N:73:SER:HB3	2.20	0.41
5:O:65:LEU:HG	5:O:69:LEU:HD11	2.03	0.41
1:A:348:ALA:HB1	1:A:352:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LYS:O	1:A:499:PRO:HD3	2.19	0.41
1:B:335:LEU:HD23	1:B:362:VAL:HB	2.01	0.41
1:B:650:LEU:HD12	1:B:650:LEU:HA	1.70	0.41
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.82	0.41
1:B:1140:PRO:O	1:B:1143:PRO:HD2	2.20	0.41
1:C:758:SER:O	1:C:762:GLN:HG3	2.20	0.41
2:J:76:SER:OG	2:J:77:SER:N	2.53	0.41
5:M:65:LEU:CD2	5:M:68:ARG:HH22	2.34	0.41
5:M:68:ARG:HE	5:M:84:MET:CG	2.33	0.41
5:O:73:LYS:HA	5:O:73:LYS:HD3	1.68	0.41
1:A:204:TYR:CD1	1:A:204:TYR:N	2.88	0.41
1:A:497:PHE:CD1	1:A:507:PRO:HD3	2.55	0.41
1:A:578:ASP:O	1:A:582:LEU:HA	2.21	0.41
1:B:280:ASN:OD1	1:B:284:THR:N	2.29	0.41
1:B:457:ARG:NH2	1:B:491:PRO:HB3	2.35	0.41
1:B:1001:LEU:HA	1:B:1001:LEU:HD12	1.76	0.41
1:C:444:LYS:O	1:C:499:PRO:HD3	2.20	0.41
3:I:4:LEU:HD23	3:I:95:CYS:SG	2.61	0.41
1:A:676:THR:HA	1:A:690:GLN:N	2.35	0.41
1:B:308:VAL:HG22	1:B:602:THR:OG1	2.21	0.41
1:C:315:THR:HG23	1:C:316:SER:N	2.35	0.41
1:C:486:VAL:HG13	1:C:487:ASN:N	2.34	0.41
1:C:810:SER:OG	1:C:811:LYS:N	2.54	0.41
2:H:49:TYR:CD2	3:I:103:GLY:HA2	2.56	0.41
3:K:72:ASP:HB2	3:K:79:TYR:CE2	2.53	0.41
5:O:89:PRO:O	5:O:92:THR:HG23	2.19	0.41
1:A:36:VAL:H	1:A:36:VAL:HG22	1.69	0.41
1:A:106:PHE:HD1	1:A:238:PHE:HB2	1.82	0.41
1:A:394:ASN:OD1	1:A:394:ASN:N	2.53	0.41
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.35	0.41
1:B:44:ARG:NH1	1:B:49:HIS:CE1	2.89	0.41
1:B:129:LYS:HE2	1:B:131:CYS:SG	2.61	0.41
1:B:359:SER:HA	1:B:524:VAL:HG13	2.03	0.41
1:C:108:THR:HG22	1:C:114:THR:HG21	2.03	0.41
1:C:128:ILE:HD12	1:C:128:ILE:N	2.36	0.41
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.55	0.41
1:C:456:PHE:CE1	3:K:33:TYR:HD2	2.38	0.41
1:C:742:ILE:O	1:C:1000:ARG:NH2	2.45	0.41
1:C:1004:LEU:HD12	1:C:1004:LEU:HA	1.78	0.41
2:H:33:LEU:HD22	2:H:71:PHE:CG	2.56	0.41
3:I:29:VAL:HG12	3:I:76:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:17:ARG:HA	4:N:76:ILE:O	2.20	0.41
1:A:115:GLN:HA	1:A:132:GLU:CB	2.51	0.41
1:B:46:SER:HA	1:B:279:TYR:O	2.21	0.41
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.56	0.41
1:B:106:PHE:HB3	1:B:235:ILE:HG21	2.03	0.41
1:B:380:TYR:CD2	1:B:380:TYR:N	2.88	0.41
1:B:513:LEU:HB3	1:B:515:PHE:HE1	1.85	0.41
1:C:330:PRO:HA	1:C:544:ASN:ND2	2.34	0.41
1:C:1024:LEU:HD12	1:C:1024:LEU:HA	1.76	0.41
3:I:93:TYR:O	3:I:111:GLY:HA2	2.20	0.41
1:A:330:PRO:CD	1:A:579:PRO:HB2	2.51	0.41
1:A:996:LEU:HA	1:A:996:LEU:HD23	1.75	0.41
1:B:294:ASP:O	1:B:297:SER:OG	2.37	0.41
1:B:331:ASN:OD1	1:B:331:ASN:N	2.46	0.41
1:B:433:VAL:HA	1:B:511:VAL:O	2.21	0.41
6:B:1303:NAG:O7	6:B:1303:NAG:O3	2.30	0.41
1:C:168:PHE:CD2	1:C:231:ILE:HD11	2.56	0.41
1:C:231:ILE:HD12	1:C:231:ILE:N	2.35	0.41
1:C:387:LEU:HA	1:C:387:LEU:HD12	1.70	0.41
1:C:444:LYS:HD3	5:O:54:TYR:CG	2.55	0.41
1:C:449:TYR:HA	1:C:494:SER:OG	2.20	0.41
1:C:1041:ASP:OD1	1:C:1041:ASP:O	2.39	0.41
2:H:61:ARG:NH2	2:H:79:GLN:HG2	2.36	0.41
3:I:3:GLN:O	3:I:4:LEU:HD12	2.21	0.41
3:I:69:ILE:HD11	3:I:78:LEU:HD11	2.02	0.41
2:J:21:LEU:O	2:J:72:THR:HA	2.20	0.41
2:J:24:ARG:NE	2:J:70:GLU:OE1	2.53	0.41
2:J:29:VAL:HG12	2:J:29:VAL:O	2.21	0.41
2:J:35:TRP:CE2	2:J:88:CYS:HB3	2.56	0.41
2:J:44:PRO:HD2	3:K:108:TRP:CE3	2.56	0.41
2:J:96:PRO:HG3	3:K:58:PHE:CD2	2.56	0.41
2:J:96:PRO:HB2	3:K:47:TRP:CH2	2.55	0.41
5:M:9:LEU:O	5:M:9:LEU:HD12	2.21	0.41
5:M:50:LEU:HD21	5:M:69:LEU:HD22	2.01	0.41
4:N:36:TRP:HA	4:N:88:TYR:O	2.20	0.41
1:A:106:PHE:CE1	1:A:238:PHE:HB2	2.54	0.41
1:A:411:ALA:HB3	1:A:414:GLN:OE1	2.21	0.41
1:A:592:PHE:HE2	1:B:857:GLY:HA2	1.86	0.41
1:B:329:PHE:N	1:B:530:SER:OG	2.37	0.41
1:B:559:PHE:HB3	1:B:577:ARG:NH1	2.36	0.41
1:B:620:VAL:O	1:B:620:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLN:HA	1:C:132:GLU:CB	2.51	0.41
2:J:94:TRP:HA	2:J:94:TRP:CE3	2.56	0.41
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.57	0.40
1:A:390:LEU:HD23	1:A:392:PHE:CE2	2.57	0.40
1:B:1045:LYS:O	1:B:1066:THR:HG21	2.22	0.40
1:B:1139:ASP:OD1	1:B:1139:ASP:N	2.45	0.40
1:C:347:PHE:CB	1:C:401:VAL:HG13	2.51	0.40
1:C:461:LEU:HD12	1:C:465:GLU:O	2.21	0.40
1:C:471:GLU:O	1:C:491:PRO:HD3	2.21	0.40
2:H:8:PRO:O	2:H:104:THR:HG22	2.21	0.40
2:H:94:TRP:HA	2:H:94:TRP:CE3	2.56	0.40
2:J:16:GLY:HA2	2:J:77:SER:OG	2.20	0.40
3:K:61:ASP:HA	3:K:64:LYS:HB2	2.03	0.40
4:N:49:ILE:HD13	4:N:49:ILE:HA	2.00	0.40
5:O:13:ARG:NE	5:O:13:ARG:HA	2.36	0.40
1:A:739:THR:H	1:A:739:THR:HG23	1.71	0.40
1:B:350:VAL:HG21	1:B:418:ILE:HG21	2.03	0.40
1:B:382:VAL:HA	1:C:983:ARG:O	2.21	0.40
1:C:117:LEU:C	1:C:118:LEU:HD12	2.42	0.40
2:H:5:THR:O	2:H:23:CYS:HA	2.22	0.40
2:H:47:LEU:HD23	2:H:58:ILE:HD12	2.03	0.40
2:H:102:GLN:NE2	2:H:103:GLY:O	2.54	0.40
3:I:61:ASP:OD1	3:I:62:SER:N	2.54	0.40
2:J:48:ILE:HG12	2:J:54:ARG:HG2	2.03	0.40
3:K:110:GLN:OE1	3:K:110:GLN:HA	2.21	0.40
5:M:62:ASN:ND2	5:M:65:LEU:HD12	2.36	0.40
4:N:28:ASN:HB3	4:N:93:ASP:CG	2.42	0.40
4:N:55:ARG:HG2	4:N:59:VAL:HB	2.04	0.40
1:B:130:VAL:HG13	1:B:130:VAL:O	2.21	0.40
1:B:1066:THR:HG22	1:B:1067:TYR:N	2.36	0.40
1:C:699:LEU:HA	1:C:699:LEU:HD23	1.90	0.40
1:C:977:LEU:HD21	1:C:1000:ARG:HH22	1.86	0.40
2:H:94:TRP:CE2	3:I:100:GLY:HA3	2.56	0.40
3:K:113:LEU:HD12	3:K:113:LEU:HA	1.88	0.40
4:L:63:PHE:CE1	4:L:76:ILE:HG22	2.57	0.40
4:N:70:THR:HG22	4:N:70:THR:O	2.21	0.40
1:A:106:PHE:HB3	1:A:235:ILE:CD1	2.51	0.40
1:A:452:ARG:HE	1:A:492:LEU:HD23	1.87	0.40
1:A:1019:ARG:NH1	1:C:1017:GLU:OE2	2.55	0.40
1:B:198:ASP:OD1	1:B:198:ASP:N	2.54	0.40
1:B:410:ILE:HD13	1:B:410:ILE:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:GLN:O	1:B:577:ARG:NH1	2.50	0.40
1:C:70:VAL:HG13	1:C:80:ASP:HA	2.02	0.40
1:C:204:TYR:CD1	1:C:204:TYR:N	2.89	0.40
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.71	0.40
2:H:27:GLU:OE1	2:H:28:SER:N	2.54	0.40
2:H:33:LEU:HG	2:H:34:ALA:H	1.87	0.40
2:H:83:SER:HA	2:H:106:LEU:O	2.22	0.40
2:H:90:GLN:O	2:H:98:TYR:HA	2.21	0.40
2:H:94:TRP:NE1	3:I:100:GLY:HA3	2.37	0.40
3:K:34:MET:HB3	3:K:78:LEU:CD2	2.50	0.40
4:L:87:TYR:CE1	4:L:107:LEU:HD23	2.56	0.40
1:A:312:ILE:HD12	1:A:598:ILE:HD11	2.03	0.40
1:B:337:PRO:HB2	1:B:340:GLU:OE2	2.22	0.40
1:B:826:VAL:CG1	1:B:1057:PRO:HG2	2.50	0.40
1:C:454:ARG:NH1	1:C:467:ASP:O	2.54	0.40
3:I:59:TYR:OH	3:I:69:ILE:HG22	2.22	0.40
5:M:100:ARG:NE	5:M:109:TYR:CZ	2.89	0.40
4:N:106:LYS:HA	4:N:106:LYS:HD3	1.82	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1008/1288 (78%)	952 (94%)	53 (5%)	3 (0%)	37	66
1	B	965/1288 (75%)	912 (94%)	51 (5%)	2 (0%)	44	71
1	C	1008/1288 (78%)	945 (94%)	57 (6%)	6 (1%)	22	53
2	H	107/109 (98%)	101 (94%)	4 (4%)	2 (2%)	6	29
2	J	107/109 (98%)	99 (92%)	6 (6%)	2 (2%)	6	29
3	I	116/118 (98%)	107 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
4	L	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
4	N	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
5	M	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
5	O	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
All	All	3883/4784 (81%)	3652 (94%)	216 (6%)	15 (0%)	32	61

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	PRO
1	B	333	THR
1	C	327	VAL
2	H	30	SER
2	H	94	TRP
2	J	94	TRP
1	A	330	PRO
1	A	334	ASN
1	B	528	LYS
1	C	228	ASP
1	C	333	THR
2	J	30	SER
1	C	527	PRO
1	C	860	VAL
1	C	332	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	811/1113 (73%)	800 (99%)	11 (1%)	62	78
1	B	776/1113 (70%)	765 (99%)	11 (1%)	62	78
1	C	810/1113 (73%)	795 (98%)	15 (2%)	52	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	88/90 (98%)	87 (99%)	1 (1%)	70	82
2	J	88/90 (98%)	86 (98%)	2 (2%)	45	68
3	I	89/94 (95%)	88 (99%)	1 (1%)	70	82
3	K	89/94 (95%)	89 (100%)	0	100	100
4	L	91/91 (100%)	91 (100%)	0	100	100
4	N	91/91 (100%)	91 (100%)	0	100	100
5	M	107/108 (99%)	106 (99%)	1 (1%)	75	85
5	O	107/108 (99%)	106 (99%)	1 (1%)	75	85
All	All	3147/4105 (77%)	3104 (99%)	43 (1%)	62	78

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ILE
1	A	333	THR
1	A	335	LEU
1	A	471	GLU
1	A	488	CYS
1	A	530	SER
1	A	538	CYS
1	A	617	CYS
1	A	760	CYS
1	A	860	VAL
1	A	861	LEU
1	B	131	CYS
1	B	166	CYS
1	B	331	ASN
1	B	432	CYS
1	B	524	VAL
1	B	617	CYS
1	B	859	THR
1	B	860	VAL
1	B	861	LEU
1	B	884	SER
1	B	886	TRP
1	C	131	CYS
1	C	166	CYS
1	C	227	VAL
1	C	228	ASP

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Mol	Chain	Res	Type
1	C	229	LEU
1	C	328	ARG
1	C	336	CYS
1	C	538	CYS
1	C	574	ASP
1	C	617	CYS
1	C	738	CYS
1	C	756	TYR
1	C	858	LEU
1	C	860	VAL
1	C	861	LEU
2	H	23	CYS
3	I	97	ARG
2	J	53	THR
2	J	109	LYS
5	M	13	ARG
5	O	16	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	165	ASN
1	A	234	ASN
1	A	370	ASN
1	A	450	ASN
1	A	477	ASN
1	A	505	HIS
1	A	657	ASN
1	A	709	ASN
1	A	801	ASN
1	A	1098	ASN
1	A	1134	ASN
1	B	49	HIS
1	B	234	ASN
1	B	282	ASN
1	B	388	ASN
1	B	394	ASN
1	B	437	ASN
1	B	506	GLN
1	B	709	ASN
1	B	801	ASN

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Mol	Chain	Res	Type
1	B	1074	ASN
1	B	1098	ASN
1	B	1134	ASN
1	C	165	ASN
1	C	282	ASN
1	C	417	ASN
1	C	439	ASN
1	C	450	ASN
1	C	544	ASN
1	C	657	ASN
1	C	801	ASN
1	C	1098	ASN
1	C	1134	ASN
2	H	6	GLN
2	H	102	GLN
3	I	81	GLN
3	K	13	GLN
3	K	81	GLN
4	L	1	GLN
4	L	6	GLN
4	L	16	GLN
4	L	32	ASN
4	L	50	HIS
5	M	79	GLN
4	N	6	GLN
4	N	52	ASN
5	O	31	ASN
5	O	78	ASN
5	O	86	ASN
5	O	99	HIS
5	O	104	HIS
5	O	105	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	B	1312	-	14,14,15	0.39	0	17,19,21	0.48	0
6	NAG	A	1307	-	14,14,15	0.25	0	17,19,21	0.49	0
6	NAG	C	1309	-	14,14,15	0.44	0	17,19,21	0.64	0
6	NAG	B	1303	-	14,14,15	0.34	0	17,19,21	0.44	0
6	NAG	B	1304	-	14,14,15	0.22	0	17,19,21	0.50	0
6	NAG	A	1311	-	14,14,15	0.49	0	17,19,21	0.63	0
6	NAG	C	1305	-	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	C	1312	-	14,14,15	0.36	0	17,19,21	0.48	0
6	NAG	A	1305	-	14,14,15	0.28	0	17,19,21	0.47	0
6	NAG	B	1310	-	14,14,15	0.32	0	17,19,21	0.59	0
6	NAG	C	1301	-	14,14,15	0.62	1 (7%)	17,19,21	0.56	0
6	NAG	C	1303	-	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	B	1305	-	14,14,15	0.24	0	17,19,21	0.49	0
6	NAG	B	1301	-	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	B	1306	-	14,14,15	0.34	0	17,19,21	0.52	0
6	NAG	A	1303	-	14,14,15	0.32	0	17,19,21	0.45	0
6	NAG	A	1306	-	14,14,15	0.29	0	17,19,21	0.70	0
6	NAG	A	1304	-	14,14,15	0.61	1 (7%)	17,19,21	0.56	0
6	NAG	A	1309	-	14,14,15	0.51	0	17,19,21	0.57	0
6	NAG	C	1308	-	14,14,15	0.29	0	17,19,21	0.53	0
6	NAG	A	1308	-	14,14,15	0.62	1 (7%)	17,19,21	0.59	0
6	NAG	C	1310	-	14,14,15	0.41	0	17,19,21	0.50	0
6	NAG	B	1307	-	14,14,15	0.53	0	17,19,21	0.63	0
6	NAG	B	1308	-	14,14,15	0.47	0	17,19,21	0.47	0
6	NAG	A	1312	-	14,14,15	0.42	0	17,19,21	0.45	0
6	NAG	B	1302	-	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	A	1310	-	14,14,15	0.27	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	1301	-	14,14,15	0.35	0	17,19,21	0.53	0
6	NAG	C	1311	-	14,14,15	0.26	0	17,19,21	0.47	0
6	NAG	C	1307	-	14,14,15	0.36	0	17,19,21	0.58	0
6	NAG	C	1306	-	14,14,15	0.64	1 (7%)	17,19,21	0.56	0
6	NAG	C	1302	-	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
6	NAG	B	1309	-	14,14,15	0.35	0	17,19,21	0.54	0
6	NAG	C	1304	-	14,14,15	0.26	0	17,19,21	0.59	0
6	NAG	A	1302	-	14,14,15	0.27	0	17,19,21	0.41	0
6	NAG	C	1313	-	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	B	1311	-	14,14,15	0.35	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1312	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1307	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1309	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	-	-	4/6/23/26	0/1/1/1
6	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1311	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1312	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1305	-	-	4/6/23/26	0/1/1/1
6	NAG	B	1310	-	-	1/6/23/26	0/1/1/1
6	NAG	C	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1305	-	-	4/6/23/26	0/1/1/1
6	NAG	B	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1306	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1304	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1309	-	-	1/6/23/26	0/1/1/1
6	NAG	C	1308	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1308	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1310	-	-	3/6/23/26	0/1/1/1
6	NAG	B	1307	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1308	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1312	-	-	4/6/23/26	0/1/1/1
6	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1310	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1311	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	-	-	3/6/23/26	0/1/1/1
6	NAG	B	1309	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1304	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1302	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1313	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1311	-	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1306	NAG	O5-C1	-2.21	1.40	1.43
6	A	1304	NAG	O5-C1	-2.12	1.40	1.43
6	A	1308	NAG	O5-C1	-2.04	1.40	1.43
6	C	1301	NAG	O5-C1	-2.02	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1302	NAG	C2-N2-C7	3.03	127.22	122.90

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1302	NAG	C1-C2-N2-C7
6	C	1309	NAG	C3-C2-N2-C7
6	C	1312	NAG	C3-C2-N2-C7
6	B	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1310	NAG	C4-C5-C6-O6
6	C	1311	NAG	C4-C5-C6-O6
6	A	1310	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	C	1304	NAG	C4-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	C	1302	NAG	O5-C5-C6-O6
6	C	1311	NAG	O5-C5-C6-O6
6	A	1305	NAG	C4-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	B	1306	NAG	C4-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	B	1308	NAG	C4-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	B	1305	NAG	C1-C2-N2-C7
6	A	1312	NAG	O5-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	A	1308	NAG	O5-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	A	1305	NAG	C1-C2-N2-C7
6	A	1312	NAG	C1-C2-N2-C7
6	B	1309	NAG	C1-C2-N2-C7
6	A	1308	NAG	C4-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1303	NAG	C4-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	C	1313	NAG	O5-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	B	1303	NAG	C1-C2-N2-C7
6	C	1307	NAG	C1-C2-N2-C7
6	C	1310	NAG	C1-C2-N2-C7
6	C	1313	NAG	C4-C5-C6-O6
6	B	1309	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	C	1301	NAG	C1-C2-N2-C7
6	B	1312	NAG	O5-C5-C6-O6
6	B	1312	NAG	C1-C2-N2-C7
6	C	1310	NAG	O5-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	A	1309	NAG	O5-C5-C6-O6
6	A	1304	NAG	C1-C2-N2-C7
6	B	1307	NAG	O5-C5-C6-O6
6	C	1304	NAG	C1-C2-N2-C7
6	B	1307	NAG	C4-C5-C6-O6
6	C	1312	NAG	C4-C5-C6-O6
6	A	1312	NAG	C4-C5-C6-O6
6	A	1302	NAG	C3-C2-N2-C7
6	A	1304	NAG	C3-C2-N2-C7
6	A	1307	NAG	C3-C2-N2-C7
6	A	1310	NAG	C3-C2-N2-C7
6	B	1303	NAG	C3-C2-N2-C7
6	B	1305	NAG	C3-C2-N2-C7
6	B	1310	NAG	C3-C2-N2-C7
6	C	1308	NAG	C3-C2-N2-C7
6	C	1312	NAG	O5-C5-C6-O6
6	C	1309	NAG	C1-C2-N2-C7
6	A	1305	NAG	C3-C2-N2-C7
6	A	1312	NAG	C3-C2-N2-C7
6	B	1309	NAG	C3-C2-N2-C7
6	B	1312	NAG	C3-C2-N2-C7
6	C	1301	NAG	C3-C2-N2-C7
6	C	1304	NAG	C3-C2-N2-C7
6	C	1307	NAG	C3-C2-N2-C7
6	C	1310	NAG	C3-C2-N2-C7

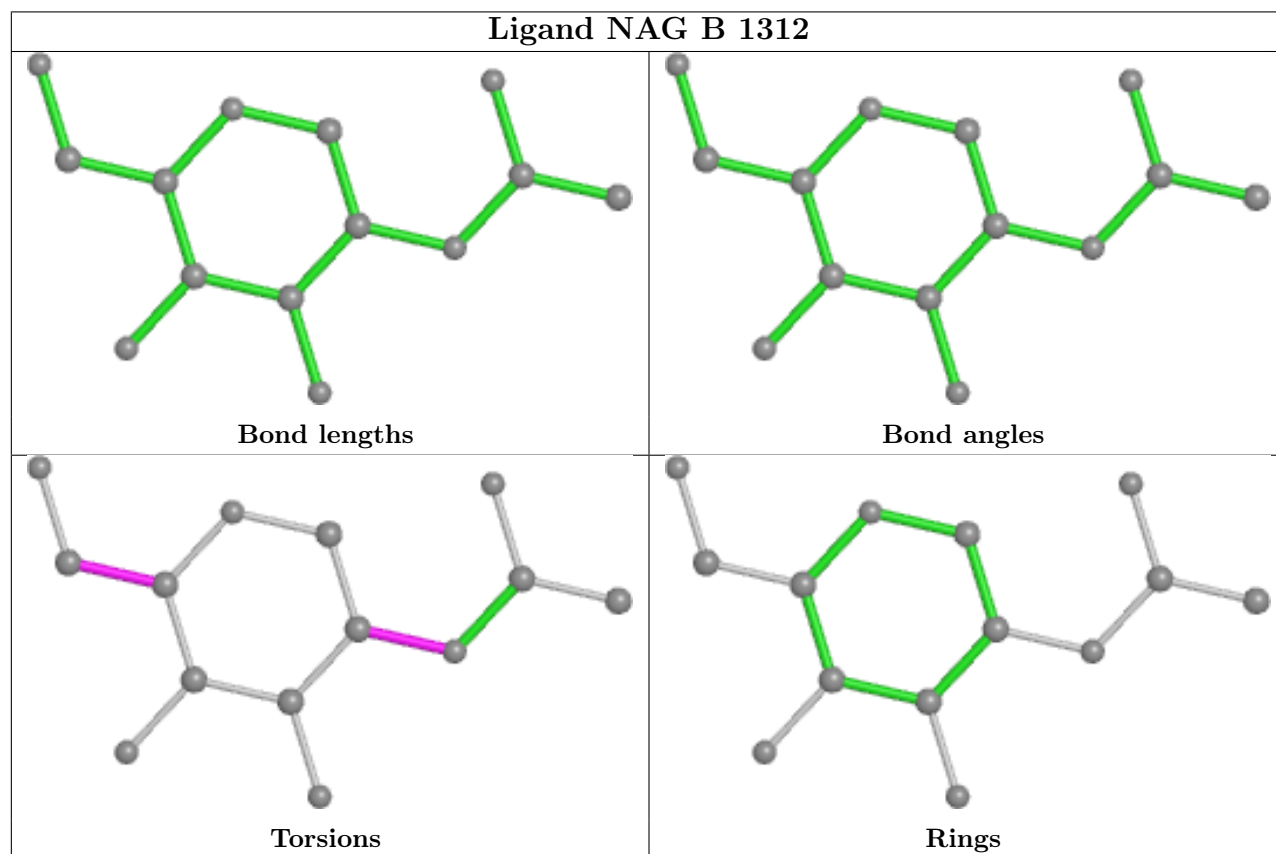
There are no ring outliers.

