



Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 09:18 PM JST

PDB ID : 7WZ1 / pdb_00007wz1
EMDB ID : EMD-32901
Title : SARS-CoV-2 Omicron Spike trimer
Authors : Zhan, W.Q.; Zhang, X.; Chen, Z.G.; Sun, L.
Deposited on : 2022-02-16
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

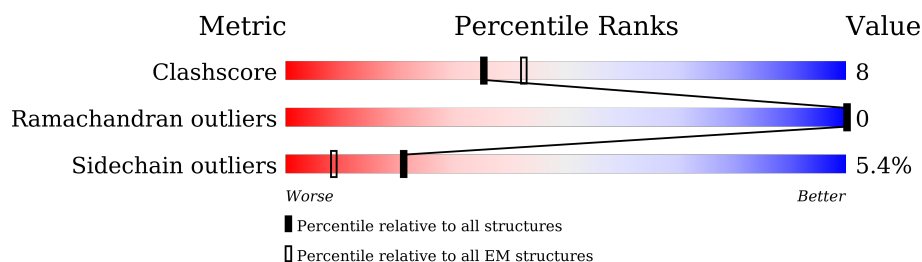
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1285	 62% 17% • 20%
1	B	1285	 61% 18% • 20%
1	C	1285	 63% 16% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24467 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	1032	Total	C	N	O	S	0	0
			8032	5149	1337	1509	37		
1	B	1027	Total	C	N	O	S	0	0
			8000	5130	1330	1503	37		
1	C	1033	Total	C	N	O	S	0	0
			8043	5158	1338	1510	37		

There are 387 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	209	ILE	-	insertion	UNP P0DTC2
A	210	VAL	-	insertion	UNP P0DTC2
A	211	ARG	ASN	conflict	UNP P0DTC2
A	212	GLU	LEU	conflict	UNP P0DTC2
A	213	PRO	VAL	conflict	UNP P0DTC2
A	214	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	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	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
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	856	LYS	ASN	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	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	209	ILE	-	insertion	UNP P0DTC2
B	210	VAL	-	insertion	UNP P0DTC2
B	211	ARG	ASN	conflict	UNP P0DTC2
B	212	GLU	LEU	conflict	UNP P0DTC2
B	213	PRO	VAL	conflict	UNP P0DTC2
B	214	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	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	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	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	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
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	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	145	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	209	ILE	-	insertion	UNP P0DTC2
C	210	VAL	-	insertion	UNP P0DTC2
C	211	ARG	ASN	conflict	UNP P0DTC2
C	212	GLU	LEU	conflict	UNP P0DTC2
C	213	PRO	VAL	conflict	UNP P0DTC2
C	214	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	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	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	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	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	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	856	LYS	ASN	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	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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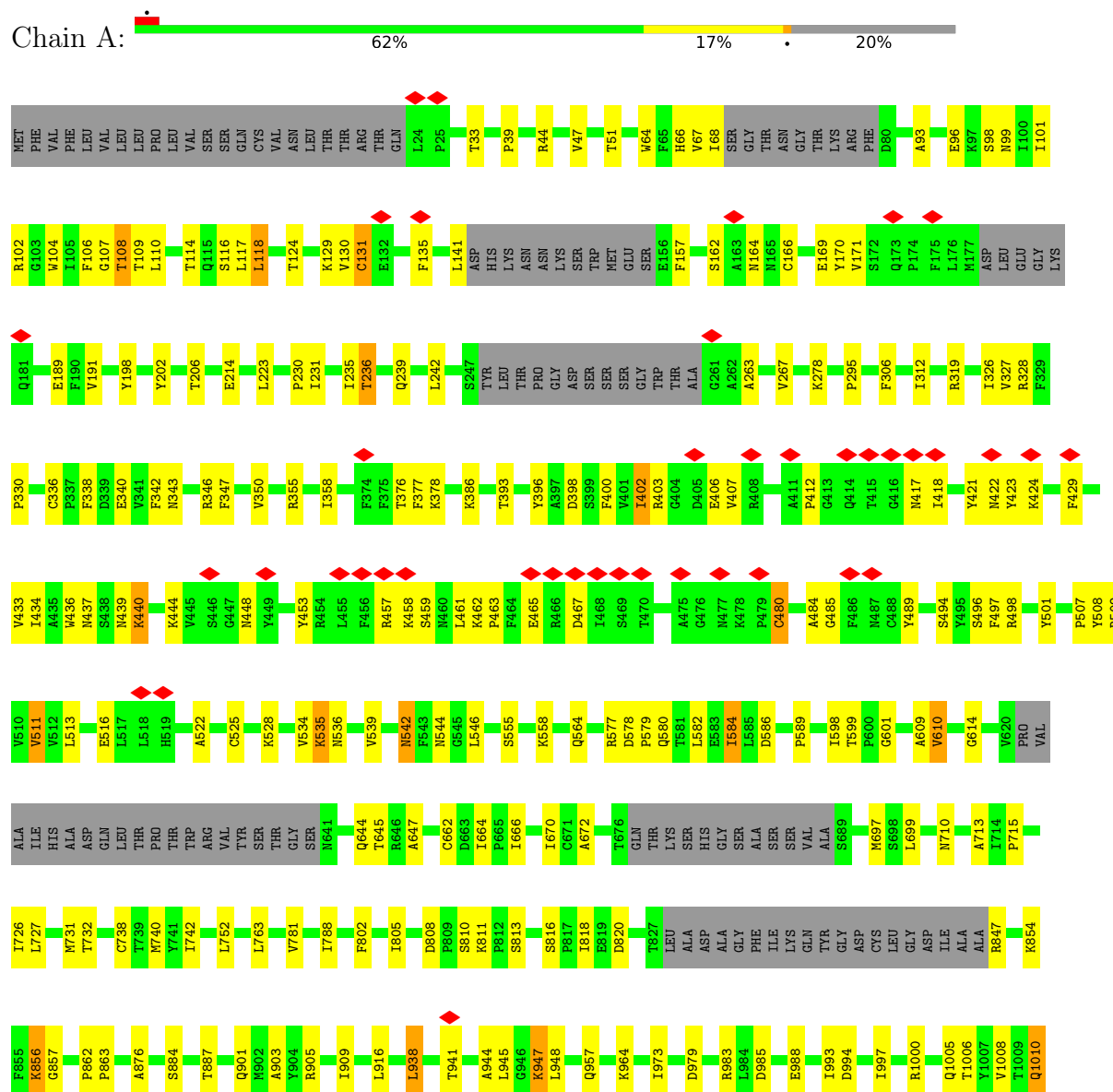
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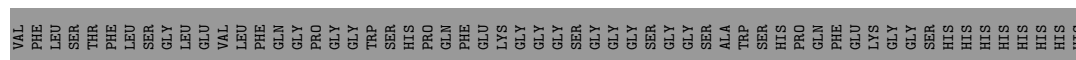
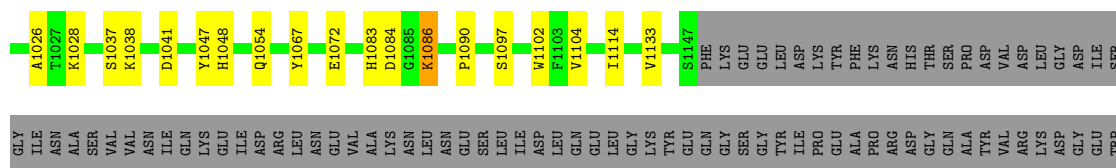
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2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

3 Residue-property plots

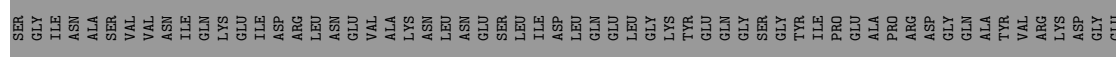
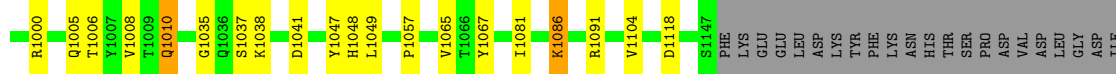
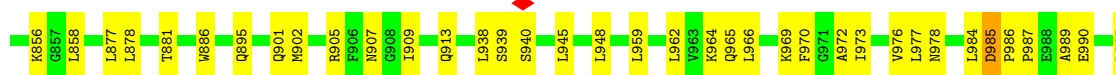
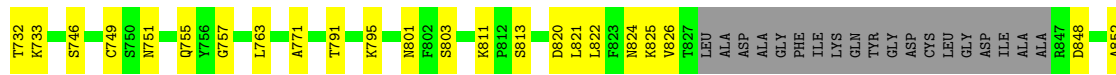
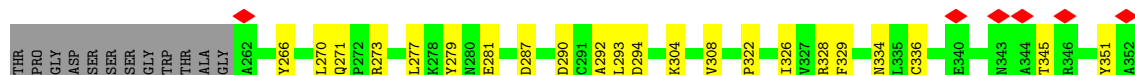
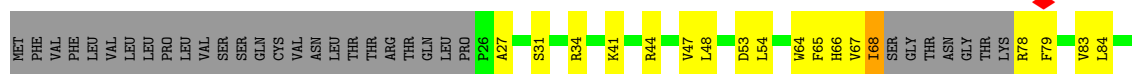
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



