



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:08 AM UTC

PDB ID : 7YVO / pdb_00007yvo
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

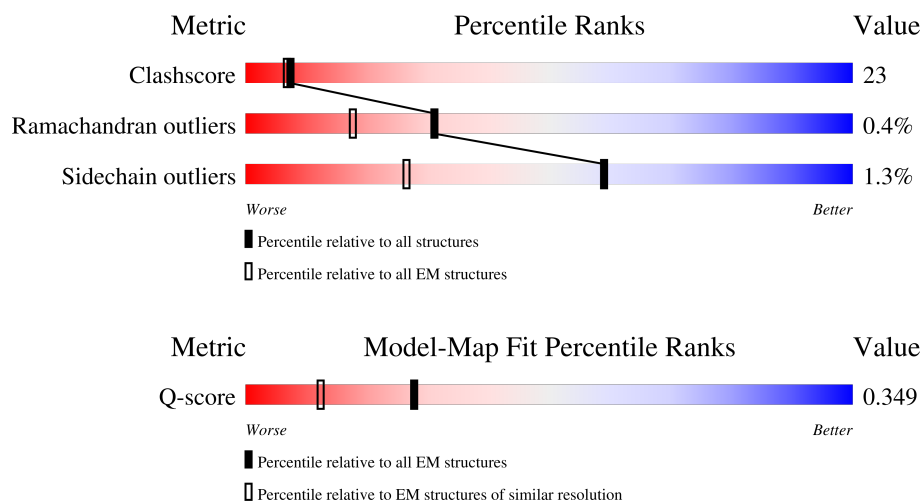
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

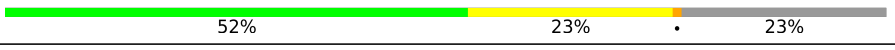
The reported resolution of this entry is 3.30 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1288	
1	B	1288	
1	C	1288	
2	H	109	

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Mol	Chain	Length	Quality of chain
2	J	109	
3	I	118	
3	K	118	
4	L	110	
4	N	110	
5	M	123	
5	O	123	

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆) (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	

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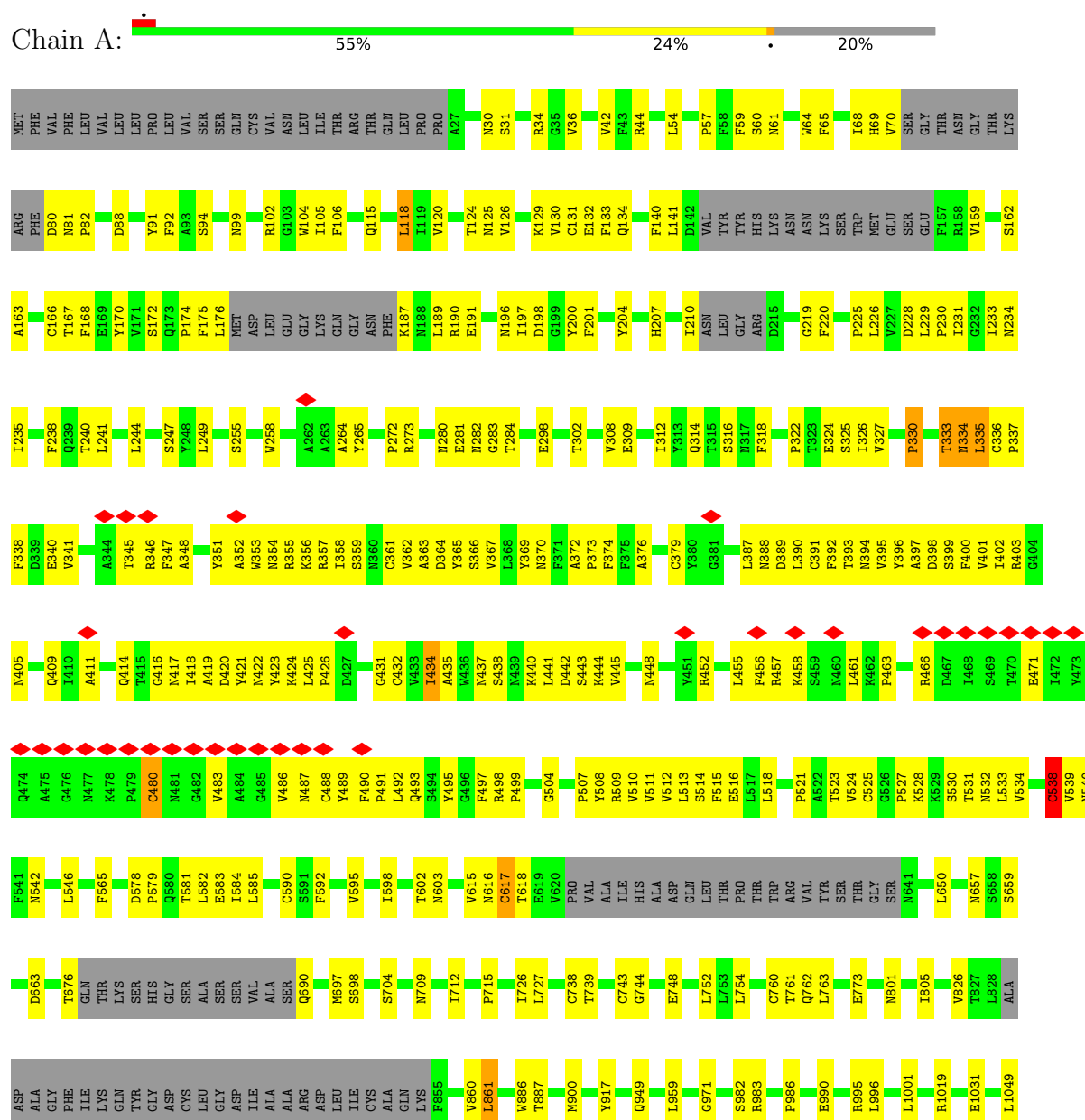
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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

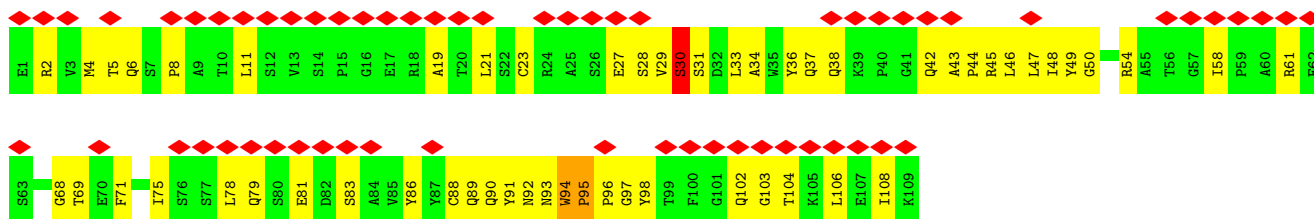


Tyr	Leu	R1000	Ala	Gly	Q564	M487	Y423	F347	F168	D80
Ile	Asp	L1001	Gly	Ser	F565	C488	K424	A243	E169	N81
Pro	Lys	L1002	Phe	Ala	Y489	F490	L425	L244	Y170	Val
GlU	Tyr	S1003	Ile	Ser	1569	P491	P426	A351	V171	Phe
Ala	Phe	L1004	Lys	Ser	P490	F491	G431	S247	S172	Leu
Pro	Lys	L1005	Gln	Val	P579	L492	K432	K353	Q173	Val
Asn	Asn	T1006	Tyr	Ala	Q493	Q493	C433	N354	P174	Leu
Asp	His	Y1007	Gly	Ser	E583	S494	Y433	K355	F175	Leu
Gly	Thr	V1008	Asp	Pro	1584	F497	I434	K356	L176	Pro
Gln	Ser	V1009	Cys	Ser	F497	R498	A435	R357	Met	Leu
Ala	Pro	E1010	Leu	Leu	C590	R498	Y436	I358	Asp	Val
Tyr	Asp	T1011	Gly	Gly	S591	P499	N437	S359	Leu	Ser
Val	Val	R1019	Asp	Asp	L699	T500	S438	N360	GlU	Ser
Arg	Asp	L1024	Ile	Ile	V695	Y501	K440	C361	Gly	Gln
Lys	Leu	L1025	Ala	Pro	Q502	Q502	L441	V362	Lys	Cys
Asp	Gly	V1040	Ala	Ala	1598	H505	D442	A363	Gln	Val
Gly	Asp	D1041	Arg	P715	T602	O506	S443	D364	Asn	Asn
GlU	Tyr	L1049	Leu	T720	N603	F507	K444	V387	Asn	Leu
Trp	Ser	L1049	Ile	Ile	Y445	Y508	Y445	R272	Phe	Ile
Val	Gly	G1059	Cys	L727	N616	R509	G446	R273	K187	Thr
Phe	Ile	E1072	Ala	S735	C617	V510	G447	N280	N188	Arg
Leu	Asn	E1072	Gln	S735	T618	V511	G447	F371	E281	Thr
Ser	Ala	E1072	Gln	S735	E619	V511	Y449	N282	R190	Gln
Thr	Ser	E1072	Lys	G744	E619	V511	Y449	P373	E191	Leu
Phe	Val	T1077	F855	C738	V620	S514	N450	T284	E191	Pro
Leu	Val	A1078	L858	T739	Pro	F515	Y451	A376	N196	
Ser	Asn	E1078	L858	I742	Val	E516	R452	F377	I197	A27
Gly	Ile	E1092	L861	C743	Ile	L517	Y453	E298	D198	
GlU	Lys	S1097	L861	G744	His	A520	L455	T302	K129	N30
Val	GlU	M1098	D867	L752	Ala	P521	F456	V308	Y200	S31
Ile	Asp	M1098	E868	L753	Asp	A522	R457	E309	F202	
Phe	Asp	W1102	L866	L754	Gln	V524	S459	V308	K202	V36
Arg	Gln	F1103	W886	Q755	Leu	C525	N460	I312	I203	Y37
Leu	Leu	V1104	W886	Y756	Thr	C525	N460	I312	Y204	
Asn	Asn	I1115	T896	G757	Pro	G526	L461	S316	S205	K41
Gly	GlU	L1115	T896	S758	Thr	P527	K462	S316	K206	
Val	Val	D1118	Y904	S758	Trp	K528	F464	V320	H207	L54
Ala	Ala	N1119	R905	Y761	Arg	K529	F464	V320	T208	
Ser	Asn	M1119	R905	Q762	Val	T531	E465	E324	P209	P57
Leu	Leu	M1125	Y934	E773	Tyr	N532	R466	S325	I210	F58
Asn	Asn	C1126	L959	E773	Tyr	L533	D467	S325	Asn	F59
Gln	Gln	D1127	L959	N801	Thr	L533	I468	I326	Leu	S80
Ser	Ser	V1128	L962	N801	Gly	V534	S469	V397	Gly	N61
Lys	Ile	V1129	L962	L806	Ser	Y534	T470	D398	Arg	
Asp	Asp	I1132	L977	L806	N641	C538	E471	F329	D215	W64
Leu	Leu	V1133	N978	S810	R657	V539	E471	P330	A222	H66
Gln	Gln	N1134	R980	K811	S659	N540	Y473	N331	L223	A67
Leu	Leu	D1139	R981	R815	F543	N544	Q475	I332	I68	H69
Gly	Gly	D1139	S982	R815	C662	N544	A475	N334	L226	
Lys	Lys	D1146	R983	R815	D663	C545	K476	L335	L227	V70
Ser	Ser	Val	R983	D820	D663	C545	K476	C336	D228	Ser
Gly	Tyr	Ser	R984	L821	T676	L546	P479	P337	L229	Gly
GlU	GlU	Phe	L822	L822	Gln	C480	C480	E340	P230	Thr
Ser	Gln	Lys	A989	L828	Lys	S555	N481	V341	I231	
Ala	Gly	Lys	Thr	L828	Thr	L560	G482	F342	G232	Gly
Trp	Ser	Trp	Ser	Ala	Ser	L560	V483	T345	I233	Thr
Gly	Gly	Trp	Asn	Asn	His	O562	V483	T345	G238	Lys
Arg	Arg	Arg	His	His	His	O562	V483	T345	F238	Arg
Phe	Phe	Phe	His	His	His	O562	V483	T345	G238	Phe

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

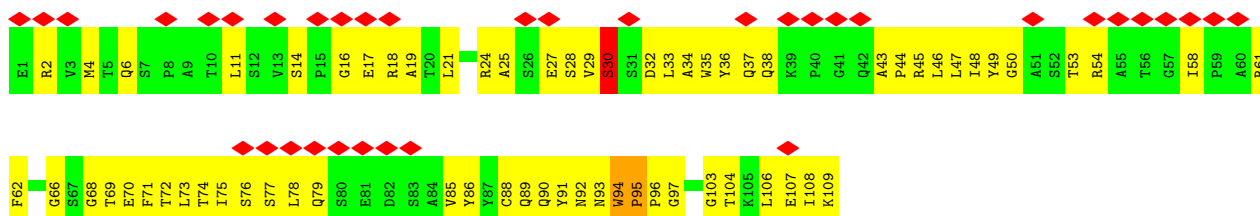
• Molecule 2: TH132 Fab light chain

Chain H: 



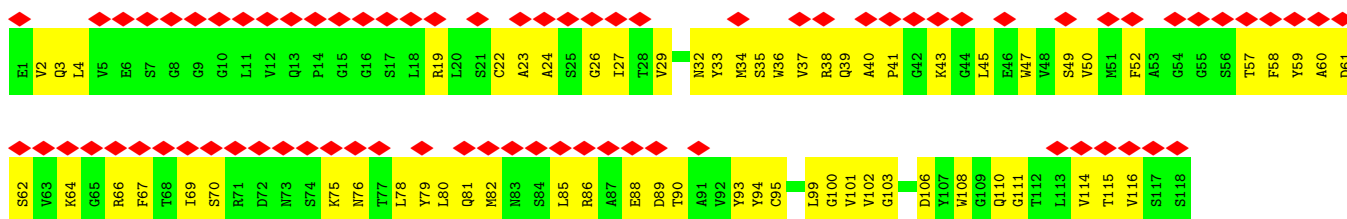
• Molecule 2: TH132 Fab light chain

Chain J: 



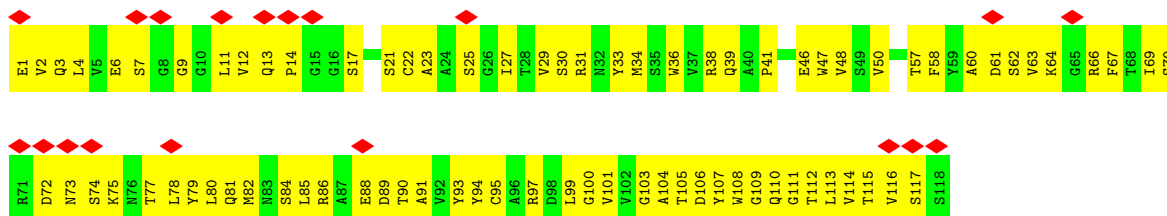
• Molecule 3: TH132 Fab heavy chain

Chain I: 

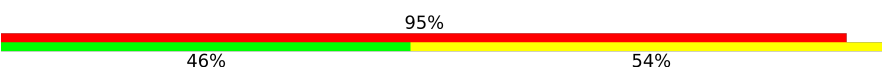


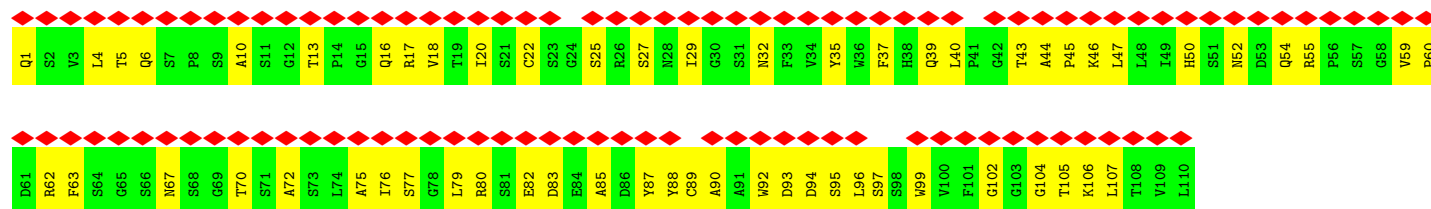
• Molecule 3: TH132 Fab heavy chain

Chain K: 

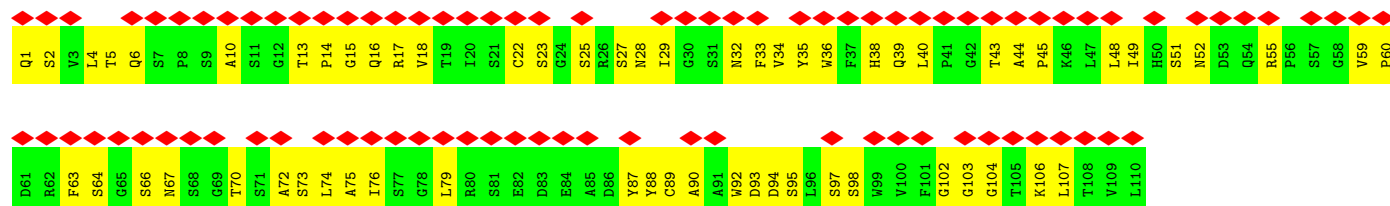
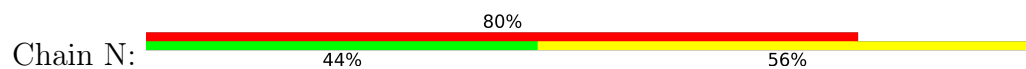