33 monomers are involved in 65 short contacts:

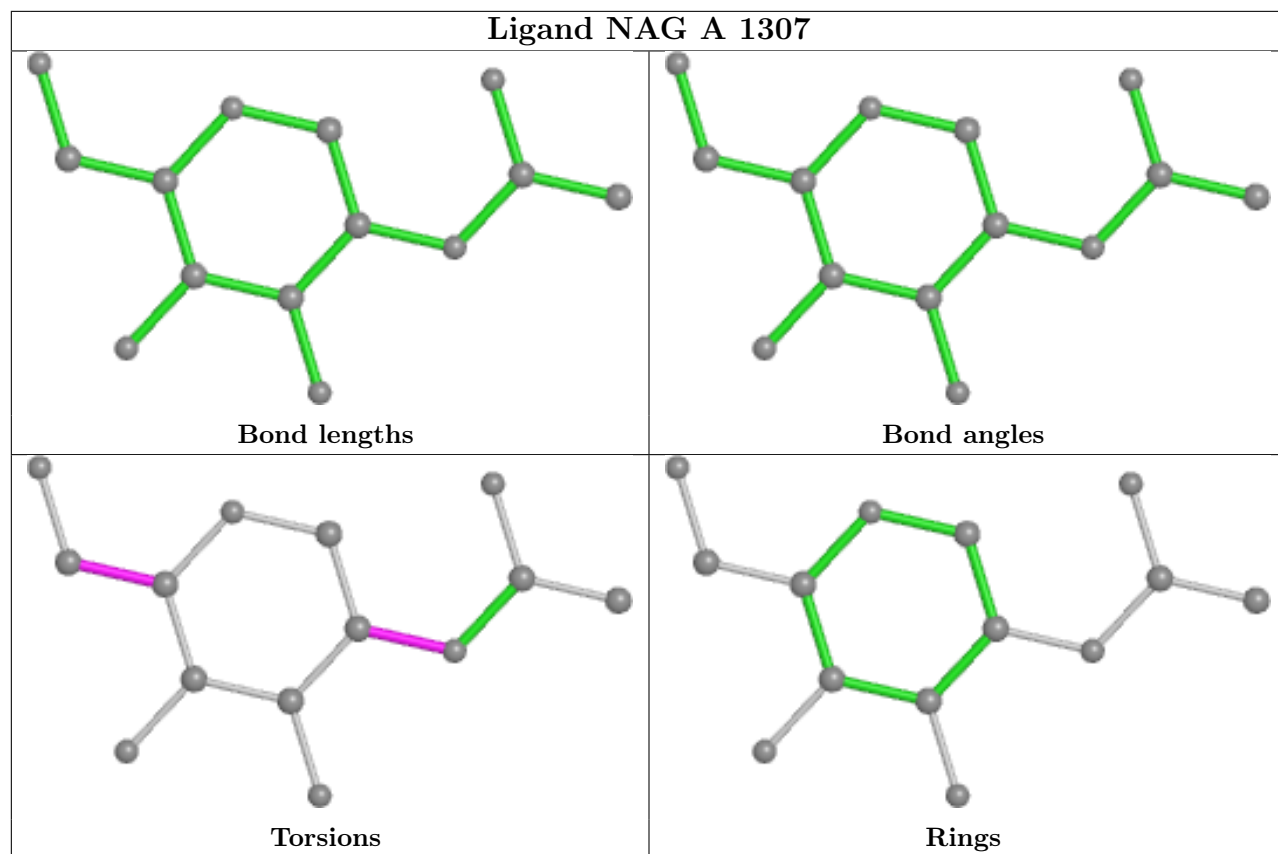
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1312	NAG	2	0
6	A	1307	NAG	2	0
6	C	1309	NAG	3	0
6	B	1303	NAG	4	0
6	B	1304	NAG	1	0
6	A	1311	NAG	4	0
6	C	1312	NAG	2	0
6	A	1305	NAG	3	0
6	B	1310	NAG	1	0
6	C	1301	NAG	3	0
6	C	1303	NAG	4	0
6	B	1305	NAG	4	0
6	B	1301	NAG	3	0
6	A	1303	NAG	1	0
6	A	1306	NAG	1	0
6	A	1304	NAG	3	0
6	A	1309	NAG	2	0
6	C	1308	NAG	1	0
6	A	1308	NAG	1	0
6	C	1310	NAG	2	0
6	B	1307	NAG	1	0
6	B	1308	NAG	2	0
6	A	1312	NAG	2	0
6	B	1302	NAG	1	0
6	A	1310	NAG	3	0
6	A	1301	NAG	2	0
6	C	1307	NAG	2	0
6	C	1306	NAG	1	0
6	C	1302	NAG	1	0
6	B	1309	NAG	1	0
6	C	1304	NAG	3	0
6	C	1313	NAG	1	0
6	B	1311	NAG	5	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

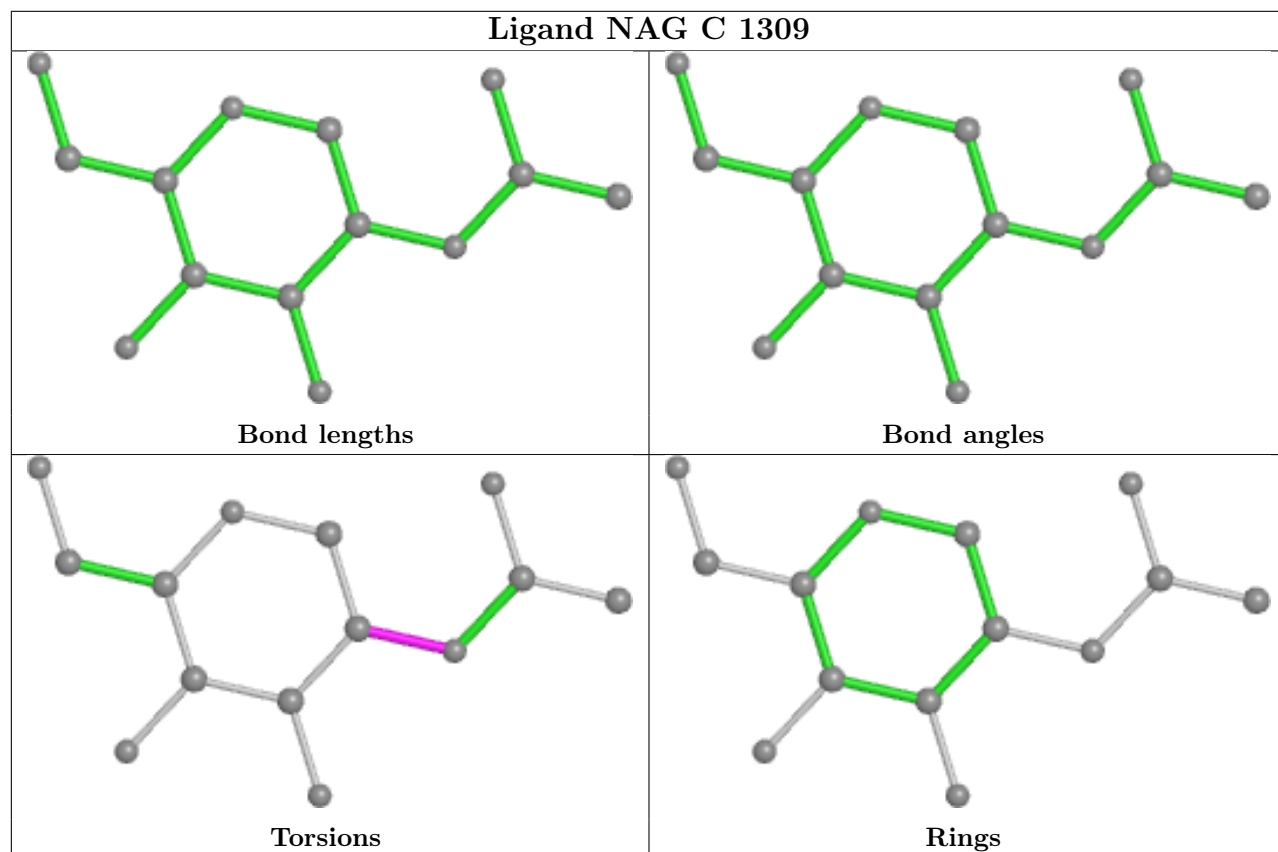
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

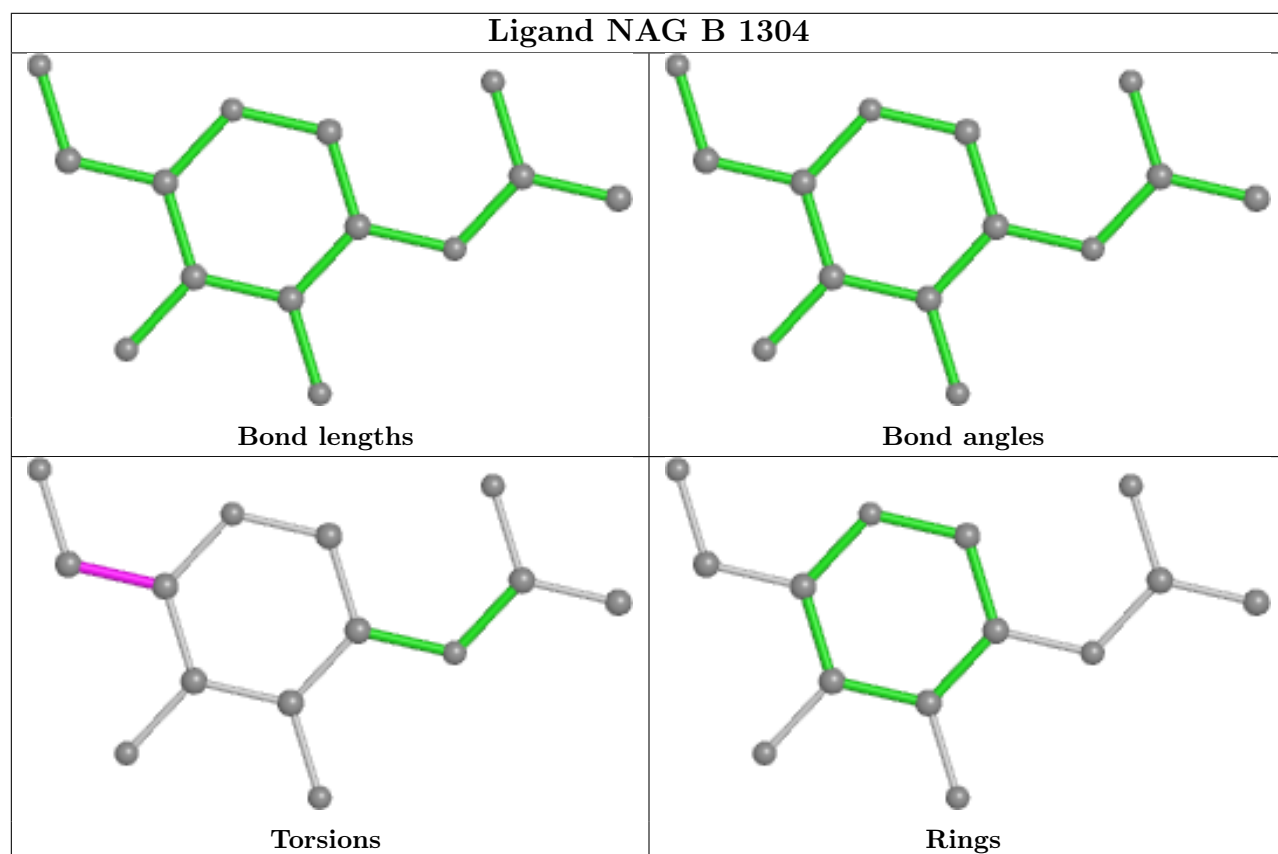
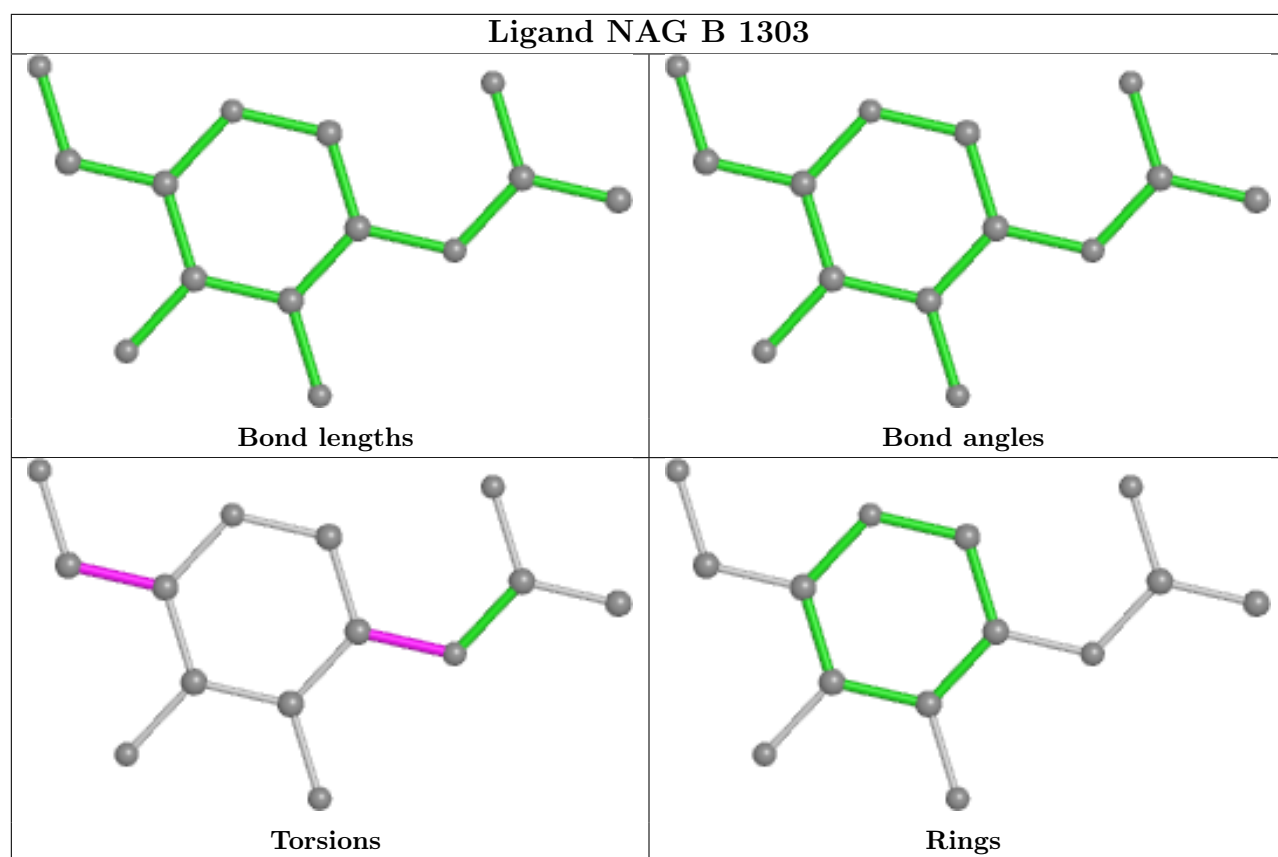