Chain C:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128589	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 ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.901	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	340.48, 340.48, 340.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/8223	0.41	1/11198 (0.0%)
1	B	0.14	0/8190	0.42	0/11151
1	C	0.15	0/8235	0.41	3/11214 (0.0%)
All	All	0.15	0/24648	0.41	4/33563 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	938	LEU	N-CA-C	-11.02	97.90	114.64
1	C	67	VAL	CB-CA-C	-5.78	104.99	111.23
1	C	79	PHE	CA-C-N	-5.41	115.36	122.99
1	C	79	PHE	C-N-CA	-5.41	115.36	122.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8032	0	7816	128	0
1	B	8000	0	7781	138	0
1	C	8043	0	7825	127	0
2	A	126	0	117	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	140	0	130	0	0
2	C	126	0	117	1	0
All	All	24467	0	23786	372	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 8.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PHE:HB2	1:C:242:LEU:HD11	1.46	0.95
1:B:107:GLY:H	1:B:235:ILE:HG13	1.55	0.71
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.72	0.71
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.74	0.69
1:B:336:CYS:N	1:B:361:CYS:SG	2.66	0.68
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.76	0.67
1:C:1037:SER:H	1:C:1048:HIS:HD2	1.43	0.67
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.75	0.67
1:B:103:GLY:HA3	1:B:241:LEU:HB2	1.78	0.66
1:A:93:ALA:HA	1:A:189:GLU:HA	1.77	0.65
1:A:1037:SER:H	1:A:1048:HIS:HD2	1.44	0.65
1:C:770:ILE:O	1:C:774:GLN:NE2	2.30	0.65
1:C:115:GLN:HG3	1:C:132:GLU:HB3	1.80	0.64
1:B:391:CYS:HA	1:B:525:CYS:HA	1.80	0.64
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.79	0.64
1:A:457:ARG:NH2	1:A:459:SER:OG	2.30	0.64
1:B:913:GLN:NE2	1:C:1090:PRO:O	2.30	0.64
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.80	0.64
1:C:302:THR:HG23	1:C:303:LEU:HD23	1.79	0.63
1:A:102:ARG:HH21	1:A:141:LEU:HG	1.64	0.63
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.79	0.63
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.80	0.63
1:A:418:ILE:O	1:A:422:ASN:ND2	2.32	0.63
1:A:577:ARG:HH21	1:A:582:LEU:HD12	1.64	0.63
1:B:308:VAL:HG12	1:B:602:THR:HG23	1.81	0.63
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.81	0.62
1:B:68:ILE:HG12	1:B:68:ILE:O	1.99	0.61
1:B:907:ASN:HD21	1:B:913:GLN:HB3	1.64	0.61
1:B:1037:SER:H	1:B:1048:HIS:HD2	1.46	0.61
1:C:336:CYS:HB2	1:C:363:ALA:HB2	1.82	0.61
1:B:452:LEU:HD13	1:B:492:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:THR:OG1	1:A:944:ALA:HB2	2.02	0.60
1:A:1006:THR:O	1:A:1010:GLN:NE2	2.33	0.60
1:B:334:ASN:ND2	1:B:360:ASN:O	2.35	0.60
1:A:1006:THR:OG1	1:C:1005:GLN:NE2	2.34	0.60
1:B:645:THR:HG23	1:B:647:ALA:H	1.66	0.60
1:B:852:ALA:O	1:B:856:LYS:NZ	2.32	0.60
1:C:403:ARG:NH1	1:C:505:HIS:O	2.35	0.60
1:C:177:MET:SD	1:C:188:ARG:NH1	2.75	0.60
1:C:599:THR:HG22	1:C:601:GLY:H	1.67	0.60
1:C:811:LYS:HE2	1:C:813:SER:HB2	1.83	0.60
1:B:820:ASP:O	1:B:824:ASN:ND2	2.30	0.60
1:B:1006:THR:O	1:B:1010:GLN:NE2	2.33	0.60
1:B:361:CYS:SG	1:B:362:VAL:N	2.74	0.59
1:C:393:THR:HG22	1:C:394:ASN:HD22	1.67	0.59
1:A:662:CYS:HB2	1:A:697:MET:HG2	1.85	0.59
1:B:31:SER:HA	1:B:216:LEU:HD23	1.84	0.59
1:B:976:VAL:HG12	1:B:978:ASN:H	1.67	0.59
1:C:79:PHE:HB2	1:C:242:LEU:CD1	2.26	0.59
1:A:437:ASN:HD22	1:A:508:TYR:HE1	1.50	0.59
1:A:726:ILE:HB	1:A:947:LYS:HD3	1.84	0.59
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.35	0.59
1:C:912:THR:OG1	1:C:1106:GLN:NE2	2.36	0.59
1:A:406:GLU:HG2	1:A:418:ILE:HB	1.85	0.58
1:B:791:THR:OG1	1:B:795:LYS:NZ	2.37	0.58
1:B:895:GLN:NE2	1:C:706:ALA:O	2.36	0.58
1:A:740:MET:HE3	1:A:857:GLY:HA2	1.85	0.58
1:B:90:VAL:HG12	1:B:192:PHE:HB2	1.85	0.58
1:B:198:TYR:OH	1:C:394:ASN:ND2	2.35	0.58
1:C:99:ASN:HB3	1:C:102:ARG:HE	1.69	0.58
1:A:599:THR:HG22	1:A:601:GLY:H	1.68	0.58
1:A:847:ARG:HH22	1:B:574:ASP:HB3	1.67	0.58
1:B:102:ARG:HD3	1:B:121:ASN:HB2	1.86	0.58
1:C:1006:THR:O	1:C:1010:GLN:NE2	2.37	0.58
1:A:393:THR:HA	1:A:522:ALA:HA	1.85	0.58
1:A:1038:LYS:HE2	1:C:1038:LYS:HZ1	1.69	0.57
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.86	0.57
1:C:184:PHE:HE2	1:C:209:ILE:HG23	1.69	0.57
1:C:563:GLN:O	1:C:577:ARG:NH1	2.36	0.57
1:A:44:ARG:HH21	1:B:567:ARG:HH21	1.53	0.57
1:A:106:PHE:O	1:A:116:SER:OG	2.21	0.57
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.68	0.57
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.85	0.57
1:A:713:ALA:HB2	1:C:895:GLN:HG2	1.87	0.57
1:B:271:GLN:OE1	1:B:273:ARG:NH2	2.37	0.57
1:B:322:PRO:HB3	1:B:539:VAL:HA	1.86	0.57
1:B:811:LYS:NZ	1:B:813:SER:OG	2.34	0.57
1:C:140:PHE:HB2	1:C:244:LEU:HD22	1.87	0.57
1:A:412:PRO:HD3	1:A:429:PHE:HD2	1.70	0.57
1:A:909:ILE:HG21	1:A:1047:TYR:HB3	1.85	0.57
1:B:1038:LYS:HB2	1:B:1038:LYS:HZ2	1.69	0.57
2:A:1308:NAG:H83	2:A:1308:NAG:H3	1.87	0.56
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.86	0.56
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.86	0.56
1:C:354:ASN:HB3	1:C:399:SER:HB3	1.87	0.56
1:B:474:GLN:NE2	1:B:478:LYS:O	2.39	0.56
1:A:135:PHE:HZ	1:A:239:GLN:HG2	1.71	0.55
1:B:47:VAL:HG12	1:C:569:ILE:HD13	1.88	0.55
1:C:393:THR:HA	1:C:522:ALA:HA	1.88	0.55
1:A:903:ALA:HB2	1:A:916:LEU:HD22	1.89	0.55
1:B:821:LEU:O	1:B:825:LYS:NZ	2.39	0.55
2:C:1306:NAG:H83	2:C:1306:NAG:H3	1.88	0.55
1:B:191:VAL:HB	1:B:202:TYR:HB2	1.88	0.55
1:C:431:GLY:HA3	1:C:514:SER:HA	1.88	0.55
1:B:345:THR:O	1:B:509:ARG:NH2	2.41	0.55
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.89	0.55
1:A:884:SER:HG	1:A:887:THR:HG1	1.55	0.54
1:B:969:LYS:NZ	1:B:972:ALA:O	2.36	0.54
1:A:964:LYS:NZ	1:C:758:SER:OG	2.40	0.54
1:A:731:MET:HG2	1:A:732:THR:H	1.72	0.54
1:A:811:LYS:NZ	1:A:820:ASP:OD1	2.41	0.54
1:B:41:LYS:HE2	1:B:225:PRO:HG3	1.88	0.54
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.40	0.54
1:B:452:LEU:HD22	1:B:492:LEU:HD13	1.89	0.54
1:C:1106:GLN:NE2	1:C:1111:GLU:OE1	2.40	0.54
1:A:295:PRO:HG2	1:A:610:VAL:HG22	1.89	0.54
1:C:818:ILE:HD12	1:C:1054:GLN:HE22	1.73	0.54
1:A:614:GLY:N	1:A:647:ALA:O	2.41	0.54
1:A:350:VAL:HG22	1:A:400:PHE:HB2	1.90	0.54
1:C:596:SER:HB2	1:C:611:LEU:HB3	1.90	0.54
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.89	0.53
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ILE:HD12	1:B:482:GLY:HA2	1.91	0.53
1:A:319:ARG:HH22	1:C:740:MET:HB2	1.74	0.53
1:A:457:ARG:NH2	1:A:465:GLU:OE1	2.42	0.53
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.90	0.53
1:B:44:ARG:HB2	1:B:279:TYR:HD2	1.74	0.53
1:A:118:LEU:HD11	1:A:129:LYS:HB2	1.90	0.53
1:B:187:LEU:HB2	1:B:208:ILE:HB	1.91	0.53
1:C:907:ASN:HD21	1:C:913:GLN:HB3	1.72	0.53
1:A:440:LYS:H	1:A:440:LYS:HD3	1.74	0.52
1:A:644:GLN:NE2	1:A:645:THR:O	2.42	0.52
1:C:96:GLU:OE2	1:C:188:ARG:NH1	2.42	0.52
1:C:454:ARG:HH22	1:C:457:ARG:HB2	1.74	0.52
1:C:615:VAL:HG11	1:C:620:VAL:HG13	1.89	0.52
1:B:96:GLU:OE1	1:B:100:ILE:N	2.43	0.52
1:B:187:LEU:HB3	1:B:206:THR:HG23	1.90	0.52
1:C:308:VAL:N	1:C:602:THR:OG1	2.41	0.52
1:A:584:ILE:HD13	1:A:584:ILE:H	1.74	0.52
1:A:752:LEU:HD22	1:A:993:ILE:HG23	1.91	0.52
1:B:96:GLU:OE2	1:B:102:ARG:NH2	2.43	0.52
1:B:119:ILE:HG22	1:B:128:ILE:HG12	1.90	0.52
1:C:332:ILE:HG23	1:C:362:VAL:HG22	1.92	0.52
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.92	0.52
1:C:735:SER:HA	1:C:767:LEU:HD13	1.92	0.52
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.92	0.51
1:B:290:ASP:OD1	1:B:293:LEU:N	2.43	0.51
1:A:117:LEU:HD23	1:A:235:ILE:HD11	1.93	0.51
1:A:1005:GLN:NE2	1:B:1006:THR:OG1	2.43	0.51
1:C:811:LYS:HD3	1:C:815:ARG:H	1.75	0.51
1:A:191:VAL:HB	1:A:202:TYR:HB2	1.92	0.51
1:C:615:VAL:HG13	1:C:619:GLU:HB3	1.92	0.51
1:C:79:PHE:CB	1:C:242:LEU:HD11	2.32	0.51
1:C:436:TRP:HE1	1:C:509:ARG:HH21	1.58	0.51
1:B:418:ILE:HG23	1:B:422:ASN:HD22	1.74	0.51
1:C:115:GLN:HA	1:C:132:GLU:HA	1.93	0.51
1:A:816:SER:OG	1:A:1054:GLN:NE2	2.43	0.51
1:C:452:LEU:HD23	1:C:492:LEU:HD12	1.93	0.51
1:A:1086:LYS:H	1:A:1086:LYS:HD2	1.77	0.50
1:A:439:ASN:HA	1:A:507:PRO:HG2	1.93	0.50
1:C:203:SER:HB2	1:C:226:LEU:HD12	1.93	0.50
1:B:187:LEU:HD13	1:B:208:ILE:HD12	1.93	0.50
1:B:909:ILE:HD13	1:B:1049:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:ASP:O	1:C:408:ARG:NE	2.44	0.50
1:A:496:SER:OG	1:A:498:ARG:NH1	2.45	0.50
1:C:94:SER:HB2	1:C:188:ARG:HG3	1.93	0.50
1:B:106:PHE:HD2	1:B:117:LEU:HB3	1.76	0.50
1:C:341:VAL:HG12	1:C:342:PHE:H	1.77	0.50
1:A:945:LEU:HB3	1:A:948:LEU:HB2	1.93	0.49
1:A:1090:PRO:O	1:C:913:GLN:NE2	2.45	0.49
1:A:403:ARG:HG2	1:A:497:PHE:HE1	1.76	0.49
1:B:34:ARG:NH1	1:B:91:TYR:OH	2.45	0.49
1:B:457:ARG:NH1	1:B:467:ASP:OD2	2.46	0.49
1:C:1037:SER:H	1:C:1048:HIS:CD2	2.27	0.49
1:A:818:ILE:HB	1:A:1054:GLN:HE22	1.78	0.49
1:C:808:ASP:OD2	1:C:810:SER:OG	2.24	0.49
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.61	0.49
1:A:96:GLU:HG2	1:A:98:SER:H	1.78	0.49
1:C:29:THR:OG1	1:C:215:ASP:OD1	2.25	0.48
1:A:278:LYS:HB2	1:A:306:PHE:HE2	1.76	0.48
1:B:473:TYR:HB2	1:B:491:PRO:HB3	1.95	0.48
1:A:319:ARG:NH1	1:C:740:MET:SD	2.83	0.48
1:C:441:LEU:HD23	1:C:441:LEU:H	1.78	0.48
1:C:541:PHE:HB3	1:C:552:LEU:HD11	1.94	0.48
1:A:64:TRP:NE1	1:A:214:GLU:OE1	2.46	0.48
1:A:191:VAL:HG23	1:A:223:LEU:HD22	1.96	0.48
1:B:351:TYR:HB2	1:B:454:ARG:HH11	1.78	0.48
1:B:751:ASN:O	1:B:755:GLN:NE2	2.45	0.48
1:C:65:PHE:HB3	1:C:80:ASP:OD2	2.14	0.48
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.96	0.48
1:A:342:PHE:HZ	1:A:513:LEU:HD11	1.79	0.48
1:A:434:ILE:HB	1:A:511:VAL:HG13	1.95	0.48
1:A:484:ALA:HA	1:A:489:TYR:HB3	1.95	0.48
1:A:727:LEU:HD11	1:A:1028:LYS:HD2	1.96	0.47
1:C:244:LEU:HG	1:C:246:ARG:HG2	1.95	0.47
1:A:994:ASP:HA	1:A:997:ILE:HG22	1.96	0.47
1:B:141:LEU:HB2	1:B:243:ALA:HB2	1.96	0.47
1:A:994:ASP:OD2	1:B:995:ARG:NH2	2.35	0.47
1:B:731:MET:HG2	1:B:732:THR:H	1.79	0.47
1:C:106:PHE:HB3	1:C:235:ILE:HD12	1.96	0.47
1:C:596:SER:O	1:C:611:LEU:N	2.42	0.47
1:C:712:ILE:HG21	1:C:1096:VAL:HG12	1.96	0.47
1:C:164:ASN:OD1	1:C:165:ASN:ND2	2.48	0.47
1:B:746:SER:O	1:B:749:CYS:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG1	1:A:114:THR:HG1	1.60	0.47
1:C:811:LYS:NZ	1:C:820:ASP:OD1	2.43	0.47
1:A:402:ILE:HG23	1:A:407:VAL:HG22	1.96	0.47
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.79	0.47
1:B:101:ILE:HG12	1:B:242:LEU:HD23	1.97	0.47
1:A:666:ILE:HD12	1:A:670:ILE:HG22	1.97	0.46
1:B:106:PHE:HB3	1:B:235:ILE:HG13	1.96	0.46
1:C:421:TYR:HA	1:C:461:LEU:HD13	1.97	0.46
1:C:440:LYS:H	1:C:440:LYS:HD3	1.80	0.46
1:C:1083:HIS:CG	1:C:1084:ASP:H	2.32	0.46
1:A:326:ILE:HD13	1:A:534:VAL:HG22	1.97	0.46
1:B:568:ASP:OD1	1:B:572:THR:N	2.45	0.46
1:B:655:TYR:OH	1:B:696:THR:OG1	2.33	0.46
1:B:858:LEU:HD13	1:B:959:LEU:HD22	1.96	0.46
1:C:533:LEU:HD21	1:C:585:LEU:HD21	1.97	0.46
1:A:710:ASN:OD1	1:A:710:ASN:N	2.48	0.46
1:B:110:LEU:HD12	1:B:110:LEU:H	1.80	0.46
1:A:162:SER:HB2	1:A:164:ASN:HD22	1.79	0.46
1:B:48:LEU:O	1:B:304:LYS:NZ	2.40	0.46
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.97	0.46
1:B:273:ARG:HD3	1:B:292:ALA:HB3	1.97	0.46
1:B:985:ASP:O	1:B:989:ALA:N	2.46	0.46
1:A:343:ASN:OD1	1:A:343:ASN:N	2.48	0.46
1:C:81:ASN:HB2	1:C:239:GLN:HE22	1.80	0.46
1:C:710:ASN:N	1:C:710:ASN:OD1	2.48	0.46
1:C:811:LYS:HG3	1:C:814:LYS:H	1.80	0.46
1:A:480:CYS:HB3	1:A:485:GLY:HA3	1.98	0.45
1:B:984:LEU:O	1:C:386:LYS:NZ	2.46	0.45
1:B:1086:LYS:H	1:B:1086:LYS:HD2	1.80	0.45
1:B:877:LEU:O	1:B:881:THR:OG1	2.31	0.45
1:C:1114:ILE:H	1:C:1114:ILE:HG13	1.54	0.45
1:B:822:LEU:HD21	1:B:938:LEU:HD13	1.97	0.45
1:C:80:ASP:OD1	1:C:80:ASP:N	2.50	0.45
1:C:551:VAL:HB	1:C:588:THR:HG23	1.98	0.45
1:C:977:LEU:HD23	1:C:993:ILE:HD11	1.97	0.45
1:A:47:VAL:HG12	1:B:569:ILE:HG12	1.99	0.45
1:A:327:VAL:HG11	1:A:528:LYS:HG2	1.99	0.45
1:A:448:ASN:HB3	1:A:494:SER:HB2	1.99	0.45
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.50	0.45
1:B:886:TRP:HB3	1:B:1035:GLY:HA2	1.99	0.45
1:C:979:ASP:HB3	1:C:983:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.98	0.45
1:B:93:ALA:HA	1:B:189:GLU:HA	1.99	0.45
1:B:129:LYS:HG3	1:B:131:CYS:H	1.82	0.45
1:B:965:GLN:HG3	1:B:970:PHE:HZ	1.82	0.45
1:C:848:ASP:OD1	1:C:848:ASP:N	2.49	0.45
1:B:41:LYS:H	1:C:519:HIS:CE1	2.34	0.45
1:C:105:ILE:HG12	1:C:241:LEU:HD11	1.99	0.45
1:B:108:THR:HG23	1:B:109:THR:H	1.81	0.44
1:B:381:GLY:HA3	1:B:430:THR:HA	1.98	0.44
1:C:65:PHE:HE2	1:C:84:LEU:HD21	1.82	0.44
1:A:788:ILE:HG23	1:A:876:ALA:HB2	1.99	0.44
1:B:858:LEU:HD21	1:B:962:LEU:HD23	2.00	0.44
1:C:393:THR:HB	1:C:516:GLU:HG3	1.99	0.44
1:A:856:LYS:HZ3	1:A:856:LYS:HB2	1.83	0.44
1:A:1083:HIS:CG	1:A:1084:ASP:H	2.36	0.44
1:B:490:PHE:HD1	1:B:491:PRO:HD2	1.82	0.44
1:C:368:LEU:H	1:C:368:LEU:HD23	1.81	0.44
1:A:330:PRO:HA	1:A:580:GLN:HB3	1.99	0.44
1:A:589:PRO:HG2	1:C:855:PHE:HB3	2.00	0.44
1:A:699:LEU:HD22	1:C:873:TYR:CZ	2.53	0.44
1:B:141:LEU:HD21	1:B:241:LEU:HD13	2.00	0.44
1:B:1005:GLN:NE2	1:C:1006:THR:OG1	2.50	0.44
1:C:139:PRO:HB2	1:C:141:LEU:HG	1.99	0.44
1:A:534:VAL:HG21	1:A:539:VAL:HG21	1.99	0.44
1:B:945:LEU:HD12	1:B:948:LEU:HD12	1.99	0.44
1:C:884:SER:OG	1:C:887:THR:OG1	2.36	0.44
1:B:193:LYS:HE2	1:B:193:LYS:HB3	1.87	0.44
1:B:661:GLU:O	1:B:695:TYR:OH	2.29	0.44
1:C:298:GLU:HG2	1:C:315:THR:HB	2.00	0.44
1:C:735:SER:OG	1:C:859:THR:OG1	2.33	0.44
1:A:198:TYR:HD1	1:A:230:PRO:HA	1.83	0.44
1:B:939:SER:OG	1:B:940:SER:N	2.51	0.44
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.30	0.43
1:A:461:LEU:HD13	1:A:467:ASP:HB3	2.00	0.43
1:B:757:GLY:HA3	1:C:965:GLN:HE22	1.84	0.43
1:A:985:ASP:OD1	1:A:988:GLU:N	2.47	0.43
1:C:82:PRO:HG2	1:C:84:LEU:HD11	1.99	0.43
1:C:538:CYS:HB2	1:C:551:VAL:HG22	1.99	0.43
1:A:938:LEU:HA	1:A:941:THR:HG21	1.98	0.43
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.52	0.43
1:B:1037:SER:H	1:B:1048:HIS:CD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLY:H	1:A:235:ILE:HG23	1.84	0.43
1:B:442:ASP:OD2	1:B:509:ARG:NH2	2.47	0.43
1:C:103:GLY:HA3	1:C:241:LEU:HB2	1.99	0.43
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.83	0.43
1:B:89:GLY:HA3	1:B:270:LEU:HD12	2.01	0.43
1:B:607:GLN:NE2	1:B:690:GLN:O	2.49	0.43
1:B:645:THR:OG1	1:B:646:ARG:N	2.51	0.43
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.99	0.43
1:C:303:LEU:HD11	1:C:308:VAL:HG23	2.00	0.43
1:C:349:SER:HA	1:C:401:VAL:HG22	2.00	0.43
1:C:994:ASP:HA	1:C:997:ILE:HG22	2.01	0.43
1:B:329:PHE:CD2	1:B:528:LYS:HB3	2.54	0.43
1:C:424:LYS:NZ	1:C:461:LEU:O	2.49	0.43
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.99	0.43
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.43
1:C:102:ARG:NH1	1:C:121:ASN:O	2.43	0.43
1:B:294:ASP:N	1:B:294:ASP:OD1	2.51	0.43
1:C:826:VAL:HG13	1:C:949:GLN:HG2	2.01	0.43
1:A:418:ILE:HG23	1:A:453:TYR:HE1	1.84	0.42
1:A:436:TRP:HE1	1:A:509:ARG:HH21	1.66	0.42
1:B:65:PHE:HE2	1:B:84:LEU:HD11	1.83	0.42
1:B:326:ILE:HD13	1:B:539:VAL:HG21	2.00	0.42
1:B:1086:LYS:HE2	1:B:1086:LYS:HB3	1.93	0.42
1:C:93:ALA:HA	1:C:189:GLU:HA	2.01	0.42
1:C:130:VAL:HG21	1:C:231:ILE:HG12	1.99	0.42
1:C:198:TYR:HA	1:C:230:PRO:HA	2.01	0.42
1:C:600:PRO:HB3	1:C:674:TYR:HB2	2.00	0.42
1:B:126:VAL:HG22	1:B:175:PHE:HA	2.02	0.42
1:C:191:VAL:HG23	1:C:223:LEU:HD22	2.01	0.42
1:C:564:GLN:HA	1:C:577:ARG:HH11	1.84	0.42
1:A:108:THR:HA	1:A:236:THR:H	1.84	0.42
1:A:535:LYS:HG3	1:A:536:ASN:H	1.85	0.42
1:B:53:ASP:OD1	1:B:54:LEU:N	2.47	0.42
1:B:121:ASN:HB3	1:B:177:MET:HB2	2.01	0.42
1:B:190:PHE:HB3	1:B:192:PHE:CE2	2.54	0.42
1:C:402:ILE:HD11	1:C:406:GLU:HB2	2.02	0.42
1:C:1031:GLU:OE1	1:C:1039:ARG:NH1	2.50	0.42
1:A:417:ASN:ND2	1:A:418:ILE:HG13	2.35	0.42
1:B:574:ASP:O	1:B:587:ILE:N	2.50	0.42
1:B:848:ASP:OD1	1:B:848:ASP:N	2.51	0.42
1:B:577:ARG:HD3	1:B:582:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ARG:HG2	1:C:459:SER:H	1.84	0.42
1:A:811:LYS:HE3	1:A:811:LYS:HB2	1.88	0.42
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.95	0.42
1:A:947:LYS:H	1:A:947:LYS:HD2	1.84	0.42
1:B:401:VAL:HG22	1:B:509:ARG:HG2	2.00	0.42
1:B:986:PRO:N	1:B:987:PRO:HD2	2.35	0.41
1:C:598:ILE:HG23	1:C:664:ILE:HG21	2.02	0.41
1:B:233:ILE:HG23	1:B:235:ILE:HG22	2.01	0.41
1:B:977:LEU:HD21	1:B:1000:ARG:NH1	2.36	0.41
1:A:424:LYS:HD2	1:A:463:PRO:HD3	2.01	0.41
1:A:542:ASN:O	1:A:542:ASN:ND2	2.48	0.41
1:A:811:LYS:HE2	1:A:813:SER:HB2	2.02	0.41
1:C:192:PHE:HB3	1:C:199:PHE:HE1	1.86	0.41
1:A:328:ARG:NE	1:A:578:ASP:OD2	2.53	0.41
1:B:733:LYS:HD2	1:B:771:ALA:HB1	2.03	0.41
1:A:98:SER:OG	1:A:99:ASN:N	2.54	0.41
1:A:117:LEU:HD21	1:A:231:ILE:HG12	2.03	0.41
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG11	2.55	0.41
1:B:223:LEU:HD13	1:B:223:LEU:HA	1.94	0.41
1:B:379:CYS:HA	1:B:432:CYS:HA	2.03	0.41
1:B:558:LYS:HE2	1:B:558:LYS:HB2	1.85	0.41
1:B:801:ASN:O	1:B:803:SER:N	2.54	0.41
1:C:468:ILE:H	1:C:468:ILE:HG13	1.48	0.41
1:B:122:ASN:OD1	1:B:124:THR:OG1	2.26	0.41
1:B:159:VAL:HG23	1:B:160:TYR:H	1.85	0.41
1:C:242:LEU:HD23	1:C:242:LEU:H	1.86	0.41
1:C:371:LEU:HG	1:C:372:ALA:H	1.86	0.41
1:A:336:CYS:HB3	1:A:338:PHE:CE2	2.55	0.41
1:A:64:TRP:HZ2	1:A:214:GLU:HB2	1.85	0.41
1:B:139:PRO:HG3	1:B:239:GLN:HE21	1.85	0.41
1:B:281:GLU:H	1:B:281:GLU:HG3	1.71	0.41
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.03	0.41
1:A:110:LEU:HB3	1:A:135:PHE:CD2	2.56	0.41
1:A:131:CYS:SG	1:A:166:CYS:N	2.93	0.41
1:A:355:ARG:HD3	1:A:396:TYR:CD1	2.55	0.41
1:B:68:ILE:O	1:B:68:ILE:CG1	2.67	0.41
1:B:158:ARG:O	1:B:158:ARG:NH1	2.54	0.41
1:B:826:VAL:HB	1:B:1057:PRO:HG2	2.03	0.41
1:B:901:GLN:HE21	1:B:905:ARG:HH21	1.67	0.41
1:A:808:ASP:OD2	1:A:810:SER:OG	2.32	0.40
1:A:979:ASP:HB3	1:A:983:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:HG13	1:B:241:LEU:HD11	2.03	0.40
1:B:856:LYS:HD2	1:B:966:LEU:HD12	2.04	0.40
1:C:108:THR:HG22	1:C:236:THR:HG22	2.02	0.40
1:A:169:GLU:HG2	1:A:170:TYR:H	1.86	0.40
1:A:191:VAL:N	1:A:202:TYR:O	2.47	0.40
1:B:202:TYR:HB3	1:B:223:LEU:HB3	2.02	0.40
1:B:403:ARG:HG2	1:B:497:PHE:CE1	2.57	0.40
1:C:29:THR:OG1	1:C:30:ASN:N	2.54	0.40
1:A:66:HIS:ND1	1:A:263:ALA:O	2.55	0.40
1:A:327:VAL:HG13	1:A:542:ASN:HB3	2.04	0.40
1:A:516:GLU:OE1	1:C:198:TYR:OH	2.36	0.40
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.69	0.40
1:B:195:ILE:HG22	1:B:196:ASP:H	1.85	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	1016/1285 (79%)	935 (92%)	81 (8%)	0	100	100
1	B	1011/1285 (79%)	928 (92%)	83 (8%)	0	100	100
1	C	1017/1285 (79%)	949 (93%)	68 (7%)	0	100	100
All	All	3044/3855 (79%)	2812 (92%)	232 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	890/1115 (80%)	836 (94%)	54 (6%)	15	40
1	B	886/1115 (80%)	842 (95%)	44 (5%)	20	46
1	C	891/1115 (80%)	845 (95%)	46 (5%)	19	45
All	All	2667/3345 (80%)	2523 (95%)	144 (5%)	21	44

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	67	VAL
1	A	68	ILE
1	A	101	ILE
1	A	104	TRP
1	A	108	THR
1	A	118	LEU
1	A	124	THR
1	A	130	VAL
1	A	131	CYS
1	A	157	PHE
1	A	171	VAL
1	A	206	THR
1	A	236	THR
1	A	242	LEU
1	A	267	VAL
1	A	312	ILE
1	A	340	GLU
1	A	346	ARG
1	A	347	PHE
1	A	358	ILE
1	A	376	THR
1	A	377	PHE
1	A	378	LYS
1	A	386	LYS
1	A	402	ILE
1	A	421	TYR
1	A	433	VAL
1	A	440	LYS
1	A	444	LYS
1	A	458	LYS

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Mol	Chain	Res	Type
1	A	462	LYS
1	A	480	CYS
1	A	501	TYR
1	A	511	VAL
1	A	525	CYS
1	A	535	LYS
1	A	542	ASN
1	A	546	LEU
1	A	558	LYS
1	A	564	GLN
1	A	584	ILE
1	A	610	VAL
1	A	738	CYS
1	A	854	LYS
1	A	856	LYS
1	A	947	LYS
1	A	957	GLN
1	A	973	ILE
1	A	1010	GLN
1	A	1041	ASP
1	A	1086	LYS
1	A	1104	VAL
1	A	1114	ILE
1	B	66	HIS
1	B	67	VAL
1	B	68	ILE
1	B	78	ARG
1	B	79	PHE
1	B	83	VAL
1	B	97	LYS
1	B	105	ILE
1	B	108	THR
1	B	119	ILE
1	B	126	VAL
1	B	133	PHE
1	B	159	VAL
1	B	177	MET
1	B	198	TYR
1	B	229	LEU
1	B	235	ILE
1	B	236	THR
1	B	242	LEU