• Molecule 4: TH27 Fab light chain

Chain L: 



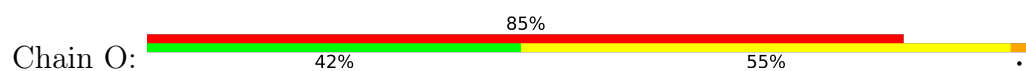
• Molecule 4: TH27 Fab light chain



• 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 (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.96	0/7912	0.87	3/10810 (0.0%)
1	B	0.97	1/7589 (0.0%)	0.88	3/10370 (0.0%)
1	C	0.98	1/7905 (0.0%)	0.91	12/10801 (0.1%)
2	H	0.32	0/837	0.86	2/1140 (0.2%)
2	J	0.37	0/837	0.87	2/1140 (0.2%)
3	I	0.27	0/881	0.66	0/1196
3	K	0.34	0/881	0.70	0/1196
4	L	0.23	0/836	0.60	0/1138
4	N	0.28	0/836	0.65	0/1138
5	M	0.29	0/981	0.63	0/1340
5	O	0.28	0/981	0.60	0/1340
All	All	0.86	2/30476 (0.0%)	0.85	22/41609 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	LEU	C-N	-5.70	1.21	1.33
1	C	886	TRP	CB-CG	-5.23	1.34	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	326	ILE	CA-C-N	7.15	134.84	121.97
1	C	326	ILE	C-N-CA	7.15	134.84	121.97
1	B	432	CYS	CA-CB-SG	6.91	130.29	114.40
2	J	30	SER	CA-C-N	-6.47	111.34	122.14
2	J	30	SER	C-N-CA	-6.47	111.34	122.14
1	A	538	CYS	CA-CB-SG	6.22	128.70	114.40
1	C	329	PHE	N-CA-C	6.16	119.22	108.82
1	C	230	PRO	N-CA-C	-6.11	106.52	114.03
1	C	886	TRP	CB-CA-C	-5.95	99.25	110.67
1	A	590	CYS	CA-CB-SG	5.88	127.93	114.40
2	H	30	SER	CA-C-N	-5.74	112.56	122.14
2	H	30	SER	C-N-CA	-5.74	112.56	122.14
1	C	538	CYS	CA-CB-SG	5.67	127.44	114.40
1	C	328	ARG	CA-C-N	-5.59	111.33	122.90
1	C	328	ARG	C-N-CA	-5.59	111.33	122.90
1	B	331	ASN	N-CA-C	-5.57	101.21	109.11
1	C	330	PRO	N-CA-C	-5.53	101.08	112.47
1	C	590	CYS	CA-CB-SG	5.48	127.01	114.40
1	B	521	PRO	N-CA-C	-5.32	97.22	113.27
1	C	521	PRO	N-CA-C	-5.31	101.53	112.47
1	A	528	LYS	CB-CA-C	-5.18	110.58	116.54
1	C	530	SER	N-CA-C	5.00	117.46	109.96

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	287	0
1	B	7413	0	7008	265	0
1	C	7719	0	7310	353	0
2	H	818	0	777	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	818	0	777	68	0
3	I	865	0	833	68	0
3	K	865	0	833	83	0
4	L	816	0	772	52	0
4	N	816	0	772	55	0
5	M	956	0	950	71	0
5	O	956	0	950	75	0
6	A	168	0	156	21	0
6	B	168	0	156	25	0
6	C	182	0	169	23	0
All	All	30285	0	28780	1373	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 (1373) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:I:59:TYR:HD1	3:I:64:LYS:HZ3	1.40	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
2:H:42:GLN:CD	2:H:43:ALA:H	2.03	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:247:SER:HG	1:C:258:TRP:CG	2.15	0.64
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
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
1:B:377:PHE:C	1:B:378:LYS:HD3	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:440:LYS:HD2	5:O:103:GLY:C	2.23	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
3:K:82:MET:HE1	3:K:114:VAL:HG11	1.80	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
4:N:93:ASP:O	4:N:97:SER:N	2.32	0.62
1:A:314:GLN:CD	1:A:314:GLN:H	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:6:GLN:HE22	4:L:88:TYR:HA	1.66	0.61
5:O:59:LYS:HZ1	5:O:71:ILE:C	2.09	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
1:C:440:LYS:HZ3	5:O:102:PRO:HB2	1.66	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:B:659:SER:OG	1:B:698:SER:HB3	2.03	0.58
1:C:91:TYR:OH	1:C:191:GLU:OE2	2.12	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:91:TYR:OH	1:A:191:GLU:OE2	2.16	0.58
1:A:616:ASN:ND2	6:A:1310:NAG:O7	2.37	0.58
1:B:393:THR:OG1	1:B:394:ASN:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.40	0.56
1:B:383:SER:HB3	1:B:386:LYS:HZ3	1.70	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
2:H:4:MET:HE2	2:H:33:LEU:HD11	1.86	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
2:J:4:MET:HE2	2:J:33:LEU:HD11	1.88	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:353:TRP:CD1	1:A:353:TRP:H	2.24	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
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:228:ASP:O	1:C:229:LEU:C	2.50	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:A:1077:THR:OG1	1:B:900:MET:HE1	2.08	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:B:792:PRO:O	1:B:795:LYS:NZ	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:616:ASN:OD1	1:C:616:ASN:C	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:616:ASN:OD1	1:A:616:ASN:C	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	3:K:106:ASP:N	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
1:B:616:ASN:OD1	1:B:616:ASN:C	2.54	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:OD1	3:I:106:ASP:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:A:1304:NAG:HO6	6:A:1311:NAG:HO6	1.51	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
3:K:86:ARG:HE	3:K:88:GLU:CD	2.19	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
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
1:B:357:ARG:HH22	1:C:230:PRO:C	2.19	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
1:B:461:LEU:HD21	1:B:465:GLU:C	2.37	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: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:A:118:LEU:C	1:A:118:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:77:SER:O	2:J:79:GLN:NE2	2.43	0.49
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
3:K:29:VAL:HG21	3:K:77:THR:C	2.37	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:383:SER:H	1:C:386:LYS:HZ3	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:40:ARG:HB3	5:O:50:LEU:HD11	1.94	0.49
1:A:448:ASN:N	1:A:497:PHE:O	2.41	0.49
1:A:900:MET:HE1	1:C:1077:THR:OG1	2.13	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
1:C:617:CYS:C	1:C:619:GLU:N	2.68	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:66:ARG:HH12	3:I:89:ASP:CG	2.22	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
1:C:603:ASN:CG	6:C:1304:NAG:H2	2.38	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:A:886:TRP:O	1:A:887:THR:C	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ILE:C	1:A:585:LEU:HD22	2.38	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
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:580:GLN:C	6:B:1305:NAG:H5	2.39	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:272:PRO:C	1:C:273:ARG:HG2	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:J:108:ILE:C	2:J:109:LYS:HG3	2.40	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
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
1:C:81:ASN:C	1:C:239:GLN:HE22	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:383:SER:H	1:C:386:LYS:HZ1	1.61	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
1:A:361:CYS:O	1:A:524:VAL:HA	2.16	0.45
1:A:704:SER:O	1:A:704:SER:OG	2.30	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: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
1:C:119:ILE:HG13	1:C:119:ILE:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:N	1:B:60:SER:O	2.32	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
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:117:LEU:C	1:C:118:LEU:HD12	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:444:LYS:HG3	1:A:448:ASN:CG	2.42	0.45
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:C:82:PRO:C	1:C:239:GLN:NE2	2.75	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
4:N:28:ASN:HB3	4:N:93:ASP:CG	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:VAL:O	2:J:30:SER:C	2.60	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
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
4:N:32:ASN:CG	4:N:33:PHE:N	2.75	0.44
1:B:353:TRP:CE3	1:B:353:TRP:C	2.96	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:616:ASN:ND2	6:C:1308:NAG:C7	2.81	0.43
1:C:617:CYS:C	1:C:619:GLU:H	2.24	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
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
3:K:25:SER:C	3:K:27:ILE:H	2.25	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:430:THR:O	1:B:430:THR:OG1	2.37	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
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:886:TRP:O	1:B:887:THR:C	2.61	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
1:C:743:CYS:O	1:C:744:GLY:C	2.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:J:93:ASN:O	2:J:94:TRP:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:442:ASP:C	1:A:448:ASN:HD22	2.27	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:69:HIS:O	1:B:70:VAL:C	2.63	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: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
4:N:32:ASN:CG	4:N:33:PHE:H	2.27	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:B:1072:GLU:CD	1:B:1072:GLU:H	2.27	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
1:C:1072:GLU:CD	1:C:1072:GLU:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:512:VAL:C	1:B:513:LEU:HD12	2.45	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
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:228:ASP:OD1	1:A:228:ASP:C	2.61	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: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
1:C:444:LYS:HZ1	5:O:56:ASP:CG	2.29	0.41
2:H:29:VAL:O	2:H:29:VAL:HG12	2.19	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:B:401:VAL:HG23	1:B:508:TYR:C	2.45	0.41
1:C:335:LEU:CG	1:C:336:CYS:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:104:ALA:O	3:K:105:THR:C	2.63	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
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
1:C:1098:ASN:CG	6:C:1307:NAG:H82	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:29:VAL:O	2:H:30:SER:C	2.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:24:ARG:NE	2:J:70:GLU:OE1	2.53	0.41
2:J:29:VAL:O	2:J:29:VAL:HG12	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:333:THR:O	1:A:334:ASN:C	2.64	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:57:PRO:HG2	1:B:271:GLN:CD	2.46	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
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
3:K:66:ARG:HH22	3:K:84:SER:C	2.29	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:A:697:MET:HE2	1:A:697:MET:HB3	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:272:PRO:C	1:B:273:ARG:HG2	2.45	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
5:O:19:THR:C	5:O:20:LEU:HD12	2.46	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
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:A:743:CYS:O	1:A:744:GLY:C	2.65	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:B:1066:THR:HG22	1:B:1067:TYR:N	2.36	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1008/1288 (78%)	952 (94%)	53 (5%)	3 (0%)	36	65
1	B	965/1288 (75%)	912 (94%)	51 (5%)	2 (0%)	43	71
1	C	1008/1288 (78%)	945 (94%)	57 (6%)	6 (1%)	21	52
2	H	107/109 (98%)	101 (94%)	4 (4%)	2 (2%)	6	28
2	J	107/109 (98%)	99 (92%)	6 (6%)	2 (2%)	6	28
3	I	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
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%)	31	60

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

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Mol	Chain	Res	Type
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%)	799 (98%)	12 (2%)	57	72
1	B	776/1113 (70%)	765 (99%)	11 (1%)	59	73
1	C	810/1113 (73%)	796 (98%)	14 (2%)	53	71
2	H	88/90 (98%)	88 (100%)	0	100	100
2	J	88/90 (98%)	87 (99%)	1 (1%)	65	76
3	I	89/94 (95%)	89 (100%)	0	100	100
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%)	105 (98%)	2 (2%)	50	68
5	O	107/108 (99%)	105 (98%)	2 (2%)	50	68
All	All	3147/4105 (77%)	3105 (99%)	42 (1%)	59	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	197	ILE
1	A	333	THR
1	A	335	LEU
1	A	434	ILE
1	A	480	CYS
1	A	488	CYS
1	A	530	SER
1	A	538	CYS

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Mol	Chain	Res	Type
1	A	617	CYS
1	A	860	VAL
1	A	861	LEU
1	B	131	CYS
1	B	166	CYS
1	B	331	ASN
1	B	398	ASP
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	C	131	CYS
1	C	166	CYS
1	C	227	VAL
1	C	228	ASP
1	C	229	LEU
1	C	327	VAL
1	C	328	ARG
1	C	336	CYS
1	C	538	CYS
1	C	617	CYS
1	C	756	TYR
1	C	858	LEU
1	C	860	VAL
1	C	861	LEU
2	J	53	THR
5	M	69	LEU
5	M	88	ASP
5	O	16	GLN
5	O	80	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) 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

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Mol	Chain	Res	Type
1	A	477	ASN
1	A	505	HIS
1	A	536	ASN
1	A	603	ASN
1	A	657	ASN
1	A	709	ASN
1	A	801	ASN
1	A	955	ASN
1	A	1098	ASN
1	A	1134	ASN
1	B	234	ASN
1	B	282	ASN
1	B	388	ASN
1	B	394	ASN
1	B	405	ASN
1	B	437	ASN
1	B	506	GLN
1	B	536	ASN
1	B	801	ASN
1	B	957	GLN
1	B	960	ASN
1	B	1005	GLN
1	B	1074	ASN
1	B	1098	ASN
1	B	1134	ASN
1	C	165	ASN
1	C	234	ASN
1	C	282	ASN
1	C	439	ASN
1	C	450	ASN
1	C	505	HIS
1	C	536	ASN
1	C	544	ASN
1	C	657	ASN
1	C	751	ASN
1	C	801	ASN
1	C	1098	ASN
1	C	1134	ASN
2	H	90	GLN
2	H	102	GLN
3	I	13	GLN
3	I	81	GLN

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Mol	Chain	Res	Type
3	I	110	GLN
2	J	42	GLN
2	J	92	ASN
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	38	HIS
4	L	50	HIS
5	M	79	GLN
5	M	104	HIS
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 [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](#)

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	1310	-	14,14,15	0.32	0	17,19,21	0.61	0
6	NAG	B	1302	-	14,14,15	0.26	0	17,19,21	0.54	0
6	NAG	C	1312	-	14,14,15	0.38	0	17,19,21	0.50	0
6	NAG	B	1306	-	14,14,15	0.37	0	17,19,21	0.54	0
6	NAG	C	1303	-	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	C	1304	-	14,14,15	0.27	0	17,19,21	0.61	0
6	NAG	C	1311	-	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	C	1305	-	14,14,15	0.24	0	17,19,21	0.46	0
6	NAG	A	1309	-	14,14,15	0.50	0	17,19,21	0.58	0
6	NAG	A	1310	-	14,14,15	0.27	0	17,19,21	0.72	0
6	NAG	B	1308	-	14,14,15	0.45	0	17,19,21	0.49	0
6	NAG	B	1307	-	14,14,15	0.51	0	17,19,21	0.65	0
6	NAG	A	1308	-	14,14,15	0.59	0	17,19,21	0.62	0
6	NAG	B	1301	-	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	A	1306	-	14,14,15	0.30	0	17,19,21	0.73	0
6	NAG	A	1305	-	14,14,15	0.28	0	17,19,21	0.49	0
6	NAG	A	1302	-	14,14,15	0.27	0	17,19,21	0.42	0
6	NAG	B	1311	-	14,14,15	0.33	0	17,19,21	0.64	0
6	NAG	C	1313	-	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	C	1310	-	14,14,15	0.41	0	17,19,21	0.47	0
6	NAG	B	1309	-	14,14,15	0.36	0	17,19,21	0.52	0
6	NAG	B	1304	-	14,14,15	0.22	0	17,19,21	0.53	0
6	NAG	B	1312	-	14,14,15	0.39	0	17,19,21	0.49	0
6	NAG	C	1302	-	14,14,15	0.54	0	17,19,21	1.01	1 (5%)
6	NAG	A	1307	-	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	B	1305	-	14,14,15	0.24	0	17,19,21	0.49	0
6	NAG	A	1304	-	14,14,15	0.58	1 (7%)	17,19,21	0.58	0
6	NAG	C	1306	-	14,14,15	0.62	1 (7%)	17,19,21	0.58	0
6	NAG	C	1309	-	14,14,15	0.42	0	17,19,21	0.65	0
6	NAG	A	1301	-	14,14,15	0.33	0	17,19,21	0.55	0
6	NAG	A	1311	-	14,14,15	0.47	0	17,19,21	0.65	0
6	NAG	C	1307	-	14,14,15	0.35	0	17,19,21	0.57	0
6	NAG	C	1308	-	14,14,15	0.28	0	17,19,21	0.55	0
6	NAG	A	1312	-	14,14,15	0.41	0	17,19,21	0.45	0
6	NAG	B	1303	-	14,14,15	0.32	0	17,19,21	0.46	0
6	NAG	A	1303	-	14,14,15	0.31	0	17,19,21	0.47	0
6	NAG	C	1301	-	14,14,15	0.59	0	17,19,21	0.57	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	1310	-	-	1/6/23/26	0/1/1/1
6	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1312	-	-	4/6/23/26	0/1/1/1
6	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1311	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1309	-	-	1/6/23/26	0/1/1/1
6	NAG	A	1310	-	-	3/6/23/26	0/1/1/1
6	NAG	B	1308	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1308	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1306	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1305	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1302	-	-	3/6/23/26	0/1/1/1
6	NAG	B	1311	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1313	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1310	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1309	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1312	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1307	-	-	3/6/23/26	0/1/1/1
6	NAG	B	1305	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1304	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1309	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1311	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1307	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1312	-	-	3/6/23/26	0/1/1/1
6	NAG	B	1303	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1303	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	-	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1306	NAG	O5-C1	-2.09	1.40	1.43
6	A	1304	NAG	O5-C1	-2.01	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	3.22	127.22	122.90

There are no chirality outliers.