## Ligand NAG A 1307

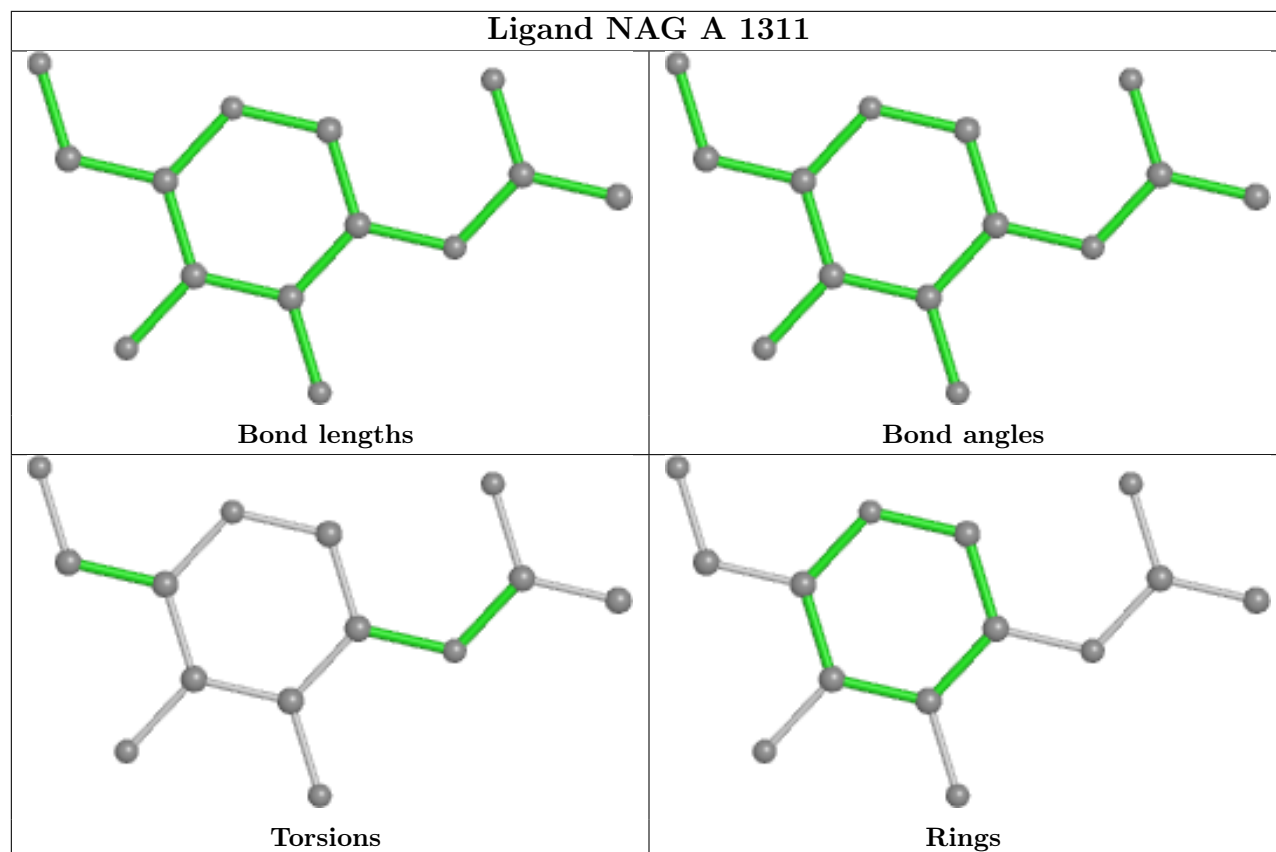


## Ligand NAG C 1309

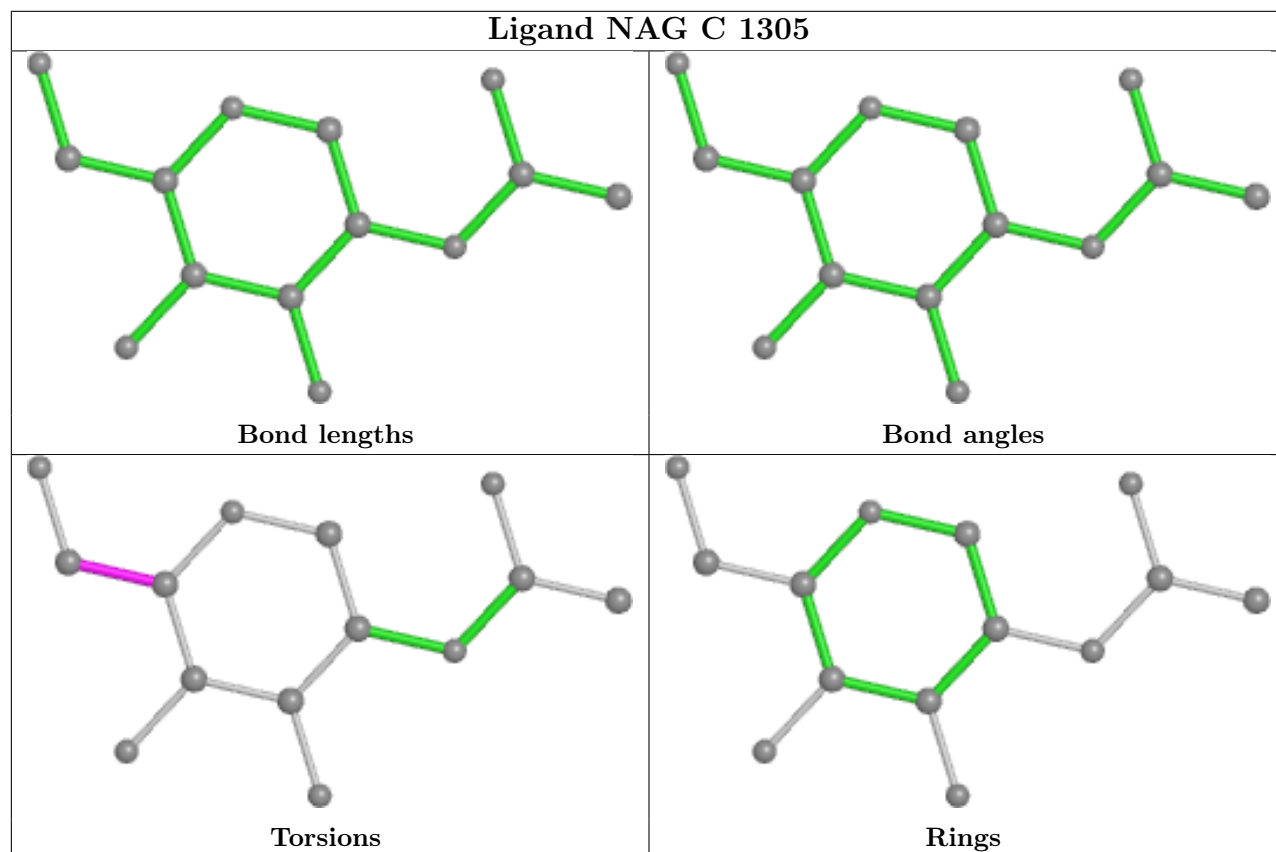




## Ligand NAG A 1311

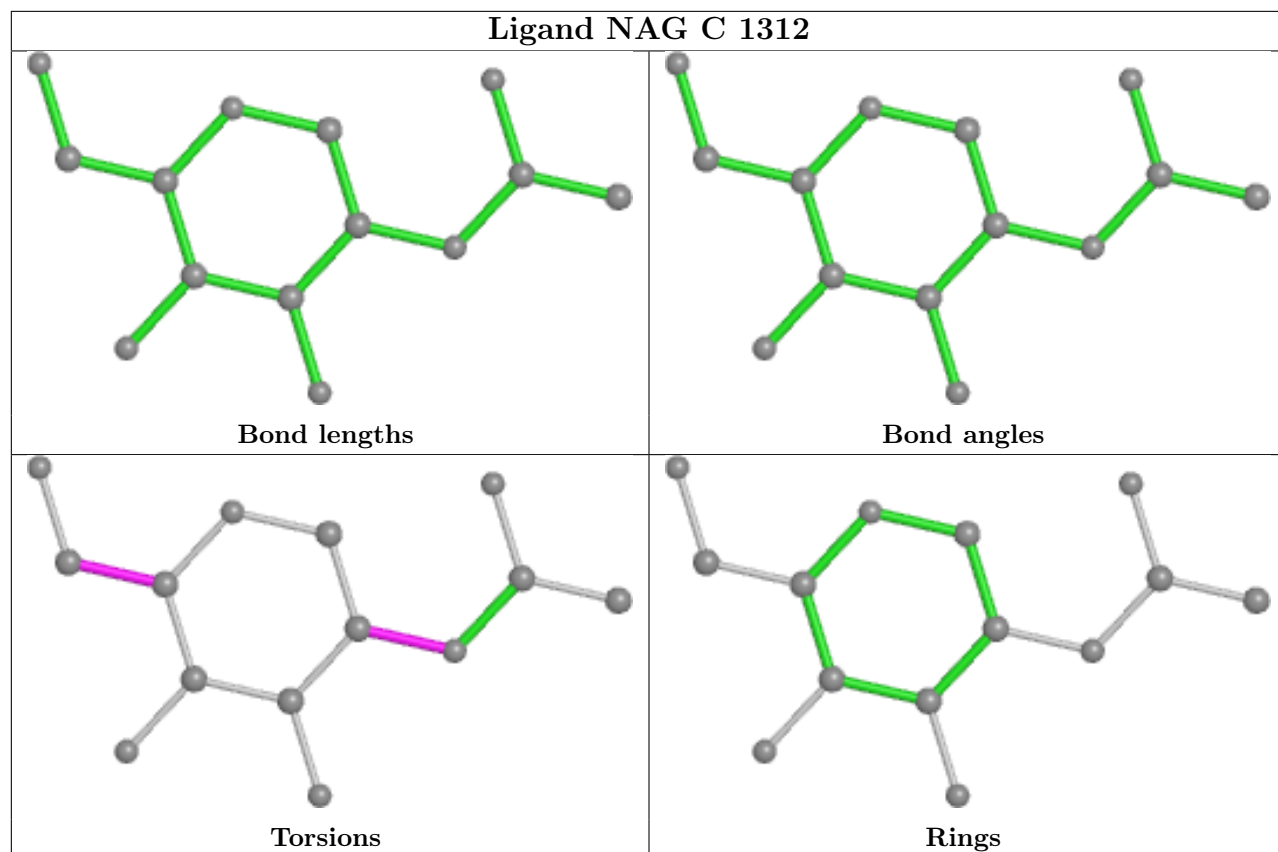


## Ligand NAG C 1305

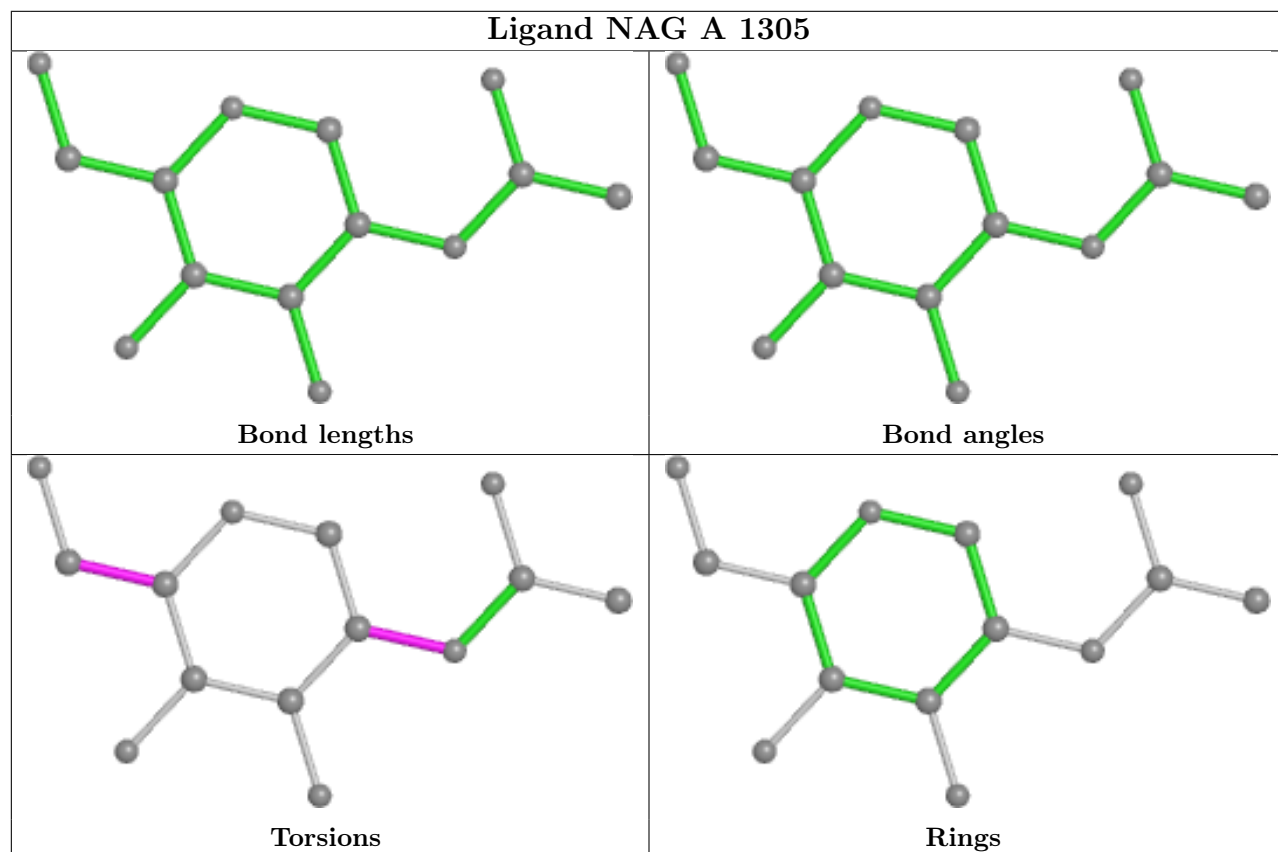




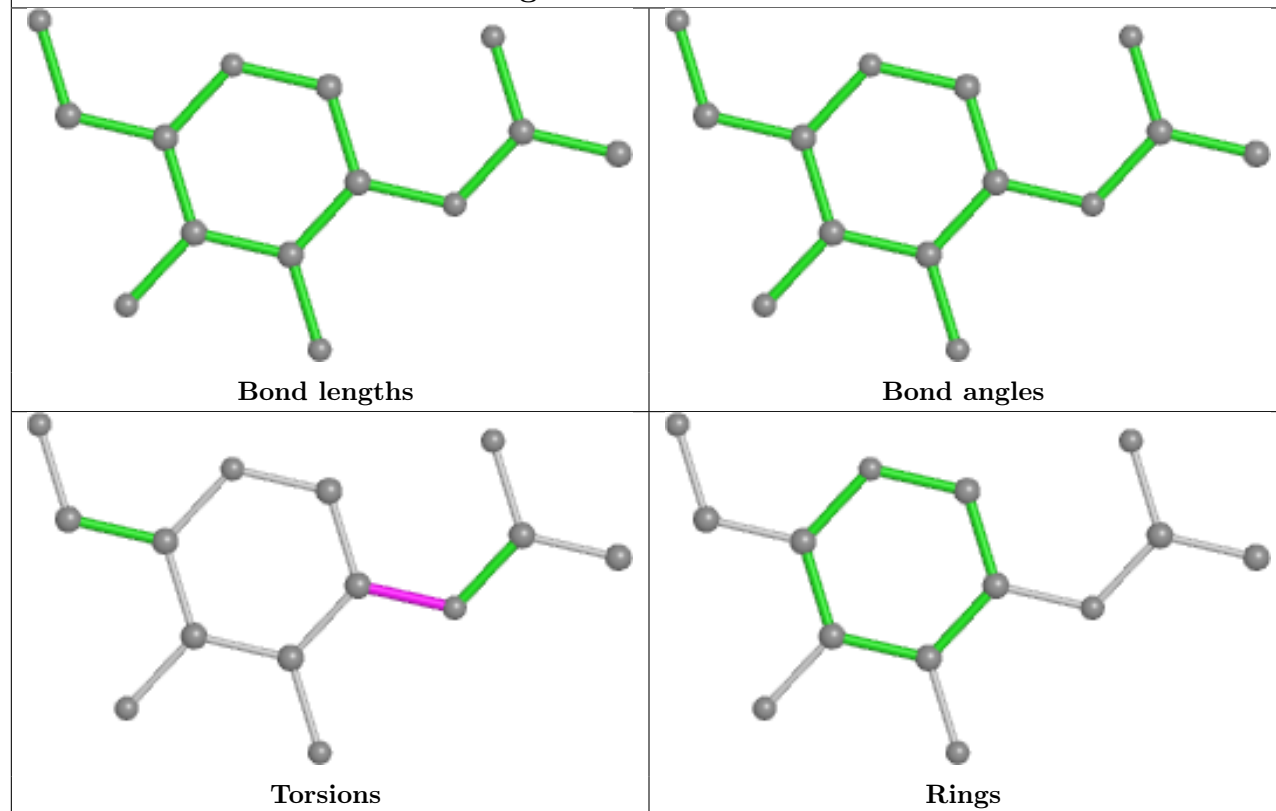
## Ligand NAG C 1312



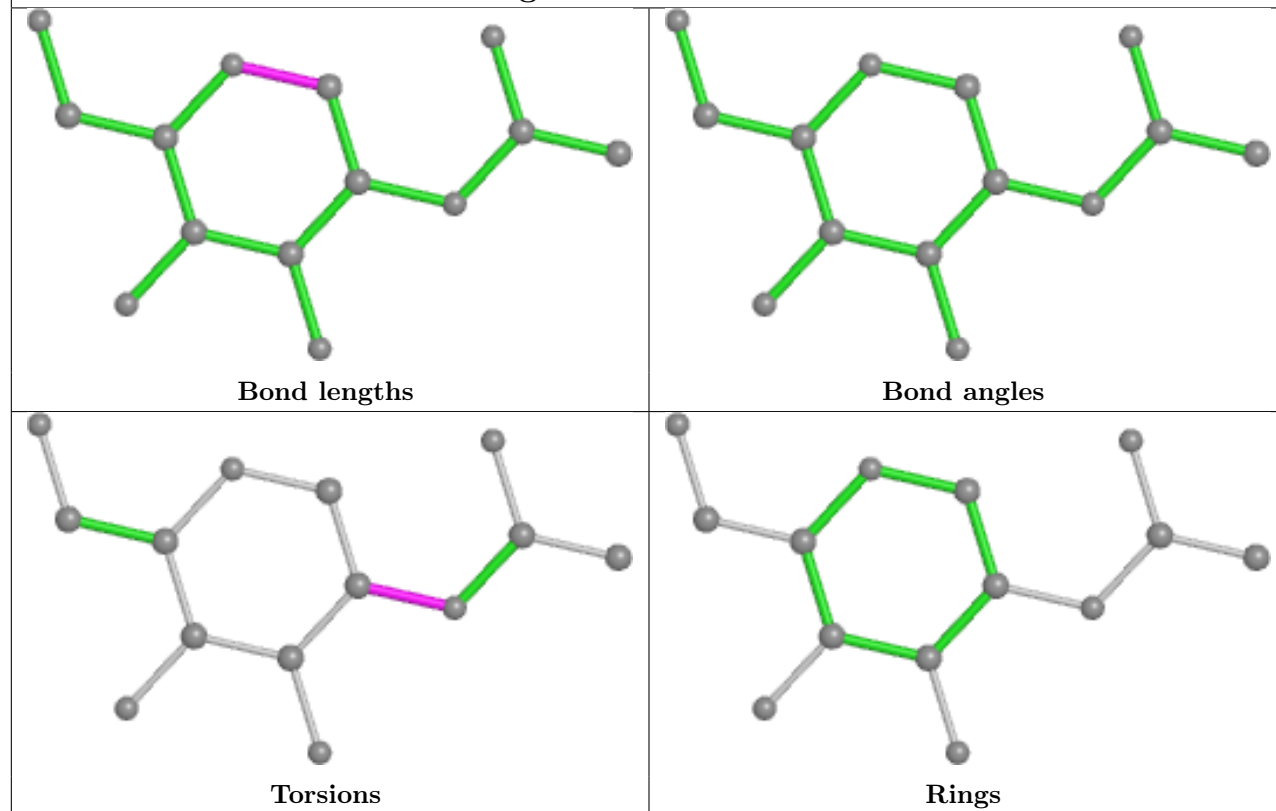
## Ligand NAG A 1305

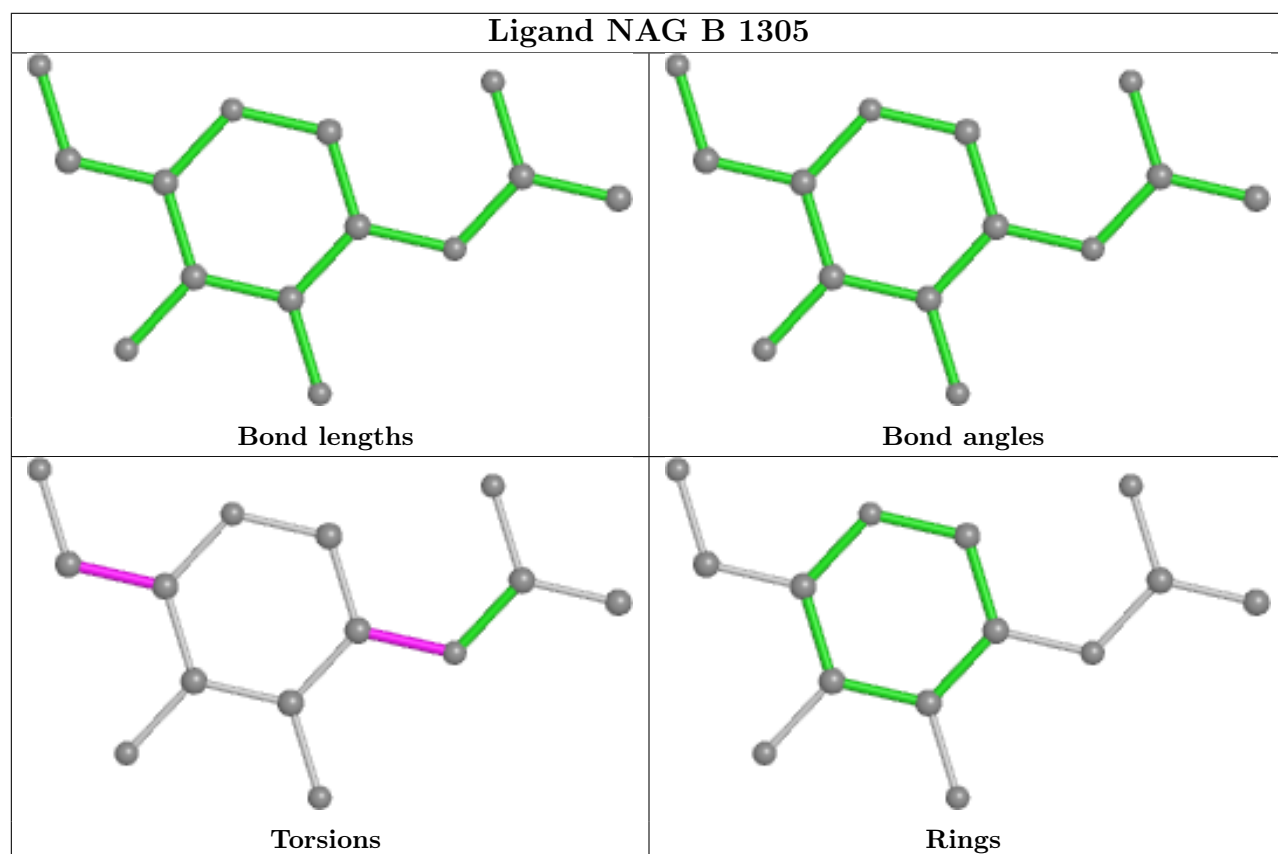
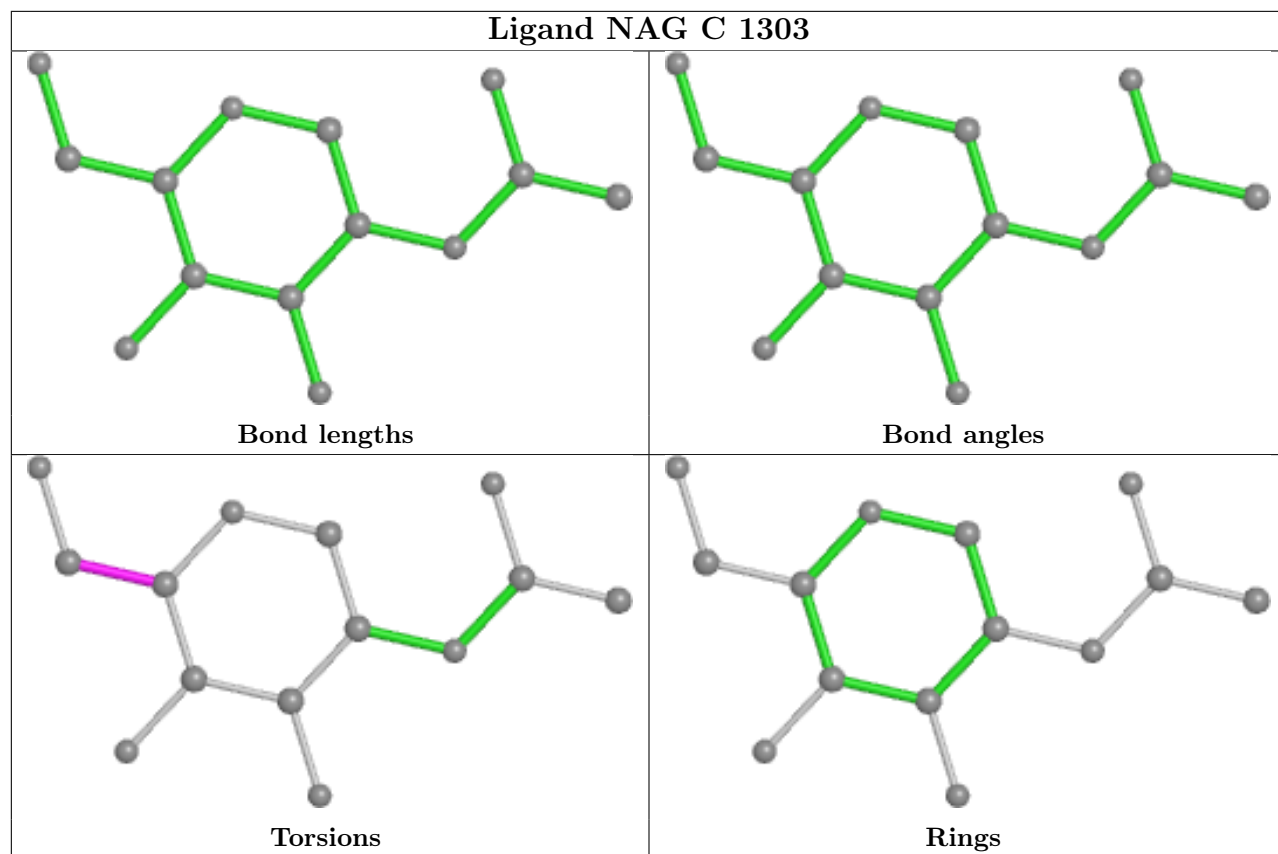


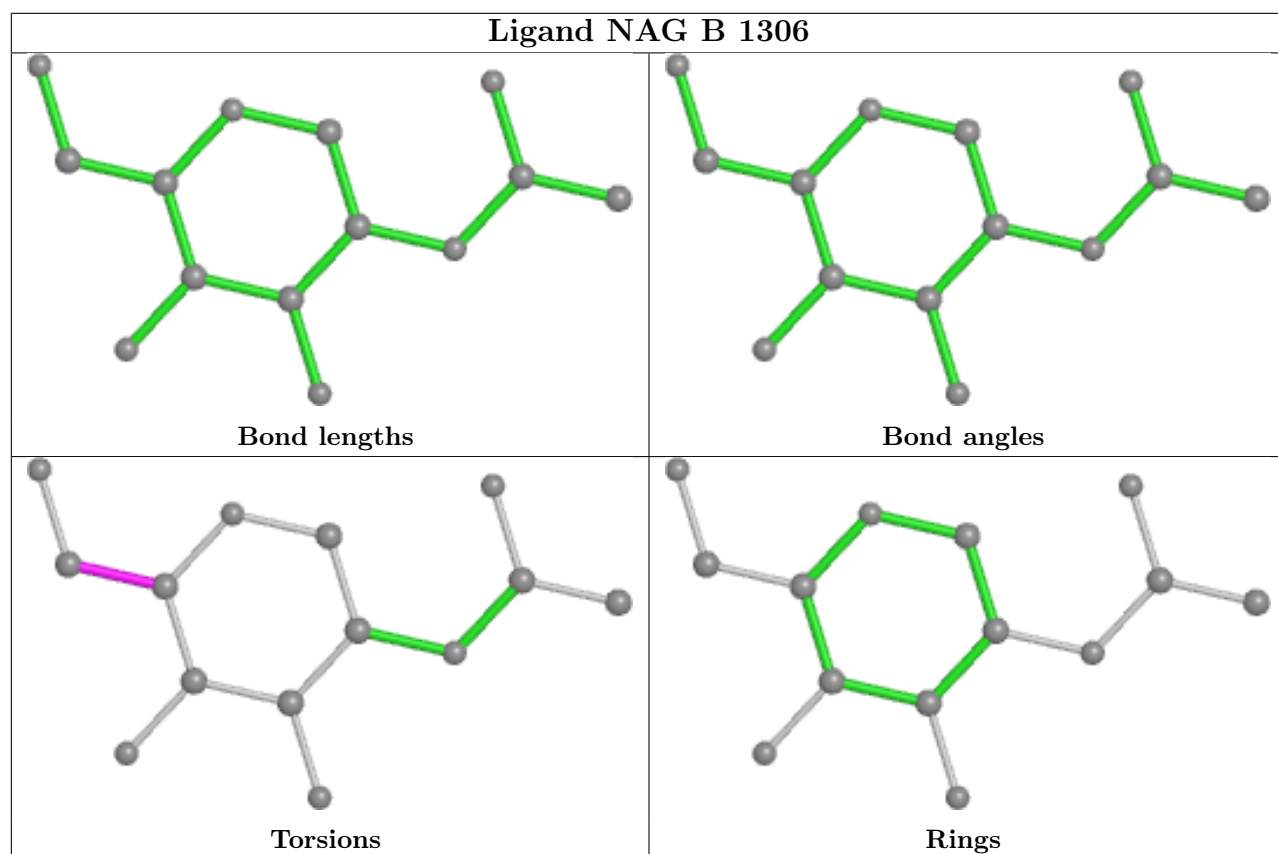
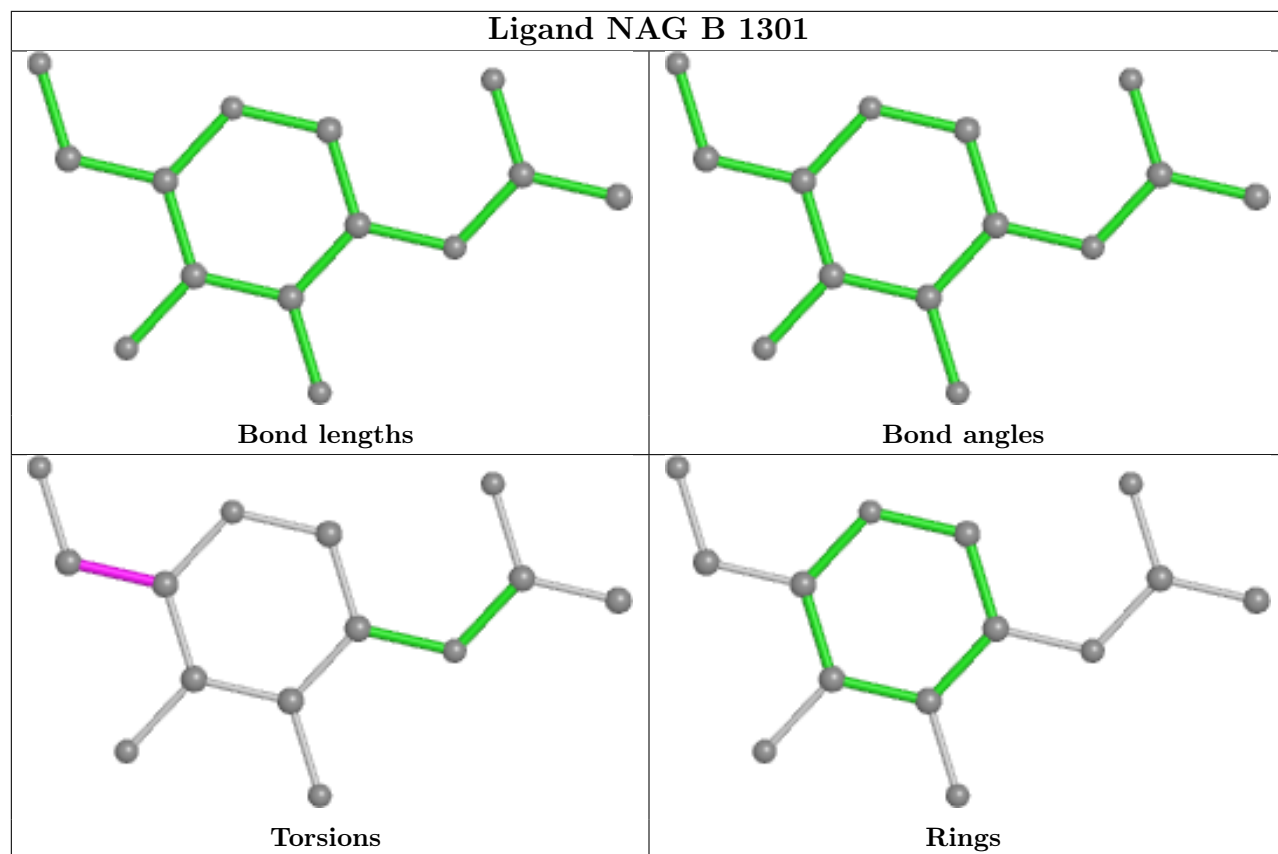
## Ligand NAG B 1310