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Mol	Chain	Res	Type
1	B	277	LEU
1	B	287	ASP
1	B	355	ARG
1	B	361	CYS
1	B	362	VAL
1	B	378	LYS
1	B	440	LYS
1	B	458	LYS
1	B	468	ILE
1	B	483	VAL
1	B	511	VAL
1	B	537	LYS
1	B	650	LEU
1	B	702	GLU
1	B	878	LEU
1	B	902	MET
1	B	964	LYS
1	B	973	ILE
1	B	985	ASP
1	B	990	GLU
1	B	1010	GLN
1	B	1041	ASP
1	B	1081	ILE
1	B	1086	LYS
1	B	1104	VAL
1	C	68	ILE
1	C	83	VAL
1	C	88	ASP
1	C	113	LYS
1	C	118	LEU
1	C	141	LEU
1	C	189	GLU
1	C	195	ILE
1	C	198	TYR
1	C	209	ILE
1	C	212	GLU
1	C	287	ASP
1	C	291	CYS
1	C	303	LEU
1	C	335	LEU
1	C	341	VAL
1	C	347	PHE

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Mol	Chain	Res	Type
1	C	356	LYS
1	C	358	ILE
1	C	362	VAL
1	C	369	TYR
1	C	377	PHE
1	C	402	ILE
1	C	440	LYS
1	C	458	LYS
1	C	468	ILE
1	C	501	TYR
1	C	518	LEU
1	C	538	CYS
1	C	542	ASN
1	C	546	LEU
1	C	558	LYS
1	C	732	THR
1	C	738	CYS
1	C	774	GLN
1	C	790	LYS
1	C	936	ASP
1	C	997	ILE
1	C	1001	LEU
1	C	1010	GLN
1	C	1018	ILE
1	C	1041	ASP
1	C	1086	LYS
1	C	1104	VAL
1	C	1114	ILE
1	C	1129	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	164	ASN
1	A	173	GLN
1	A	181	GLN
1	A	234	ASN
1	A	271	GLN
1	A	314	GLN
1	A	409	GLN
1	A	414	GLN

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Mol	Chain	Res	Type
1	A	417	ASN
1	A	437	ASN
1	A	506	GLN
1	A	540	ASN
1	A	544	ASN
1	A	563	GLN
1	A	564	GLN
1	A	603	ASN
1	A	641	ASN
1	A	644	GLN
1	A	774	GLN
1	A	853	GLN
1	A	872	GLN
1	A	901	GLN
1	A	955	ASN
1	A	1005	GLN
1	A	1010	GLN
1	A	1011	GLN
1	A	1048	HIS
1	A	1054	GLN
1	A	1108	ASN
1	B	81	ASN
1	B	99	ASN
1	B	165	ASN
1	B	218	GLN
1	B	321	GLN
1	B	360	ASN
1	B	370	ASN
1	B	540	ASN
1	B	580	GLN
1	B	641	ASN
1	B	784	GLN
1	B	853	GLN
1	B	901	GLN
1	B	928	ASN
1	B	965	GLN
1	B	1005	GLN
1	B	1010	GLN
1	B	1011	GLN
1	B	1048	HIS
1	B	1071	GLN
1	C	52	GLN

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Mol	Chain	Res	Type
1	C	81	ASN
1	C	121	ASN
1	C	165	ASN
1	C	173	GLN
1	C	239	GLN
1	C	321	GLN
1	C	394	ASN
1	C	414	GLN
1	C	422	ASN
1	C	505	HIS
1	C	540	ASN
1	C	563	GLN
1	C	564	GLN
1	C	613	GLN
1	C	644	GLN
1	C	762	GLN
1	C	853	GLN
1	C	901	GLN
1	C	965	GLN
1	C	1005	GLN
1	C	1011	GLN
1	C	1048	HIS
1	C	1119	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 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	$\# Z > 2$
2	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.52	0
2	NAG	B	1306	1	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	C	1303	1	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	A	1309	1	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	A	1303	1	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	B	1303	1	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	B	1301	1	14,14,15	0.26	0	17,19,21	0.54	0
2	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	B	1302	1	14,14,15	0.31	0	17,19,21	0.55	0
2	NAG	A	1308	1	14,14,15	0.43	0	17,19,21	1.27	1 (5%)
2	NAG	B	1310	1	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	C	1307	1	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	B	1304	1	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.36	0
2	NAG	C	1306	1	14,14,15	0.42	0	17,19,21	1.27	2 (11%)
2	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	C	1309	1	14,14,15	0.23	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	5/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	5/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1308	NAG	C2-N2-C7	4.32	129.05	122.90
2	C	1306	NAG	C2-N2-C7	4.31	129.04	122.90
2	C	1306	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1302	NAG	C4-C5-C6-O6
2	B	1309	NAG	O5-C5-C6-O6
2	B	1304	NAG	C4-C5-C6-O6
2	C	1303	NAG	C4-C5-C6-O6
2	C	1301	NAG	O5-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	C	1305	NAG	O5-C5-C6-O6
2	B	1309	NAG	C4-C5-C6-O6
2	A	1303	NAG	O5-C5-C6-O6
2	C	1309	NAG	O5-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	B	1308	NAG	O5-C5-C6-O6
2	B	1305	NAG	O5-C5-C6-O6
2	C	1308	NAG	O5-C5-C6-O6
2	C	1303	NAG	O5-C5-C6-O6
2	C	1306	NAG	O5-C5-C6-O6
2	A	1308	NAG	C8-C7-N2-C2
2	A	1308	NAG	O7-C7-N2-C2
2	A	1309	NAG	C8-C7-N2-C2
2	A	1309	NAG	O7-C7-N2-C2
2	C	1306	NAG	C8-C7-N2-C2
2	C	1306	NAG	O7-C7-N2-C2
2	C	1308	NAG	C4-C5-C6-O6
2	B	1305	NAG	C4-C5-C6-O6
2	A	1308	NAG	O5-C5-C6-O6
2	C	1301	NAG	C4-C5-C6-O6
2	C	1305	NAG	C4-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6
2	A	1303	NAG	C4-C5-C6-O6
2	C	1306	NAG	C4-C5-C6-O6
2	C	1309	NAG	C4-C5-C6-O6
2	B	1308	NAG	C4-C5-C6-O6
2	A	1304	NAG	O5-C5-C6-O6
2	A	1307	NAG	C4-C5-C6-O6
2	B	1303	NAG	O5-C5-C6-O6
2	B	1310	NAG	C4-C5-C6-O6
2	A	1306	NAG	O5-C5-C6-O6
2	C	1307	NAG	O5-C5-C6-O6
2	B	1306	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	1302	NAG	C4-C5-C6-O6
2	A	1307	NAG	O5-C5-C6-O6
2	B	1310	NAG	O5-C5-C6-O6
2	A	1307	NAG	C3-C2-N2-C7
2	B	1301	NAG	C3-C2-N2-C7
2	B	1302	NAG	C3-C2-N2-C7
2	A	1309	NAG	O5-C5-C6-O6
2	A	1308	NAG	C3-C2-N2-C7
2	C	1306	NAG	C3-C2-N2-C7

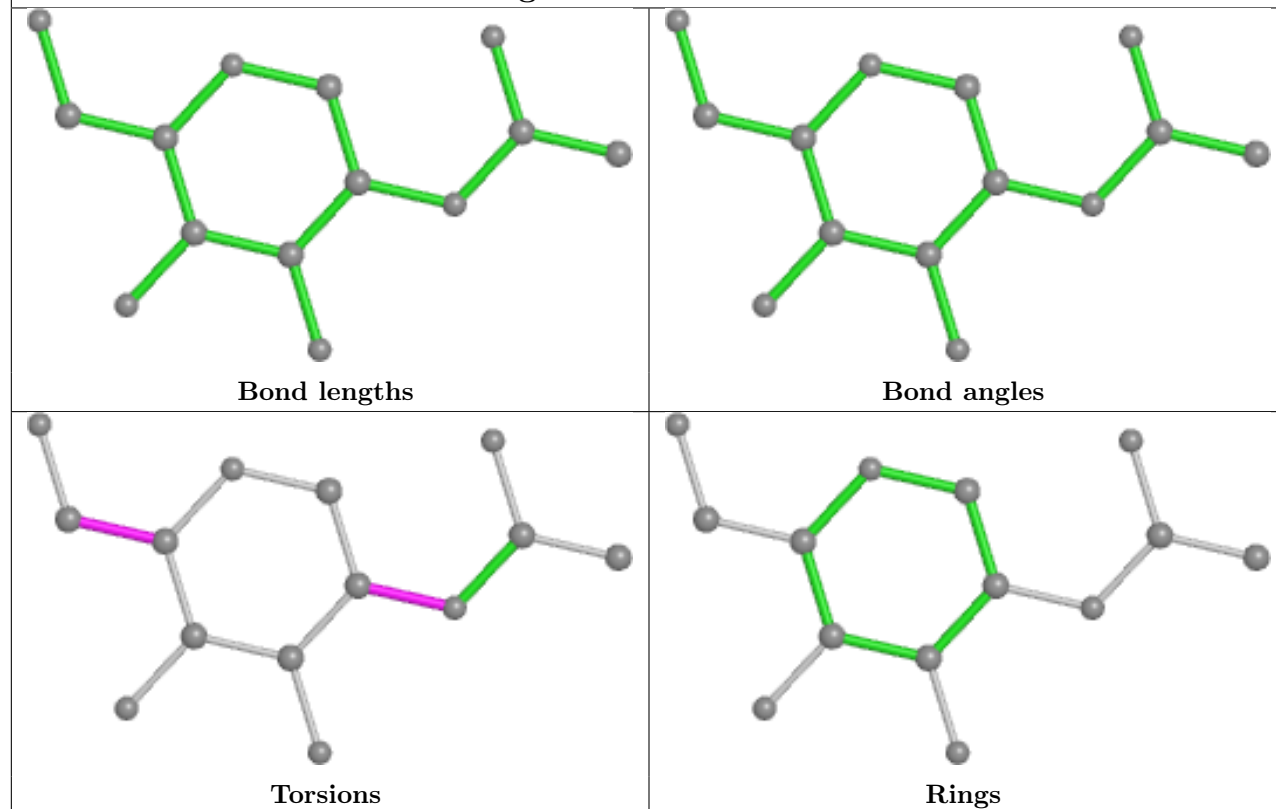
There are no ring outliers.

2 monomers are involved in 2 short contacts:

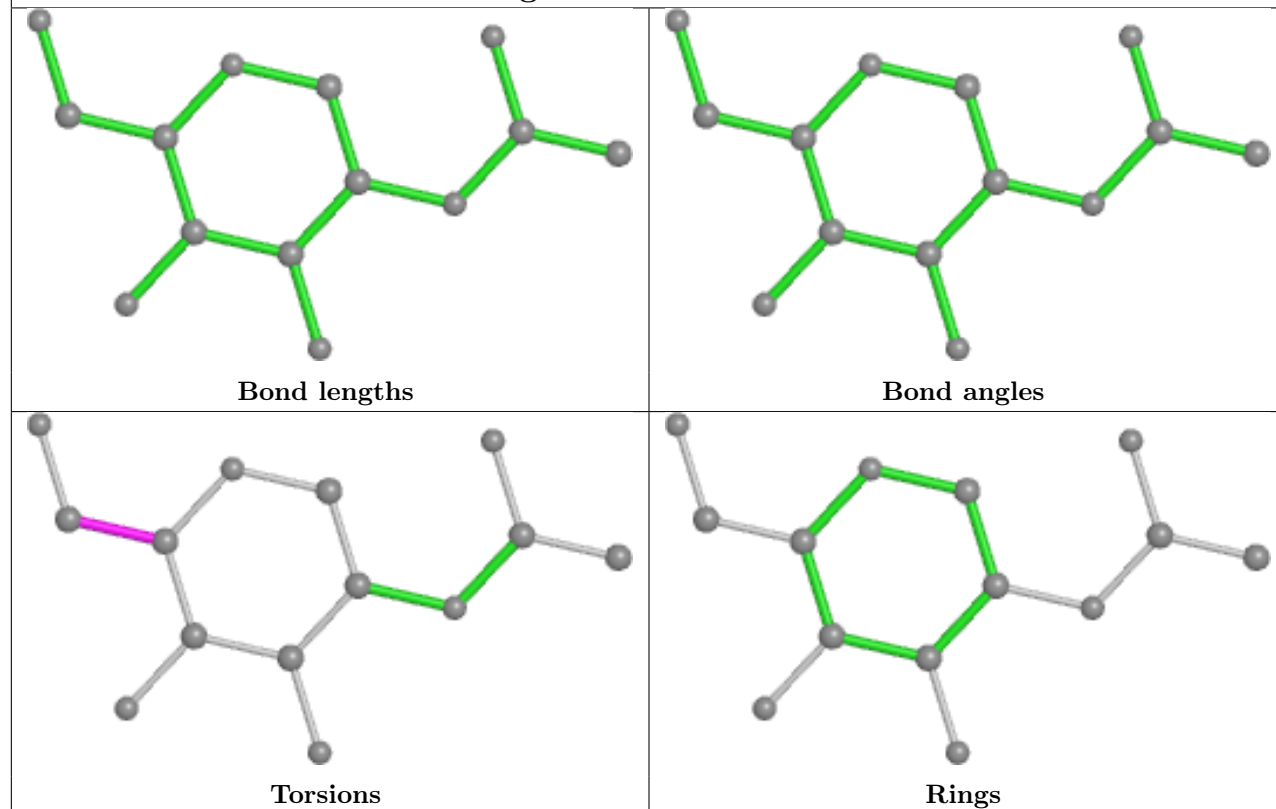
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1308	NAG	1	0
2	C	1306	NAG	1	0

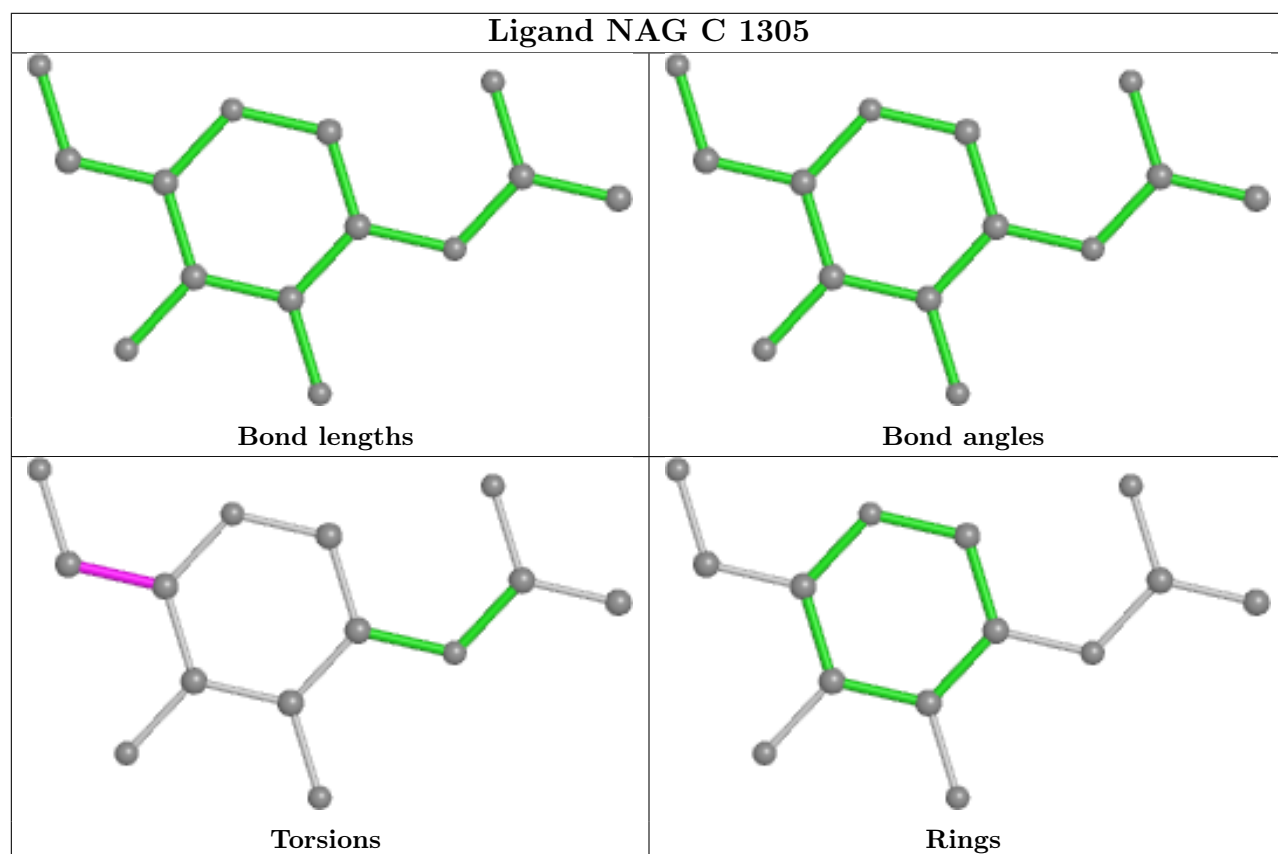
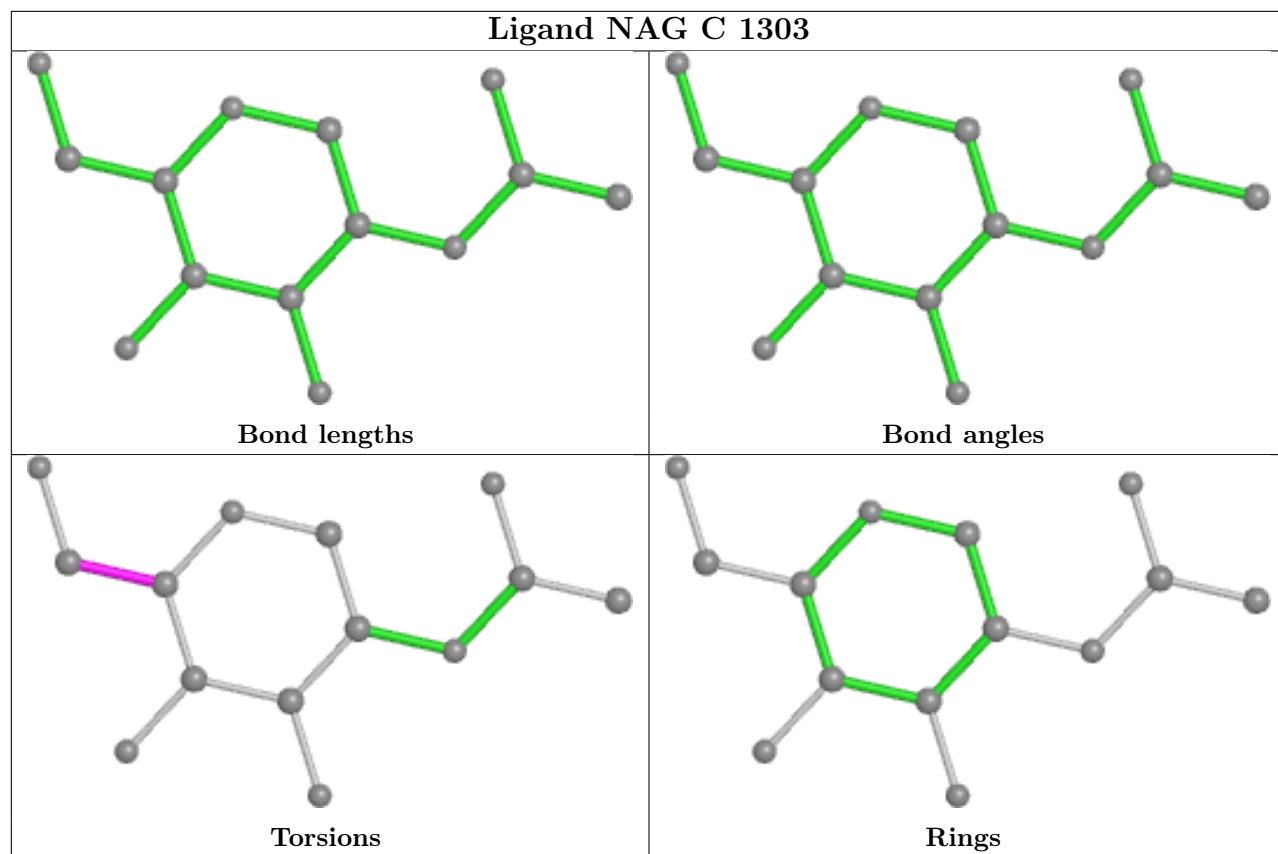
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAG A 1307