All (76) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
6	C	1305	NAG	O5-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	1303	NAG	C4-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	A	1312	NAG	O5-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6
6	A	1308	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	A	1308	NAG	C4-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	C	1313	NAG	O5-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
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	B	1312	NAG	O5-C5-C6-O6
6	C	1310	NAG	O5-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	C	1309	NAG	C3-C2-N2-C7
6	C	1312	NAG	C3-C2-N2-C7
6	A	1309	NAG	O5-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	B	1307	NAG	C4-C5-C6-O6
6	C	1309	NAG	C1-C2-N2-C7
6	C	1312	NAG	C1-C2-N2-C7
6	C	1312	NAG	C4-C5-C6-O6
6	A	1312	NAG	C4-C5-C6-O6
6	A	1310	NAG	C3-C2-N2-C7
6	B	1303	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
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	A	1302	NAG	C1-C2-N2-C7
6	A	1307	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 66 short contacts:

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

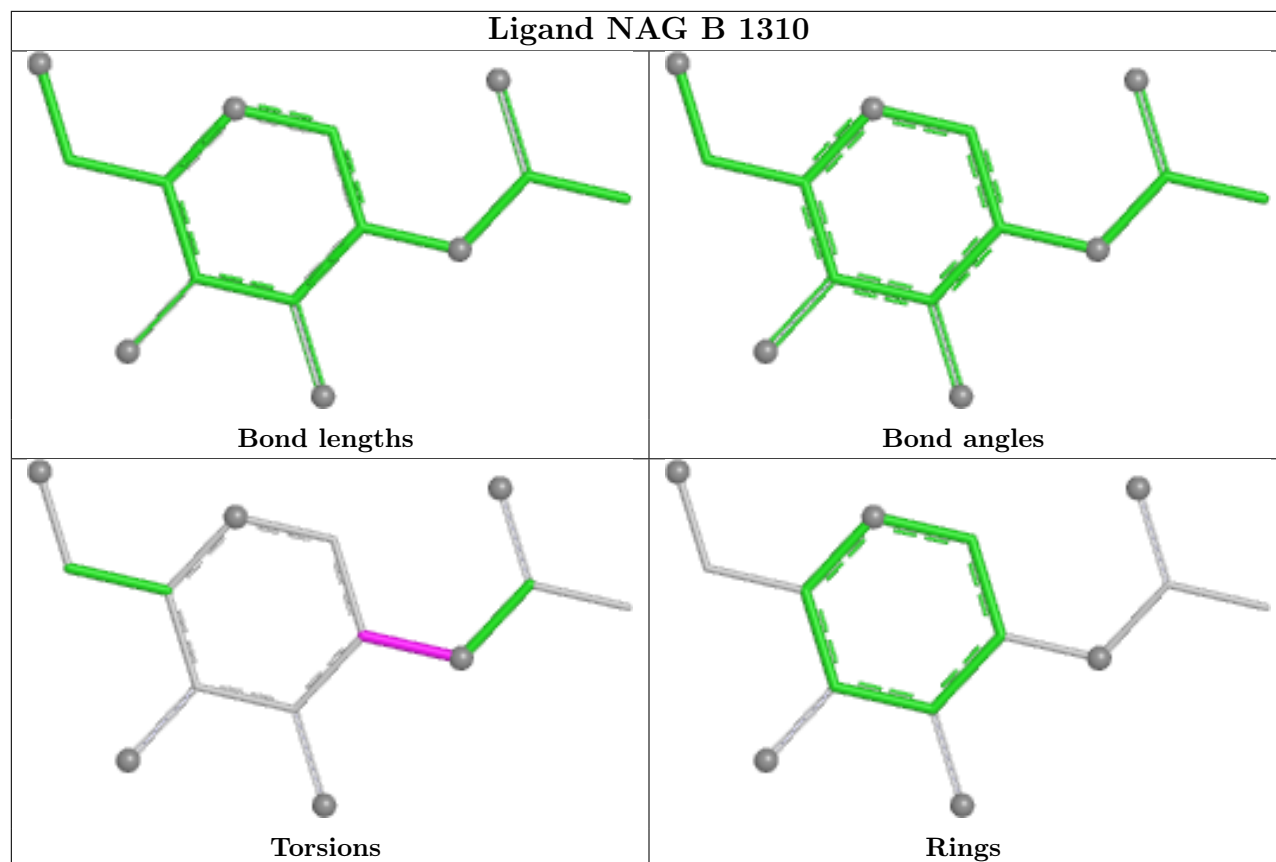
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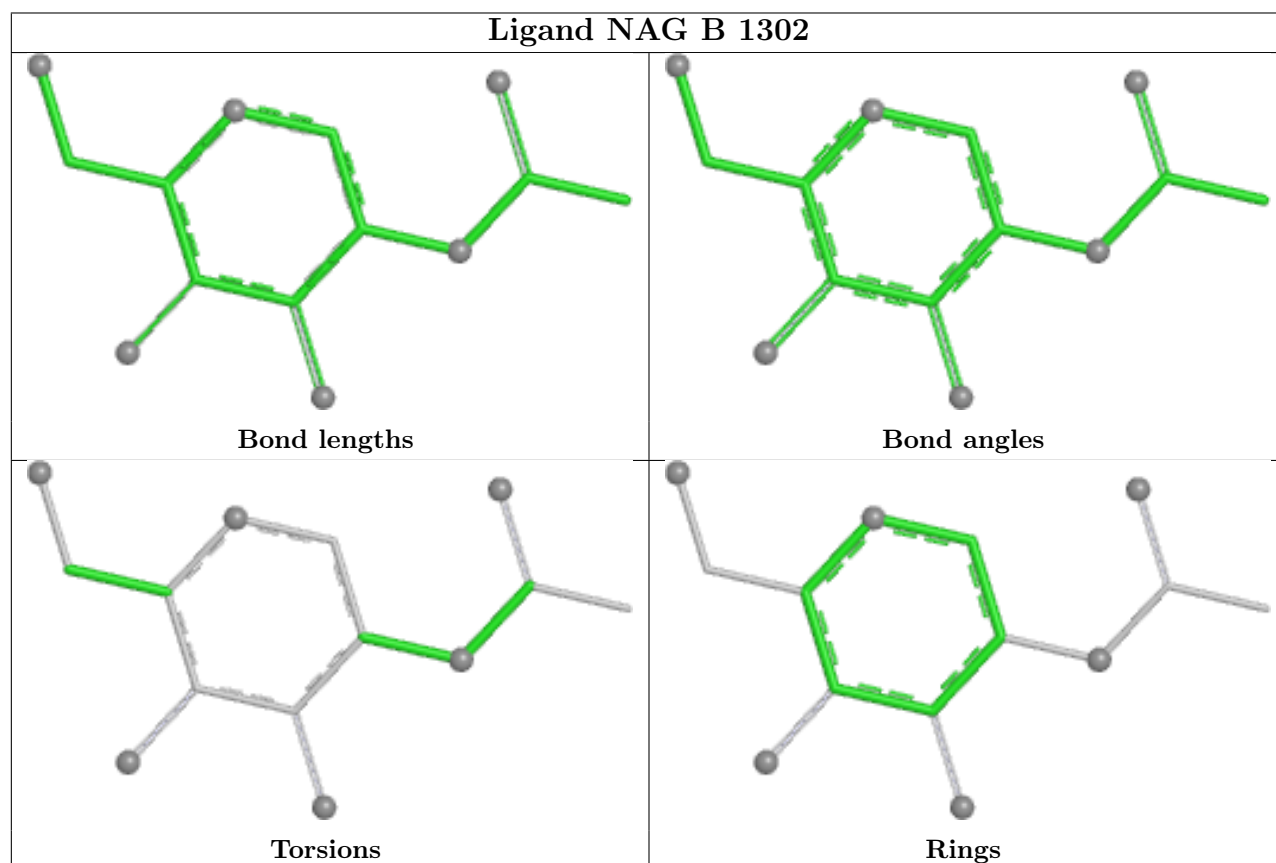
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1306	NAG	1	0
6	C	1309	NAG	3	0
6	A	1301	NAG	2	0
6	A	1311	NAG	4	0
6	C	1307	NAG	3	0
6	C	1308	NAG	1	0
6	A	1312	NAG	2	0
6	B	1303	NAG	4	0
6	A	1303	NAG	1	0
6	C	1301	NAG	3	0

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.