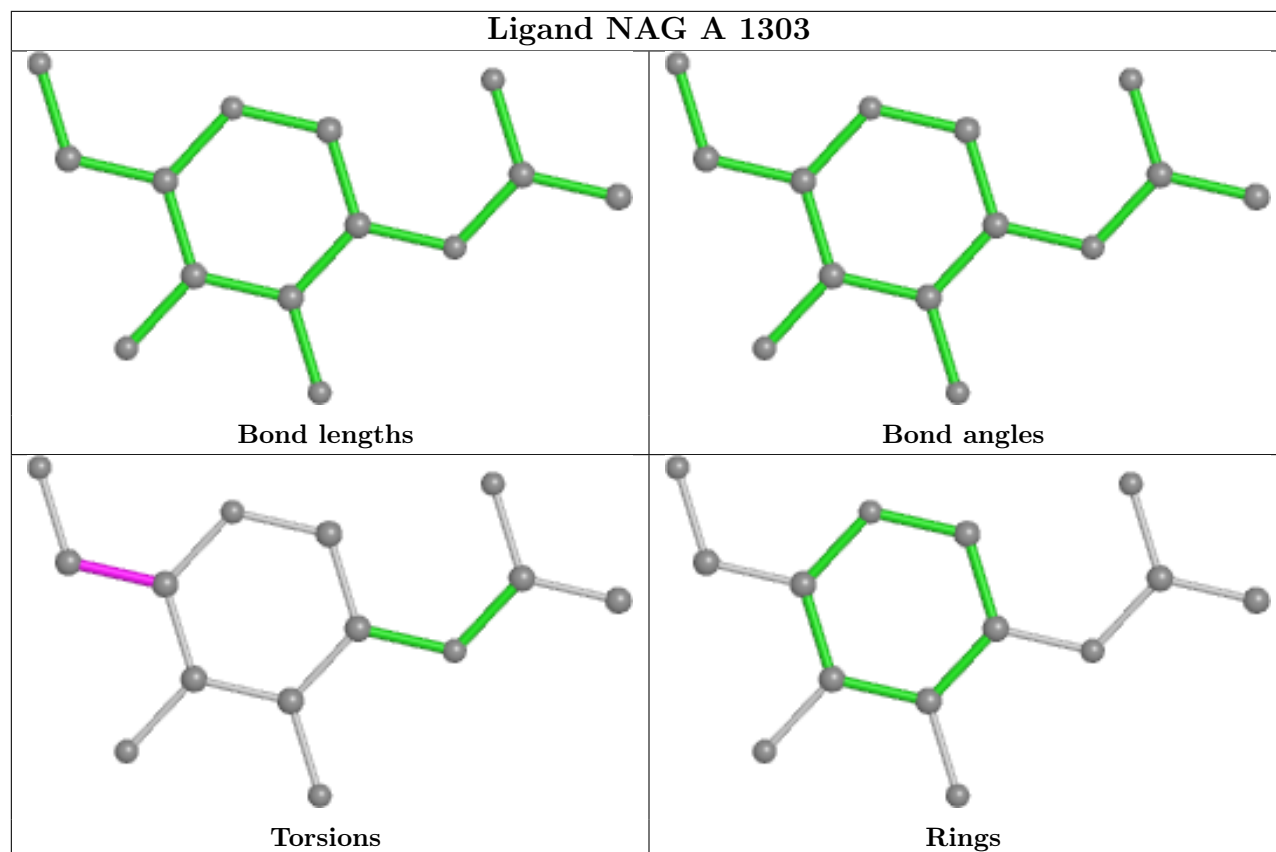
## Ligand NAG C 1301



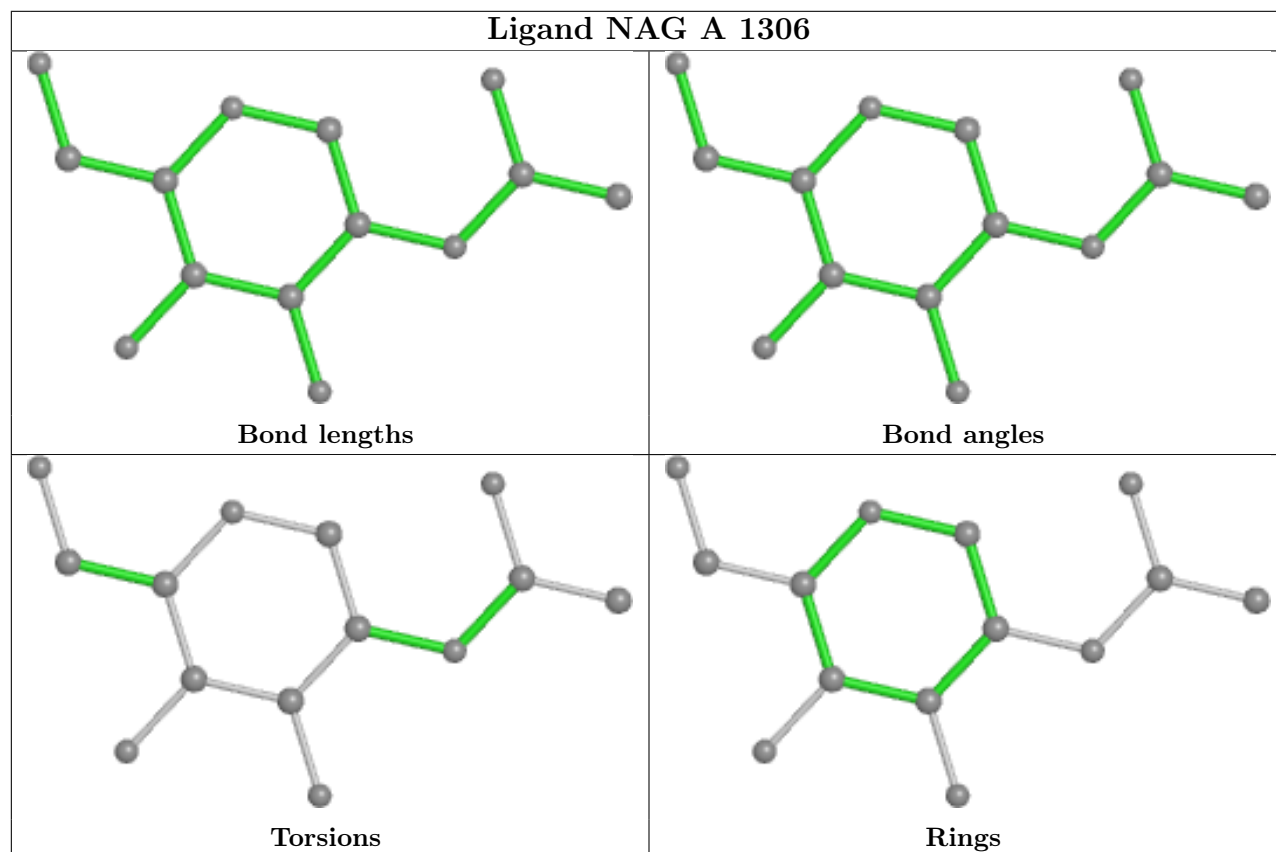




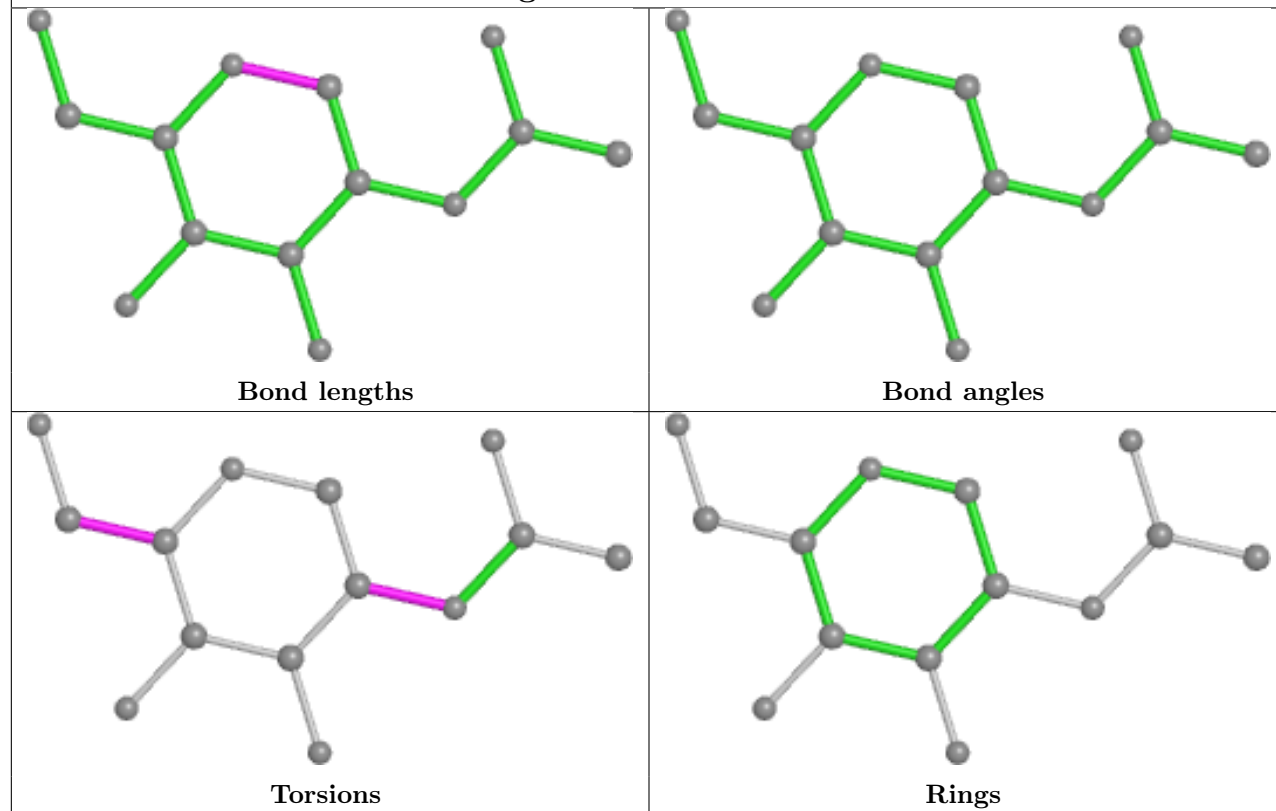
## Ligand NAG A 1303



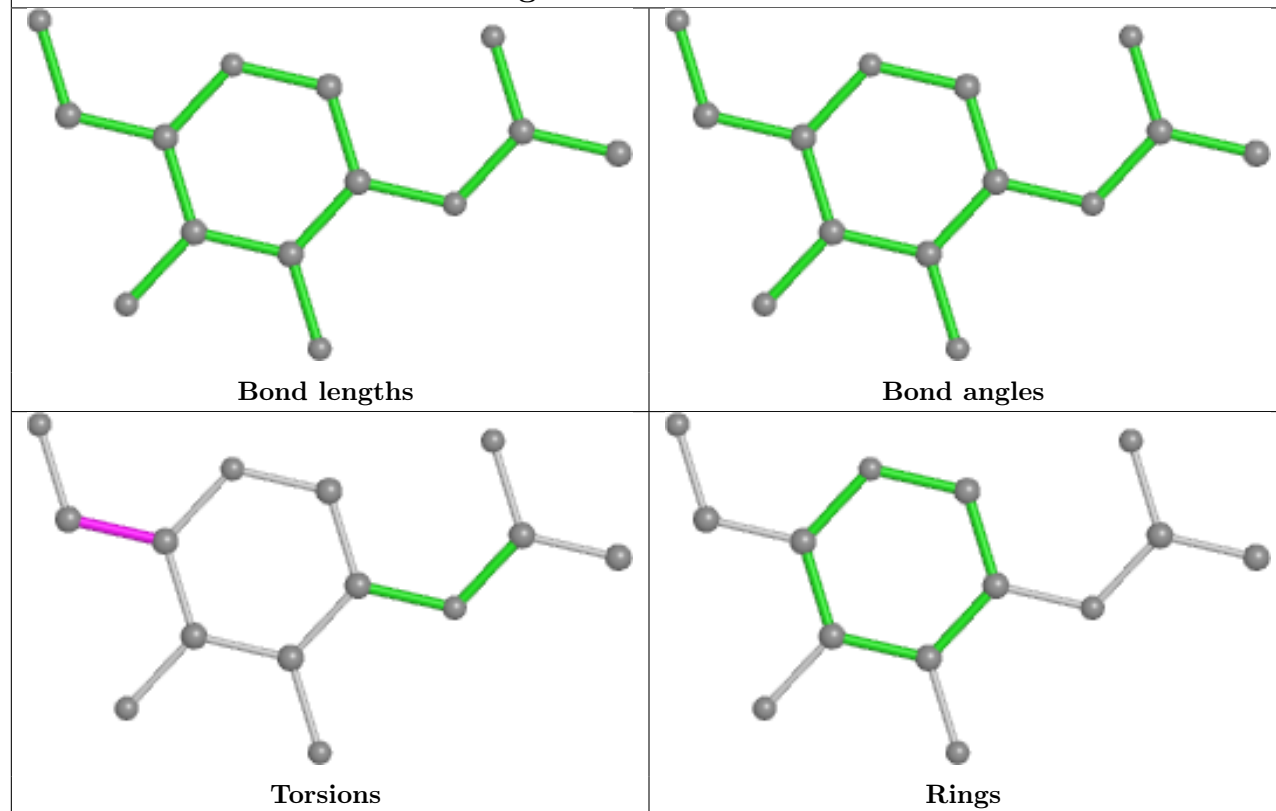
## Ligand NAG A 1306



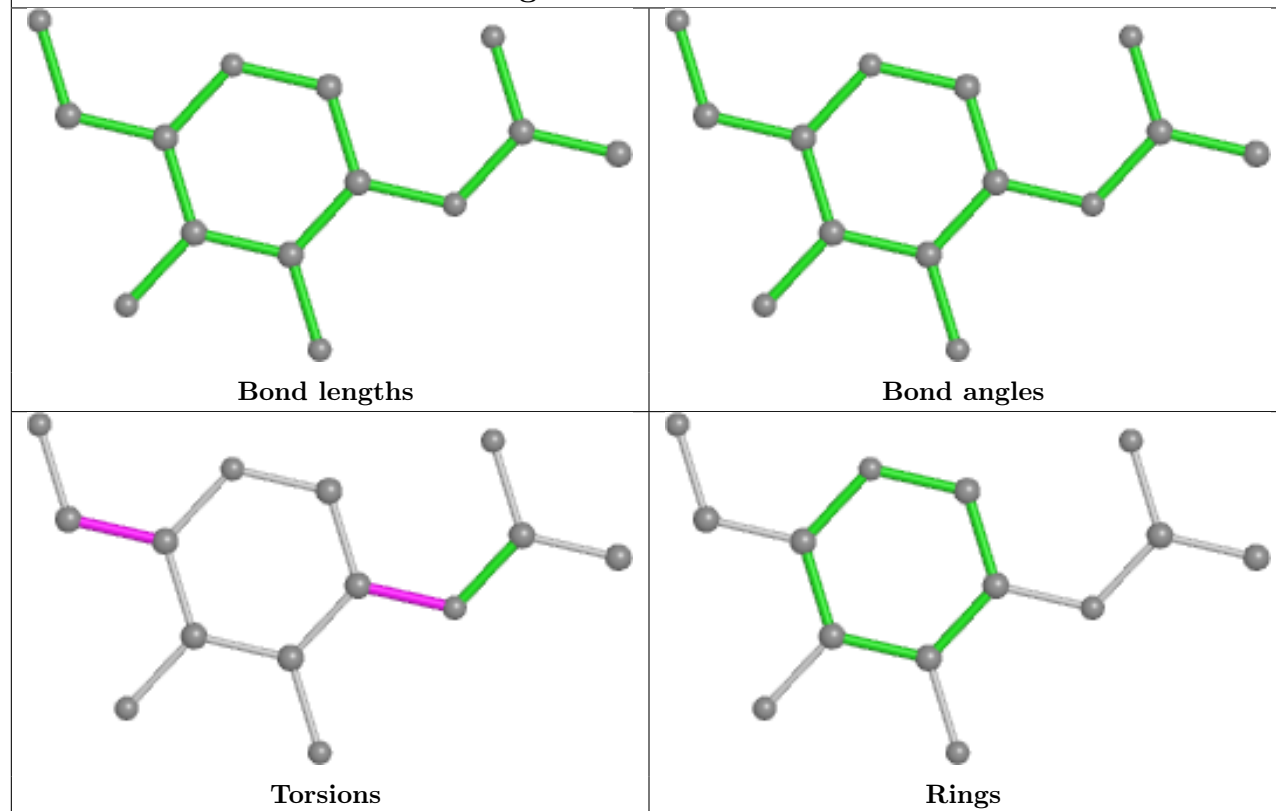
## Ligand NAG A 1304



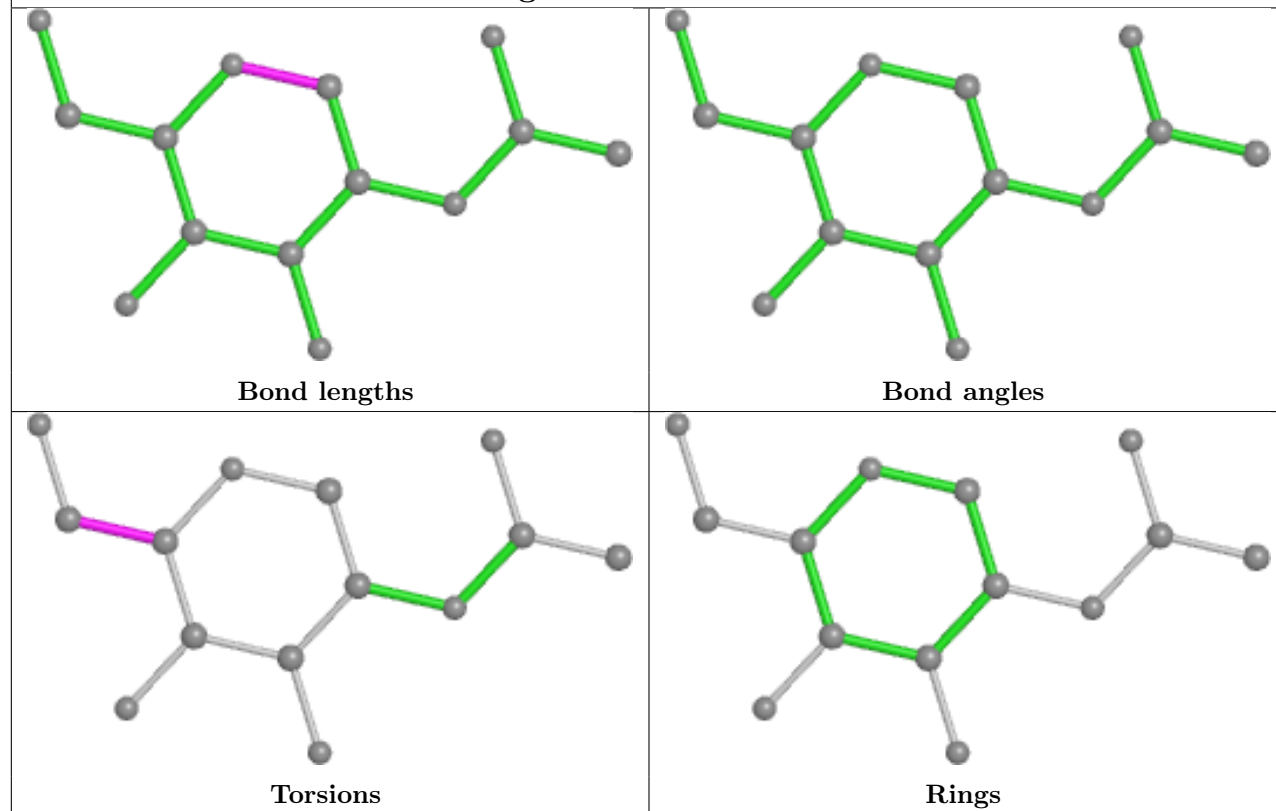