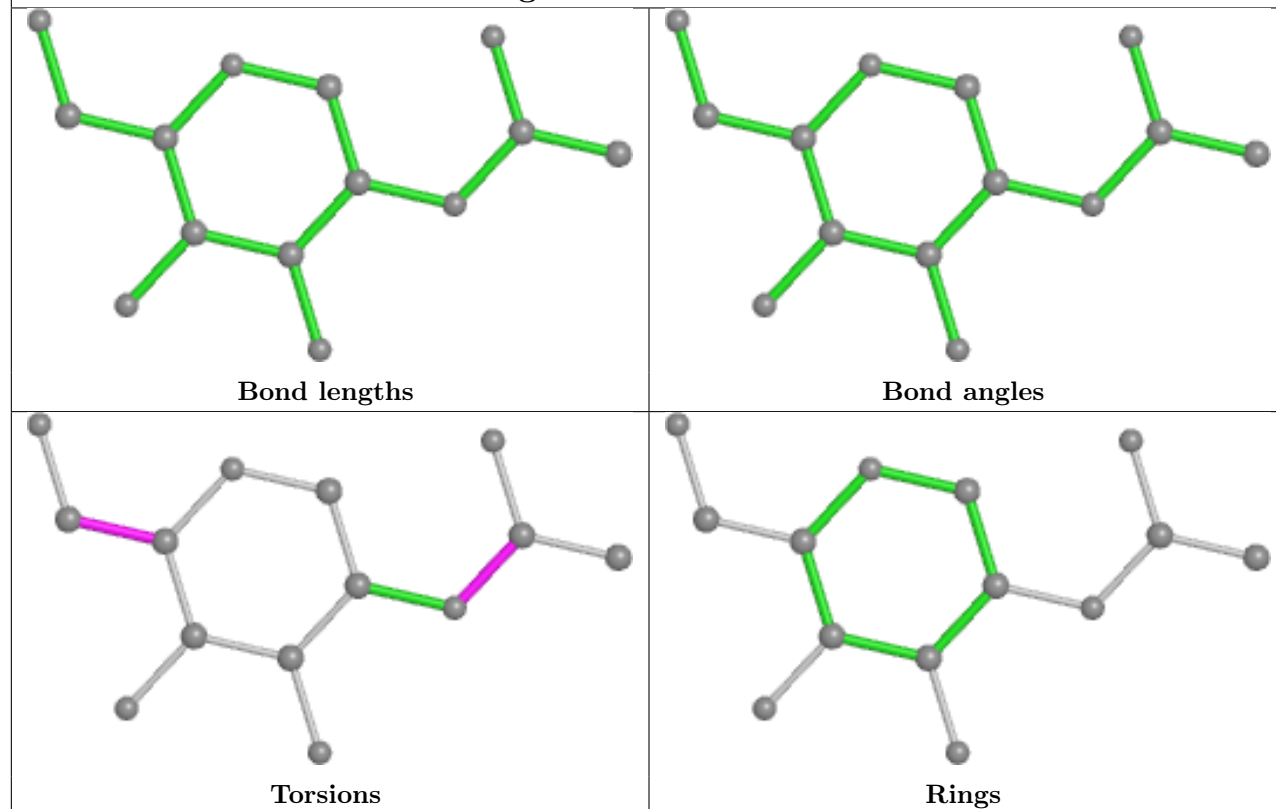


Ligand NAG B 1306

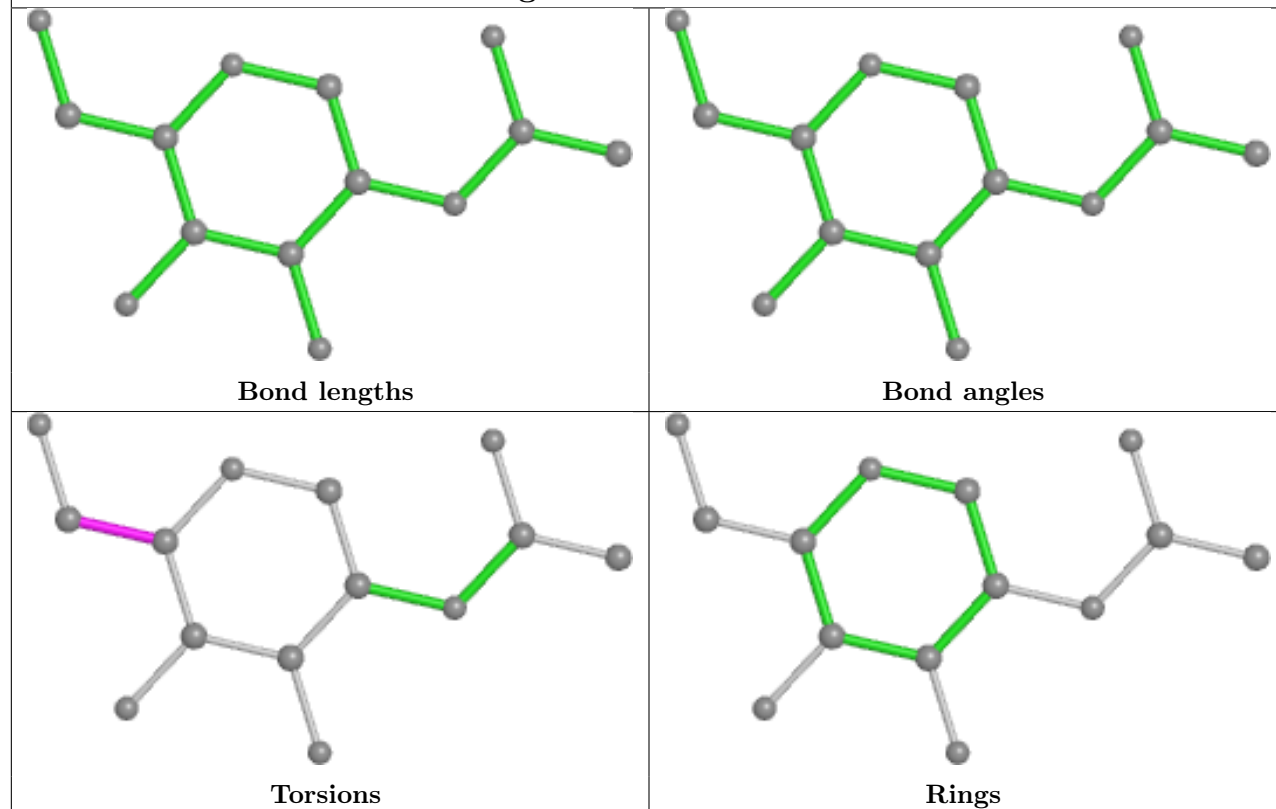


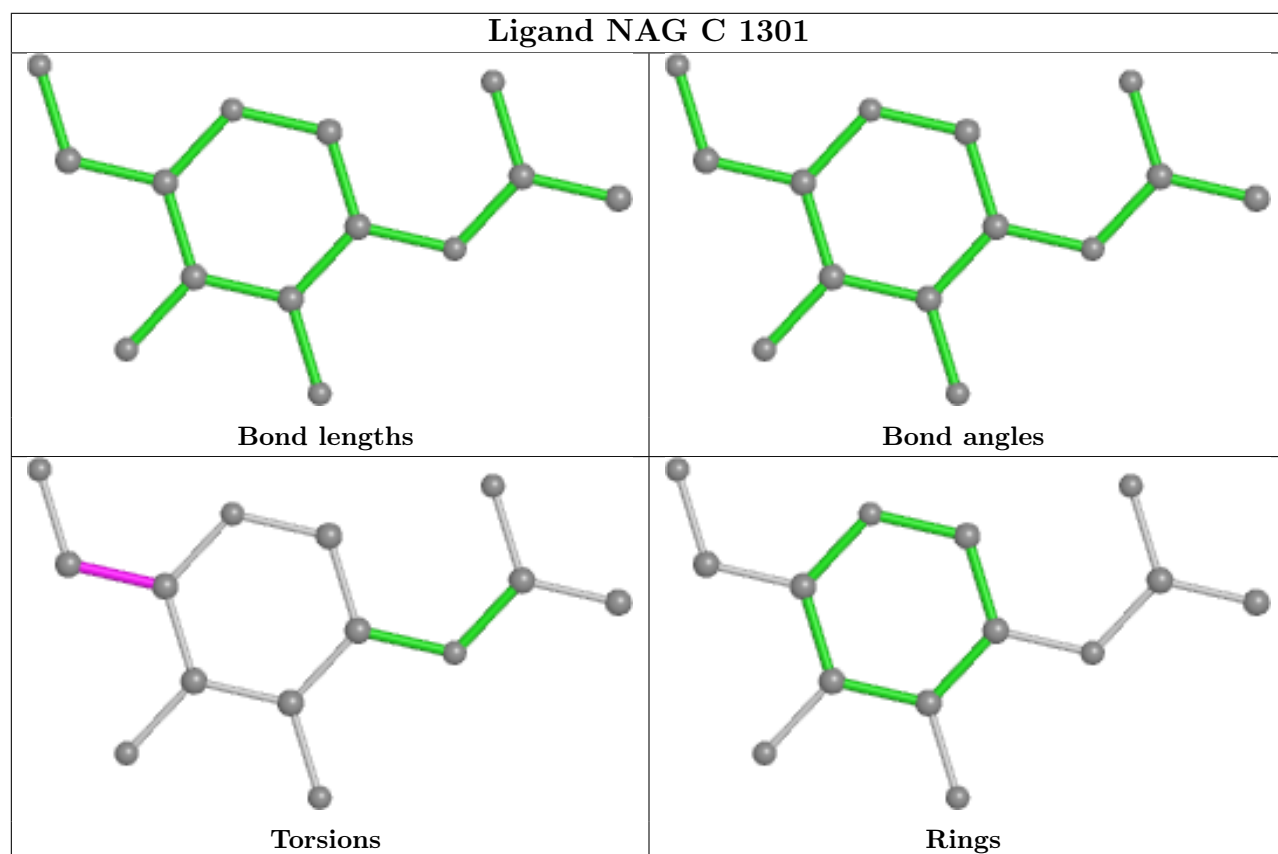
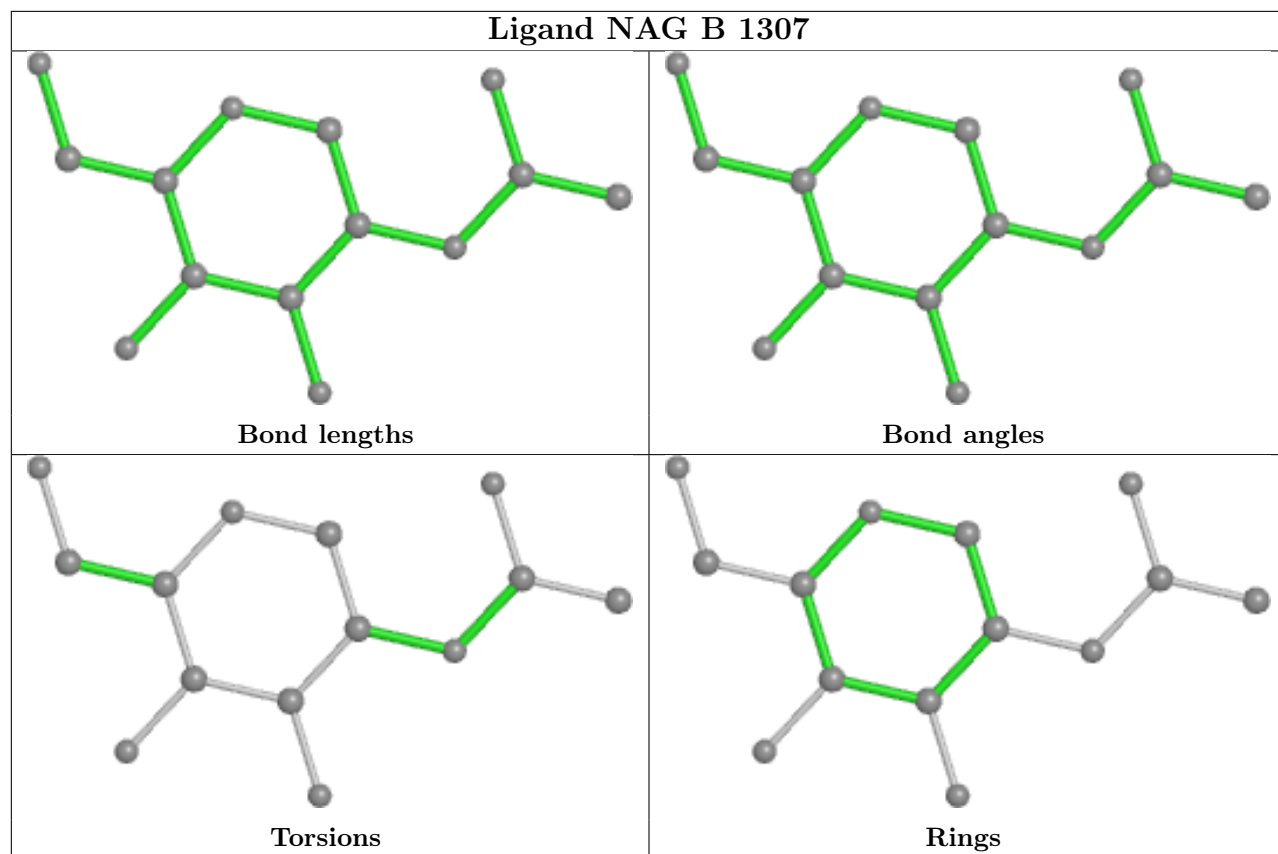


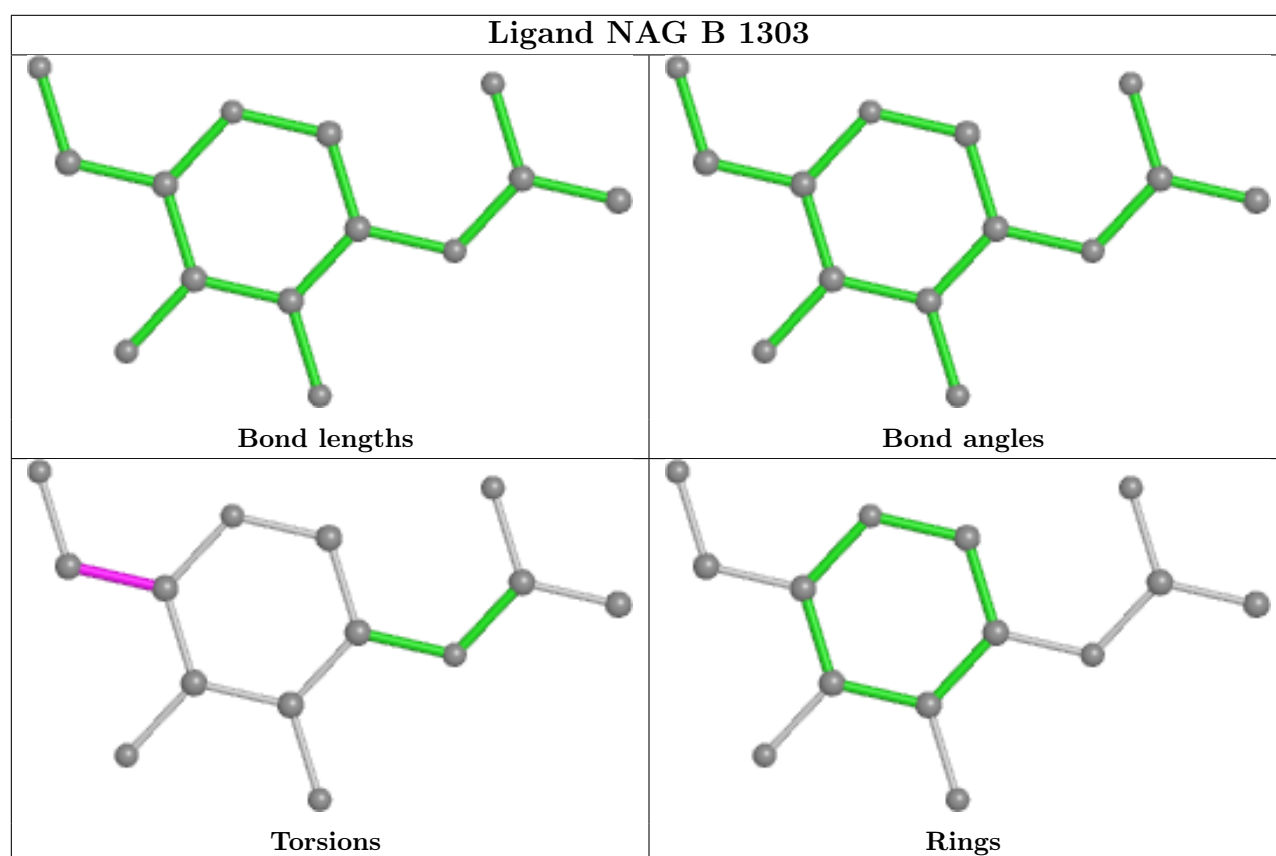
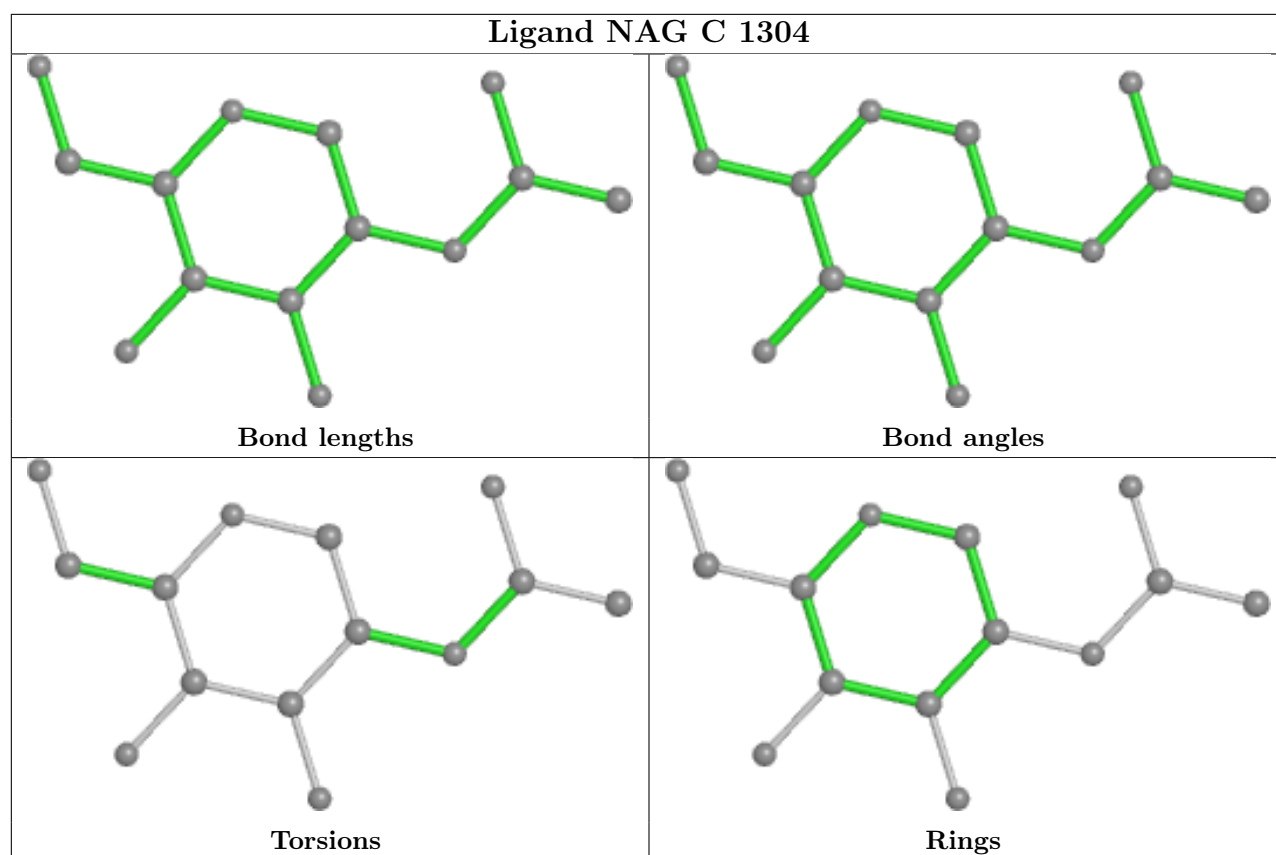
Ligand NAG A 1309