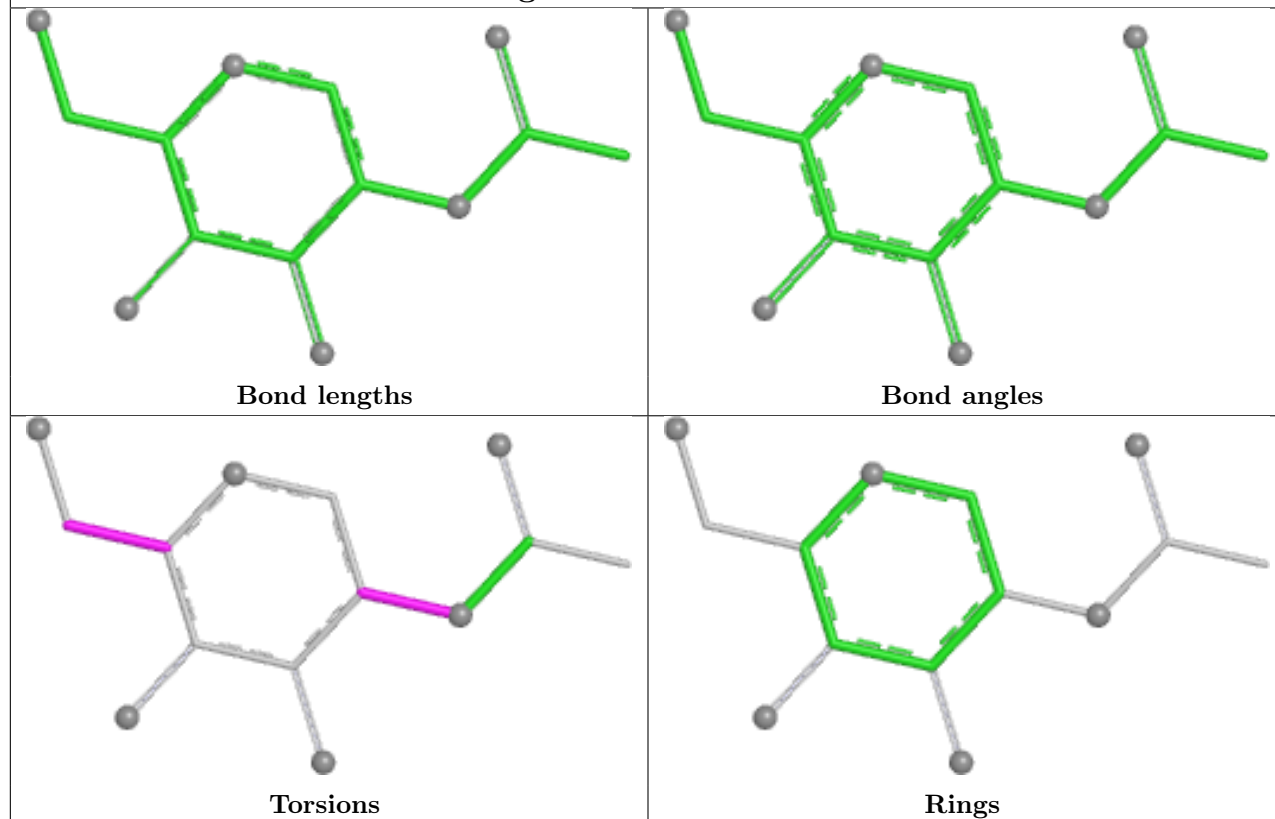
Ligand NAG B 1310



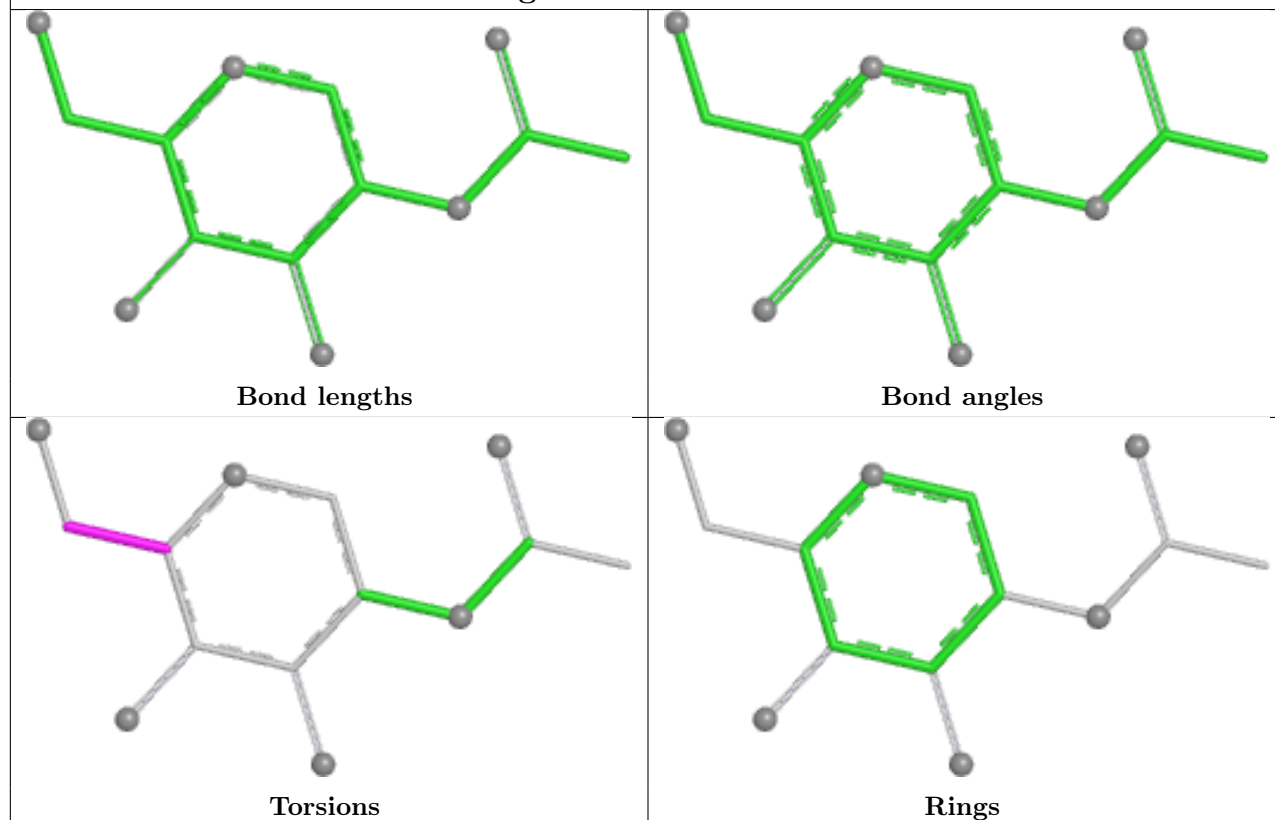
Ligand NAG B 1302

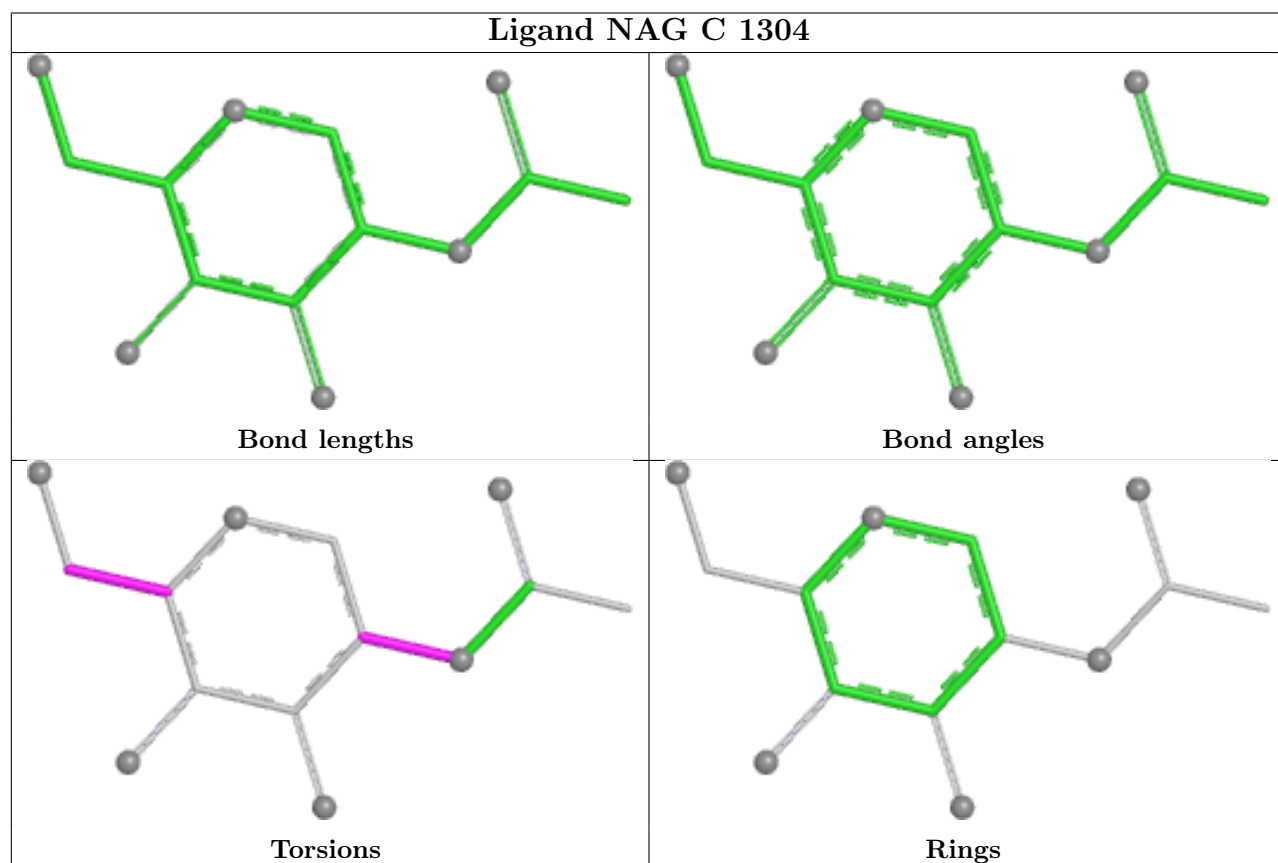
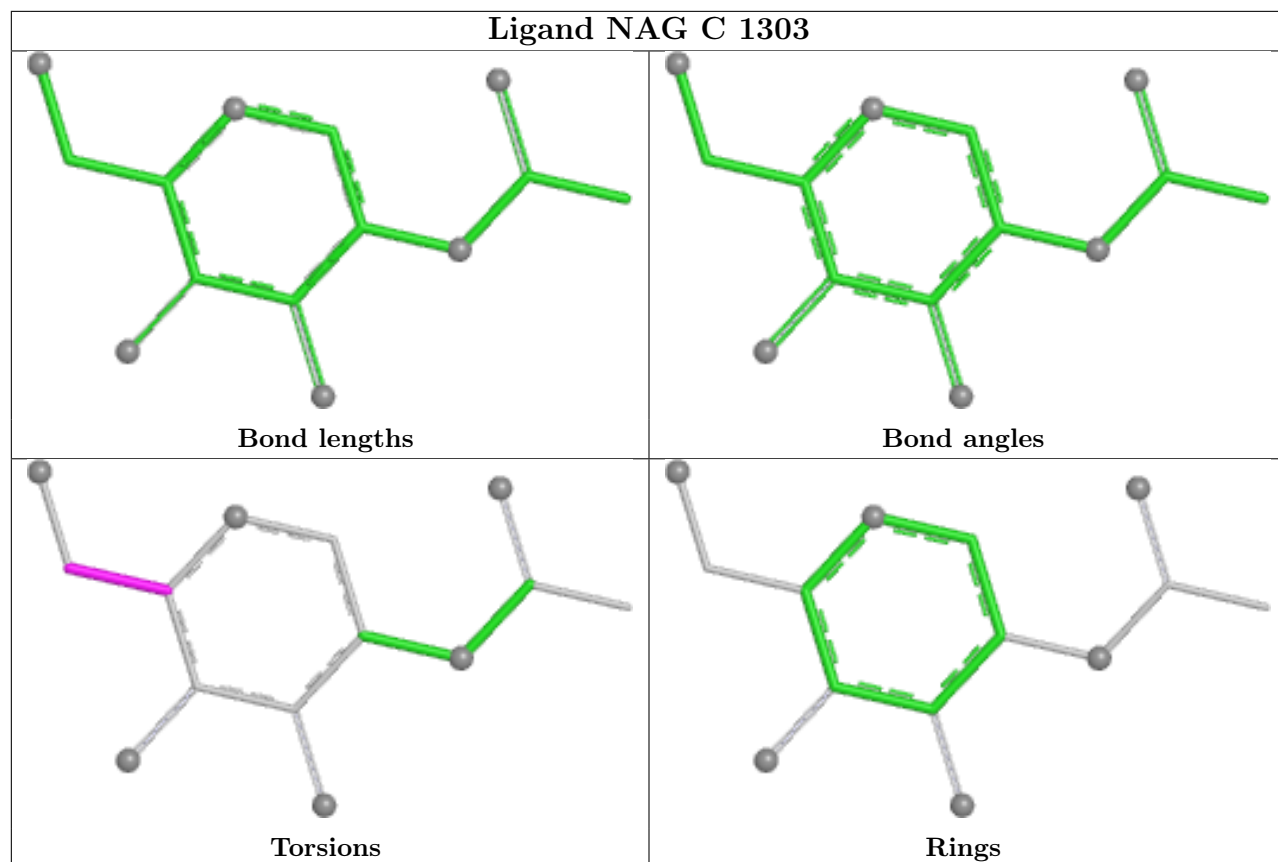


Ligand NAG C 1312

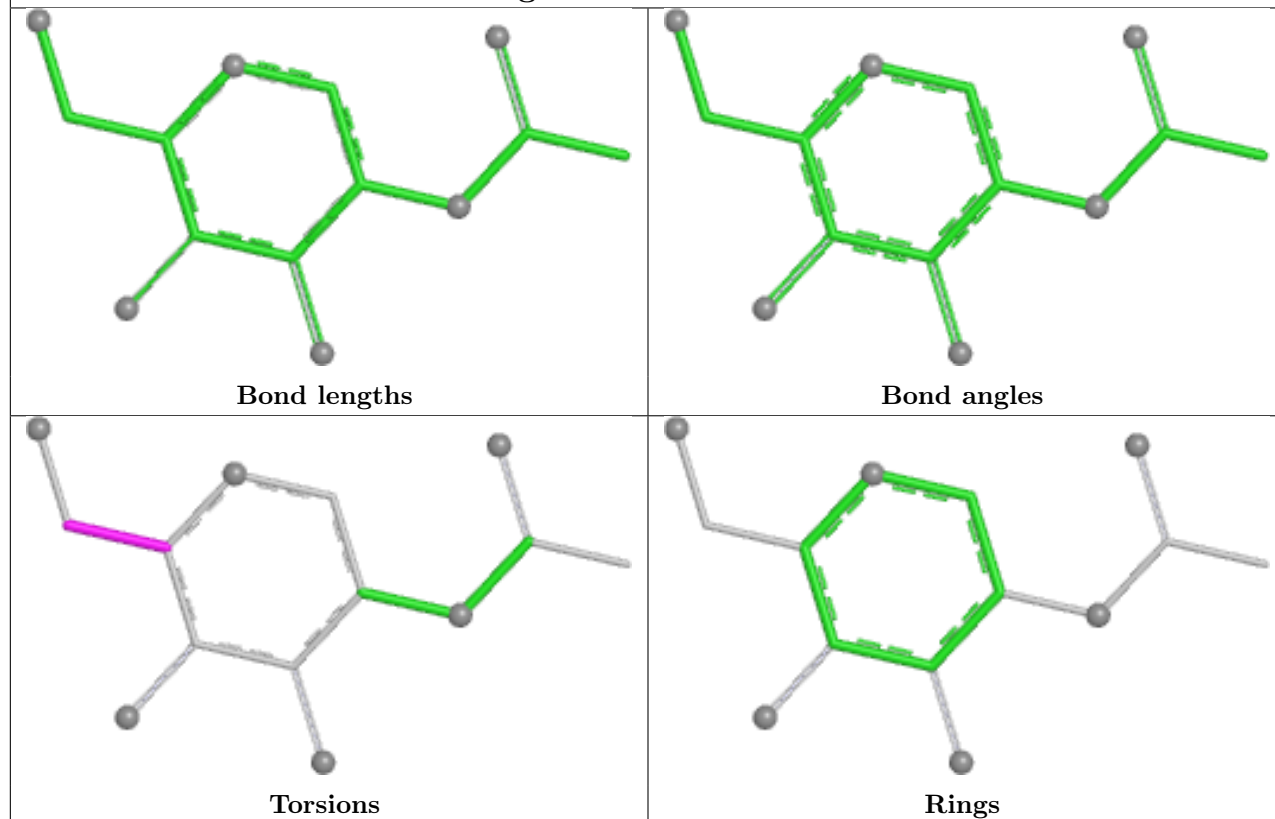


Ligand NAG B 1306

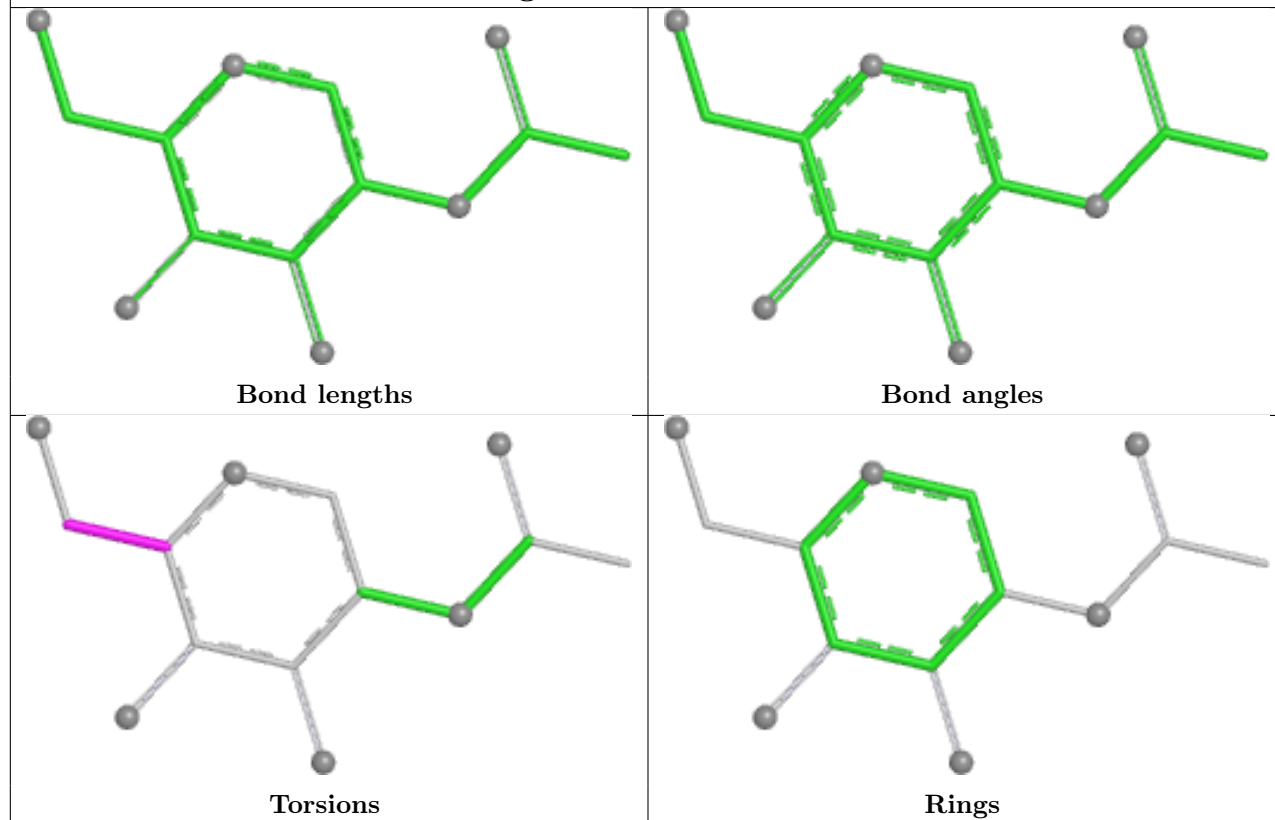


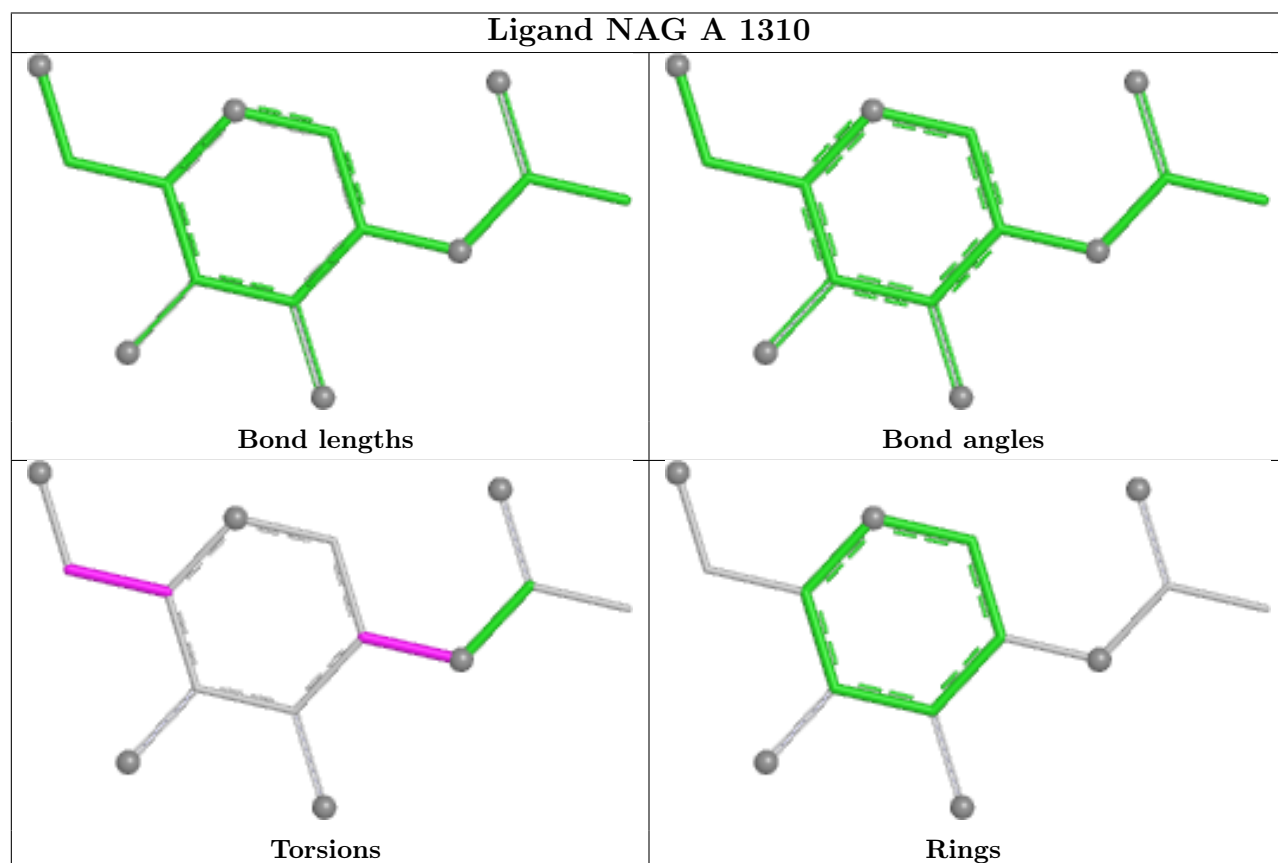
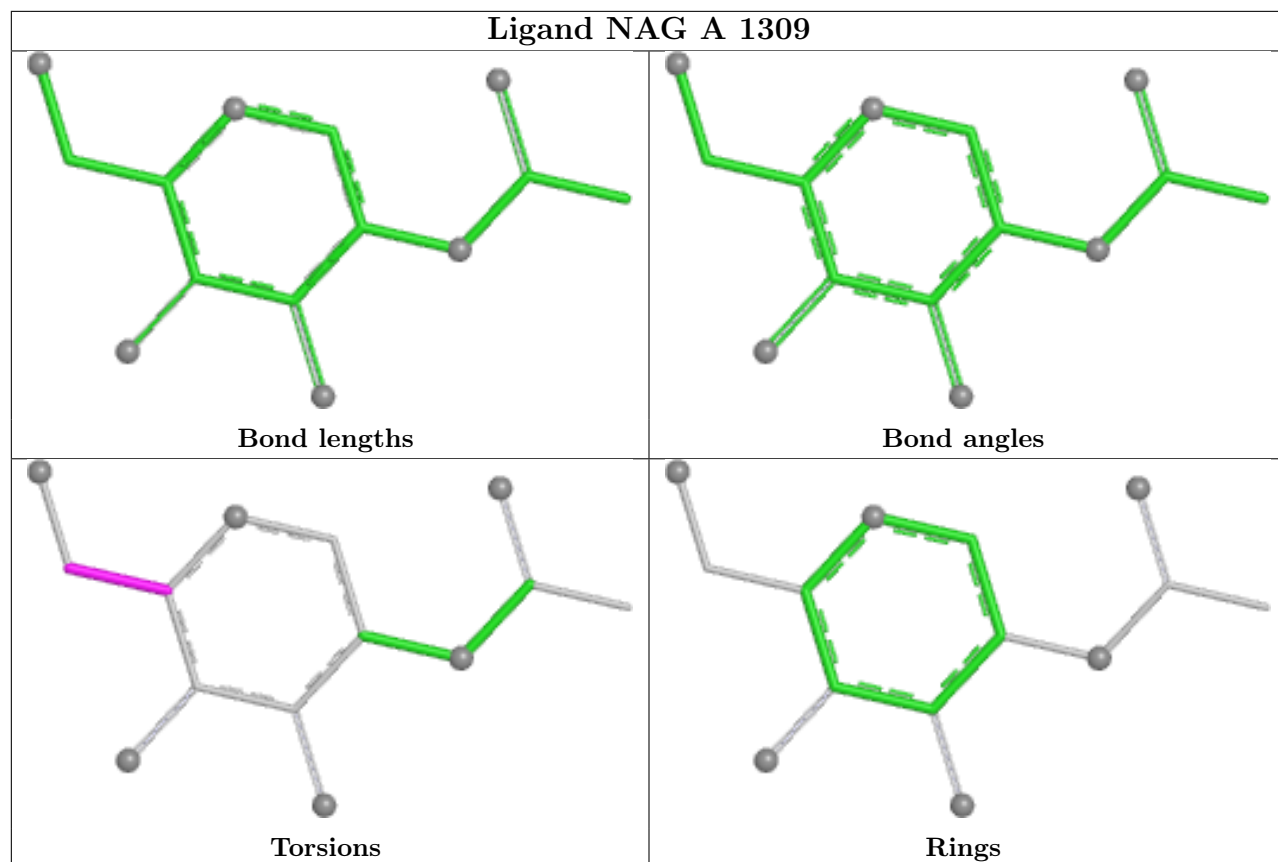