## Ligand NAG A 1309



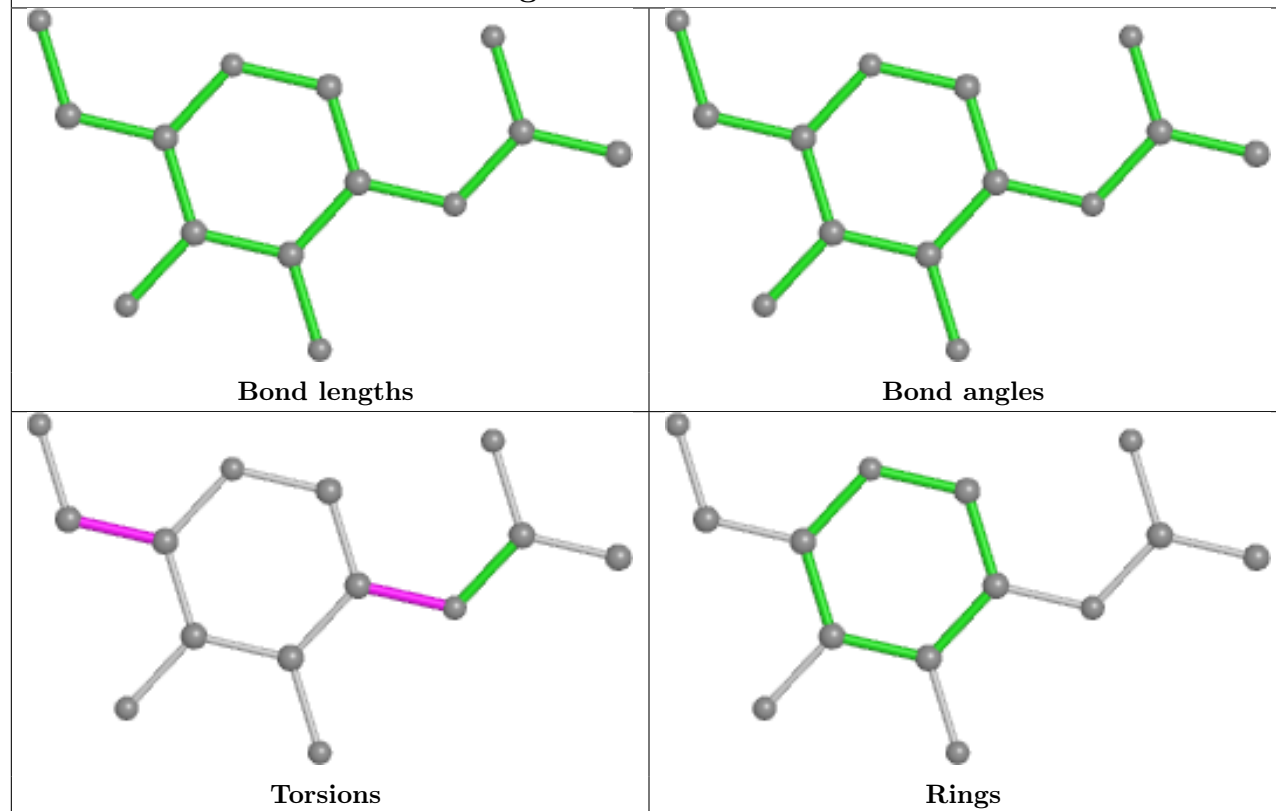
## Ligand NAG C 1308



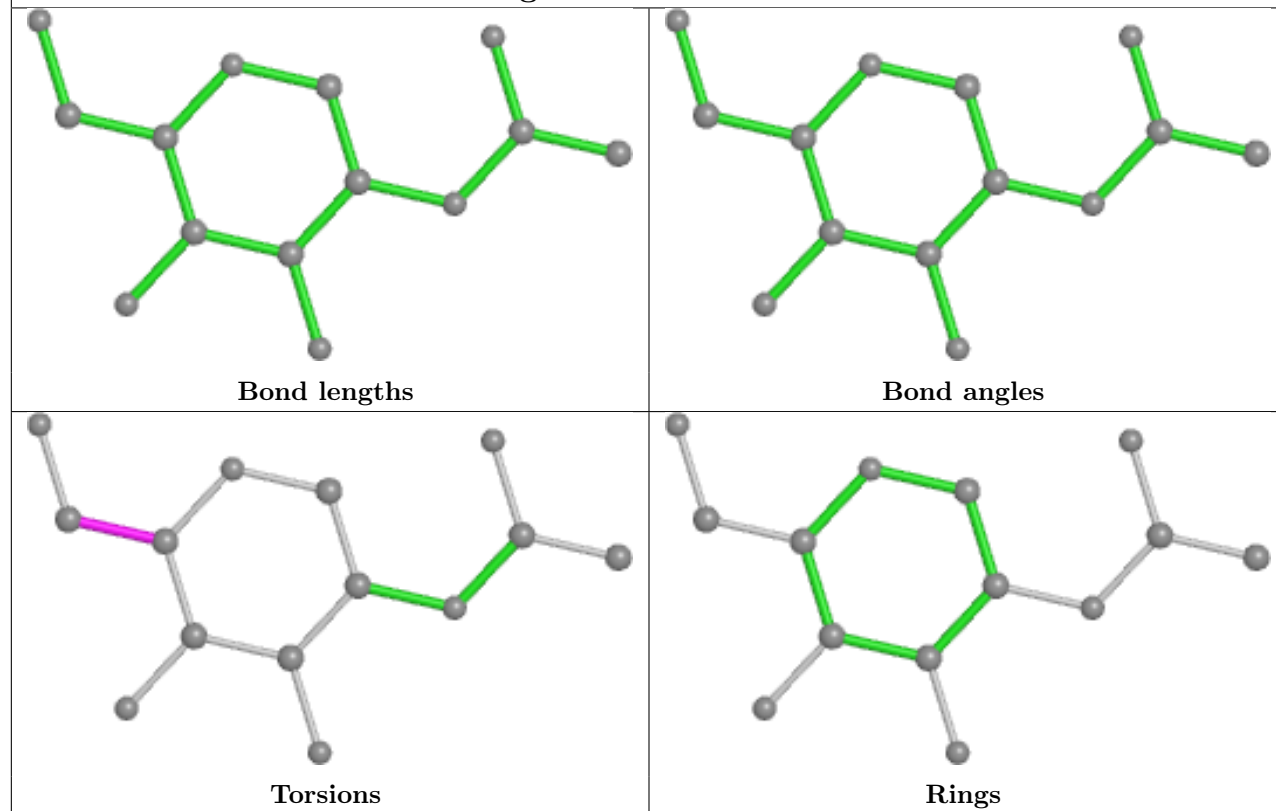
## Ligand NAG A 1308



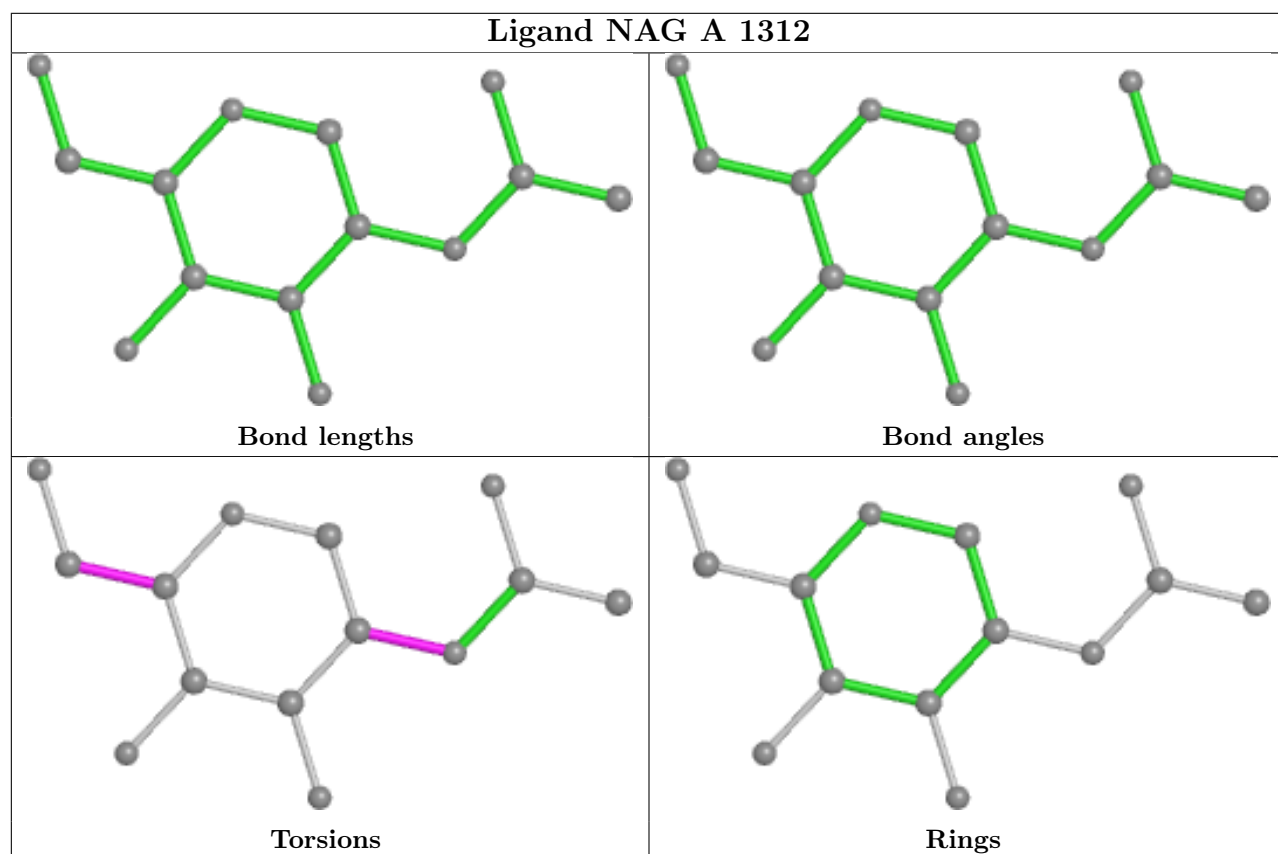
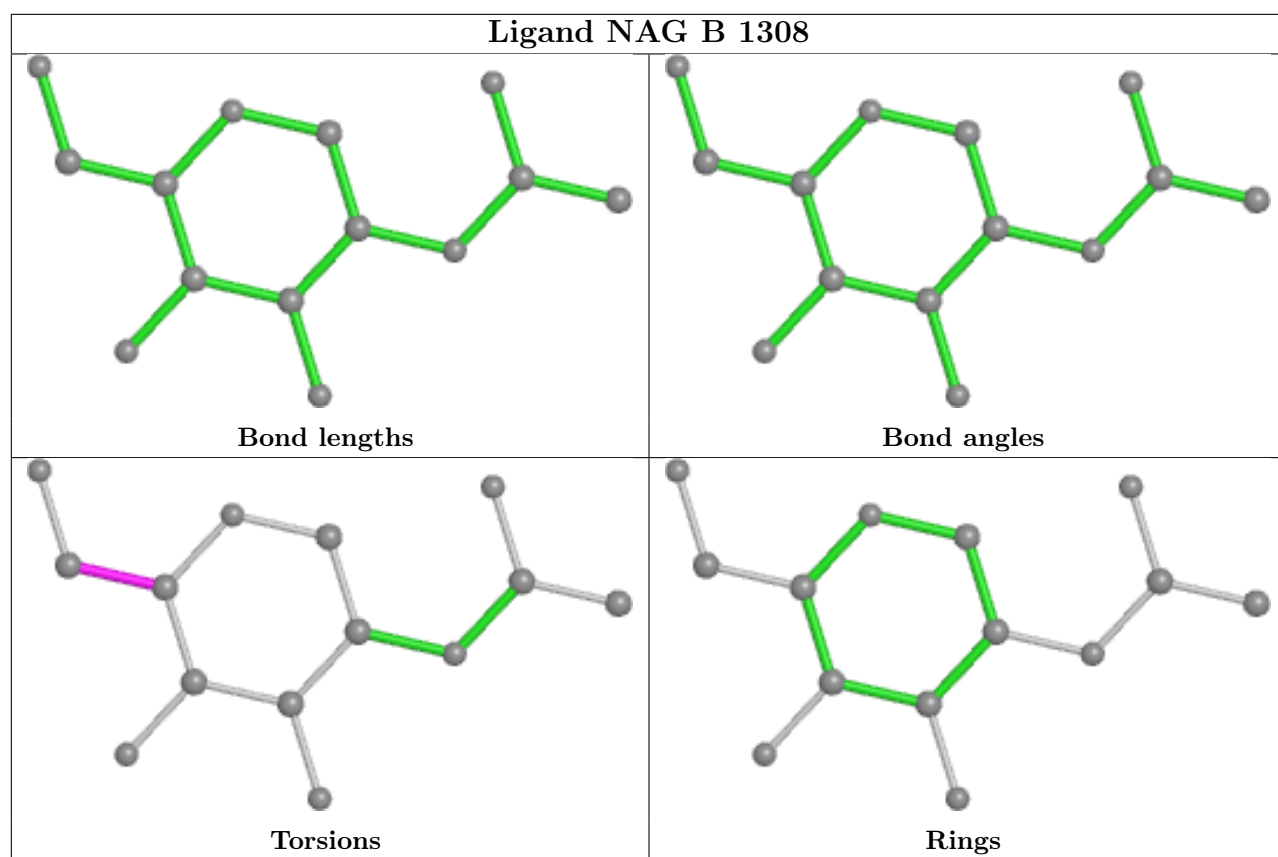
## Ligand NAG C 1310

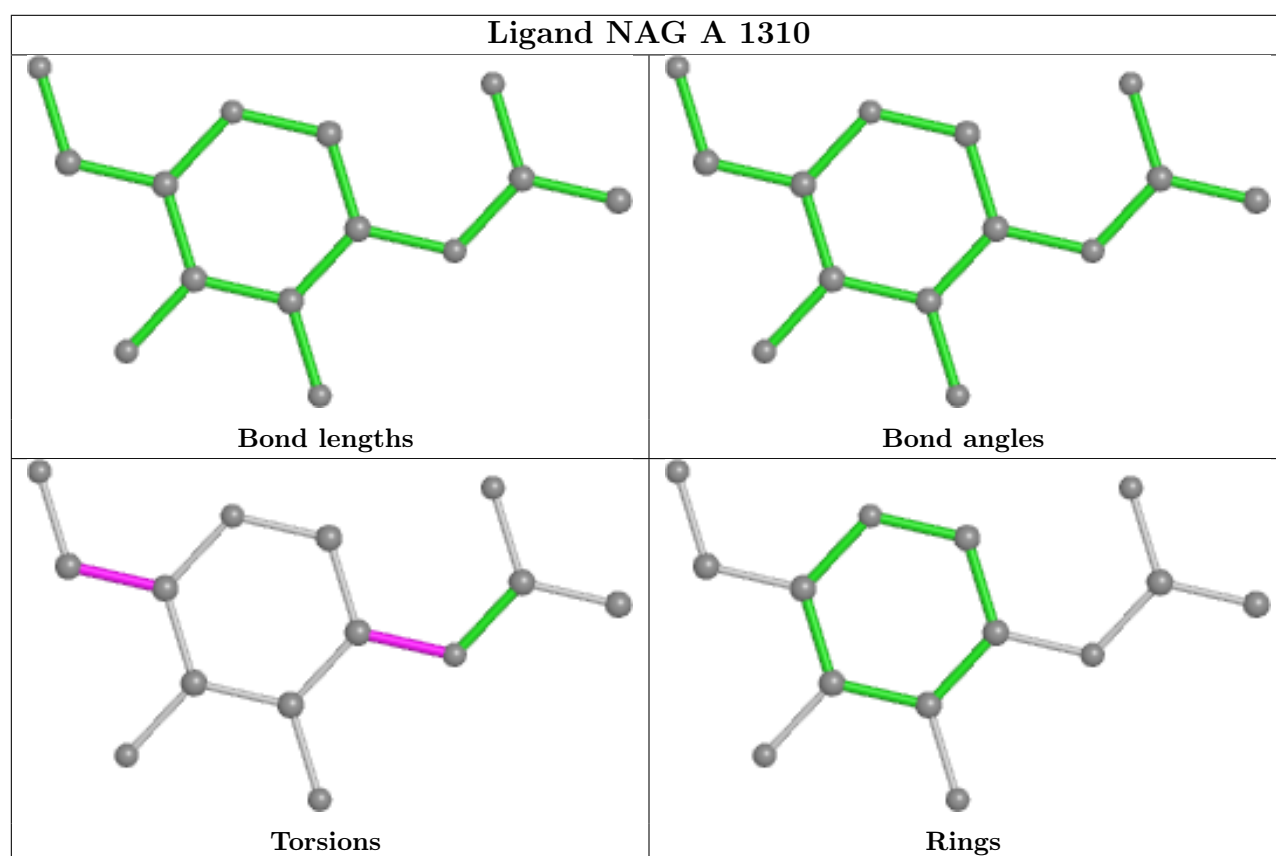
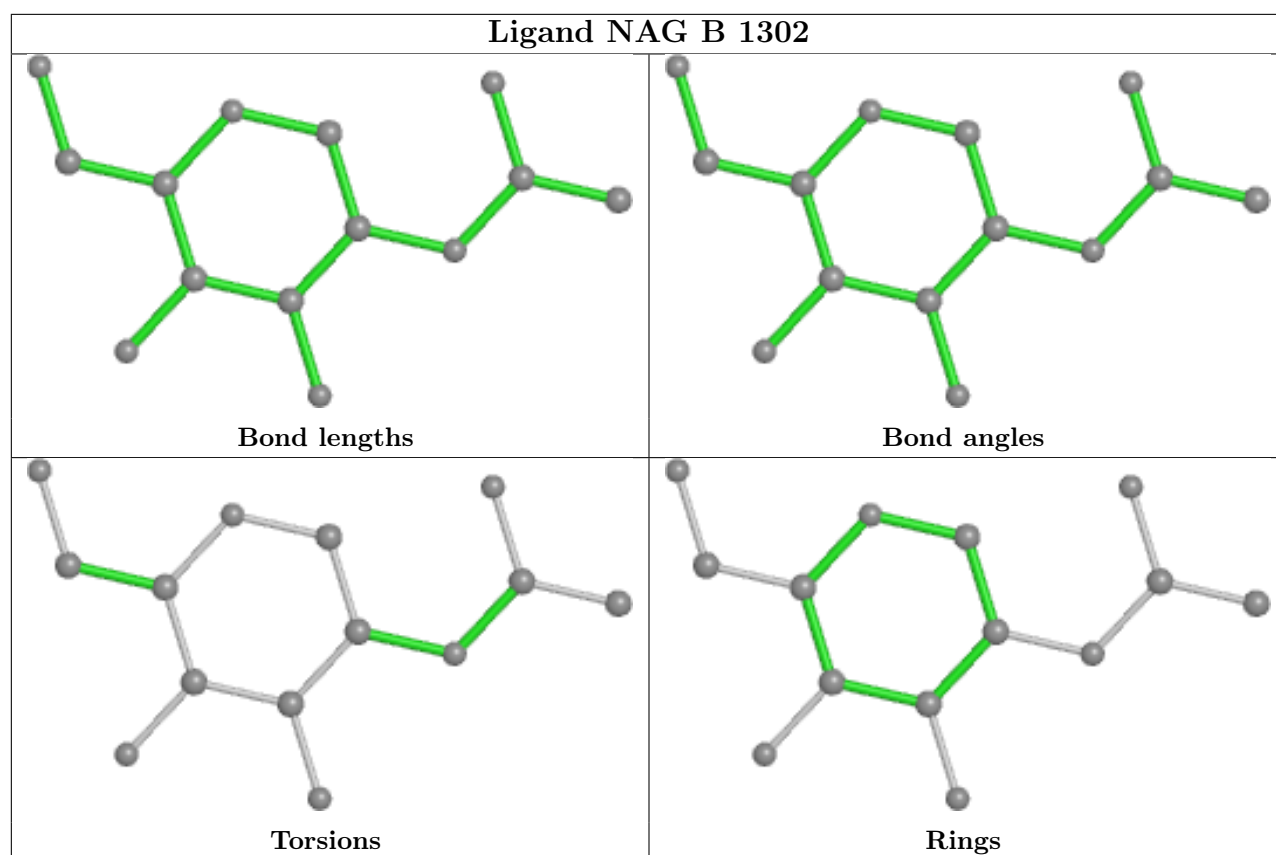