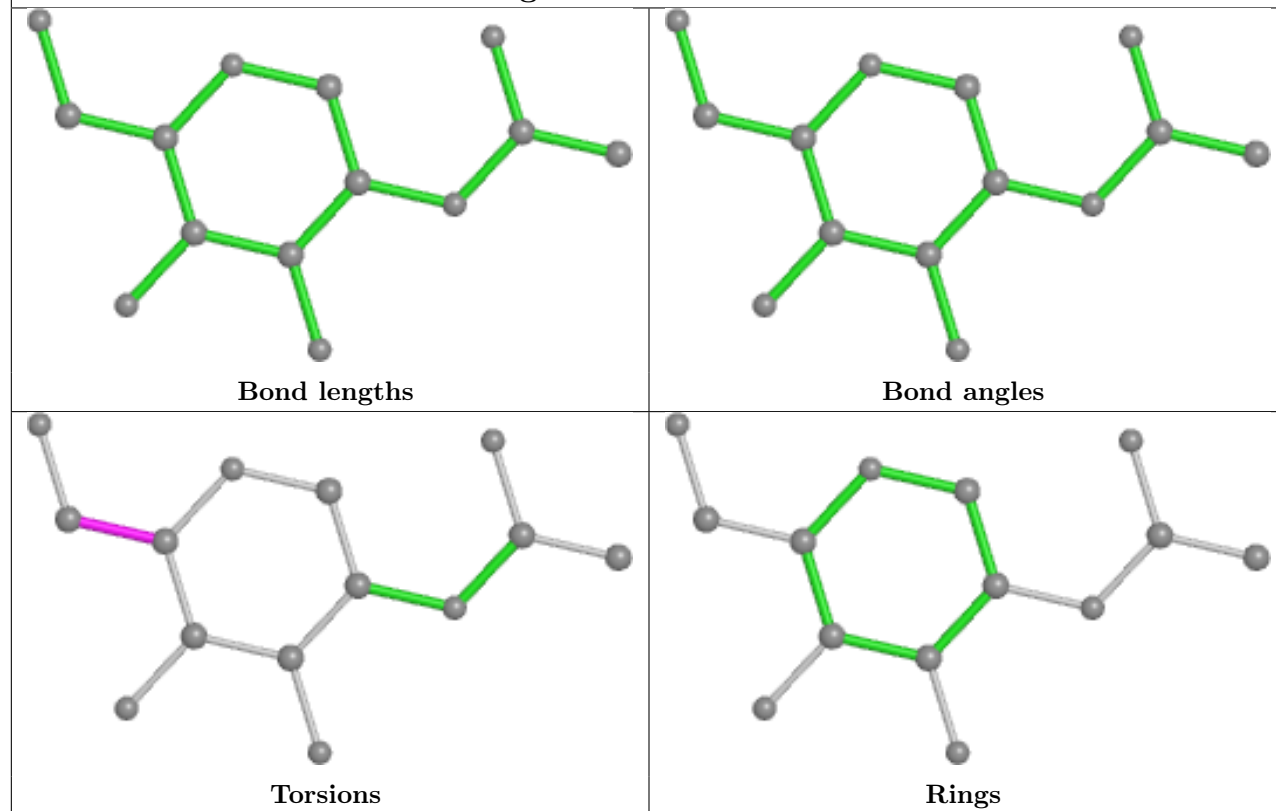
Ligand NAG A 1303



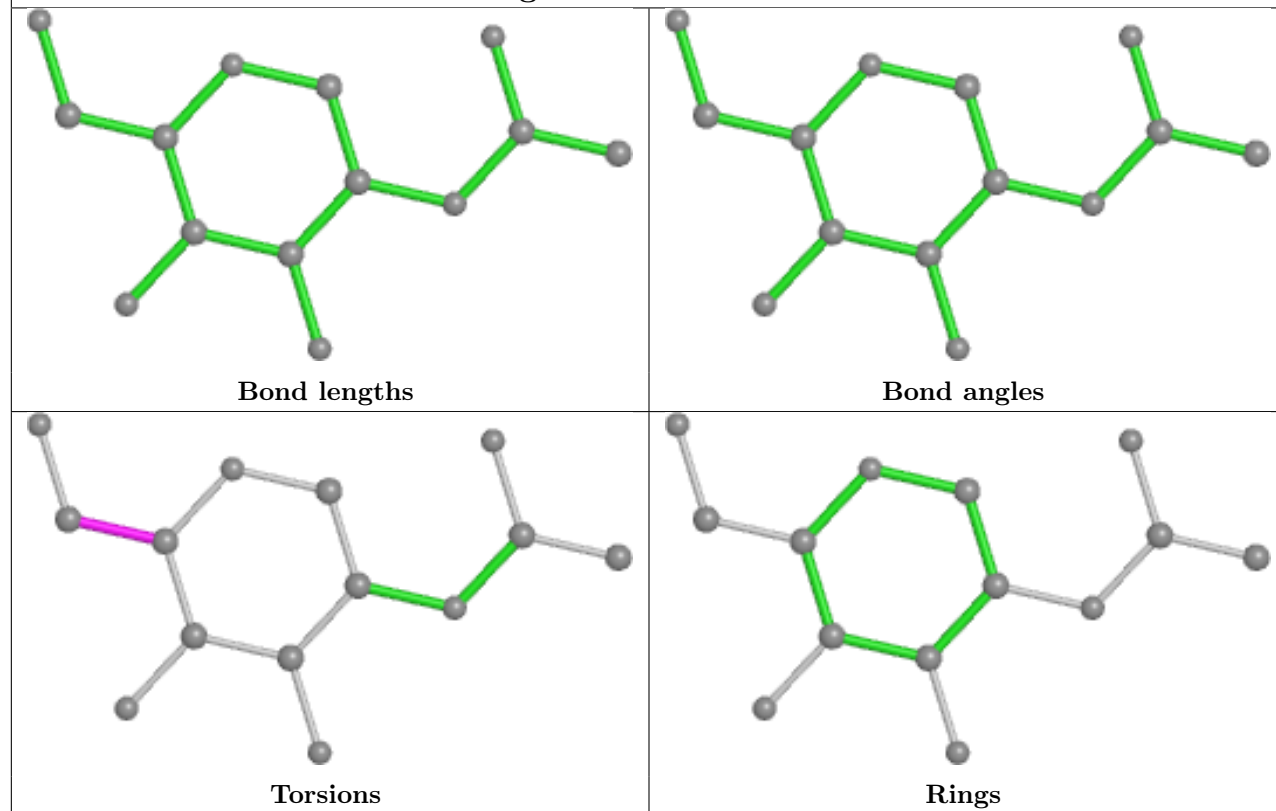




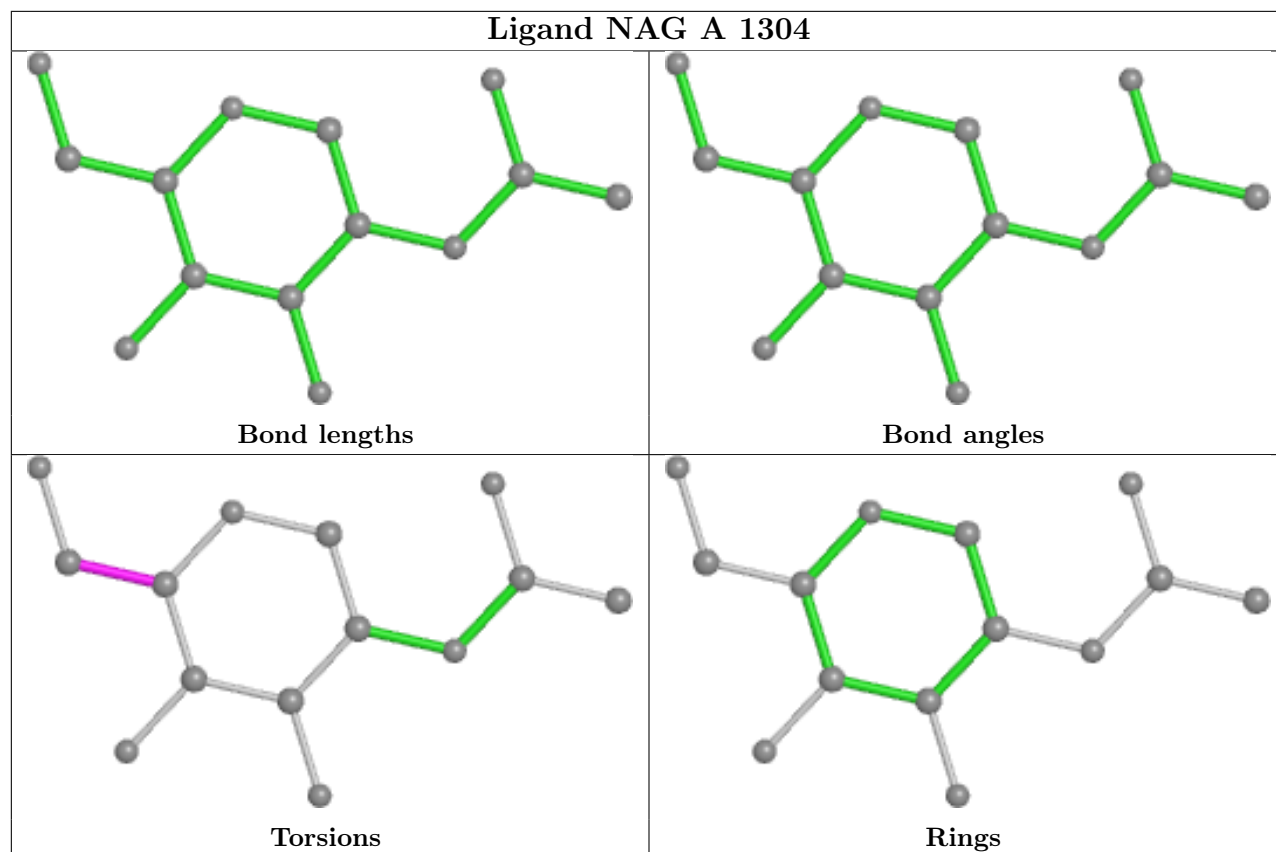
Ligand NAG B 1309



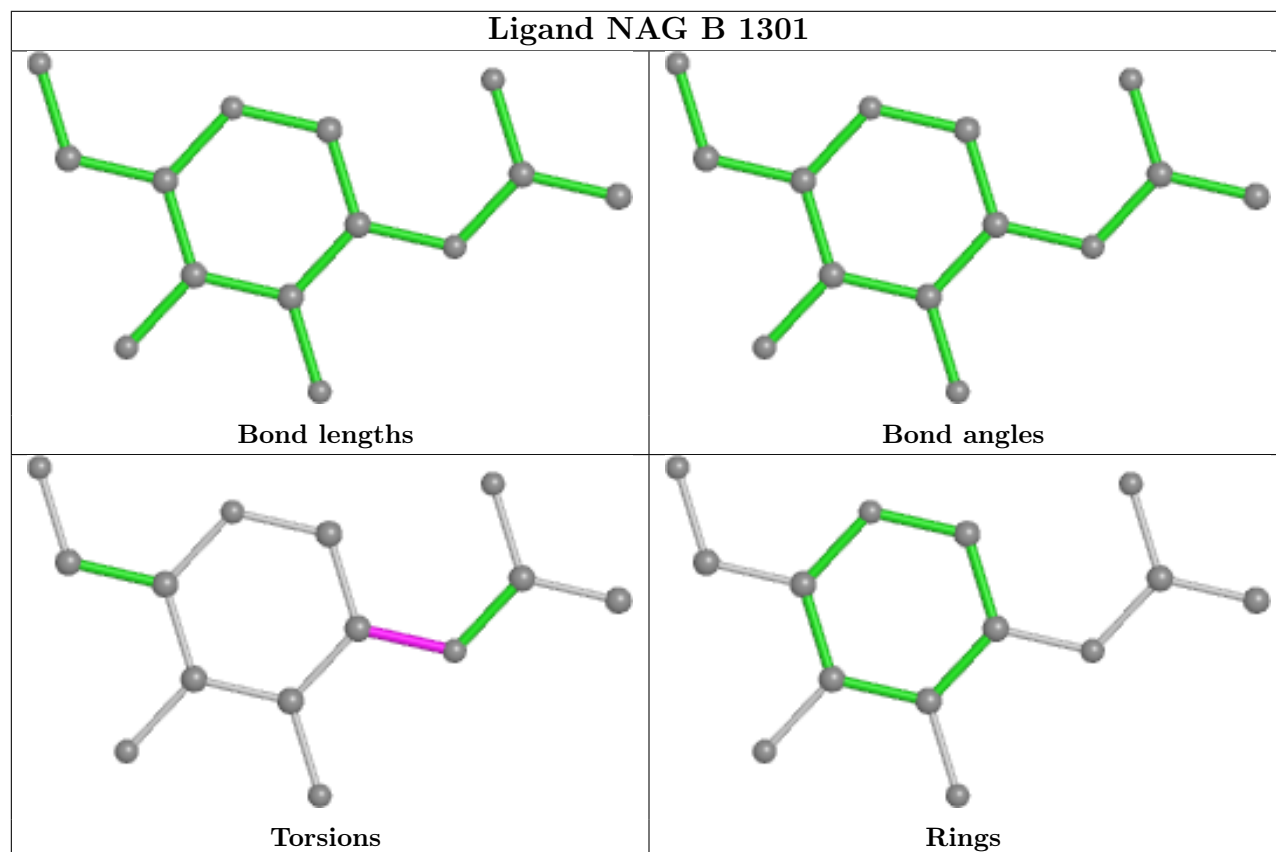
Ligand NAG C 1302



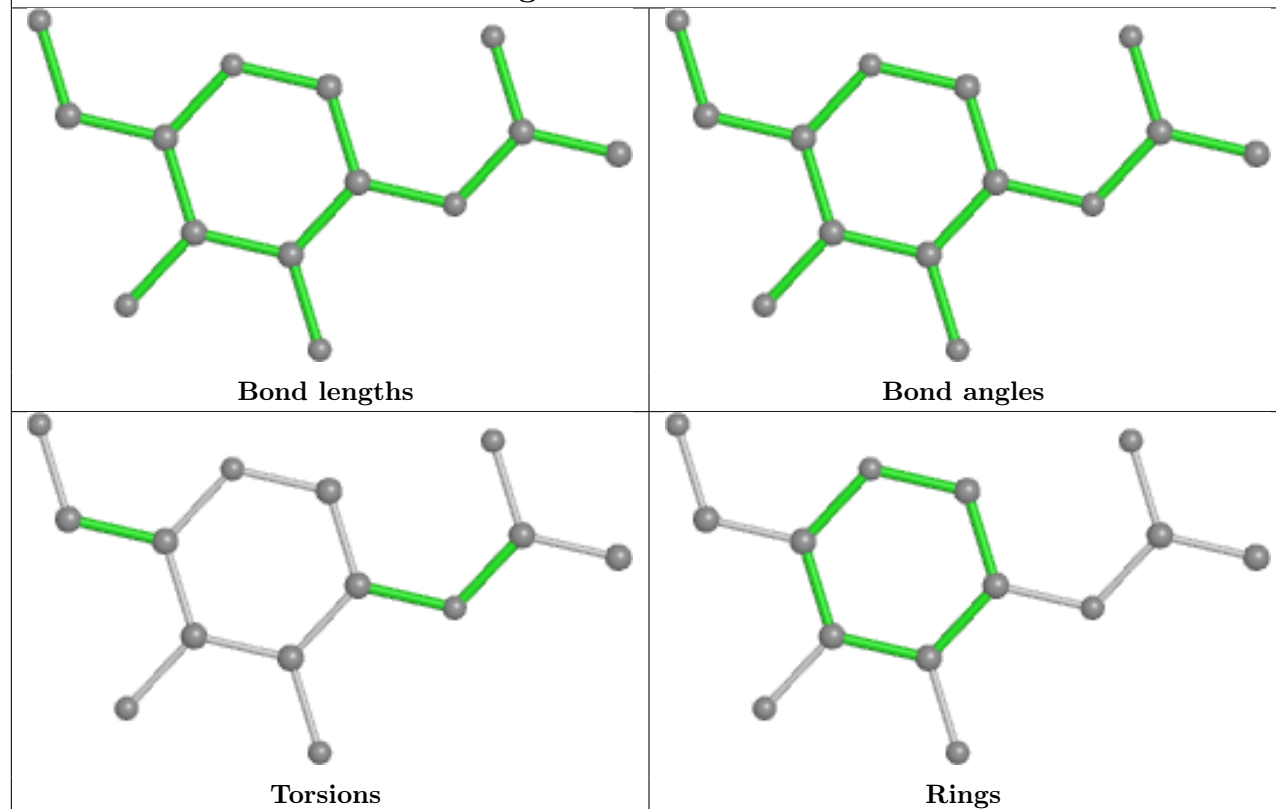
Ligand NAG A 1304



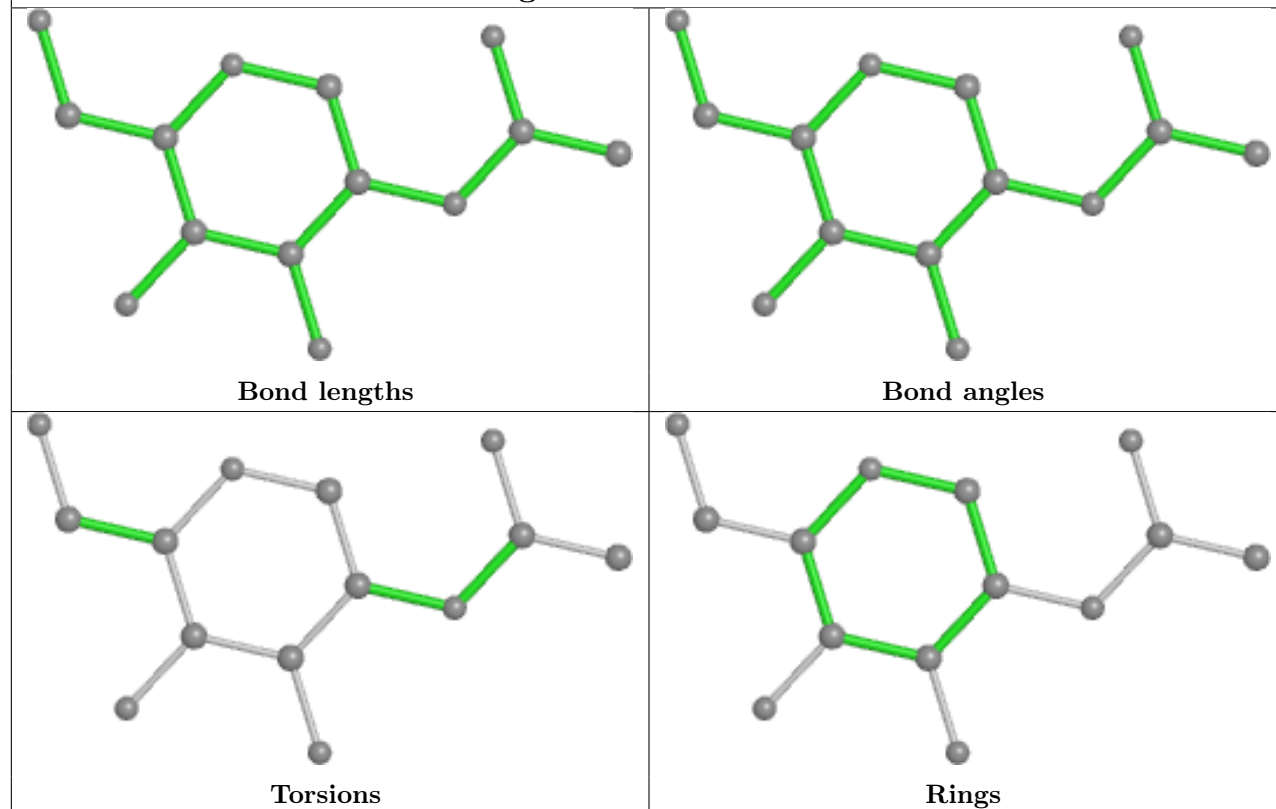
Ligand NAG B 1301



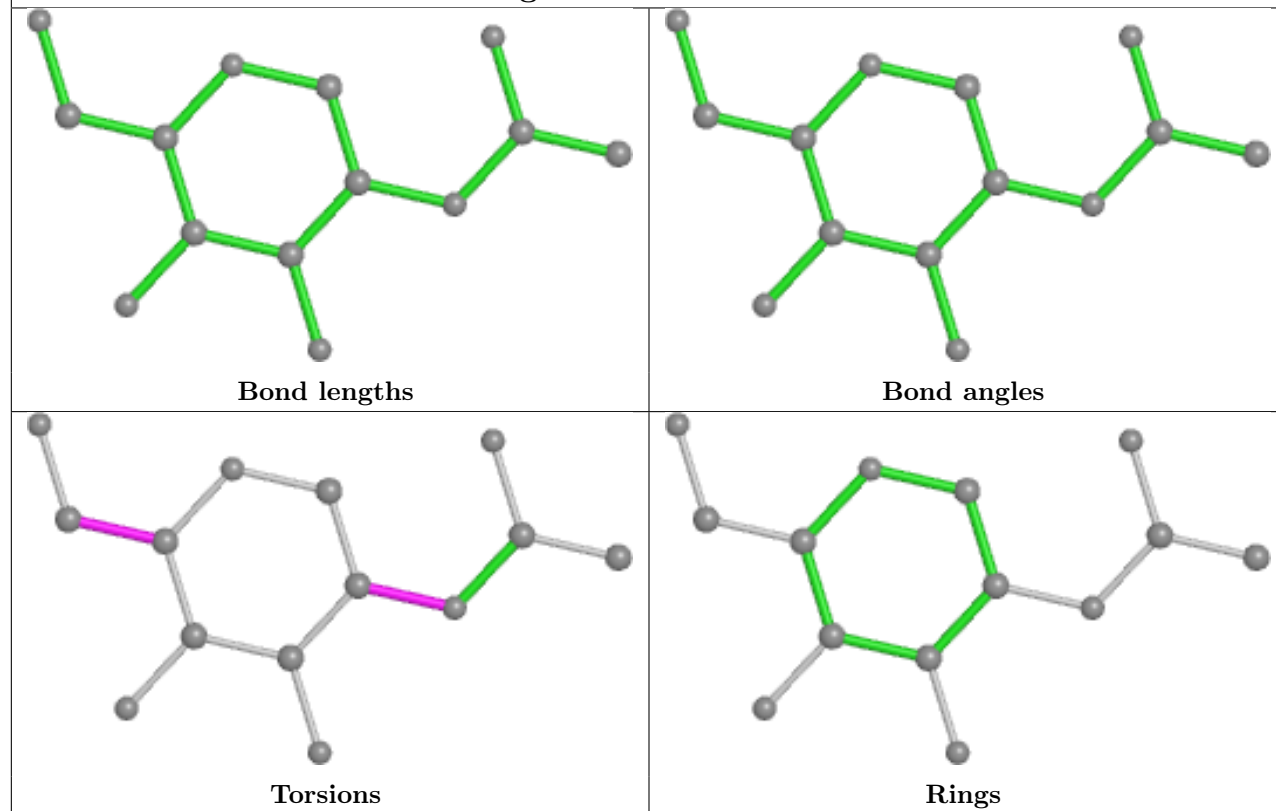
Ligand NAG A 1305



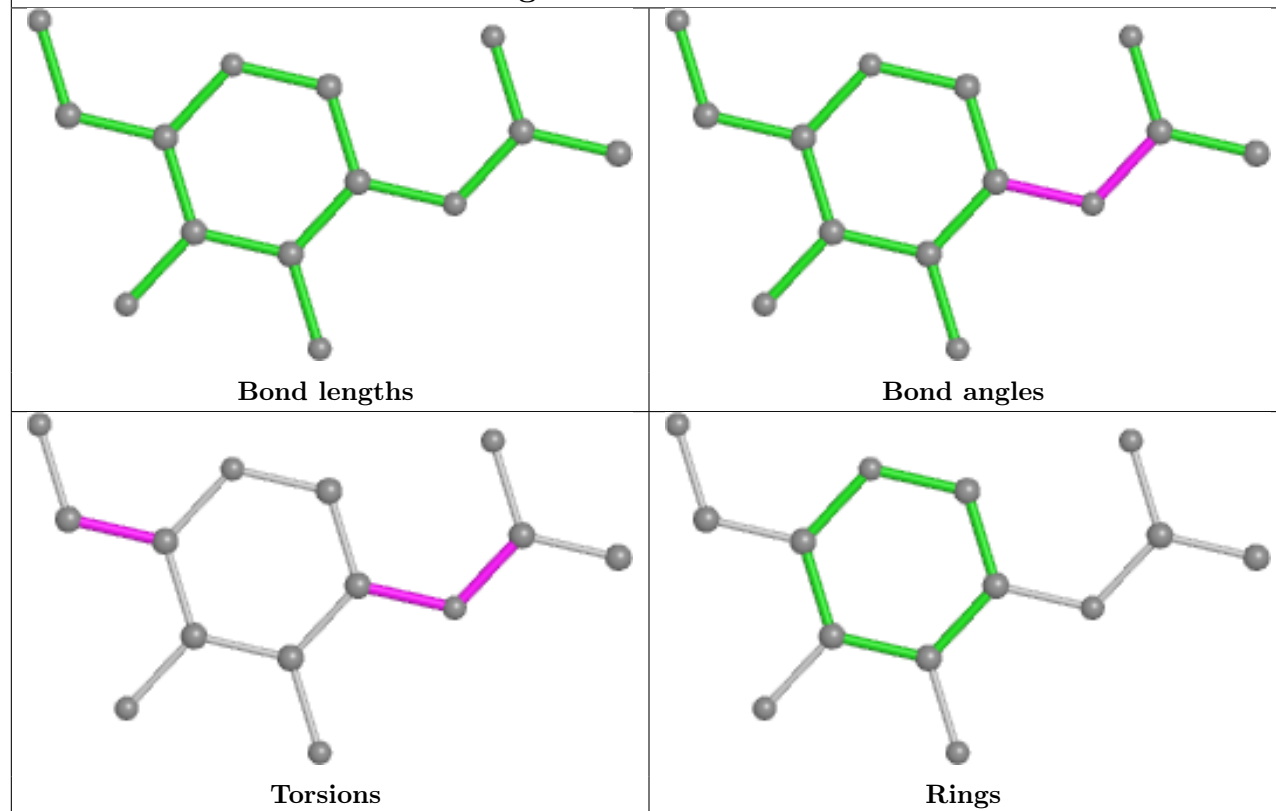
Ligand NAG A 1301



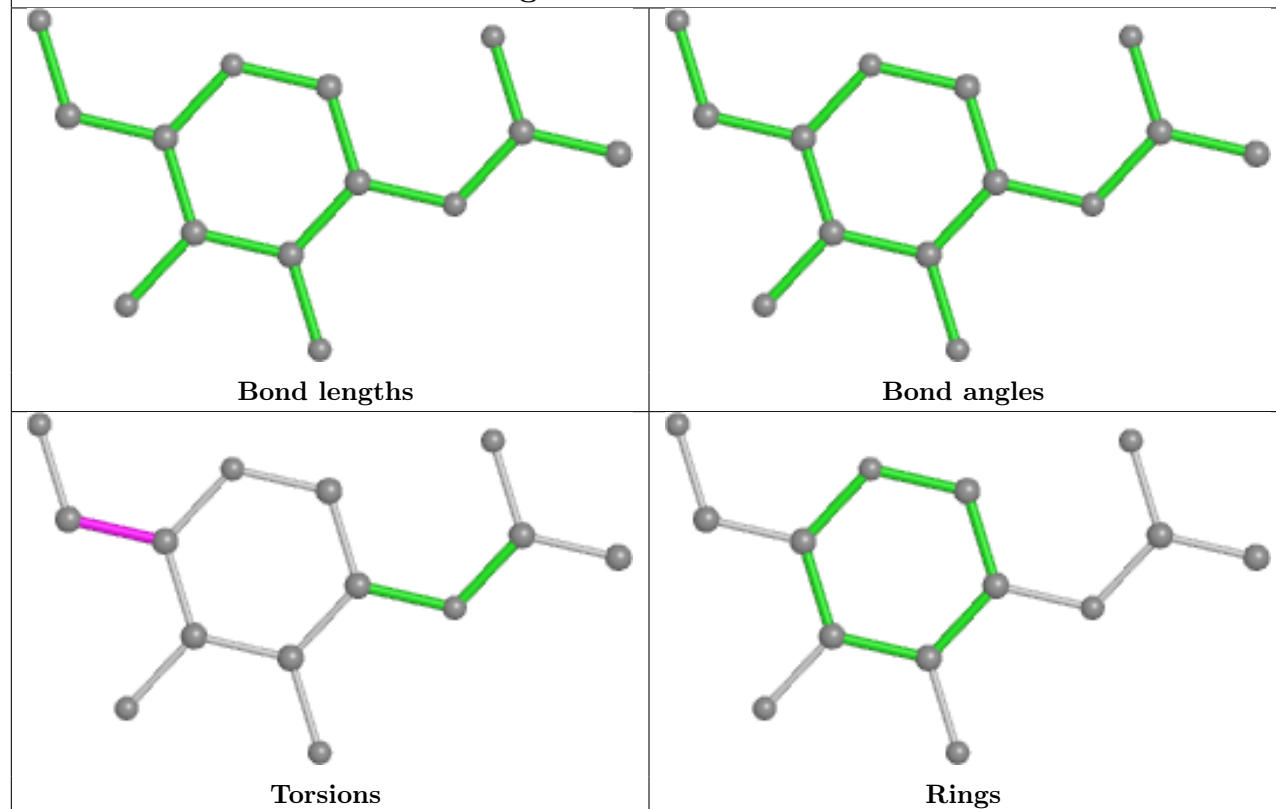
Ligand NAG B 1302



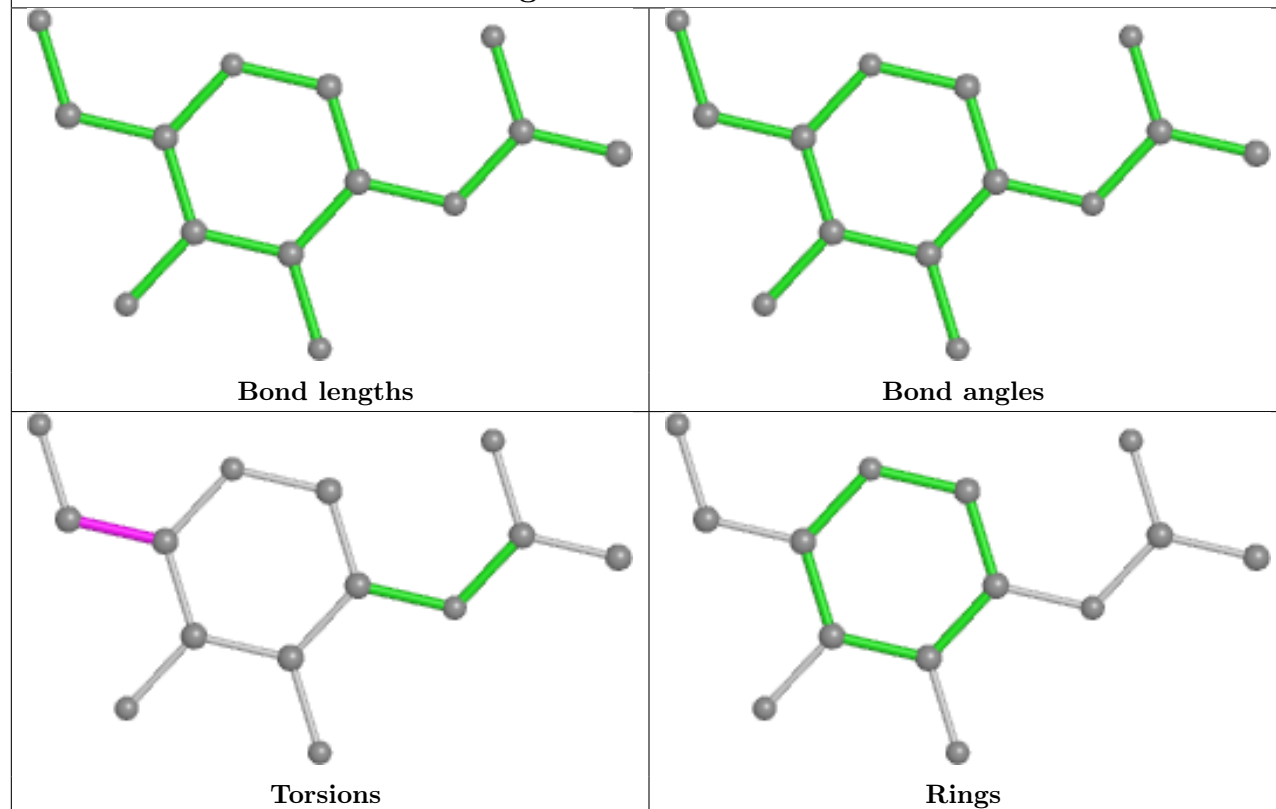