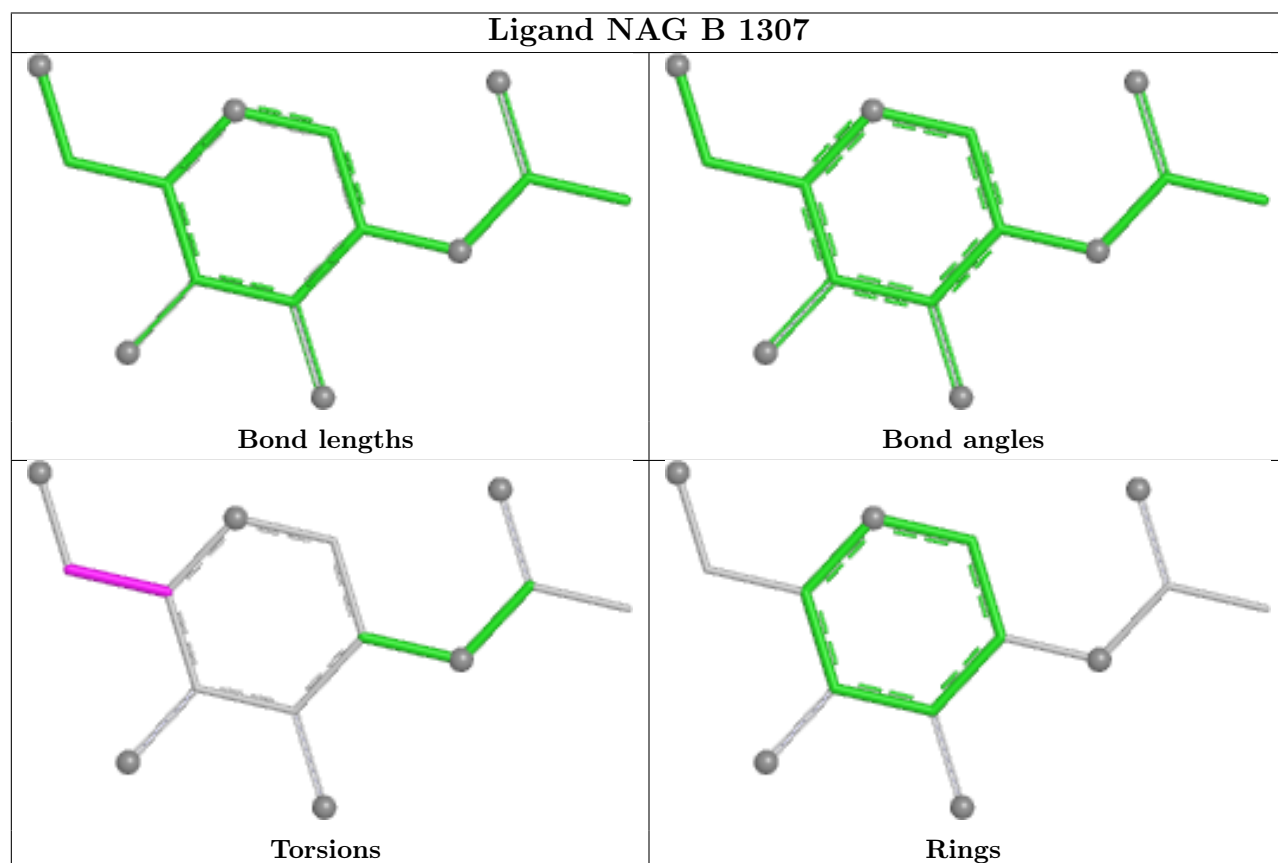
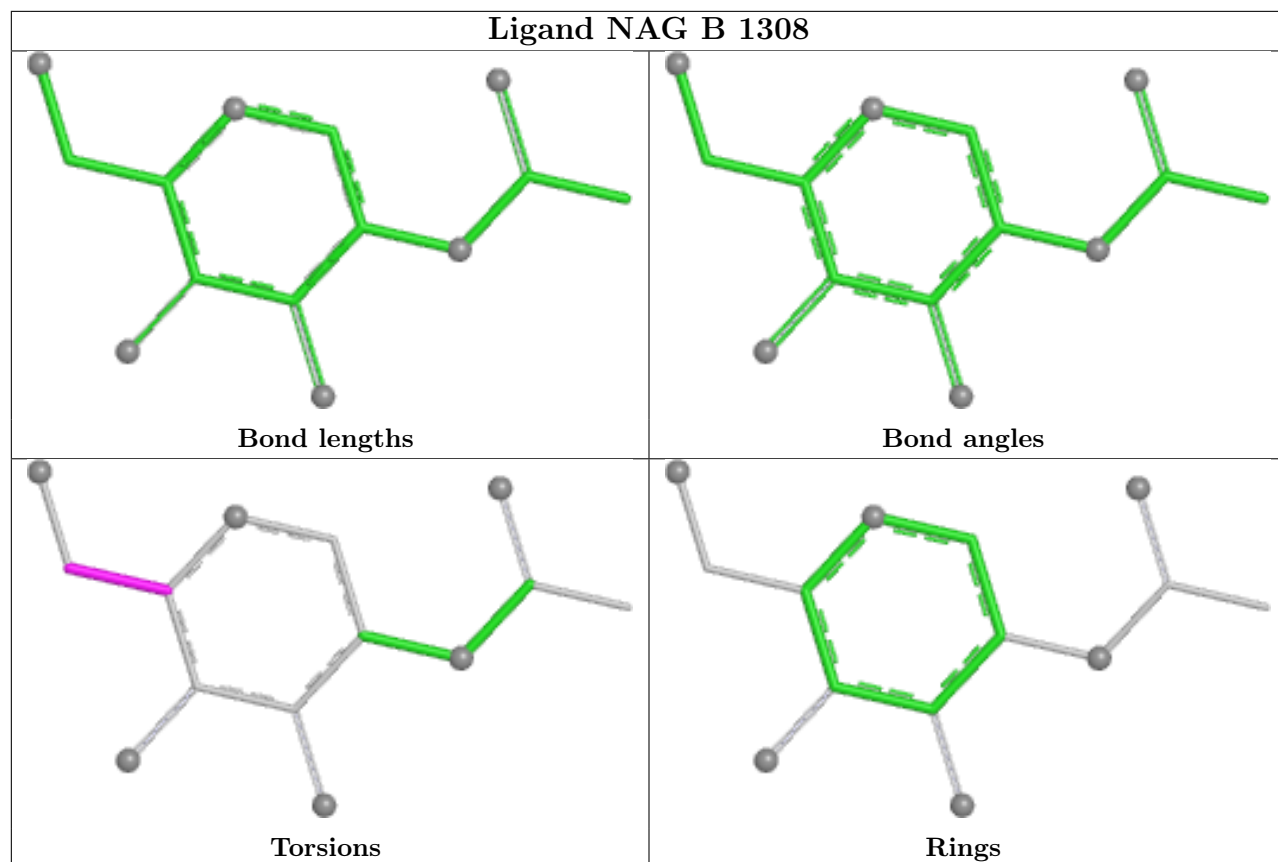
Ligand NAG C 1311