## Ligand NAG B 1307

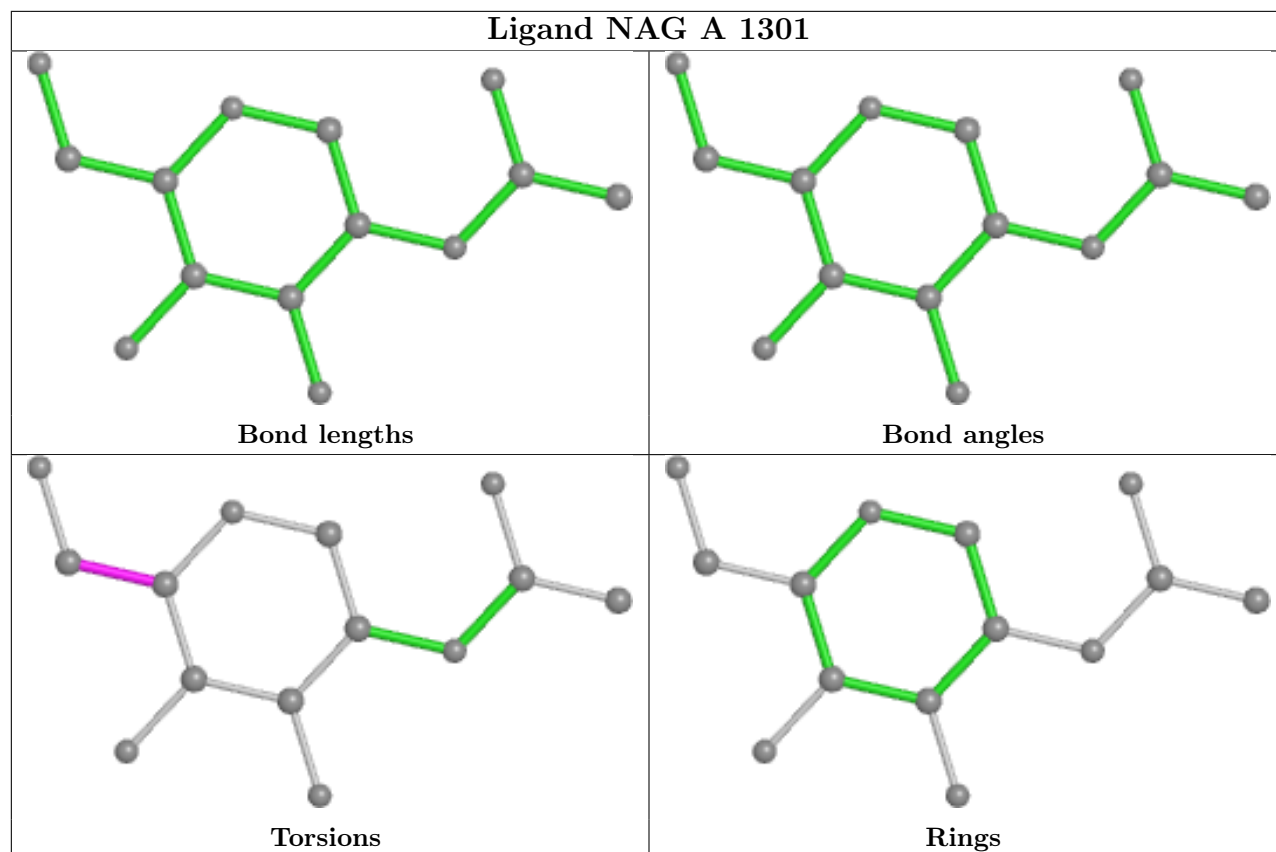




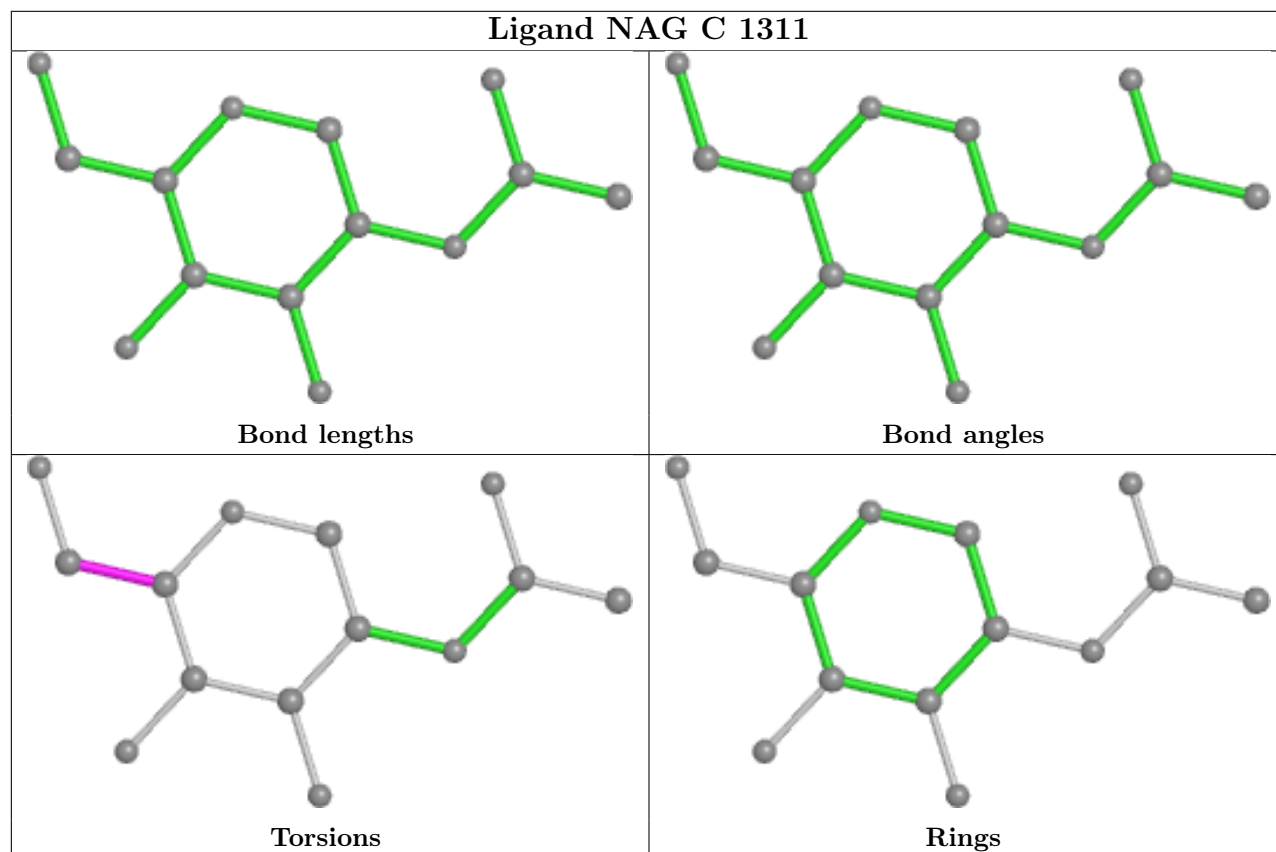


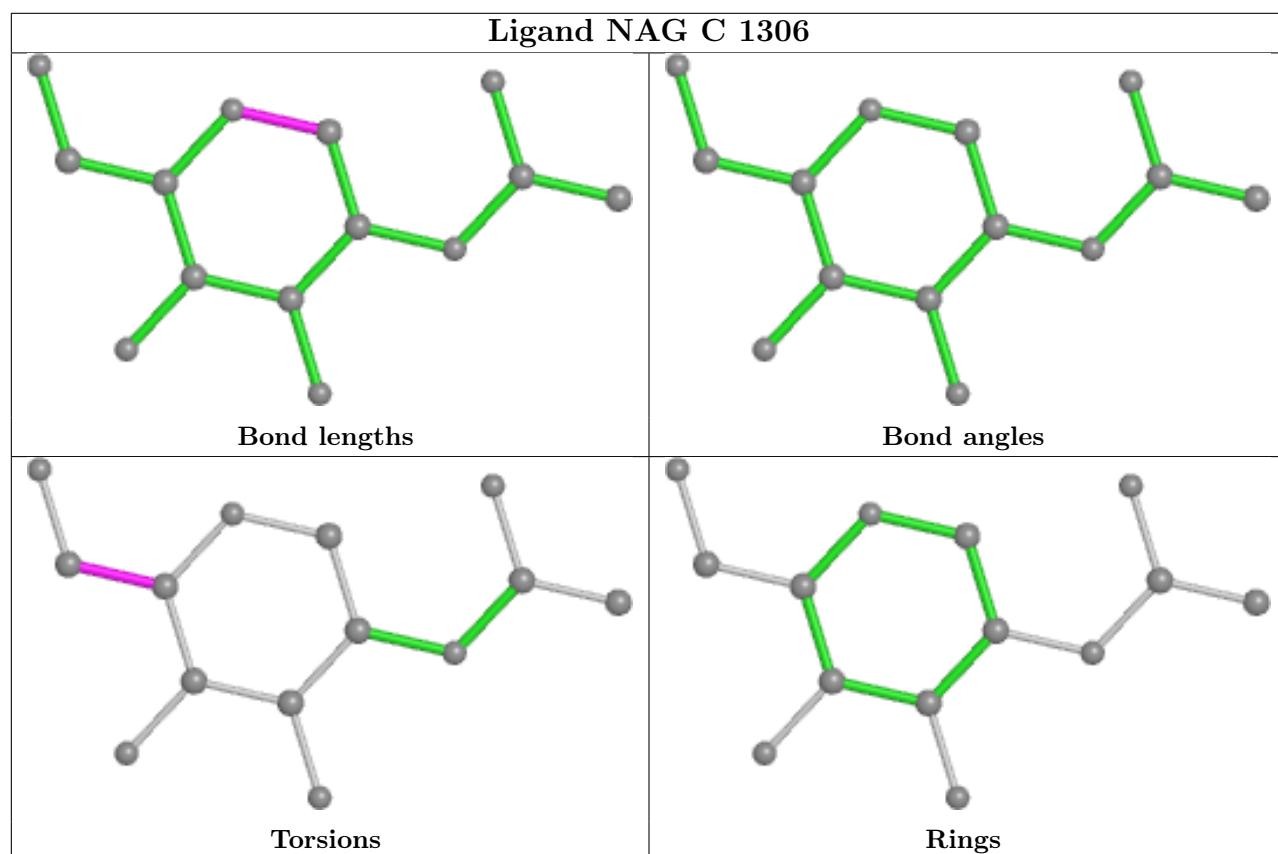
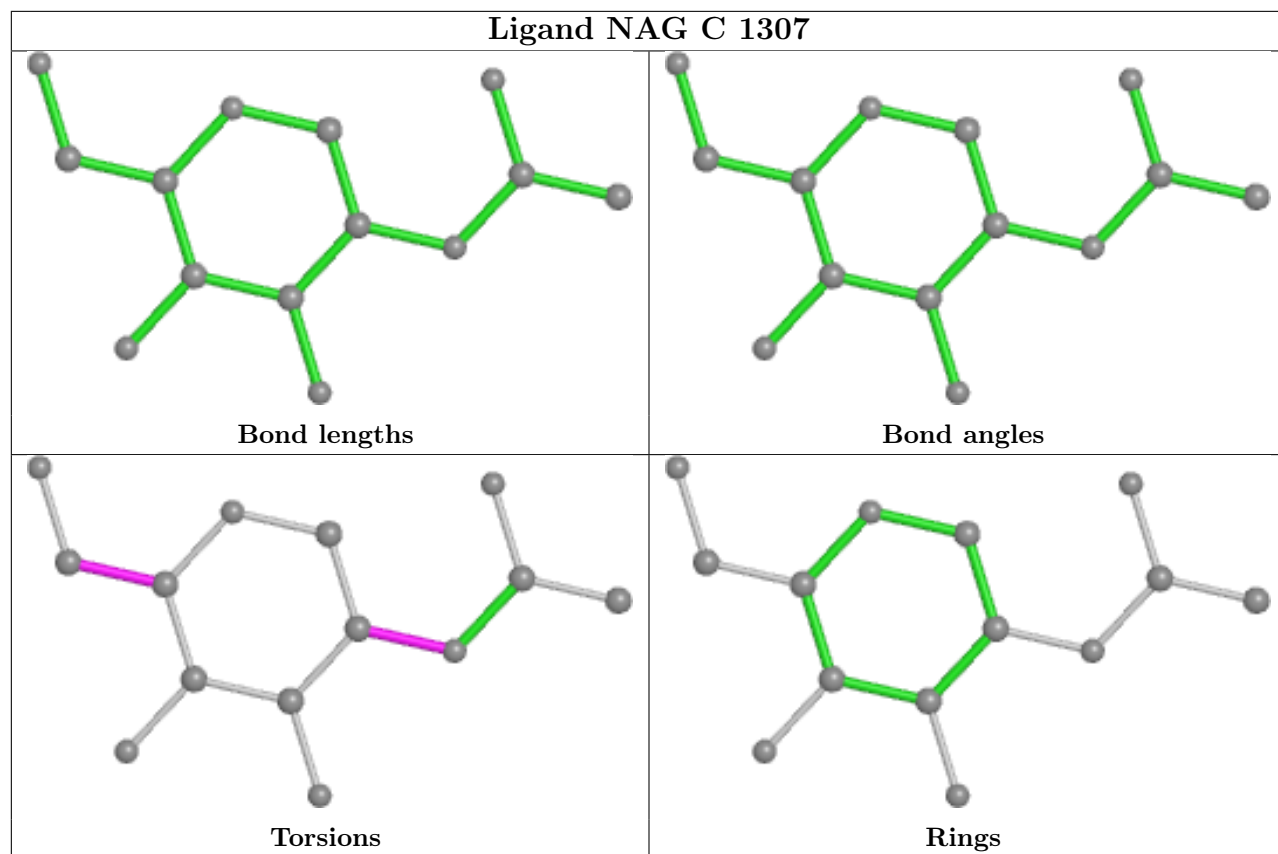