Ligand NAG A 1308



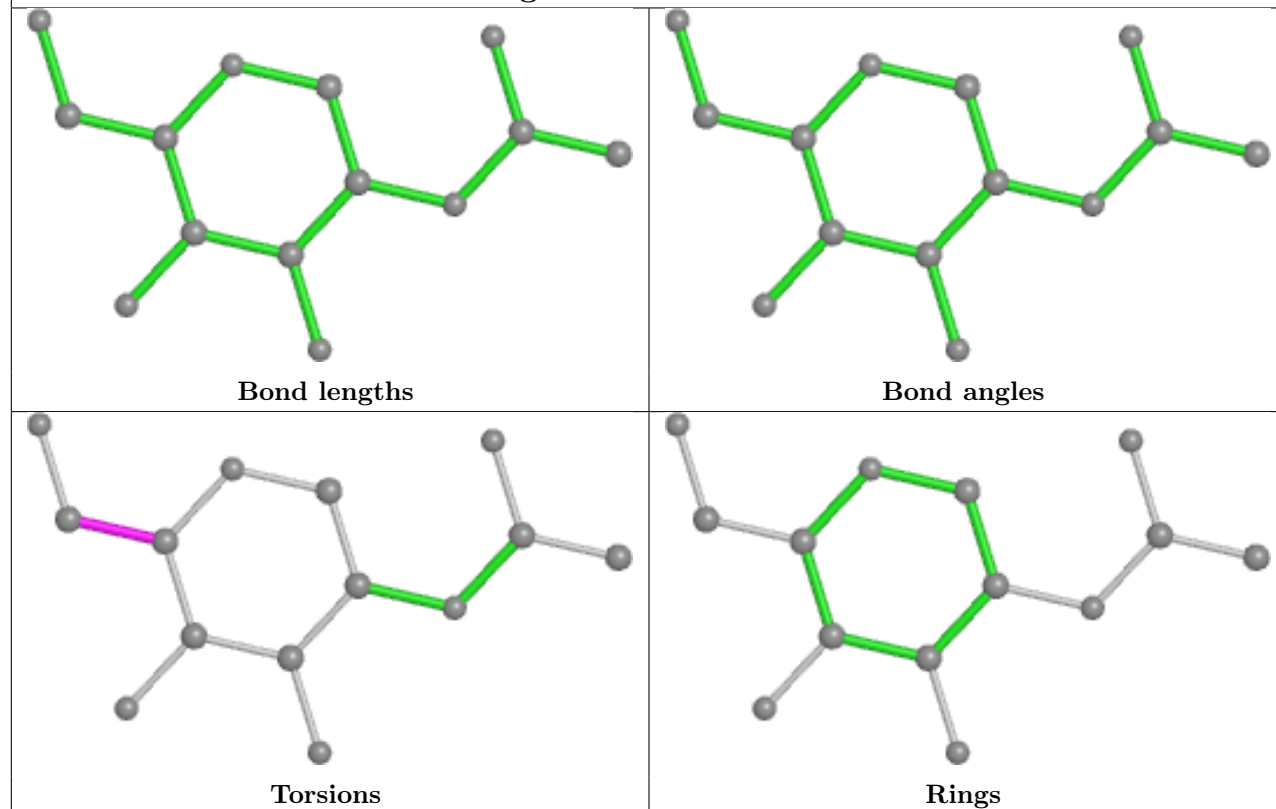
Ligand NAG B 1310



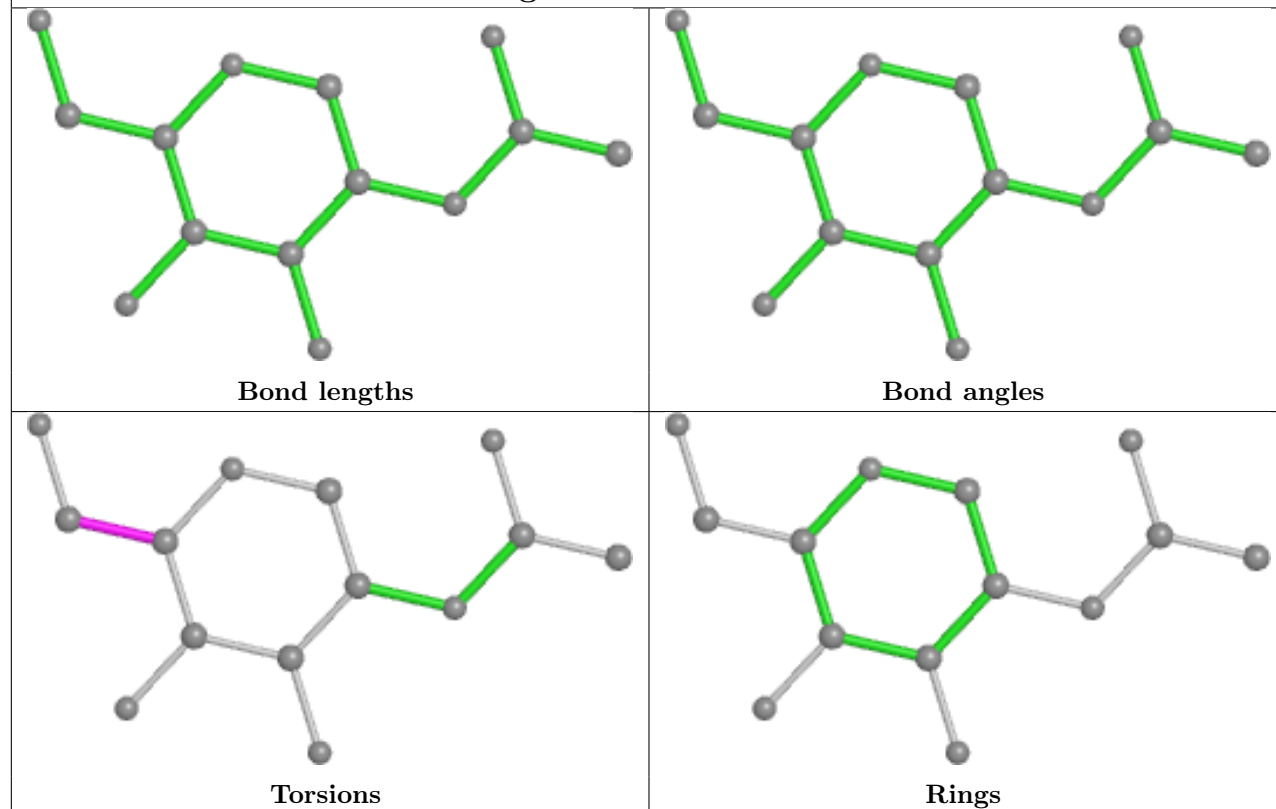
Ligand NAG C 1307



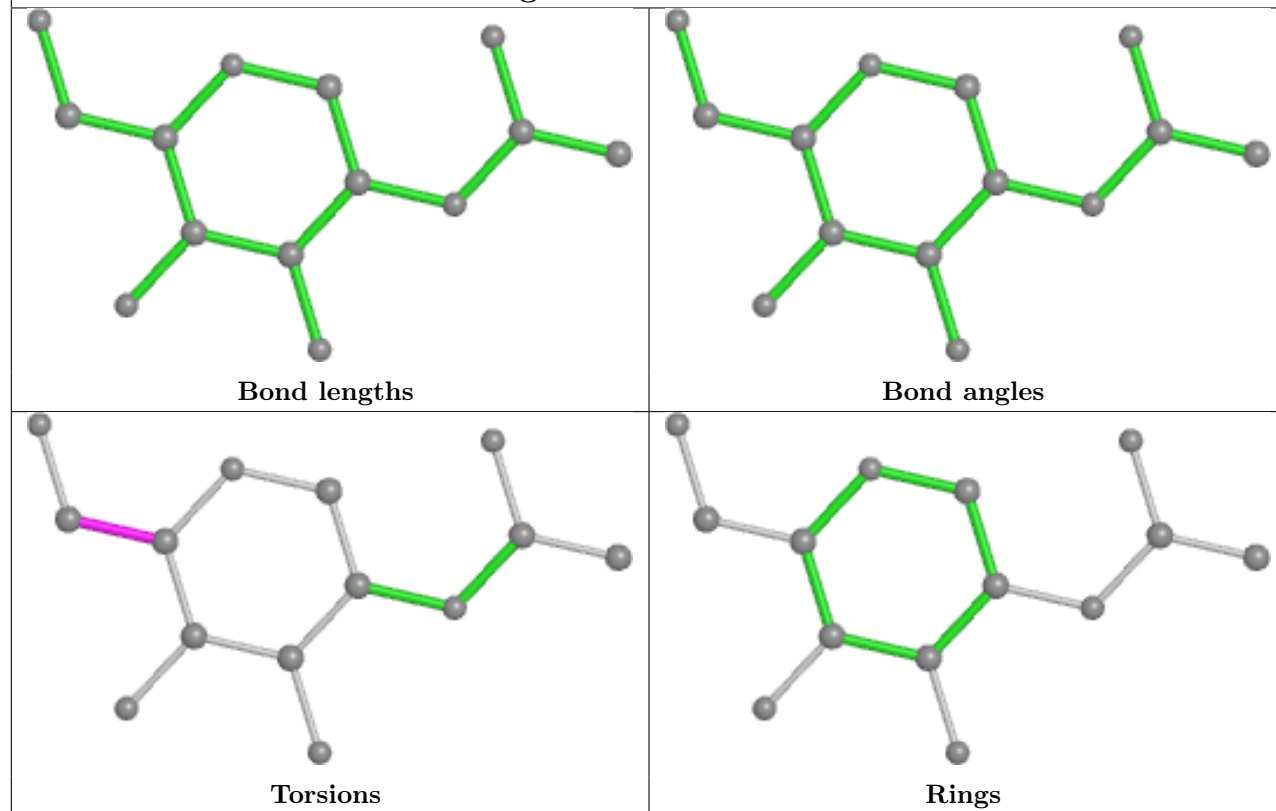
Ligand NAG B 1304



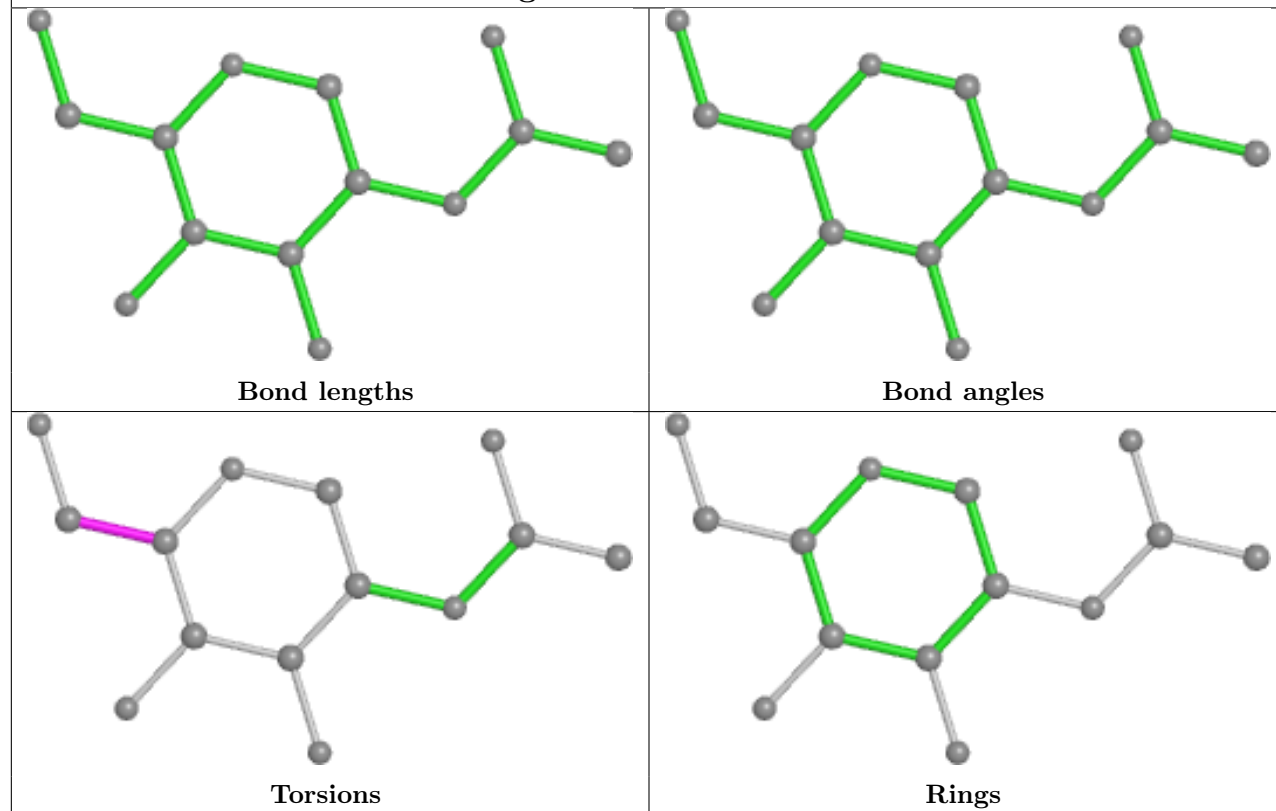
Ligand NAG C 1308



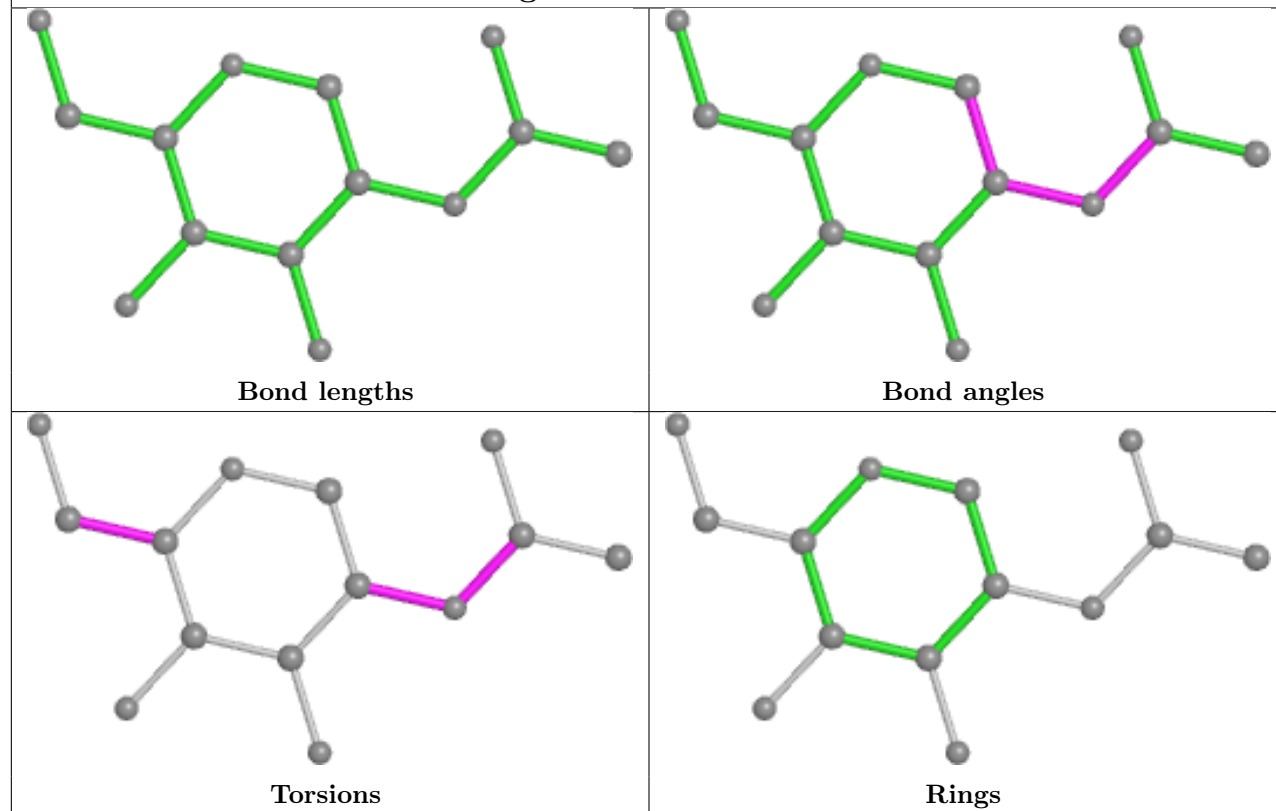
Ligand NAG B 1308



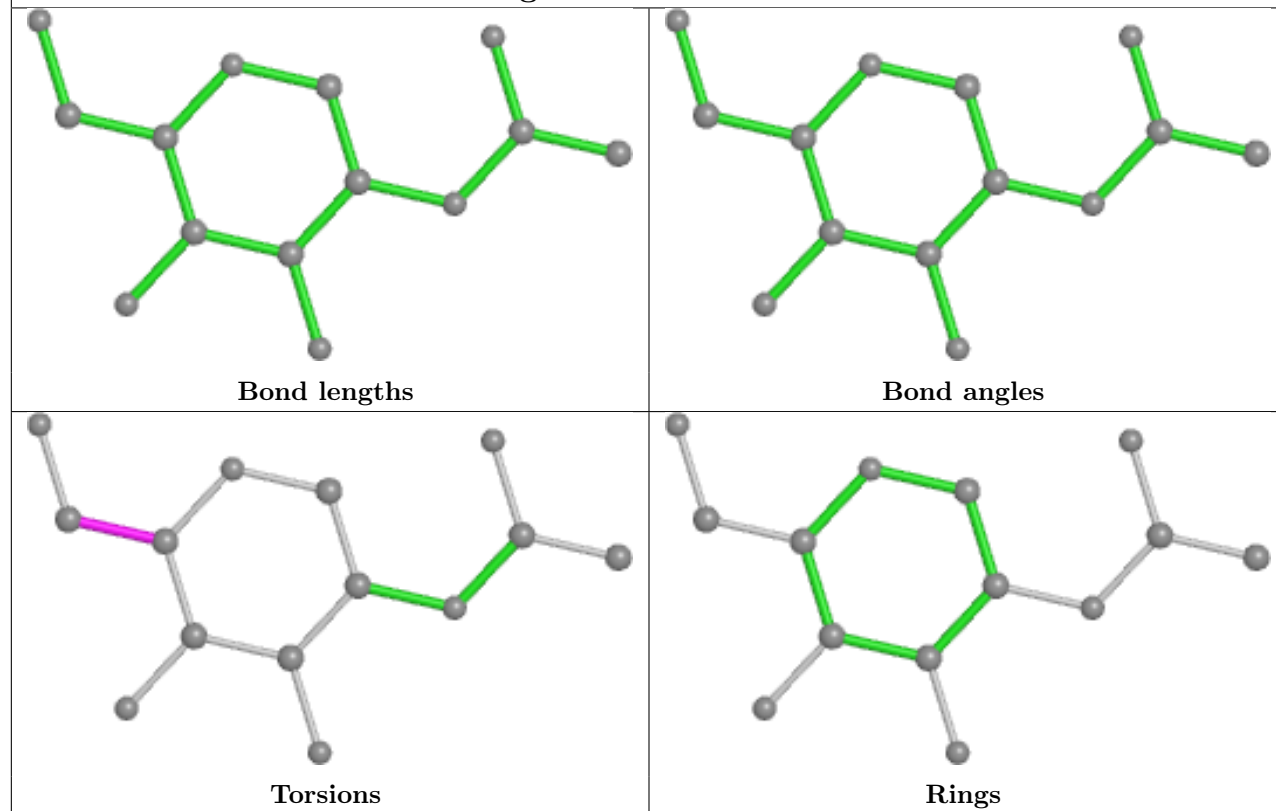
Ligand NAG A 1302



Ligand NAG C 1306



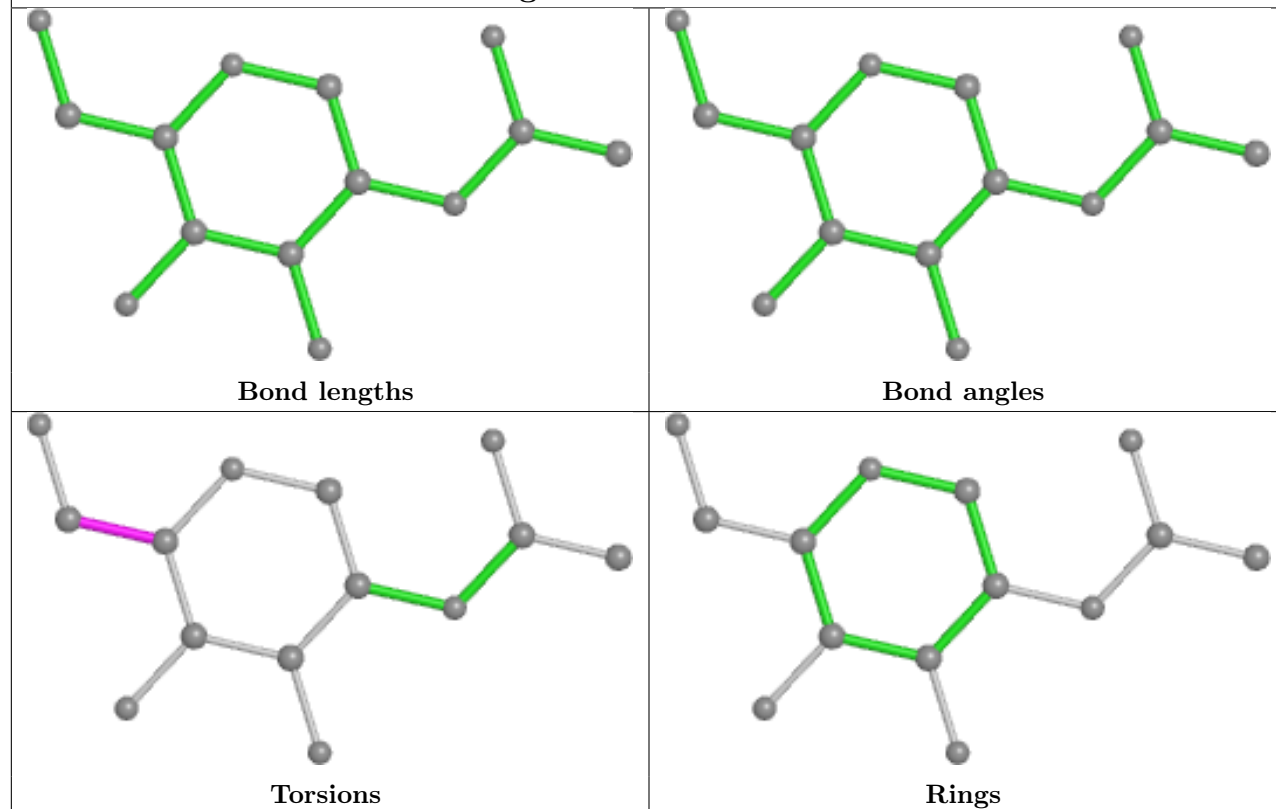
Ligand NAG B 1305



Ligand NAG A 1306



Ligand NAG C 1309



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.