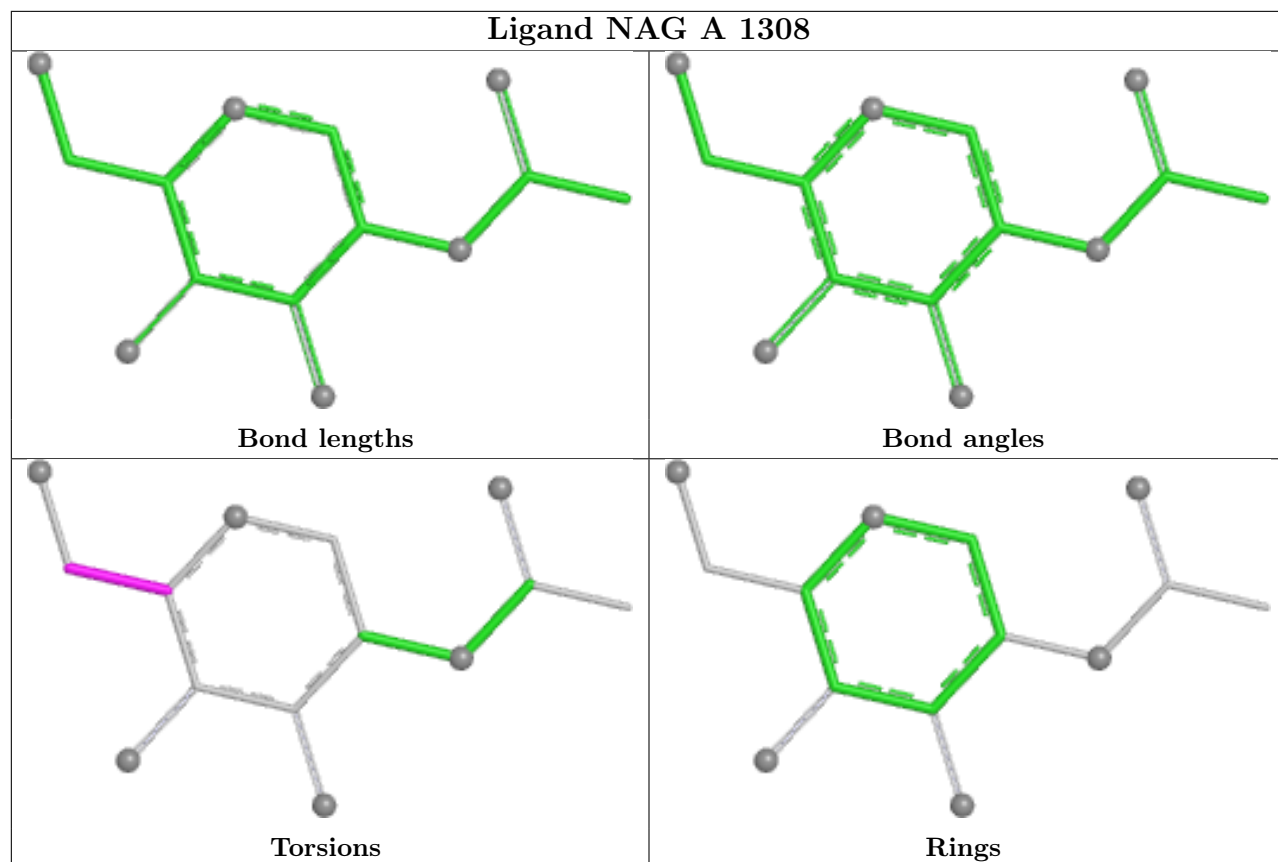
Ligand NAG C 1305



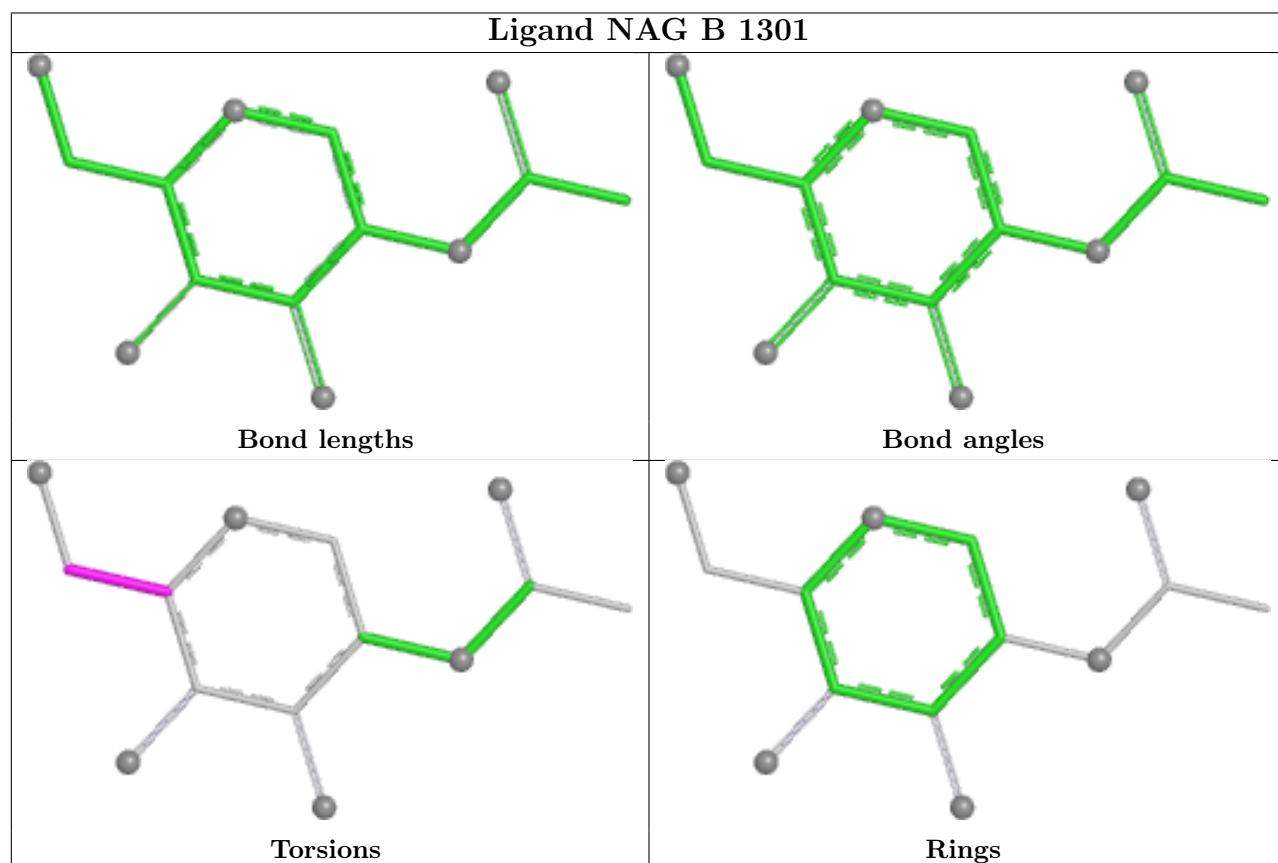


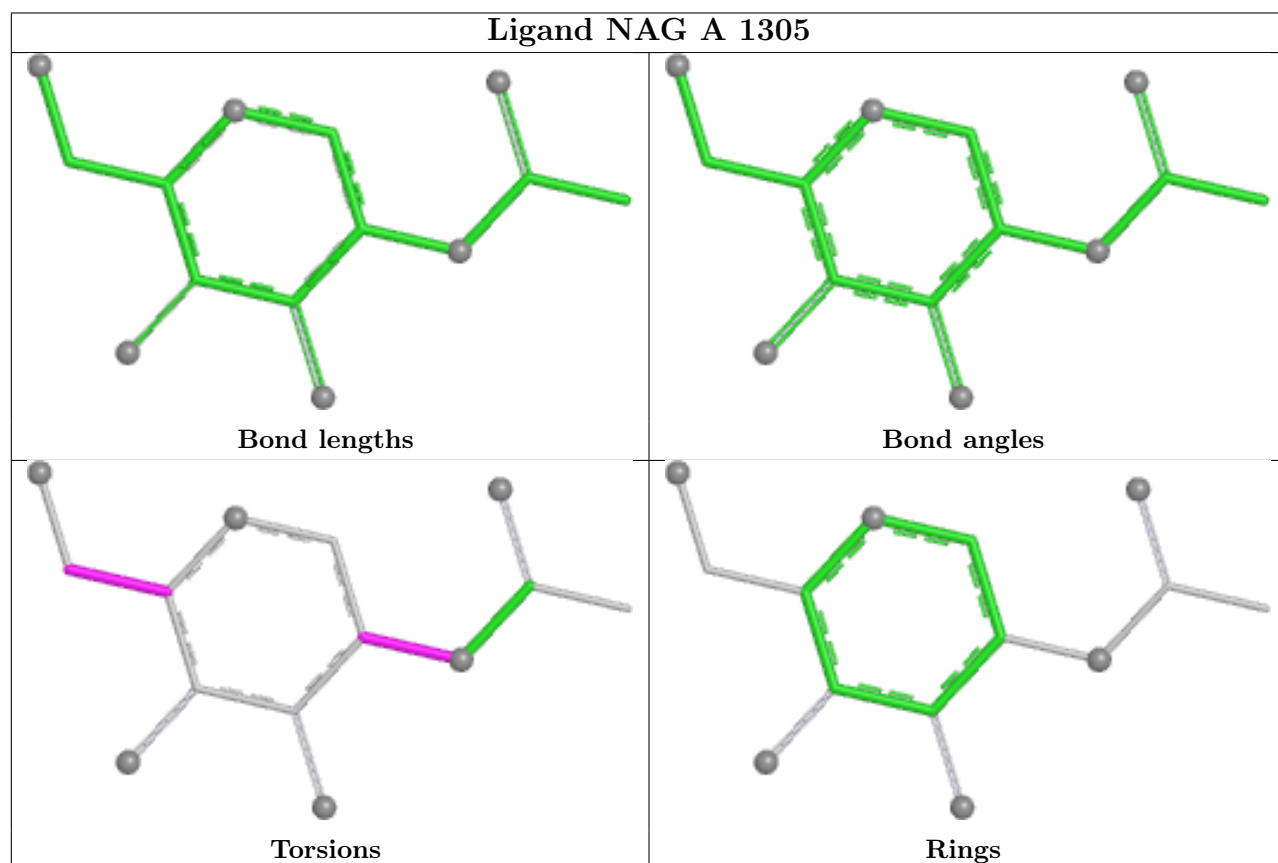
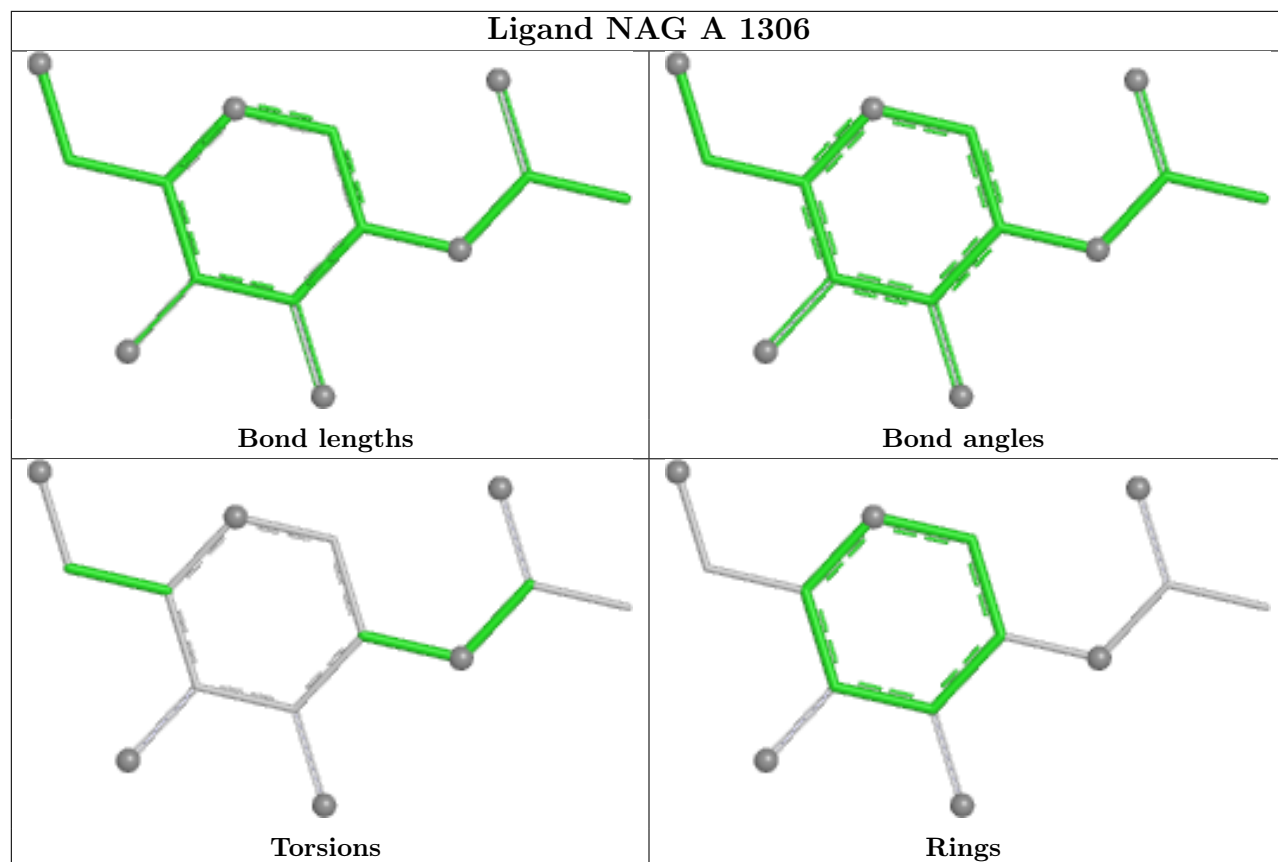


Ligand NAG A 1308

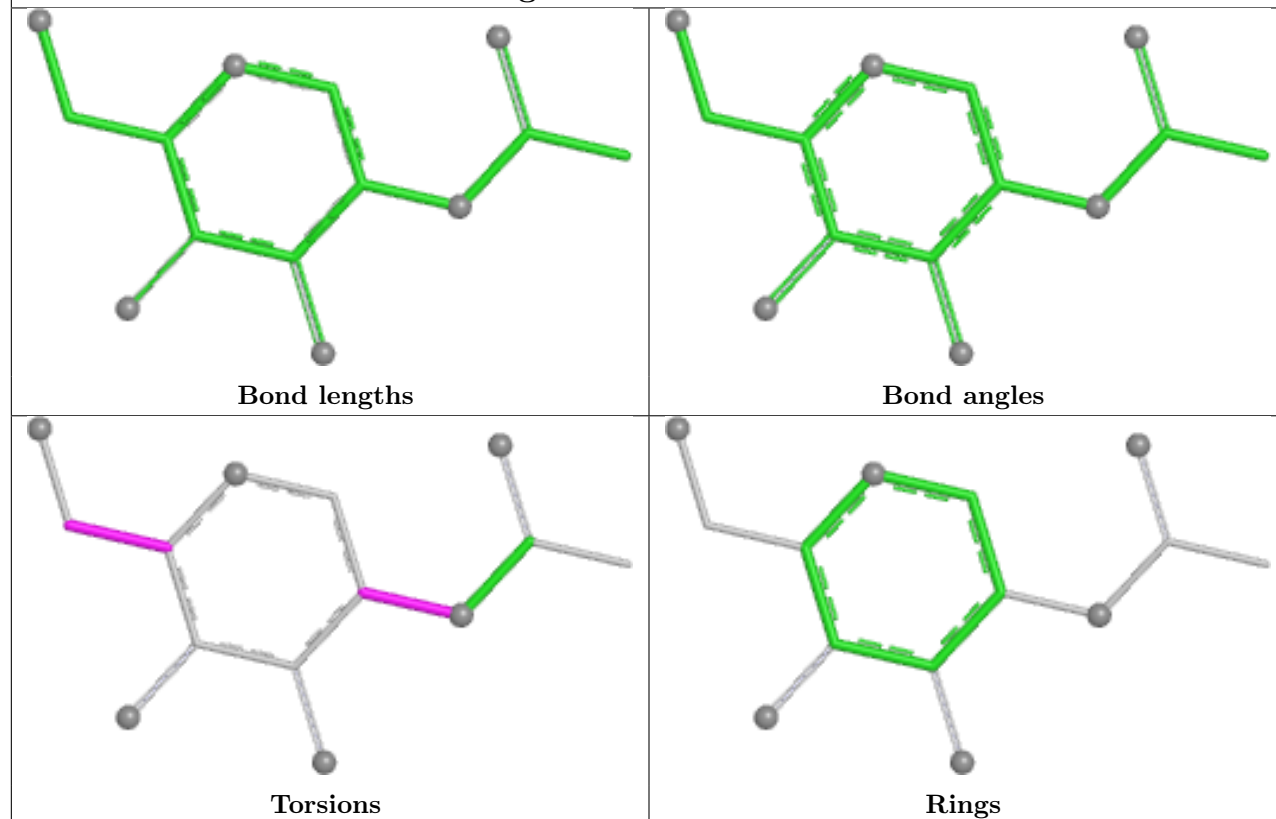


Ligand NAG B 1301

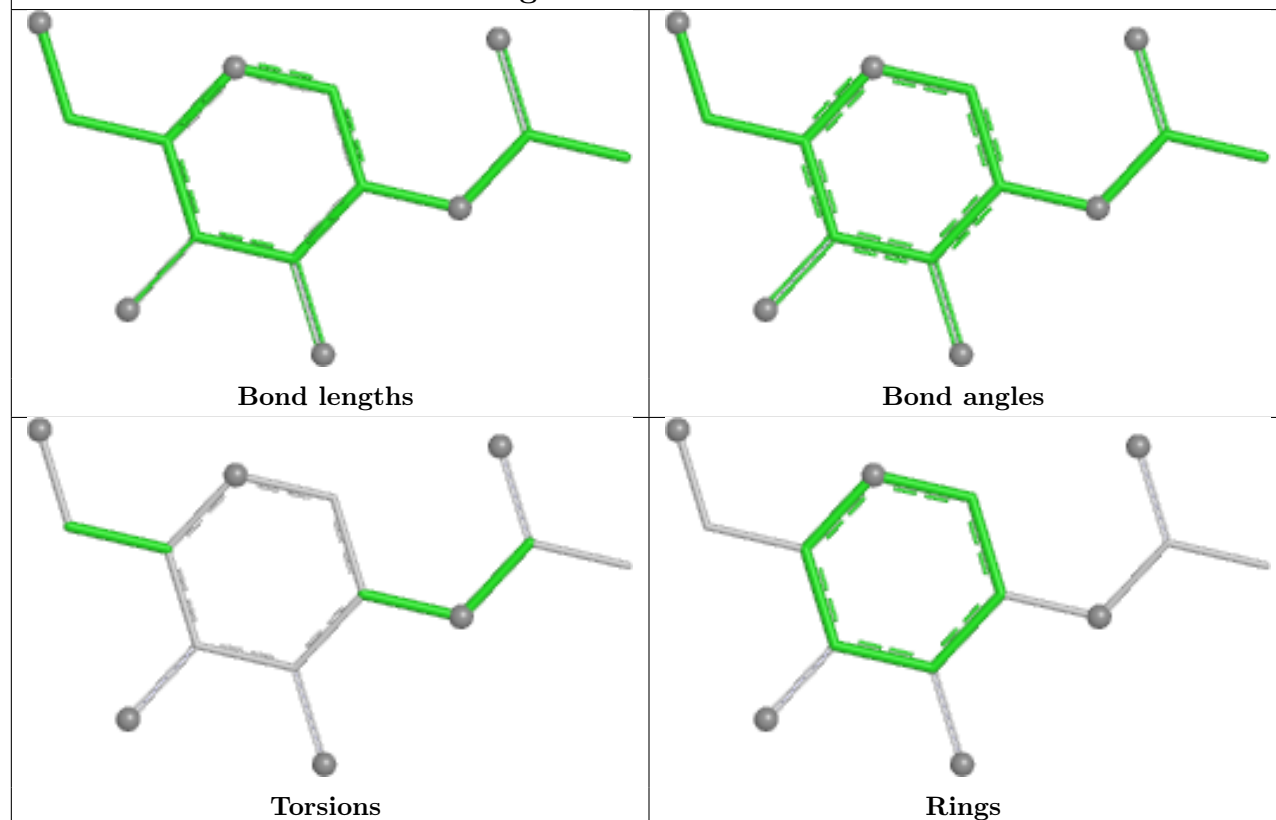


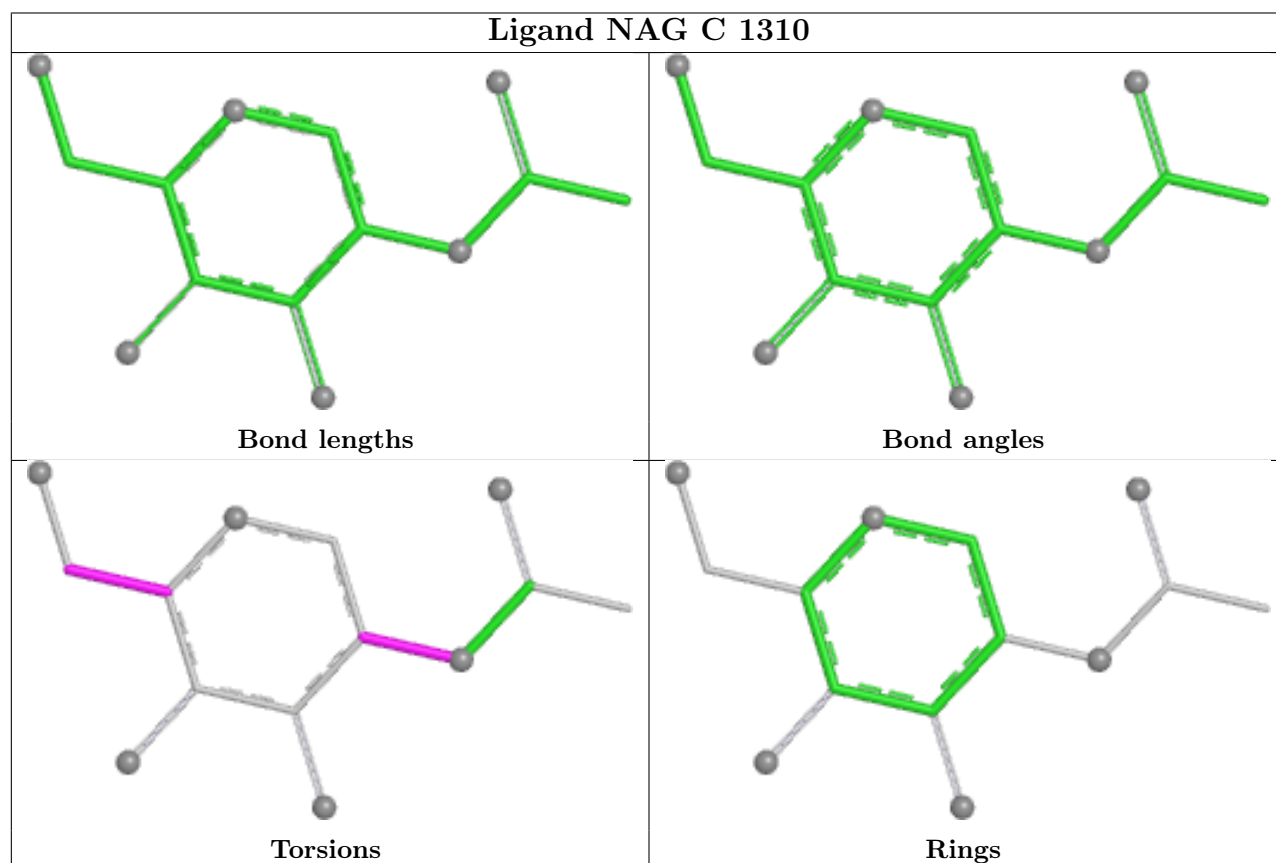
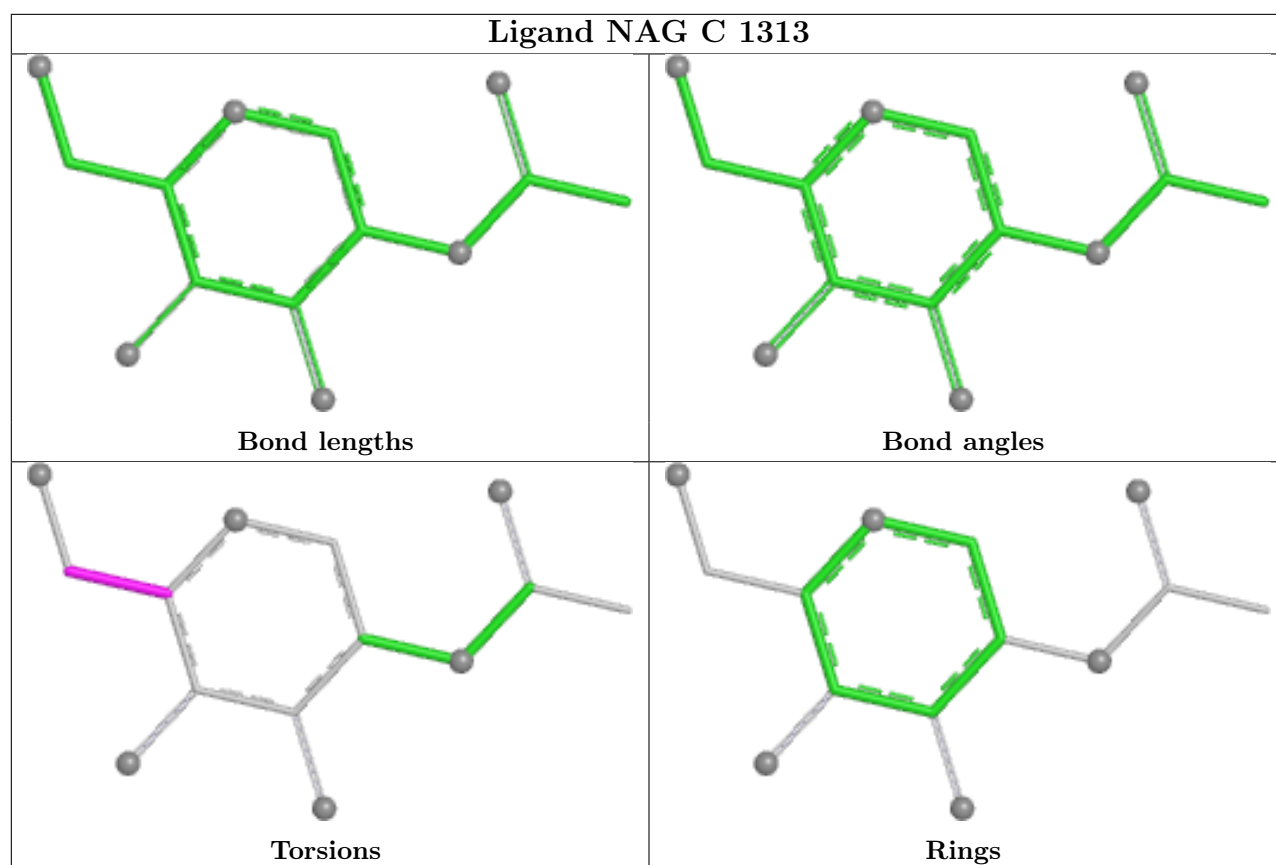