## Ligand NAG A 1301

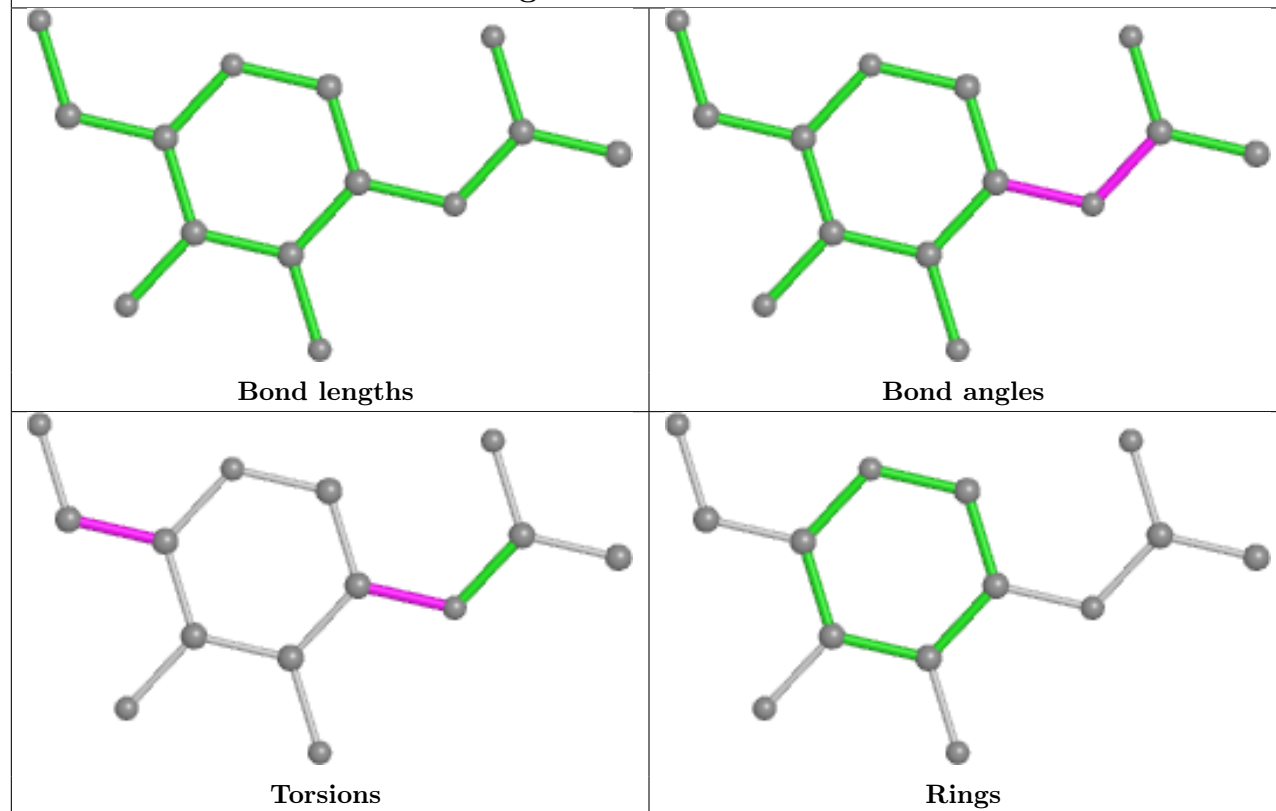


## Ligand NAG C 1311

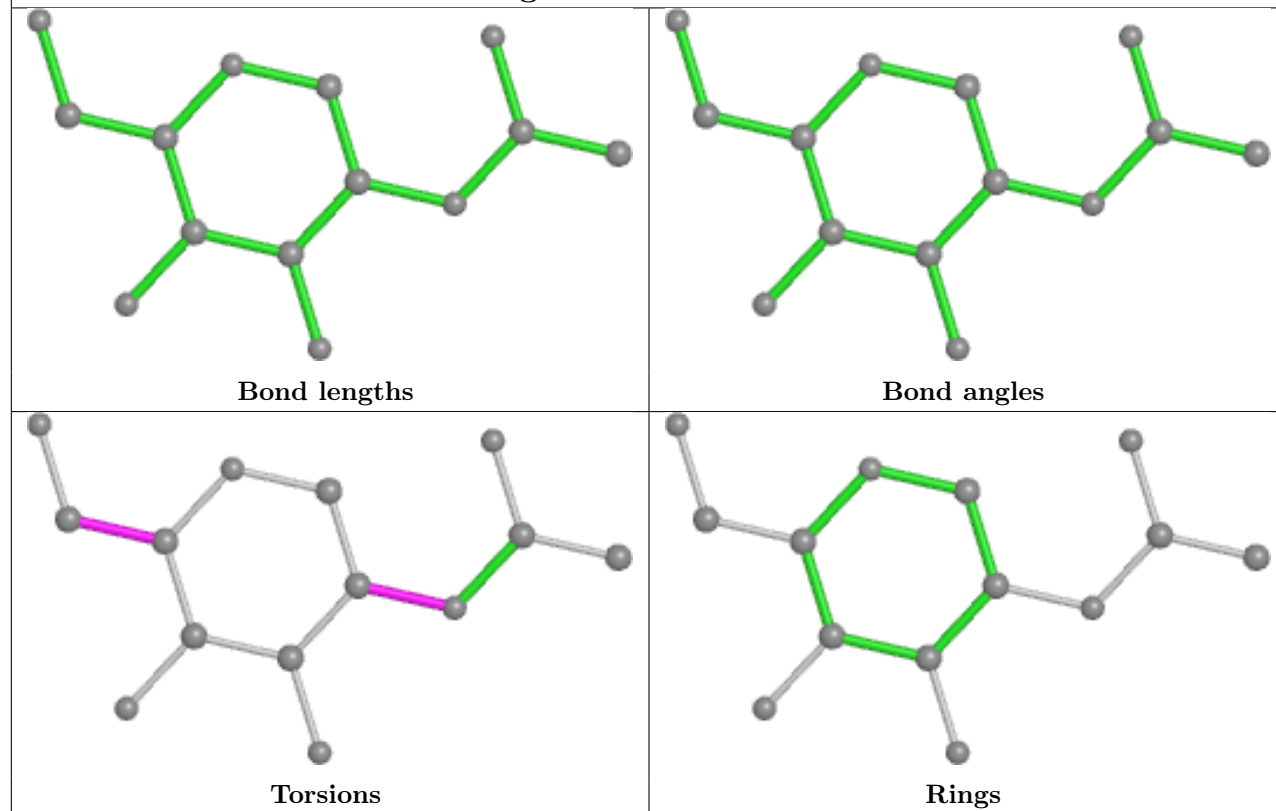




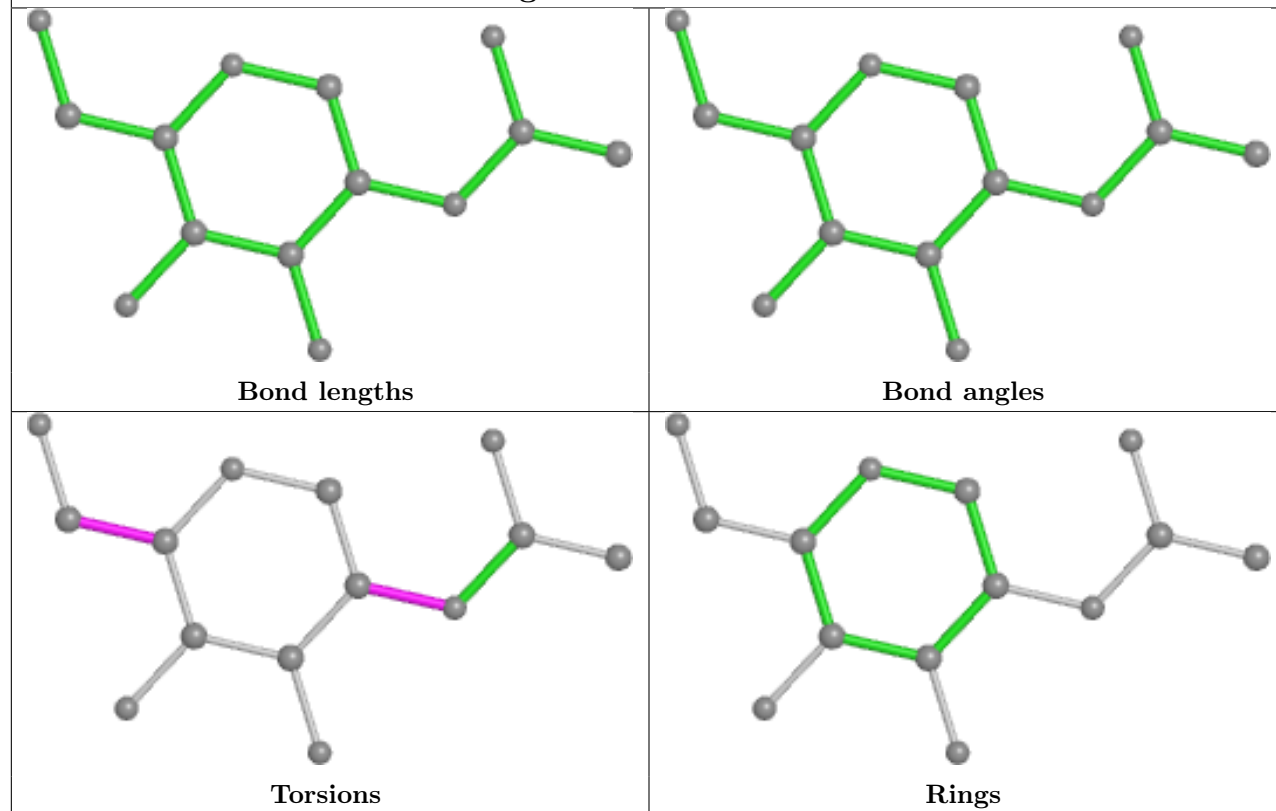
## Ligand NAG C 1302



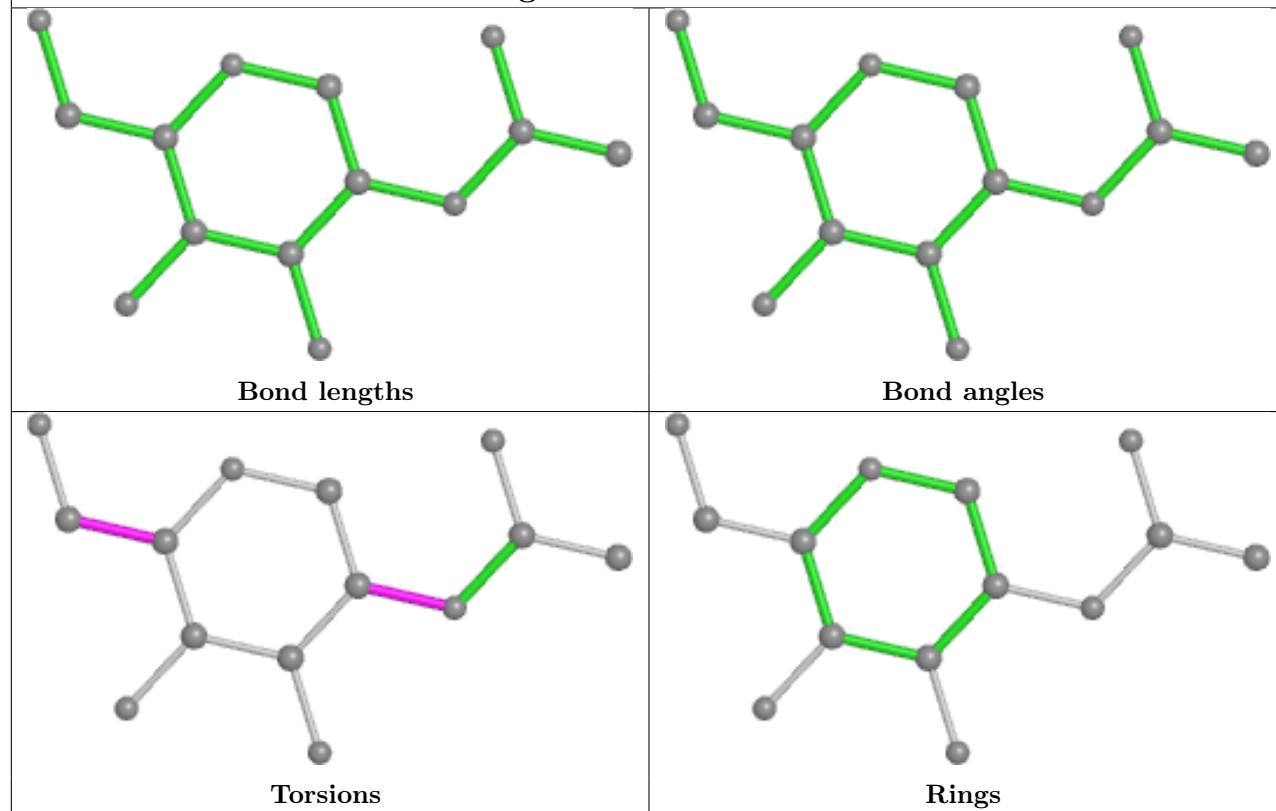
## Ligand NAG B 1309

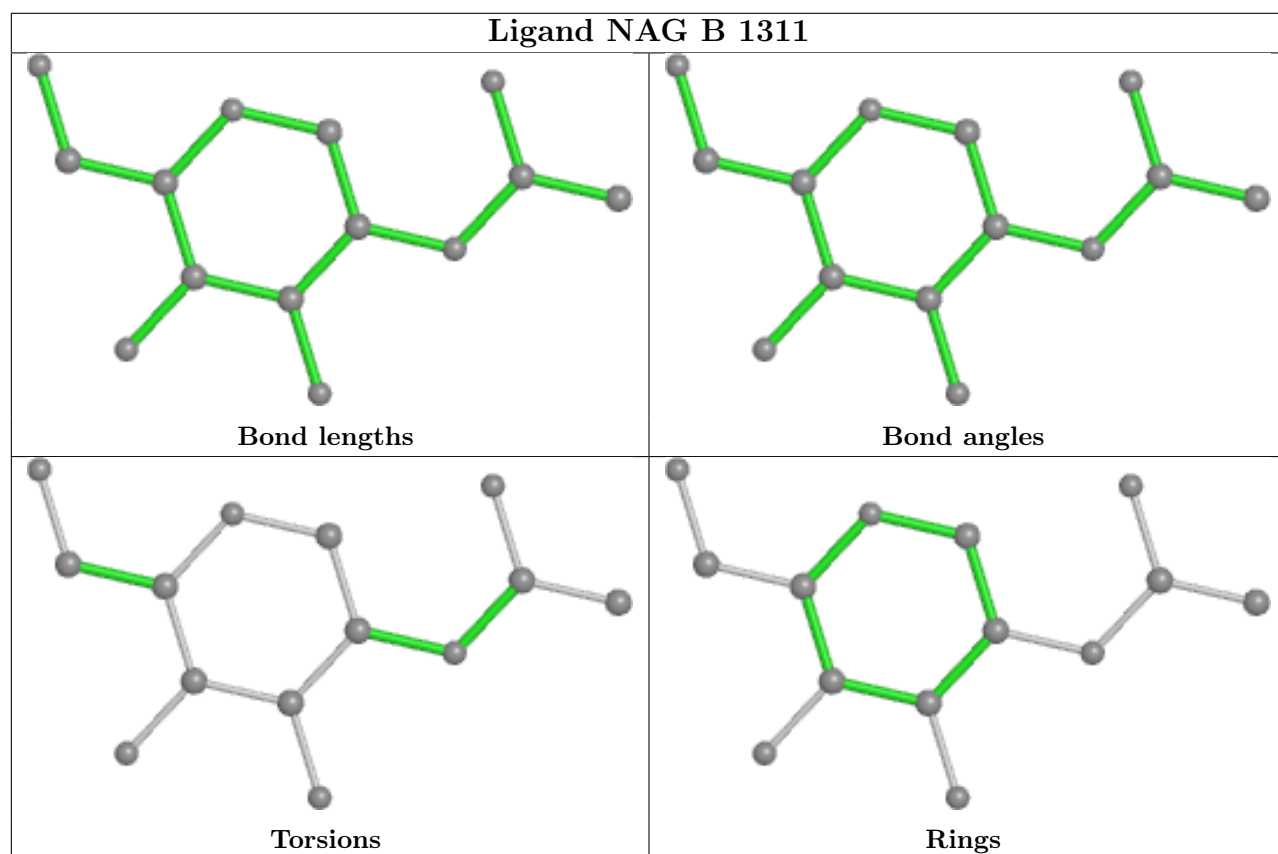
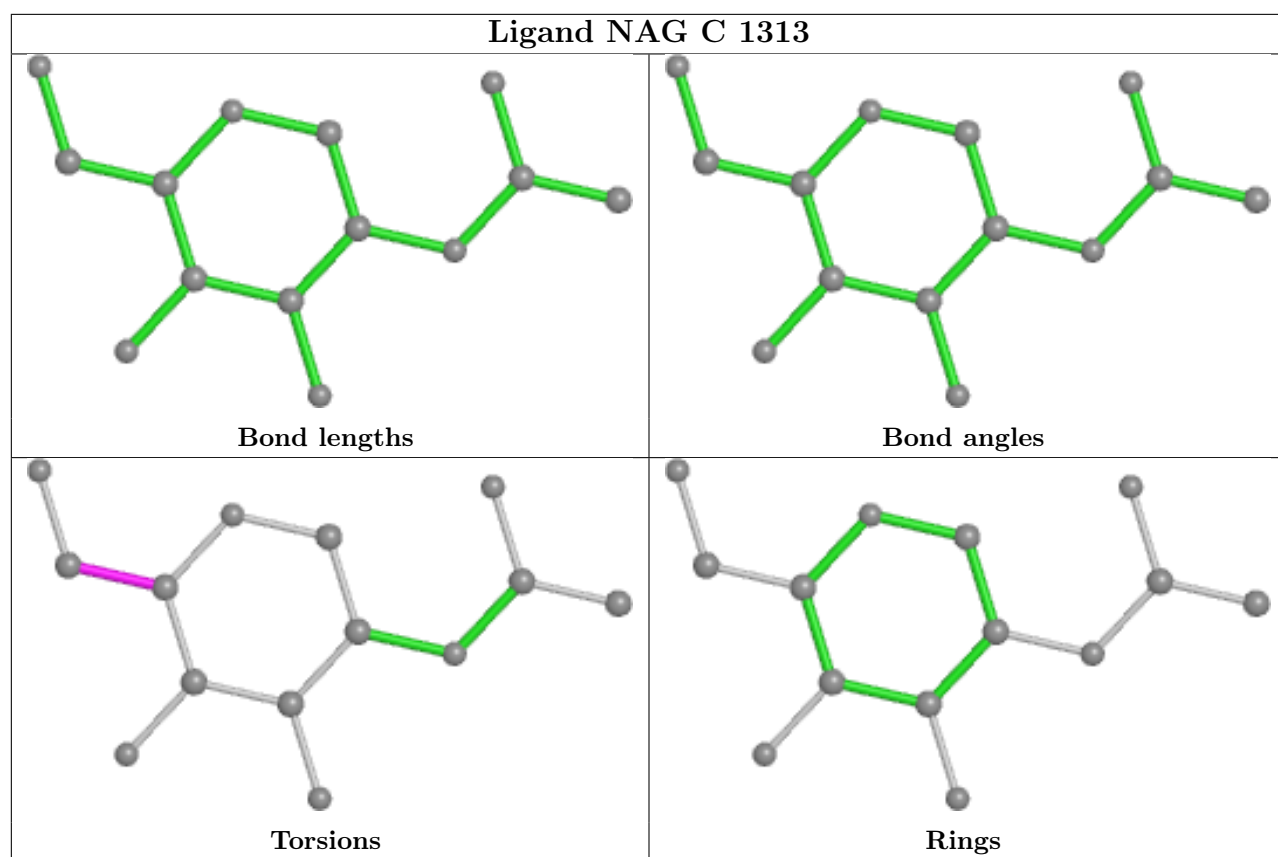


## Ligand NAG C 1304



## Ligand NAG A 1302





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



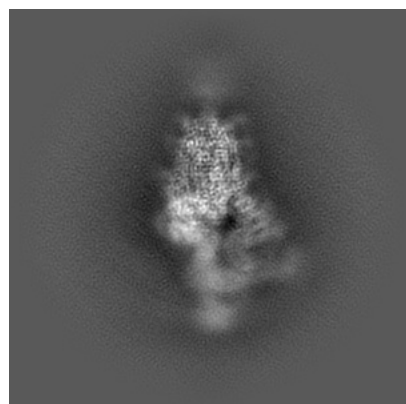
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34134. These allow visual inspection of the internal detail of the map and identification of artifacts.

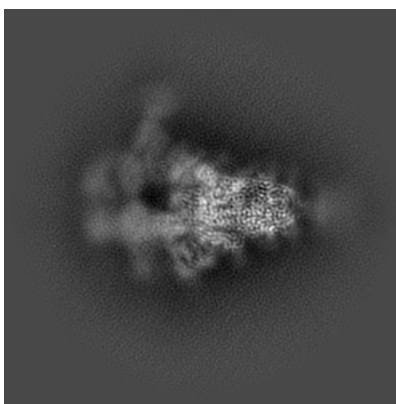
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

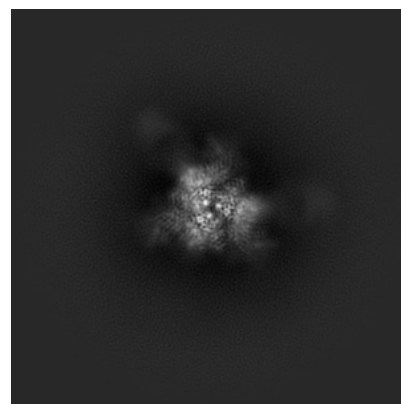
#### 6.1.1 Primary map



X

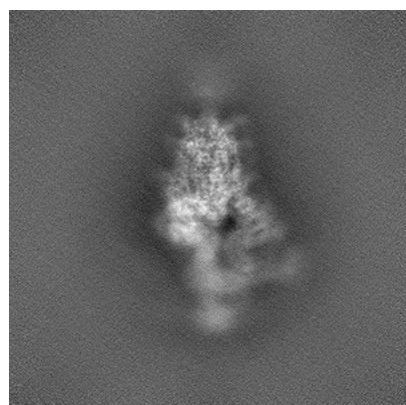


Y

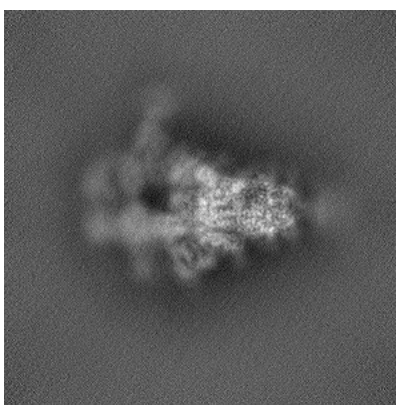


Z

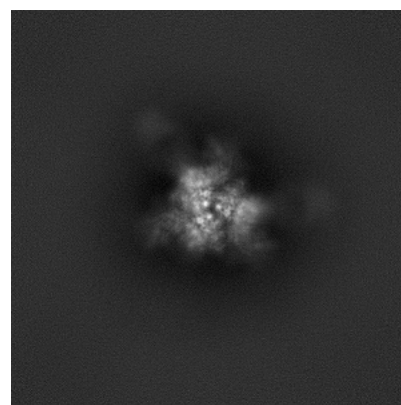
#### 6.1.2 Raw map



X



Y

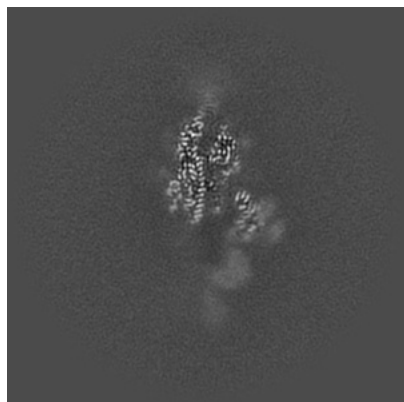


Z

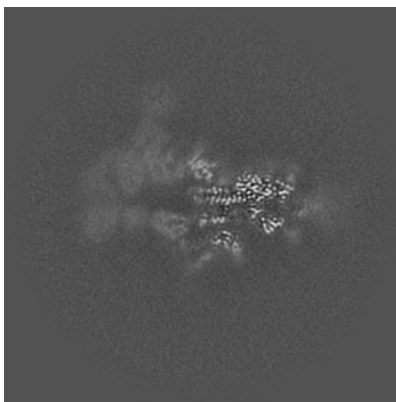
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

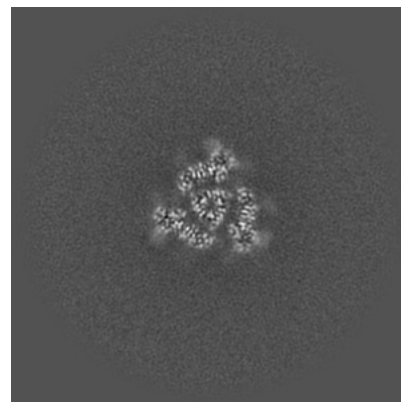
### 6.2.1 Primary map



X Index: 256

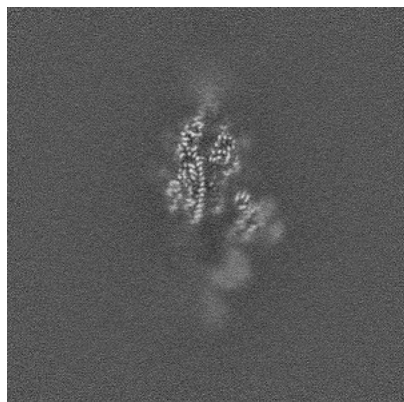


Y Index: 256



Z Index: 256

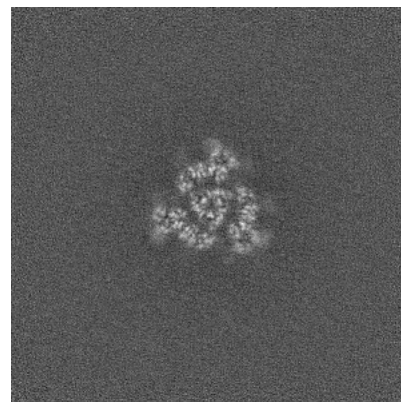
### 6.2.2 Raw map



X Index: 256



Y Index: 256

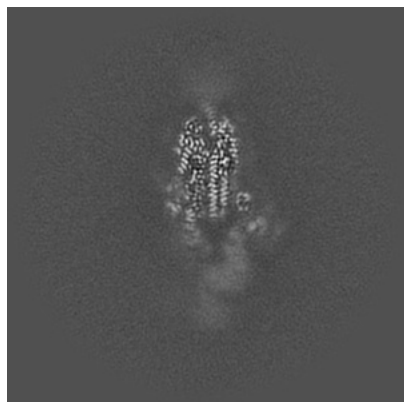


Z Index: 256

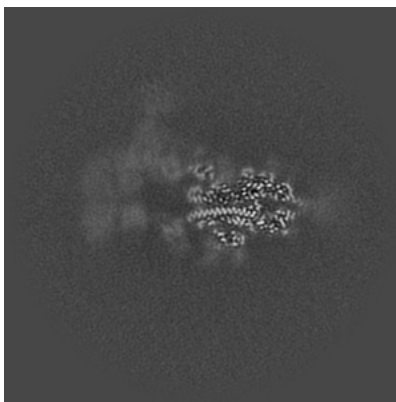
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

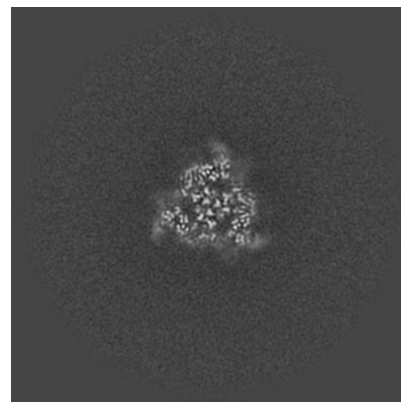
### 6.3.1 Primary map



X Index: 249

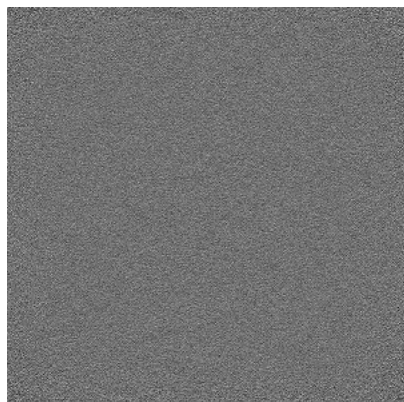


Y Index: 264

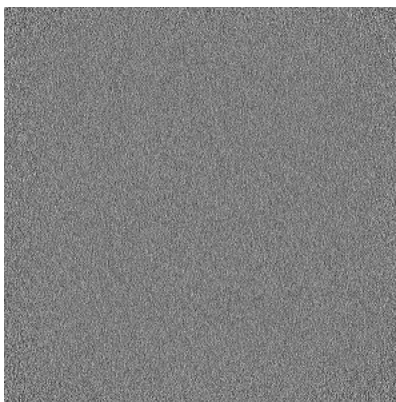


Z Index: 265

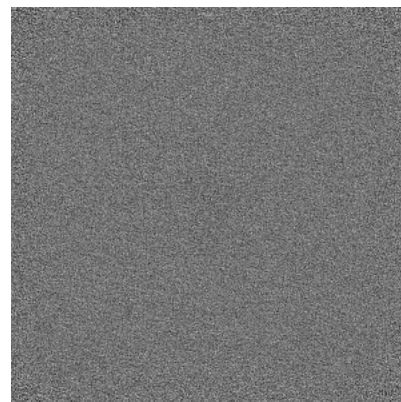
### 6.3.2 Raw map



X Index: 0



Y Index: 0



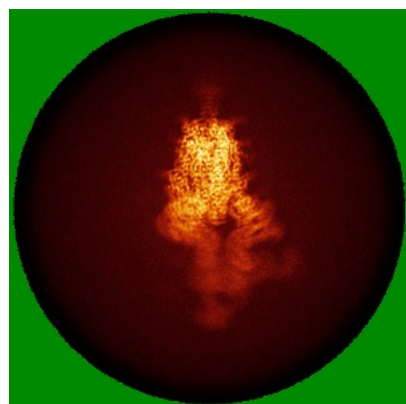
Z Index: 0

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

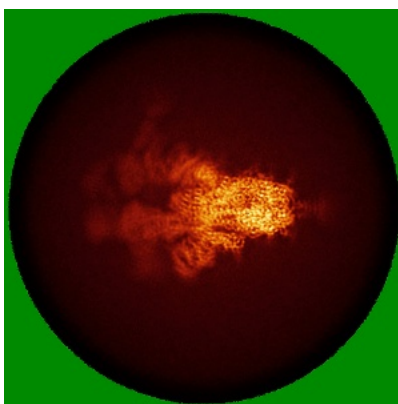


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

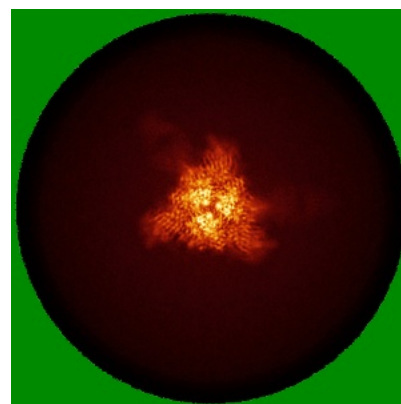
### 6.4.1 Primary map



X

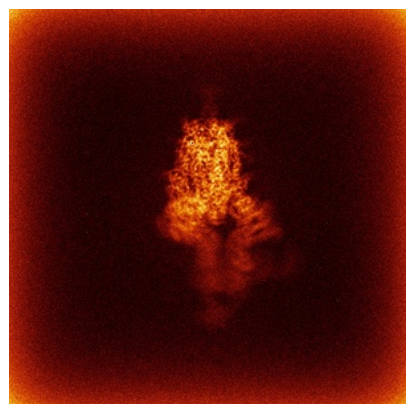


Y

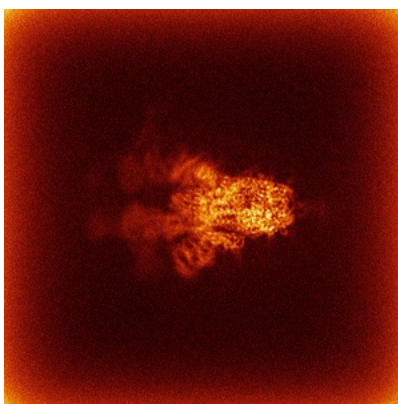


Z

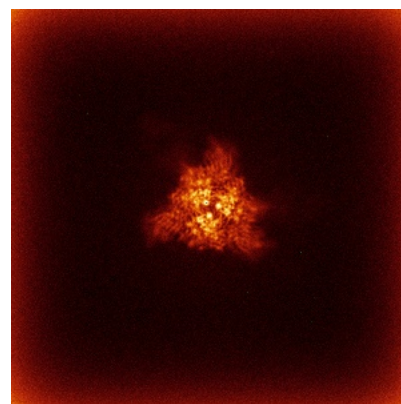
### 6.4.2 Raw map



X



Y

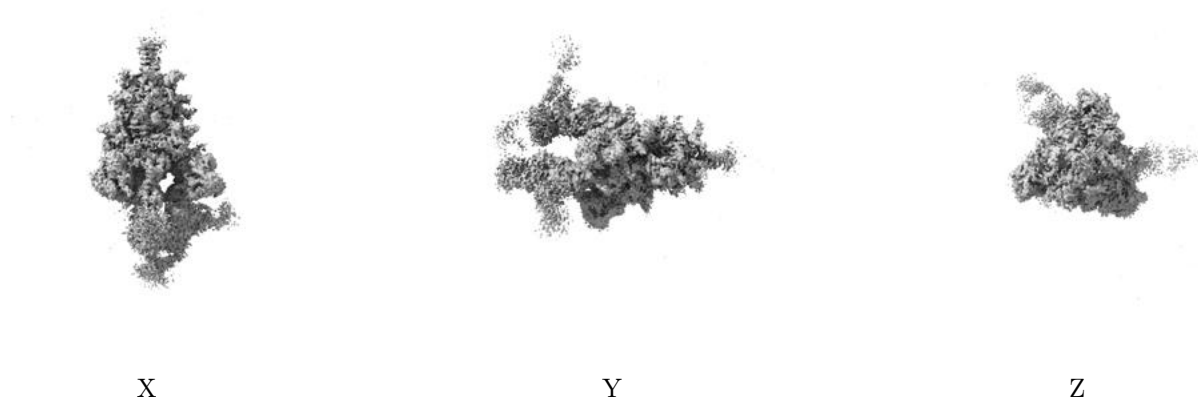


Z

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

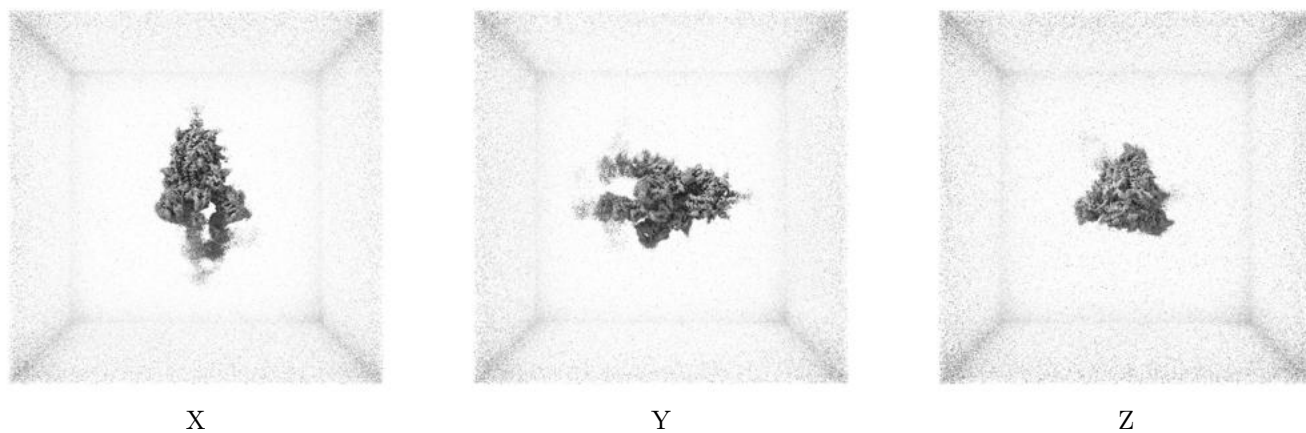
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

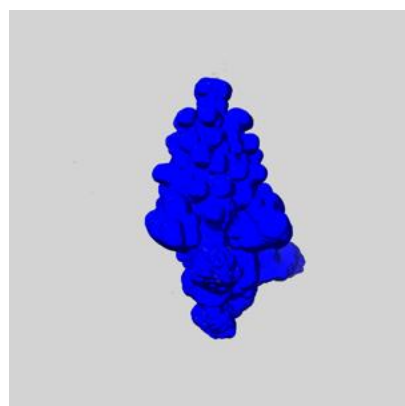
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

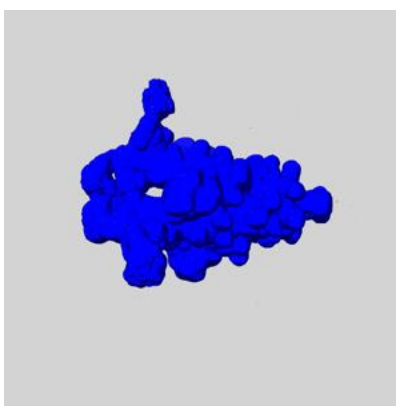
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

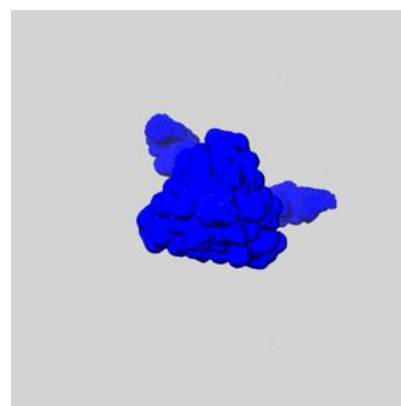
### 6.6.1 emd\_34134\_msk\_1.map [i](#)