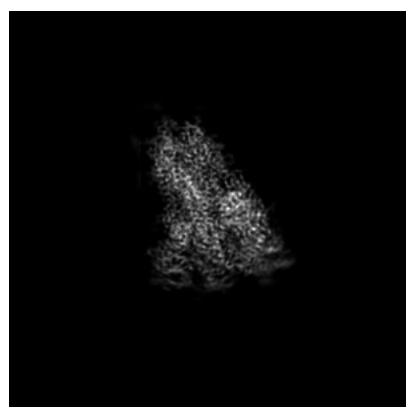
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32901. These allow visual inspection of the internal detail of the map and identification of artifacts.

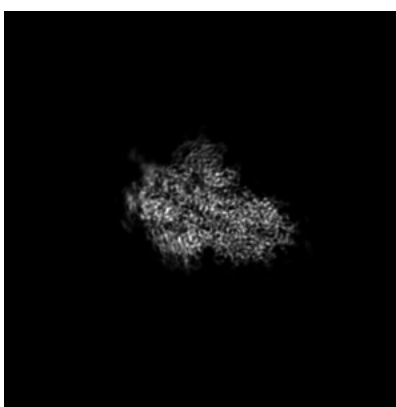
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

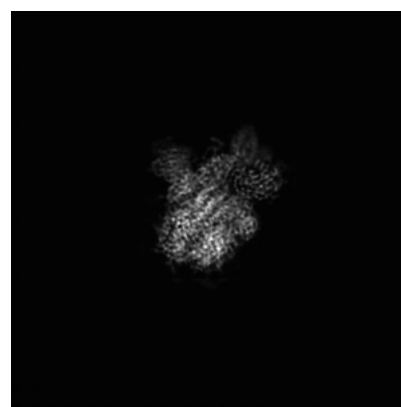
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 155



Y Index: 144

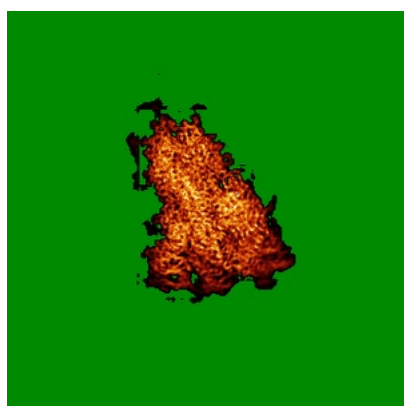


Z Index: 149

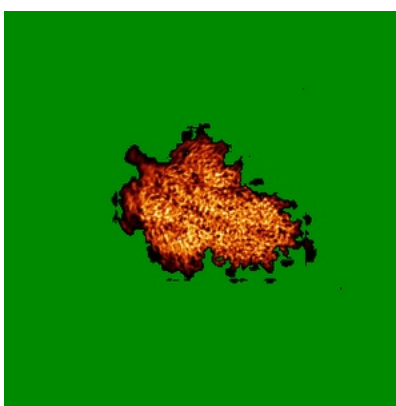
The images above show the largest variance slices of the map in three orthogonal directions.