Ligand NAG A 1302

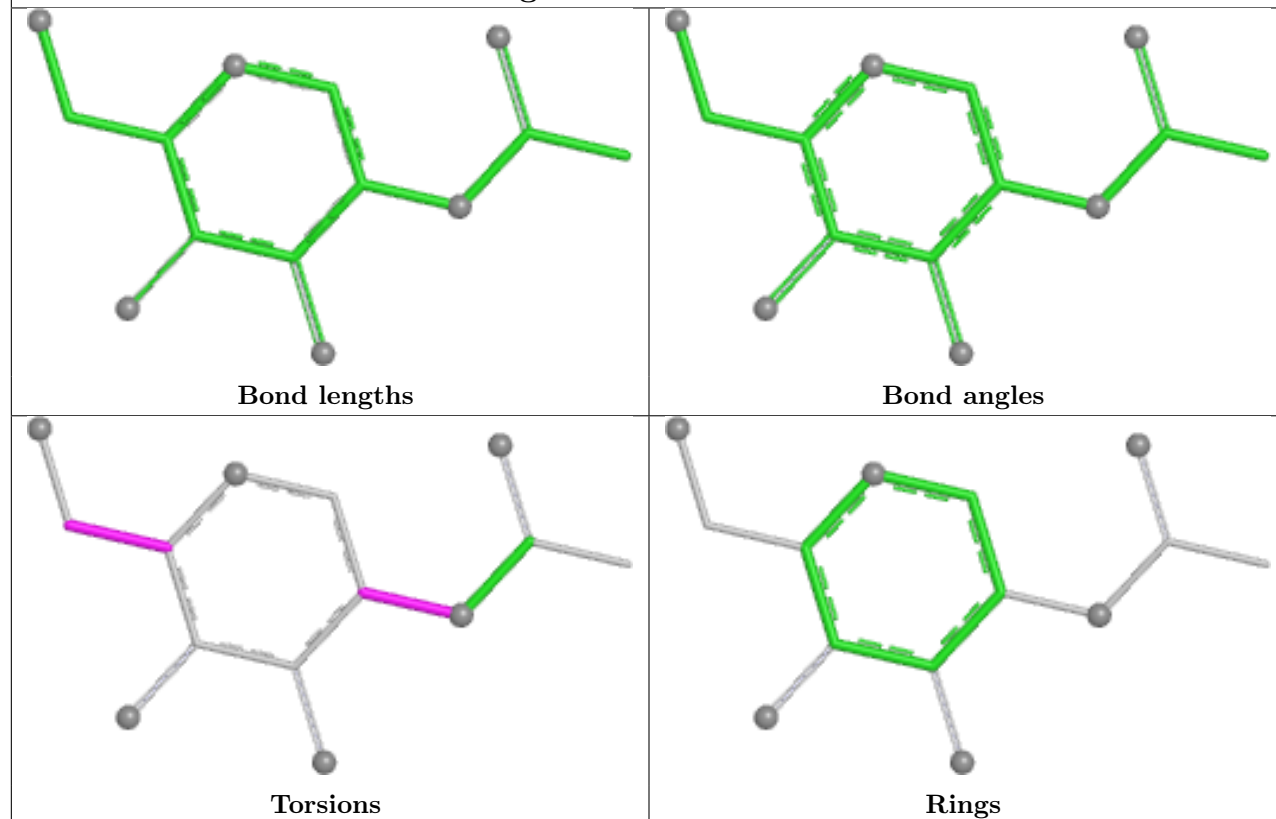


Ligand NAG B 1311

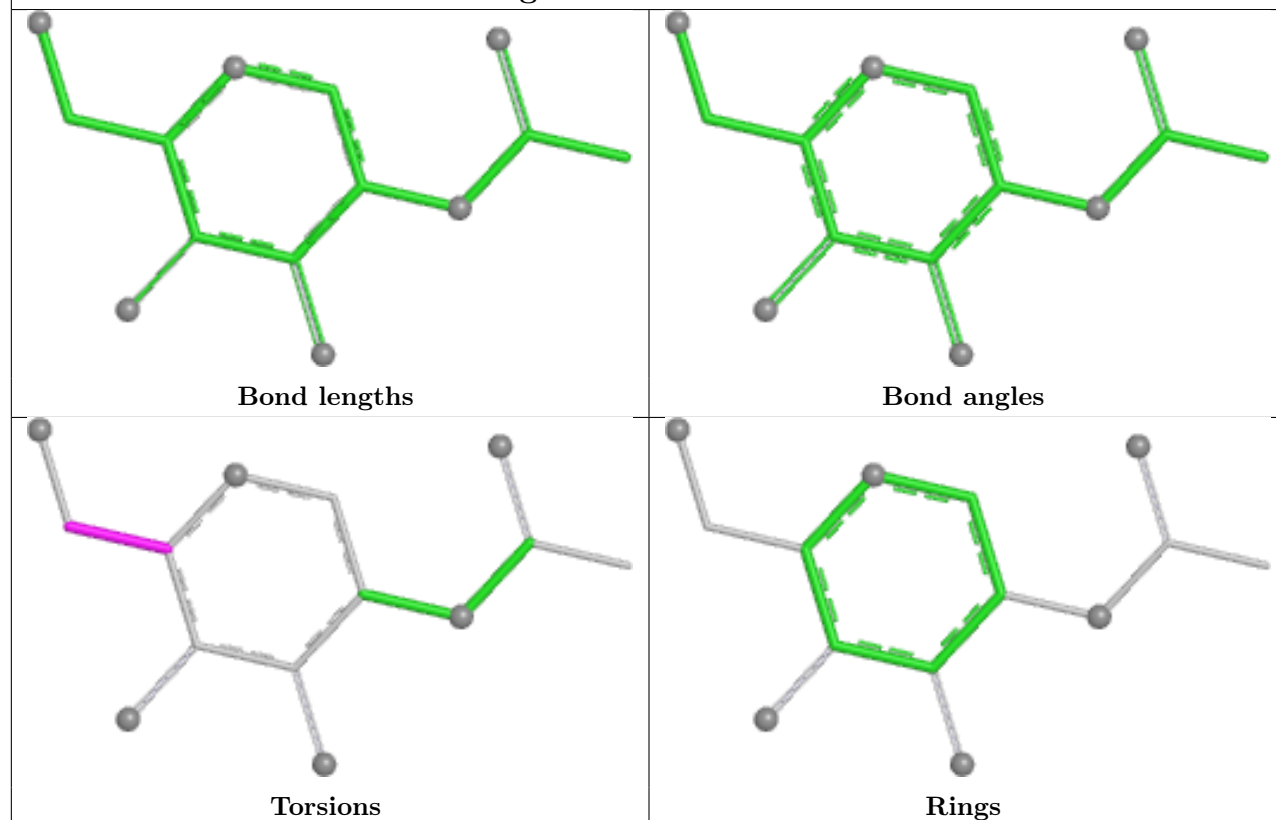




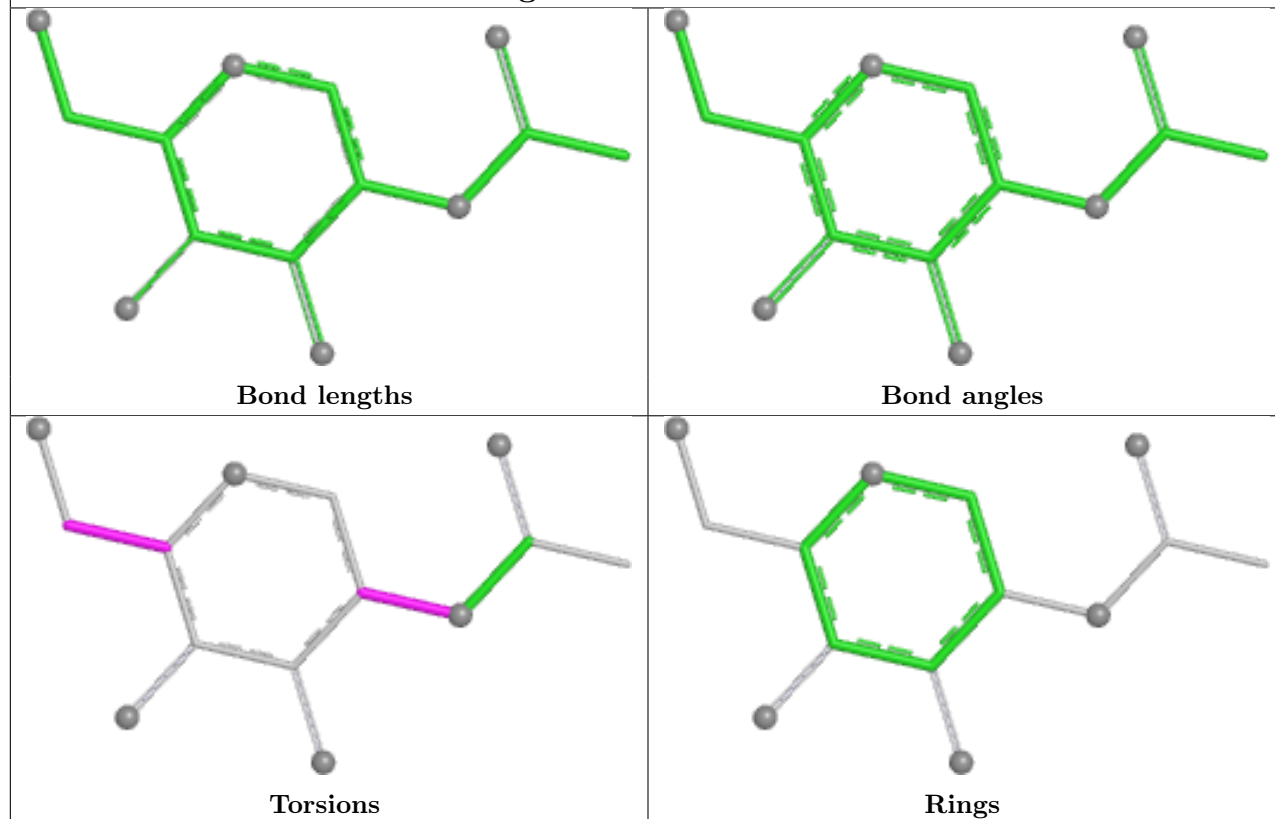
Ligand NAG B 1309



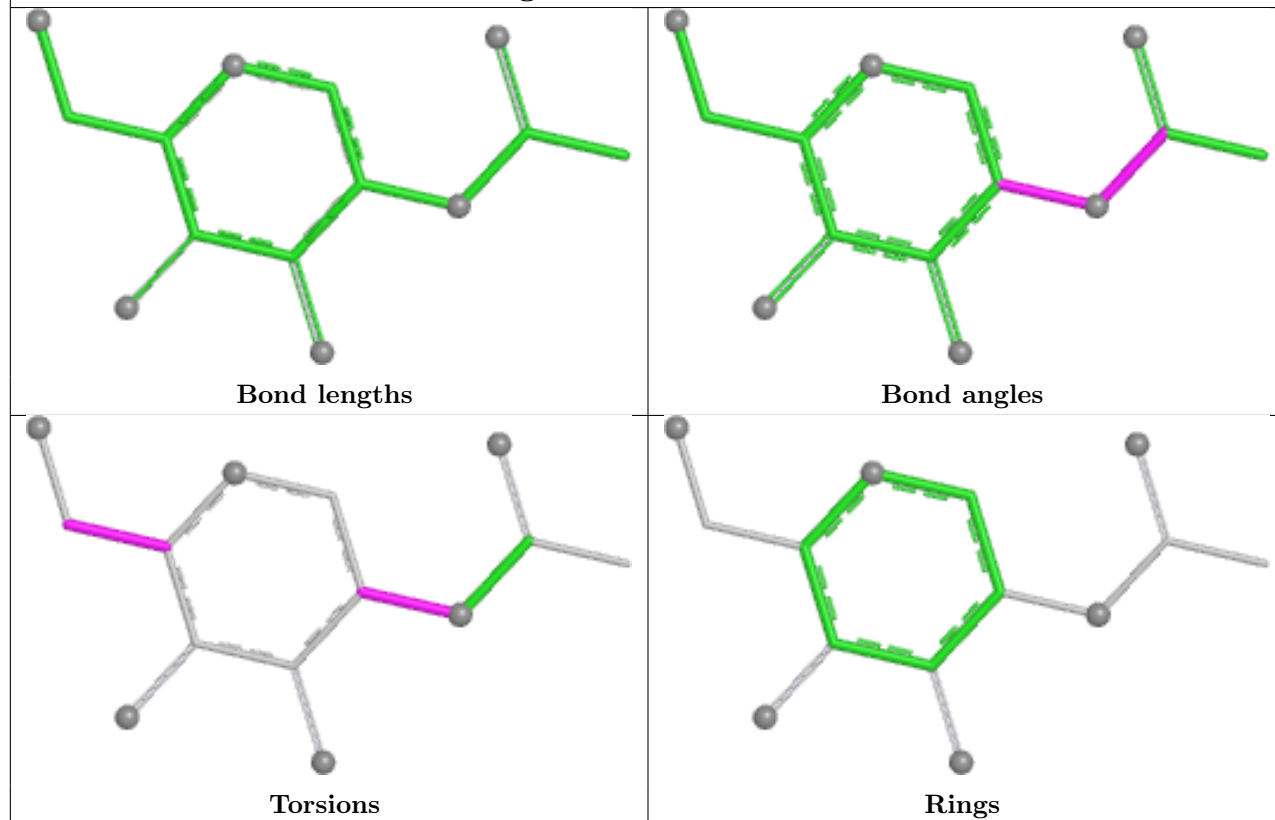
Ligand NAG B 1304



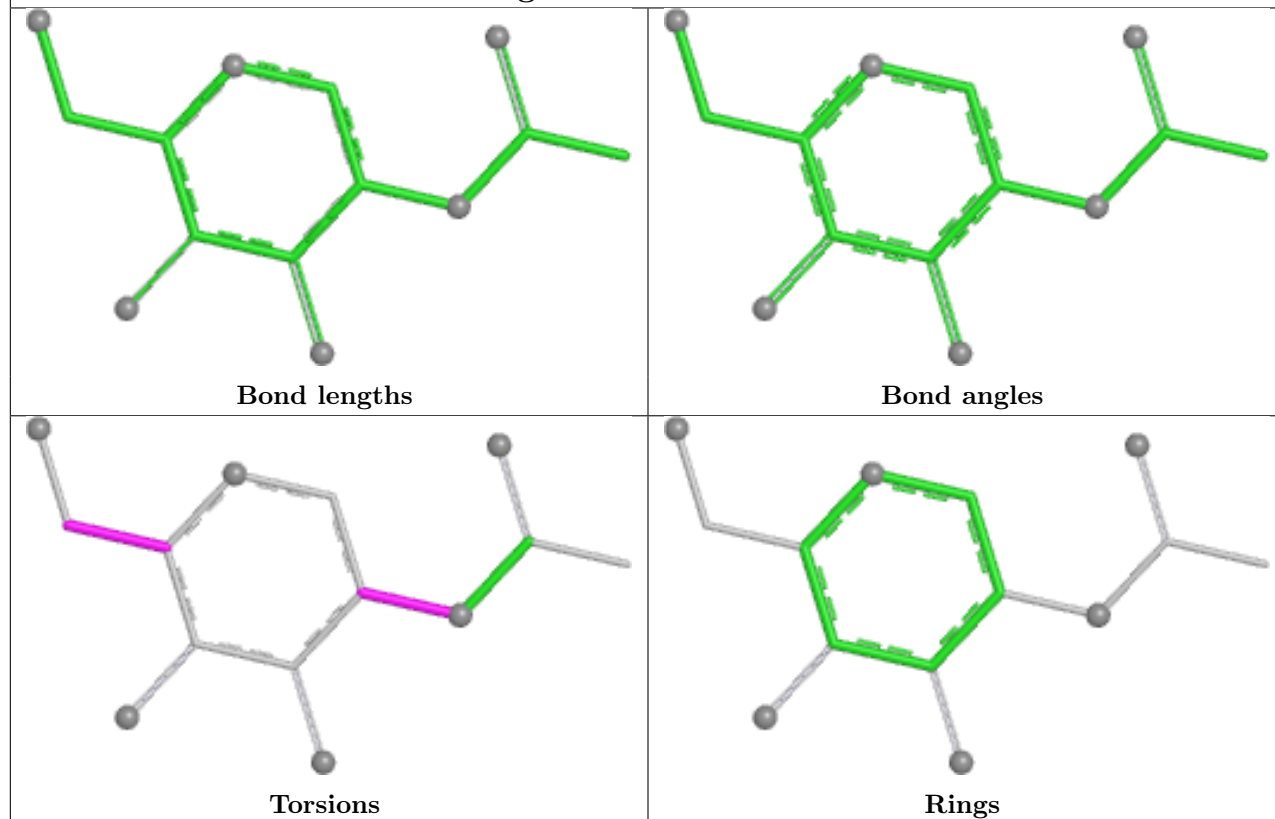
Ligand NAG B 1312