X



Y

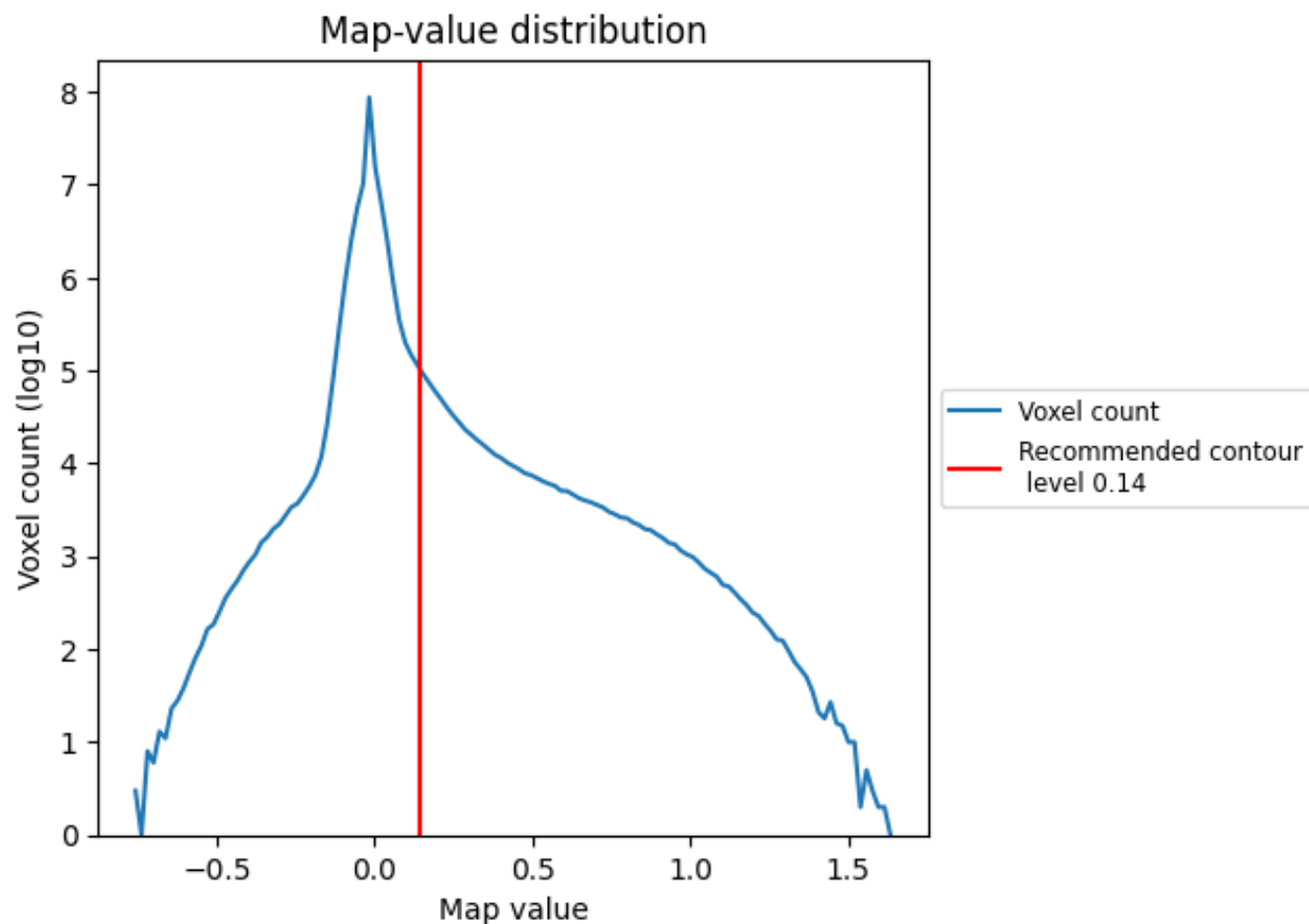


Z

## 7 Map analysis [i](#)

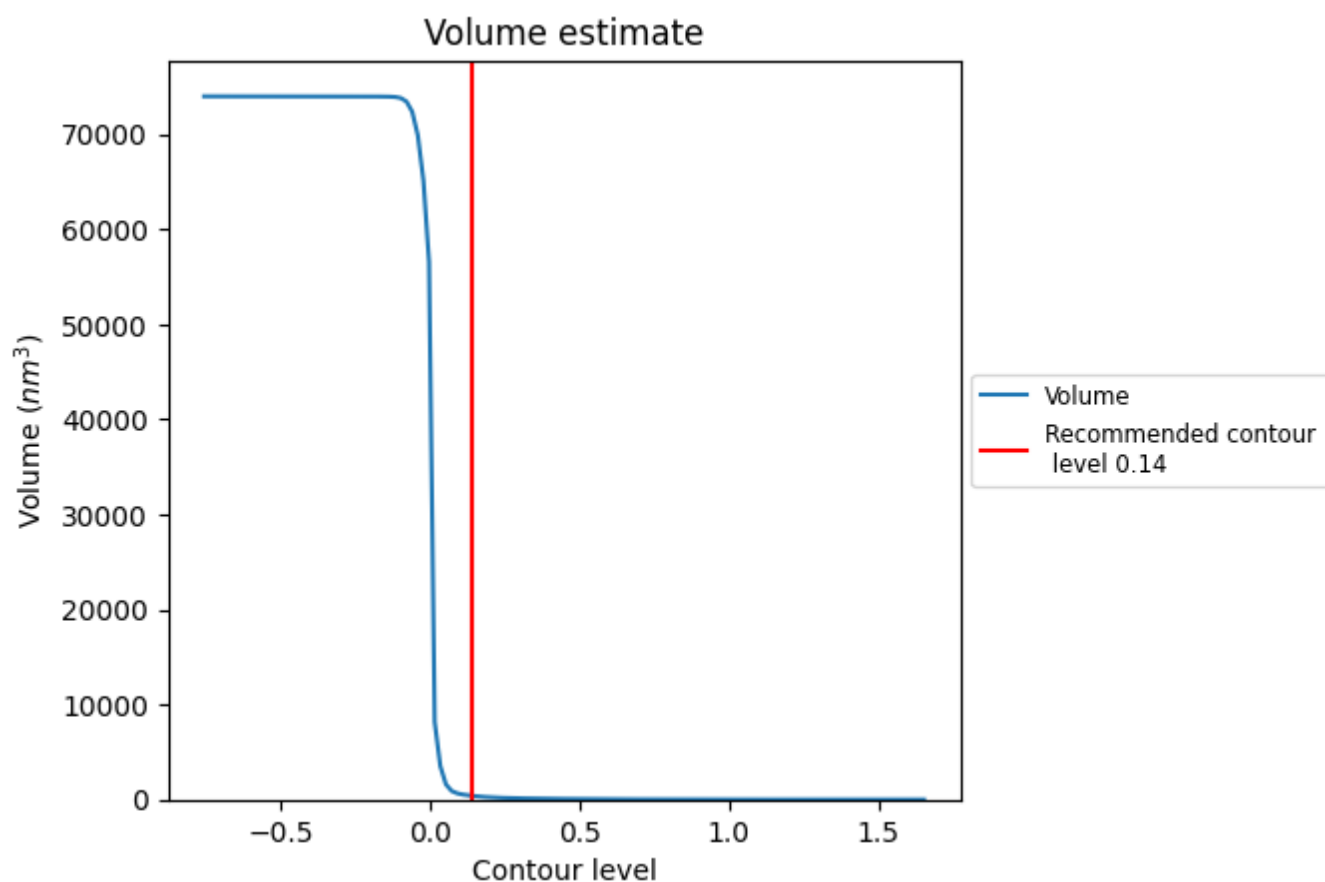
This section contains the results of statistical analysis of the map.

### 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](#)

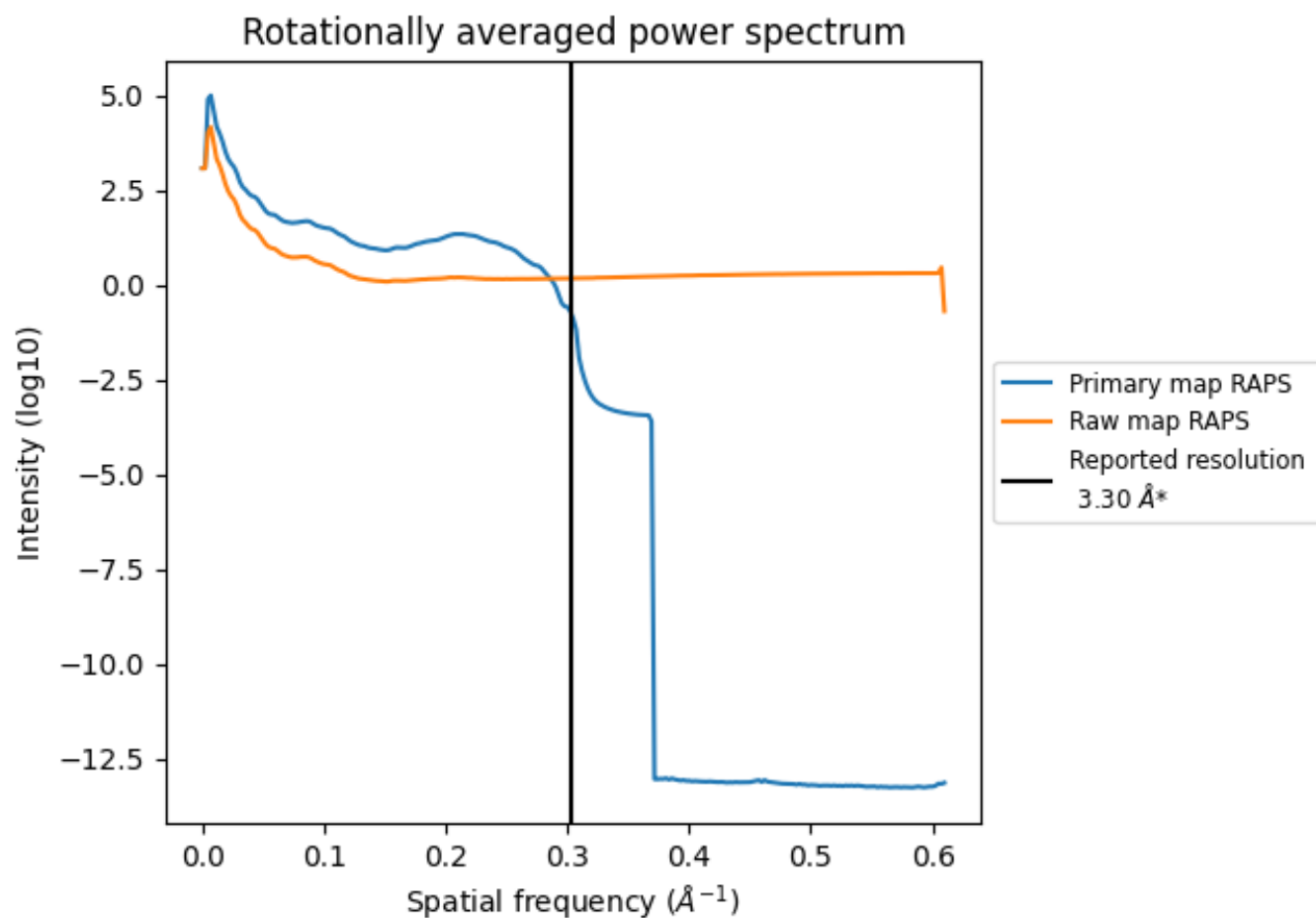


The volume at the recommended contour level is 393  $\text{nm}^3$ ; this corresponds to an approximate mass of 355 kDa.

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 ⓘ

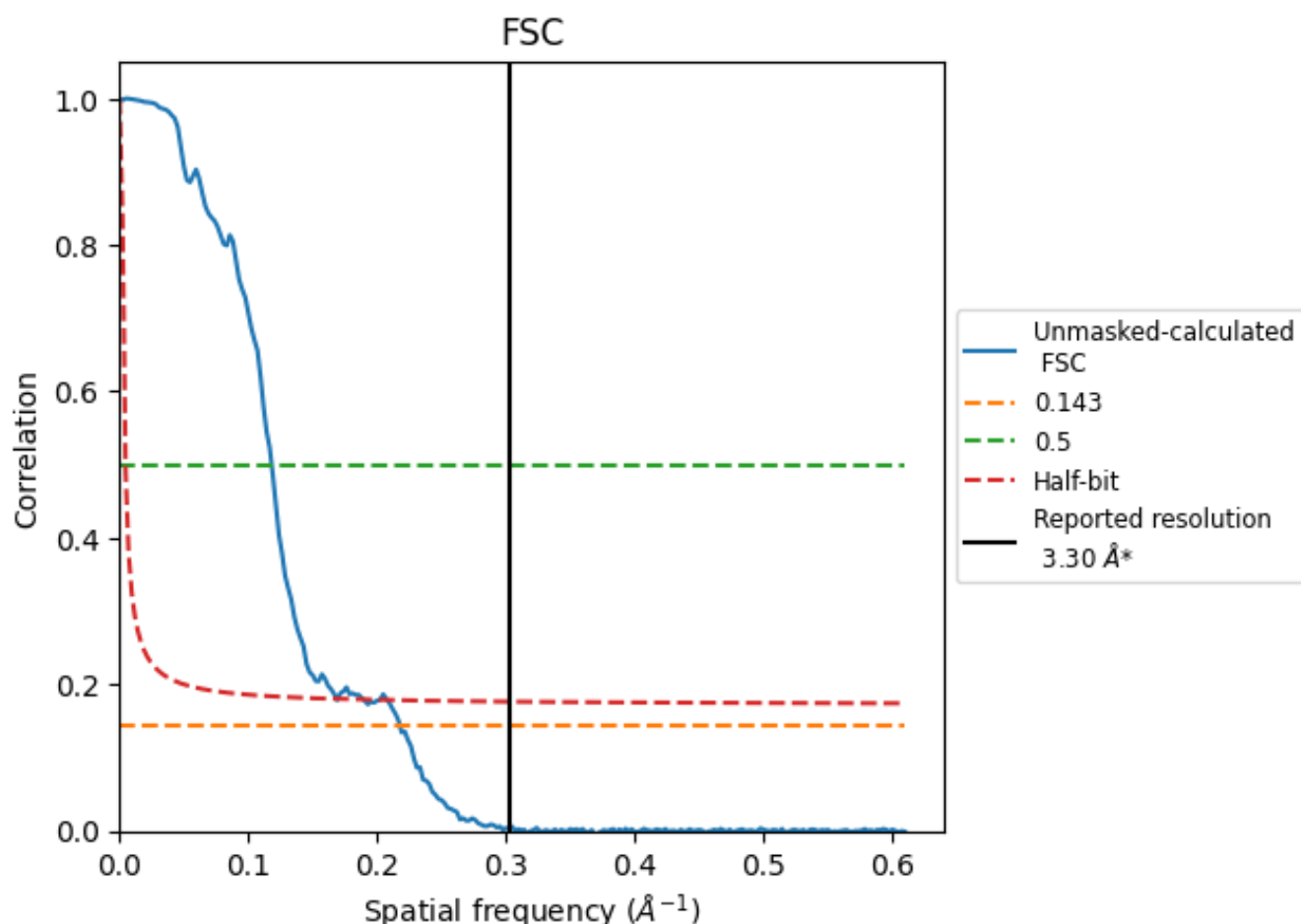


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

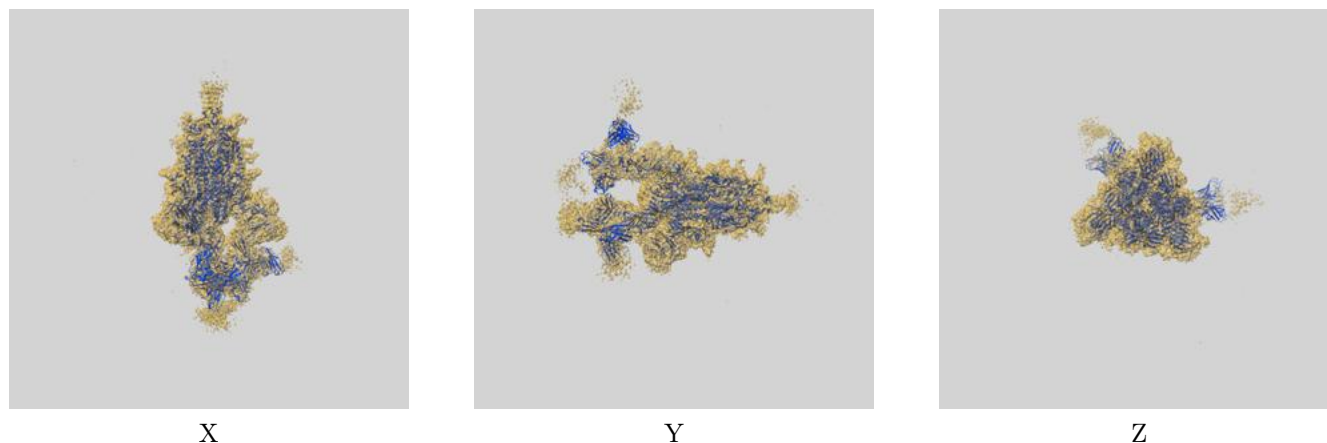
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.59	8.47	5.93

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.59 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

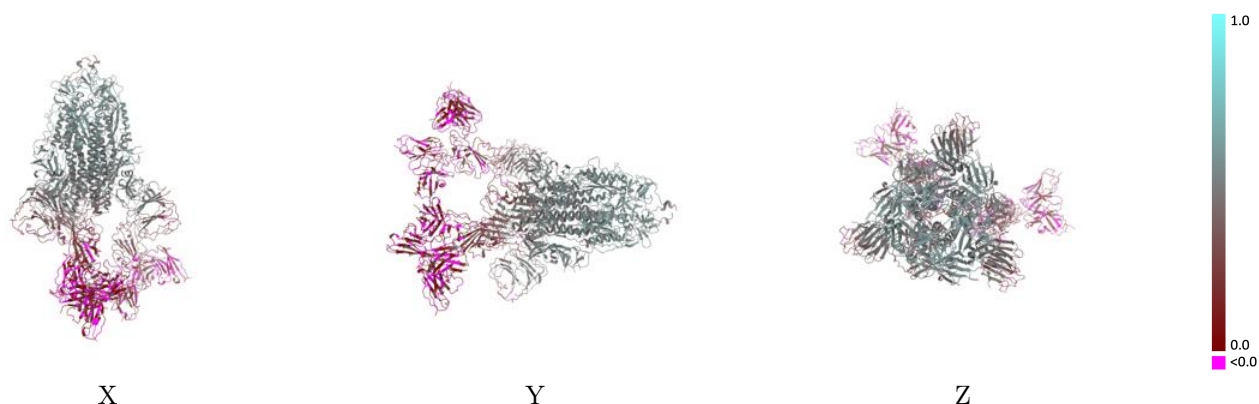
This section contains information regarding the fit between EMDB map EMD-34134 and PDB model 7YVO. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

### 9.1 Map-model overlay [i](#)



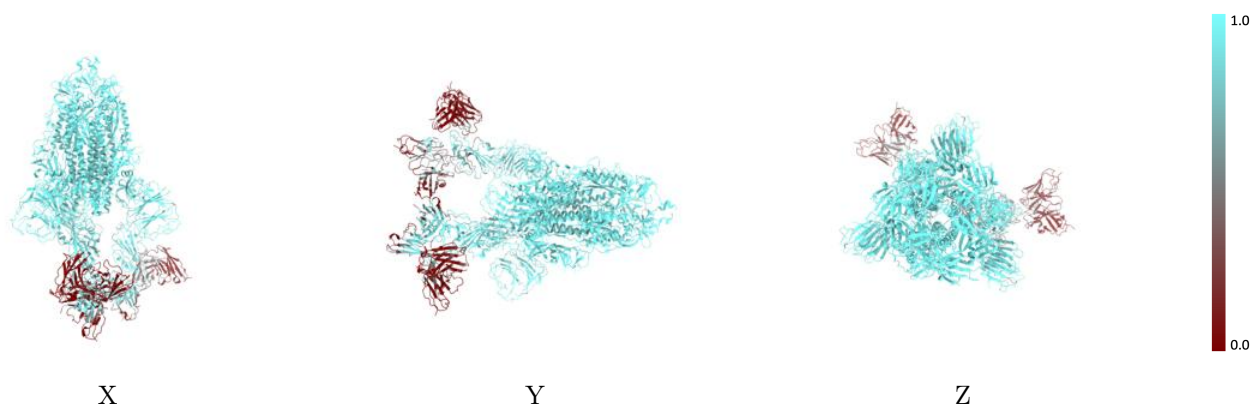
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



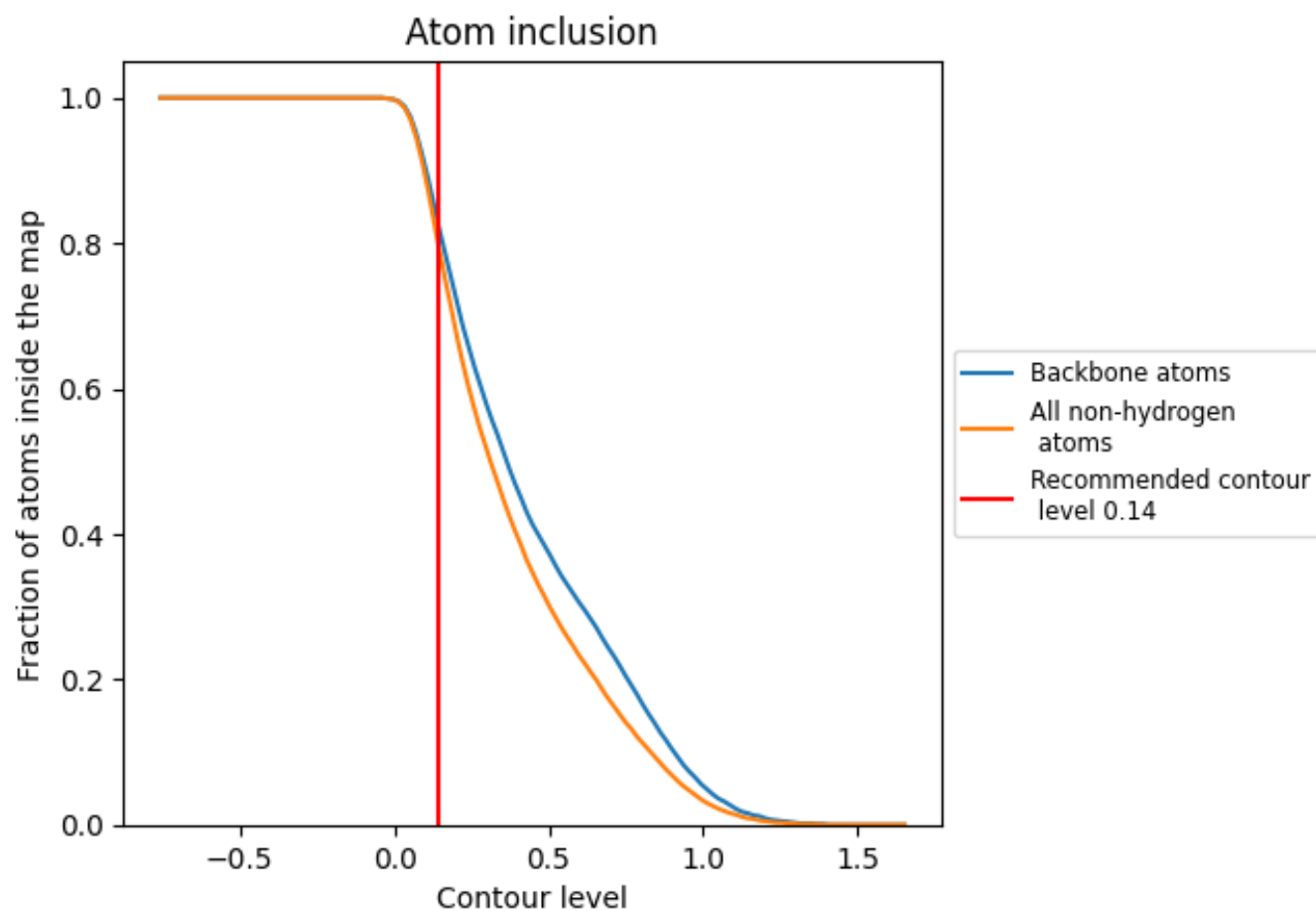
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8040	<div></div> 0.3490
A	<div></div> 0.9240	<div></div> 0.4130
B	<div></div> 0.9510	<div></div> 0.4330
C	<div></div> 0.9610	<div></div> 0.4320
H	<div></div> 0.4110	<div></div> 0.0940
I	<div></div> 0.3140	<div></div> 0.0760
J	<div></div> 0.6300	<div></div> 0.0980
K	<div></div> 0.7250	<div></div> 0.0890
L	<div></div> 0.0650	<div></div> 0.0770
M	<div></div> 0.0900	<div></div> 0.0910
N	<div></div> 0.1960	<div></div> 0.0980
O	<div></div> 0.1960	<div></div> 0.0890

1.0

0.0

<0.0