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

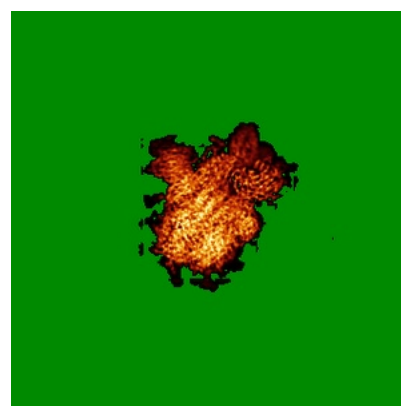
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

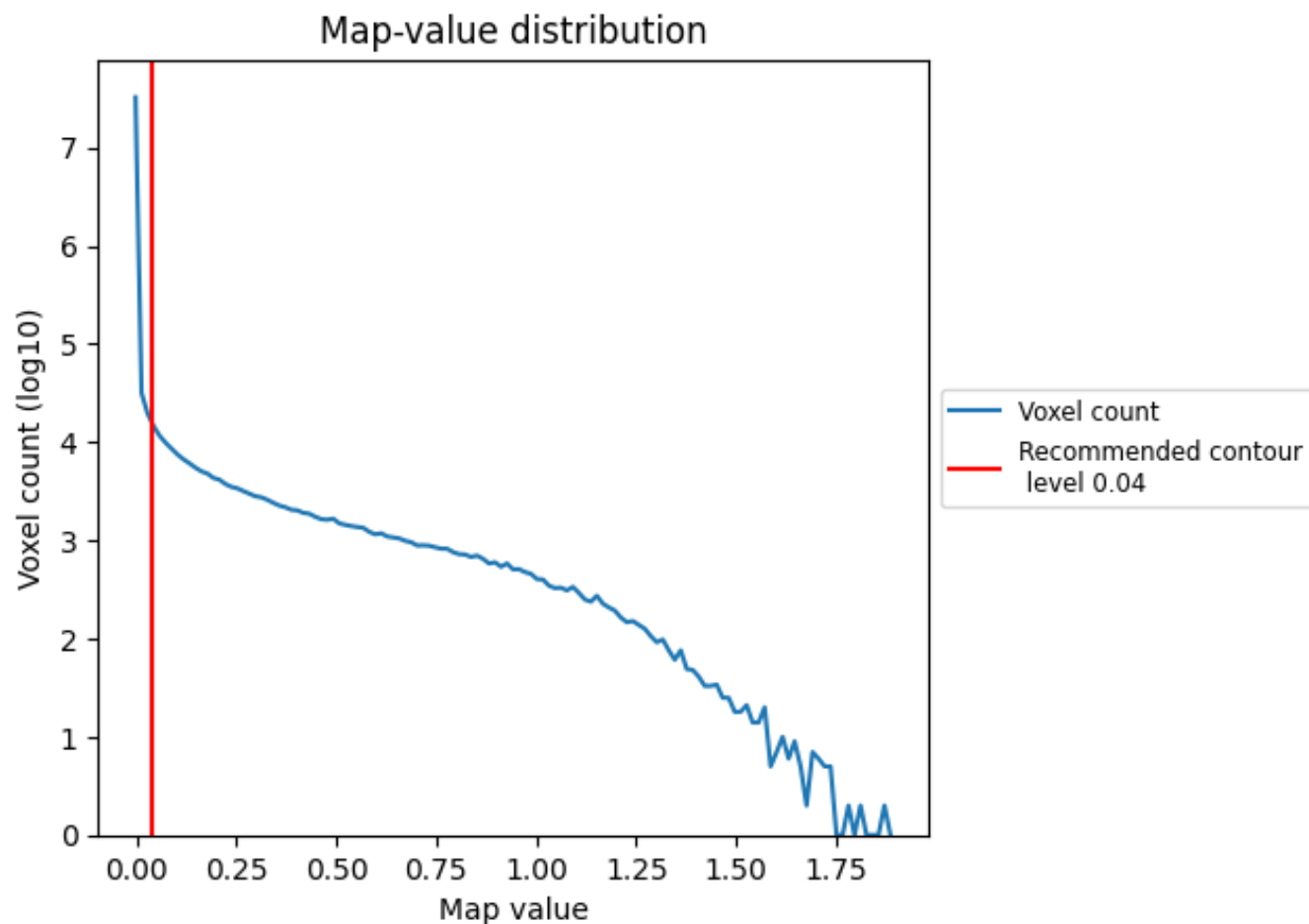
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

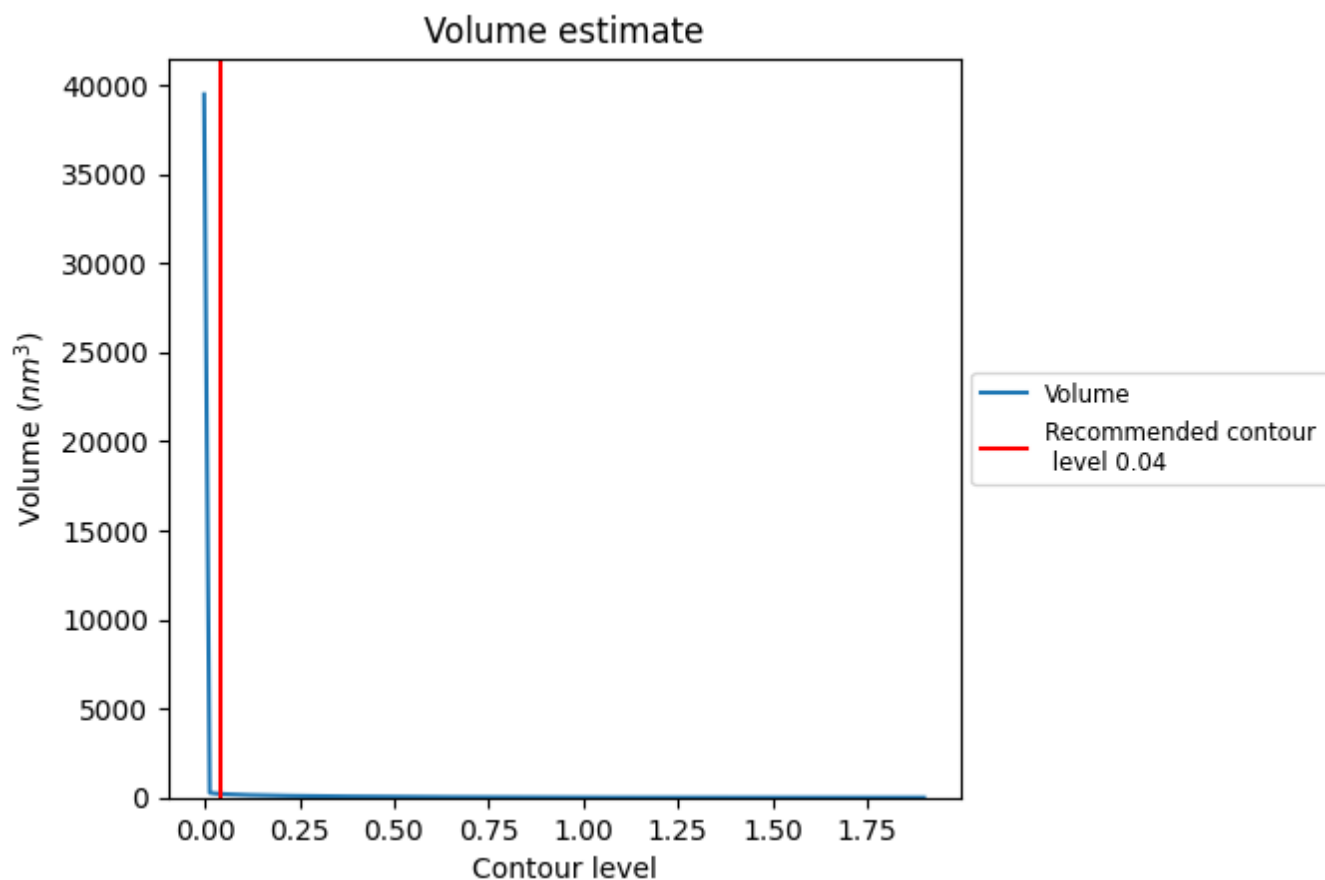
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

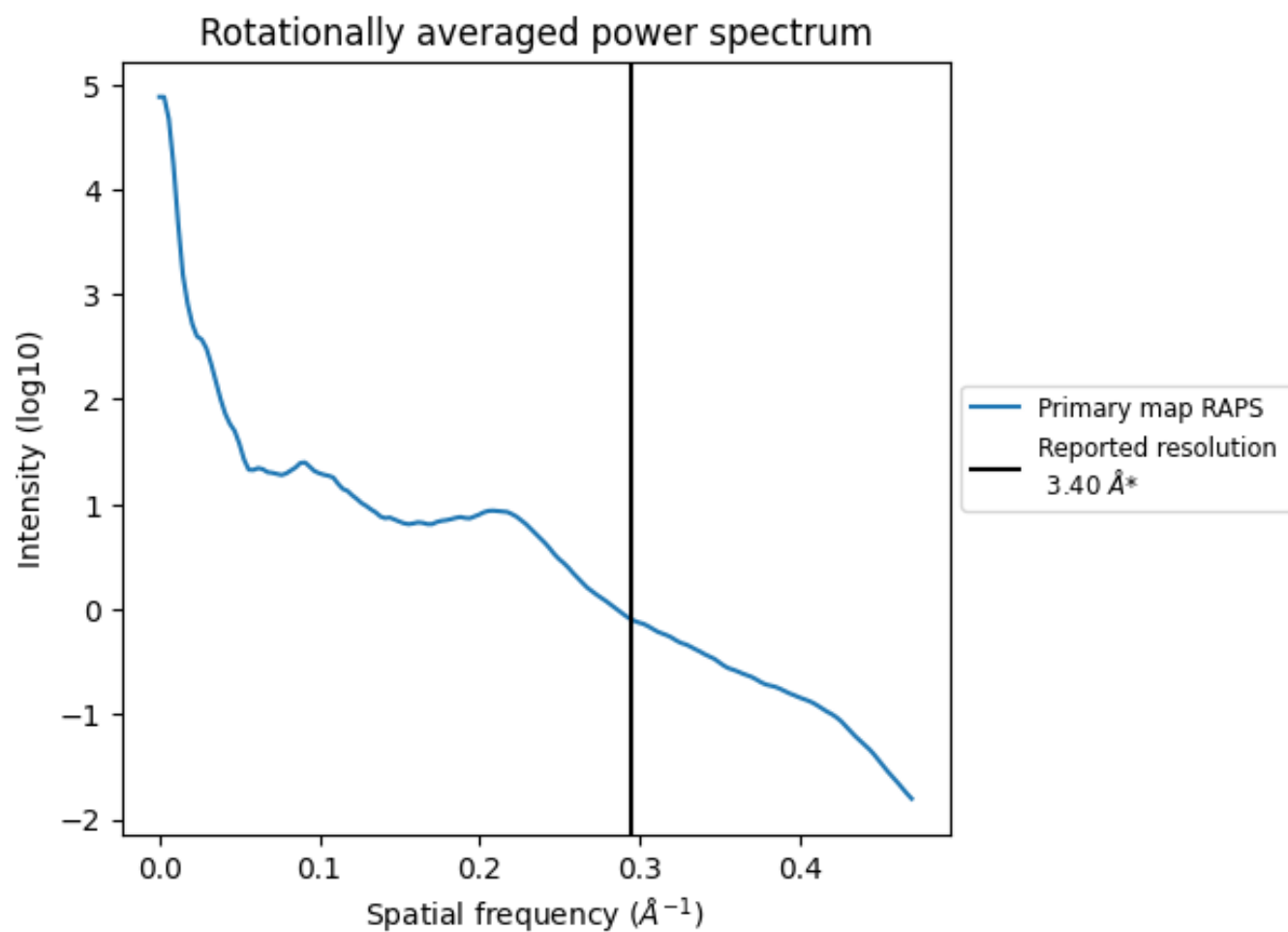
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 190 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 0.294 Å⁻¹

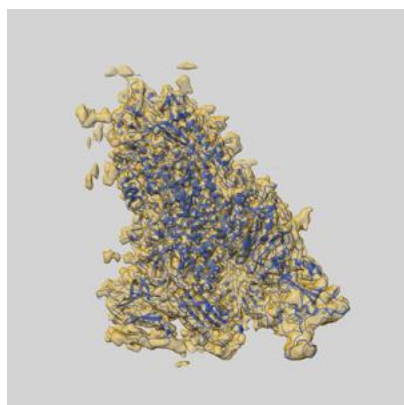
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

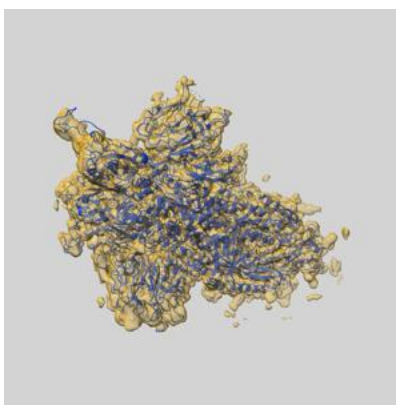
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32901 and PDB model 7WZ1. Per-residue inclusion information can be found in section 3 on page 15.

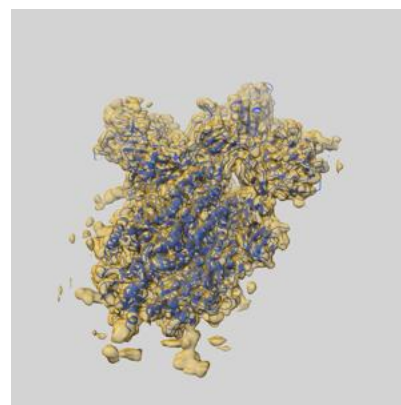
9.1 Map-model overlay [i](#)



X



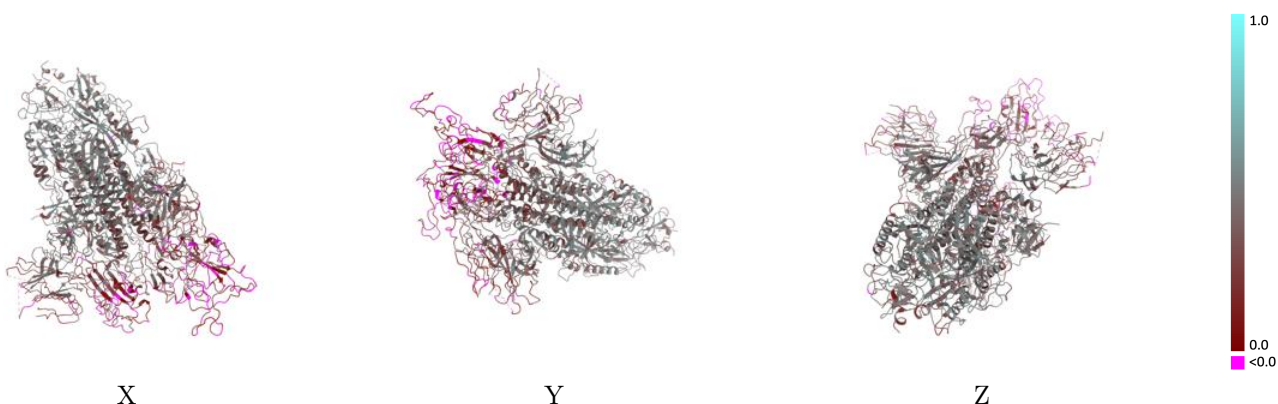
Y



Z

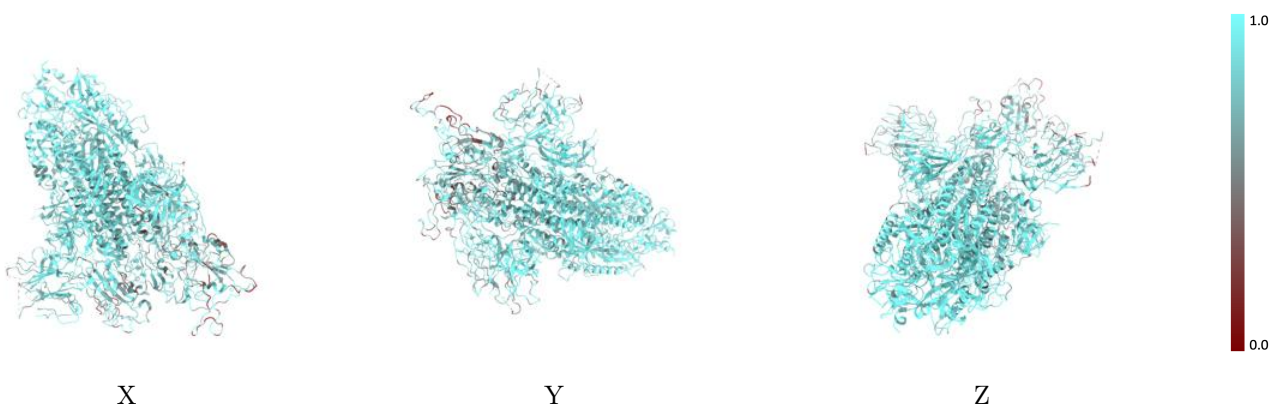
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



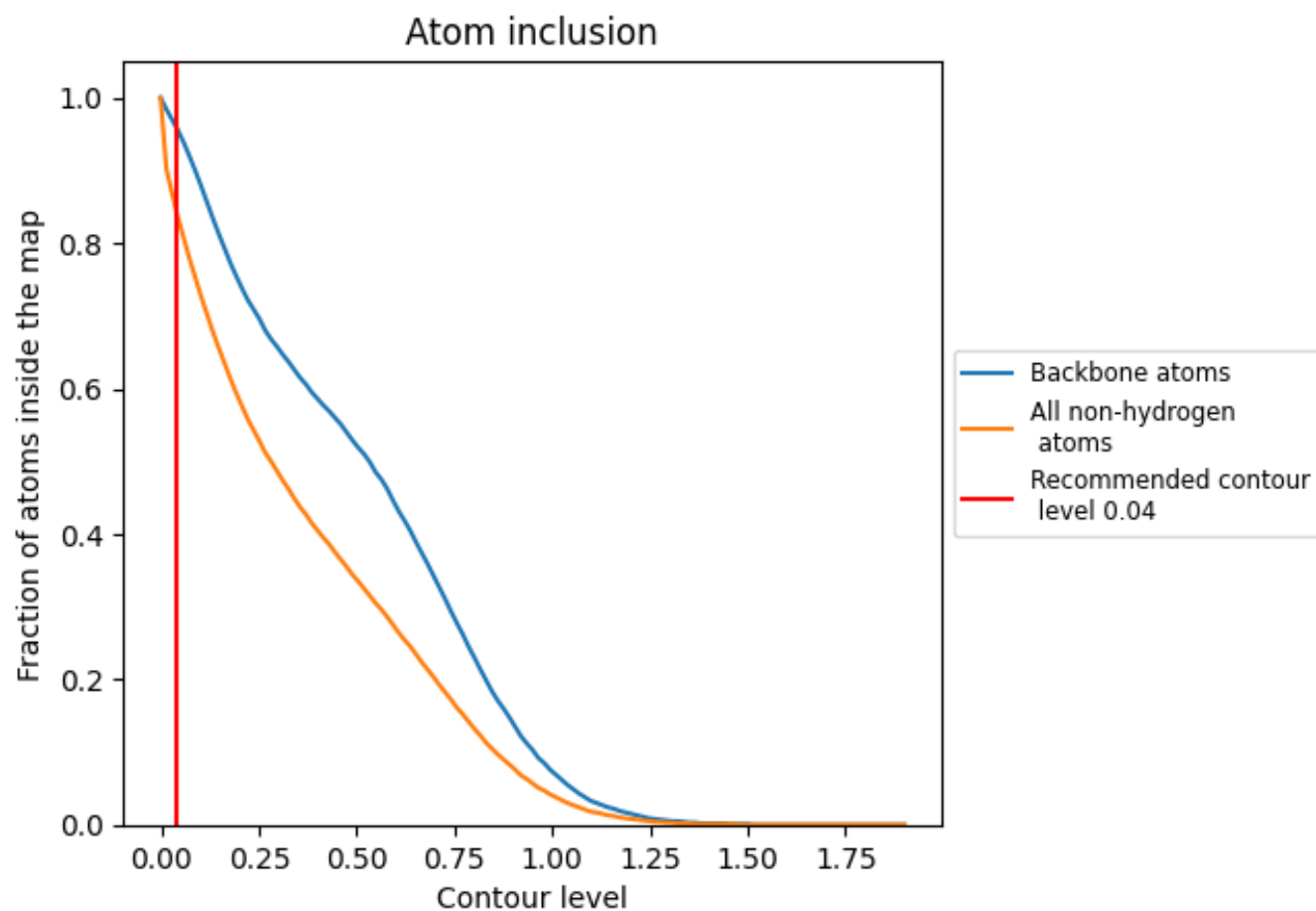
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8400	<div></div> 0.3430
A	<div></div> 0.8340	<div></div> 0.3410
B	<div></div> 0.8350	<div></div> 0.3330
C	<div></div> 0.8520	<div></div> 0.3550