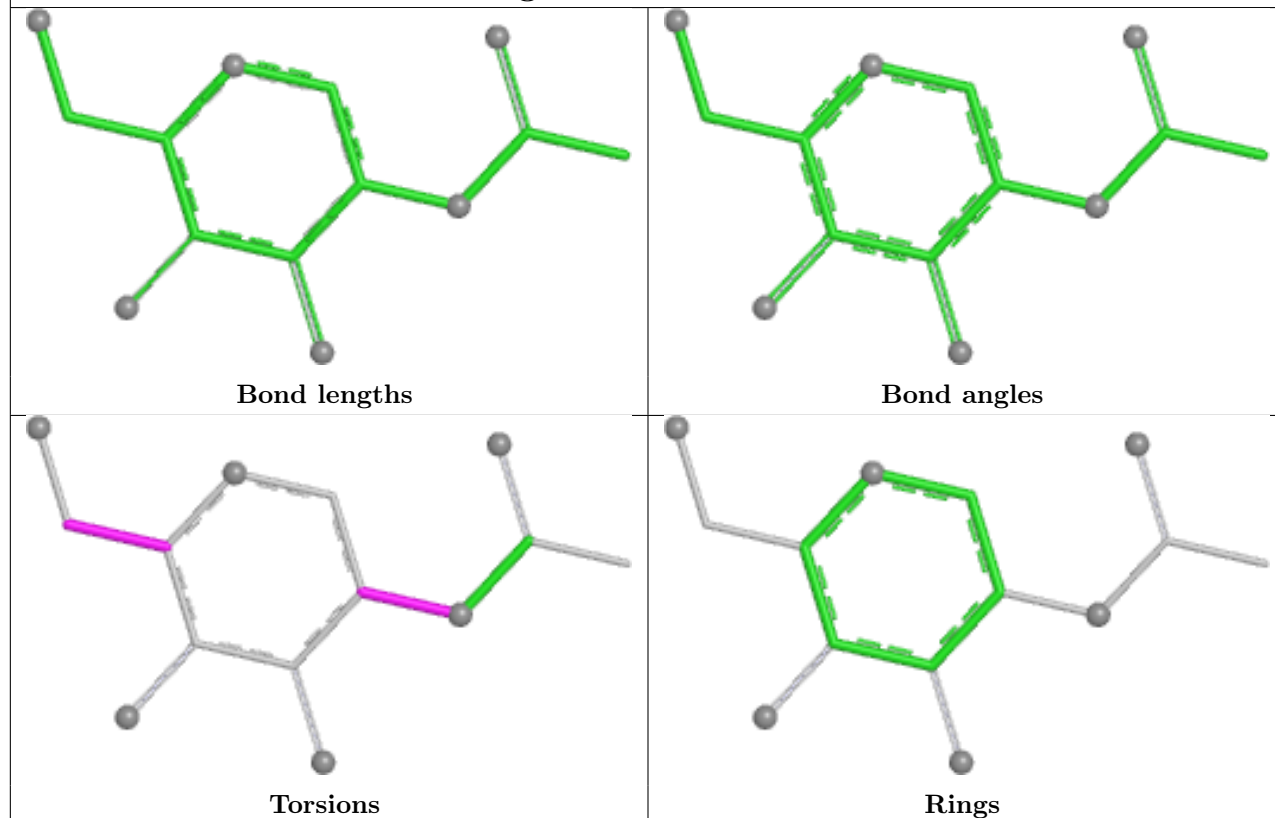
Ligand NAG C 1302



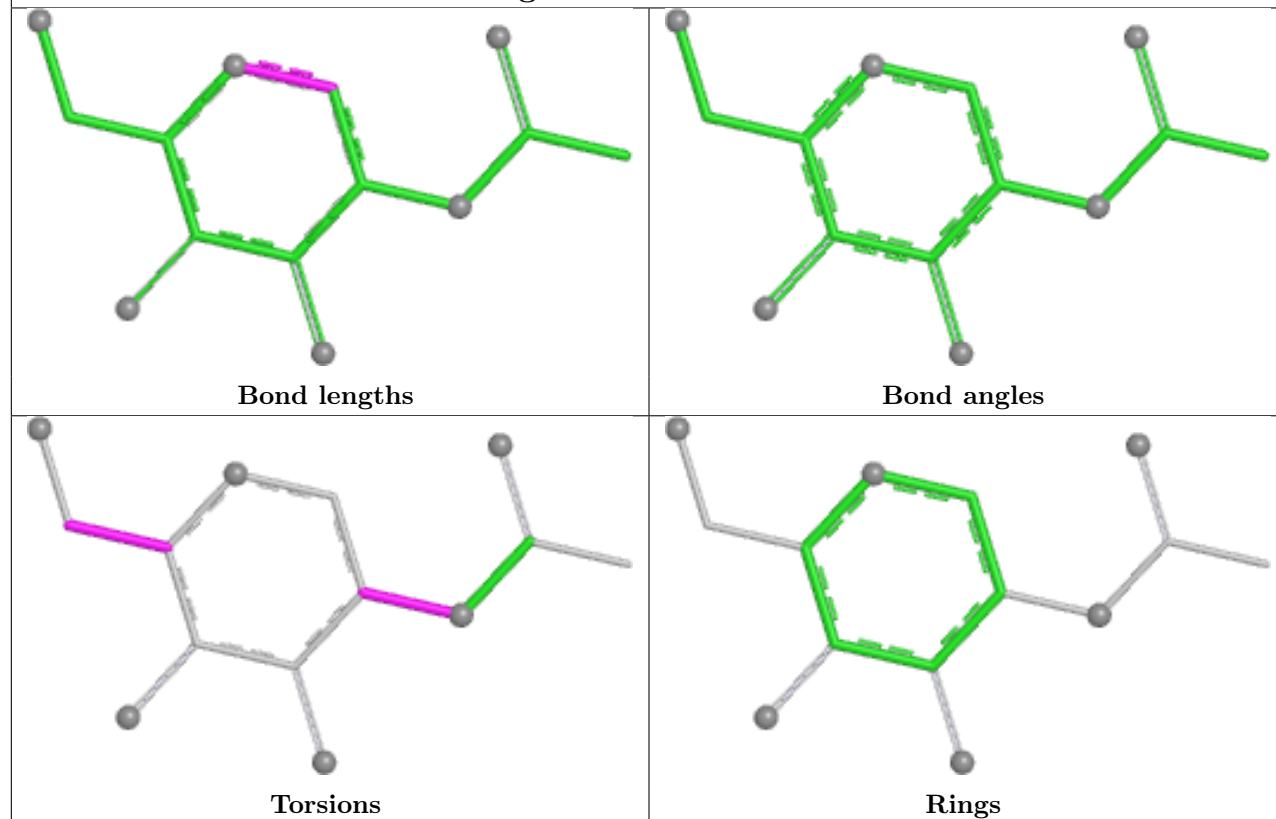
Ligand NAG A 1307



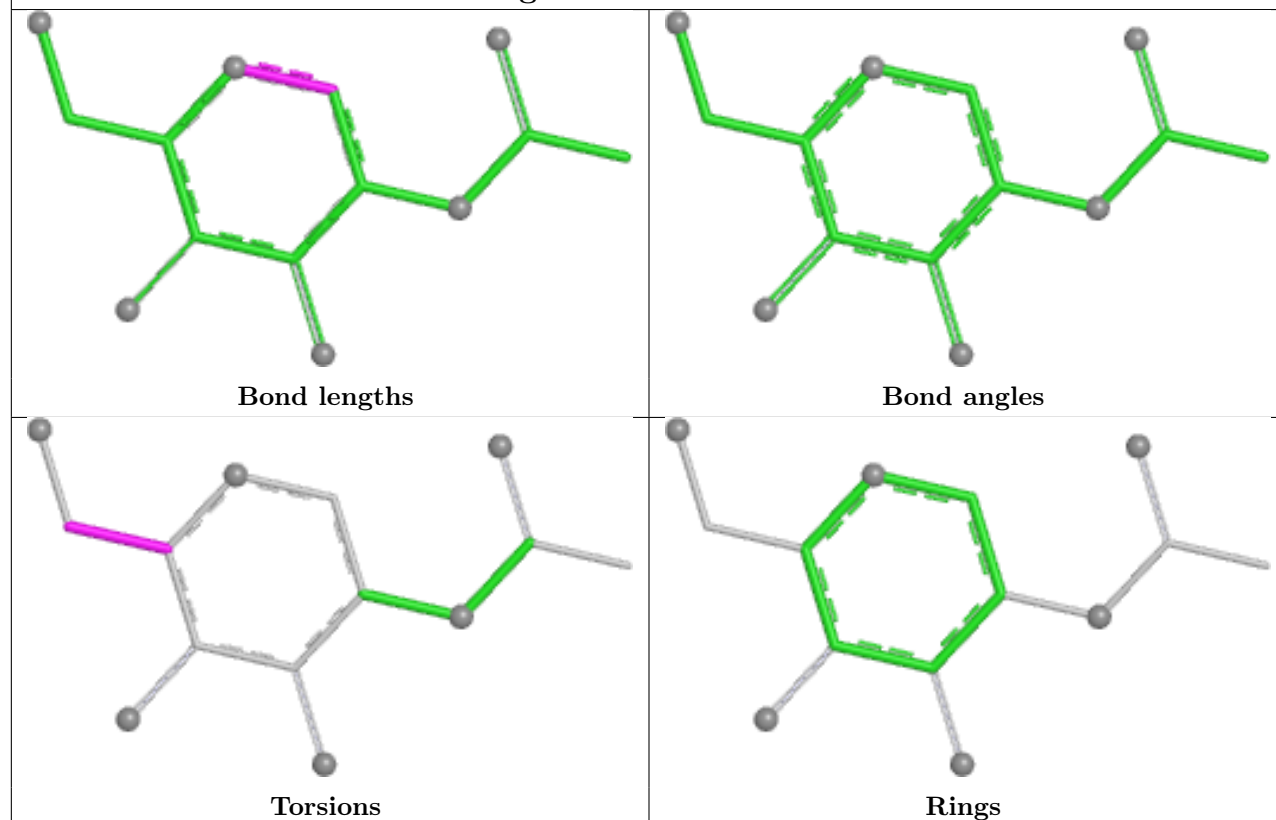
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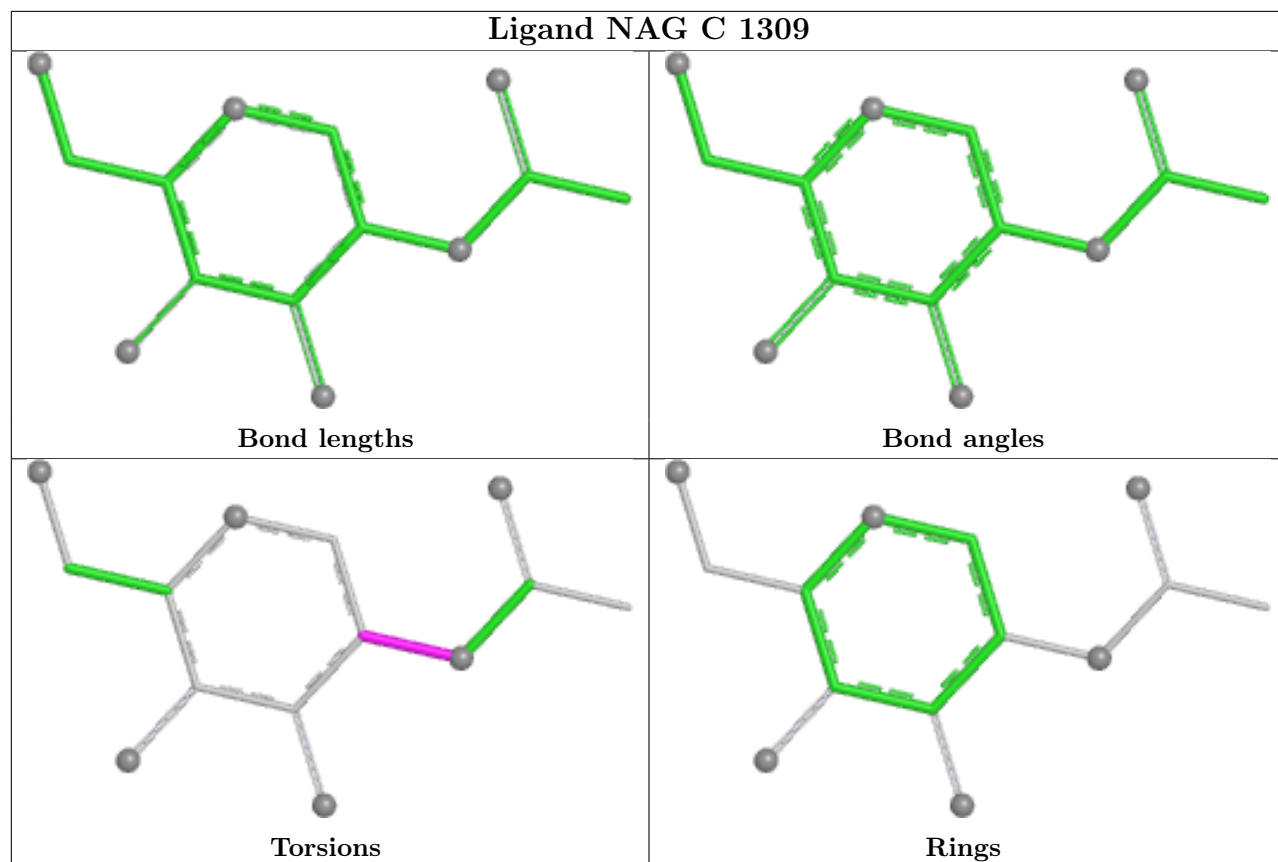
Ligand NAG A 1304



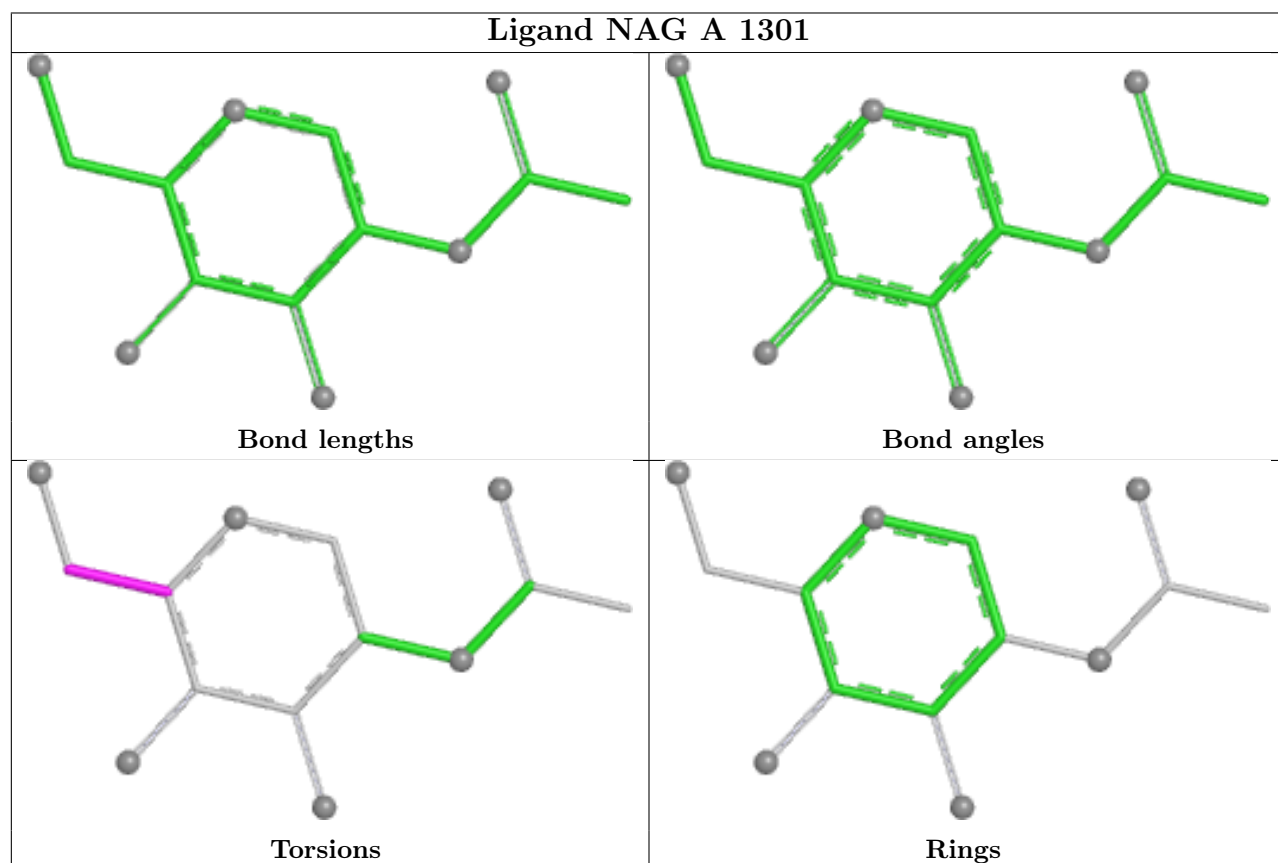
Ligand NAG C 1306



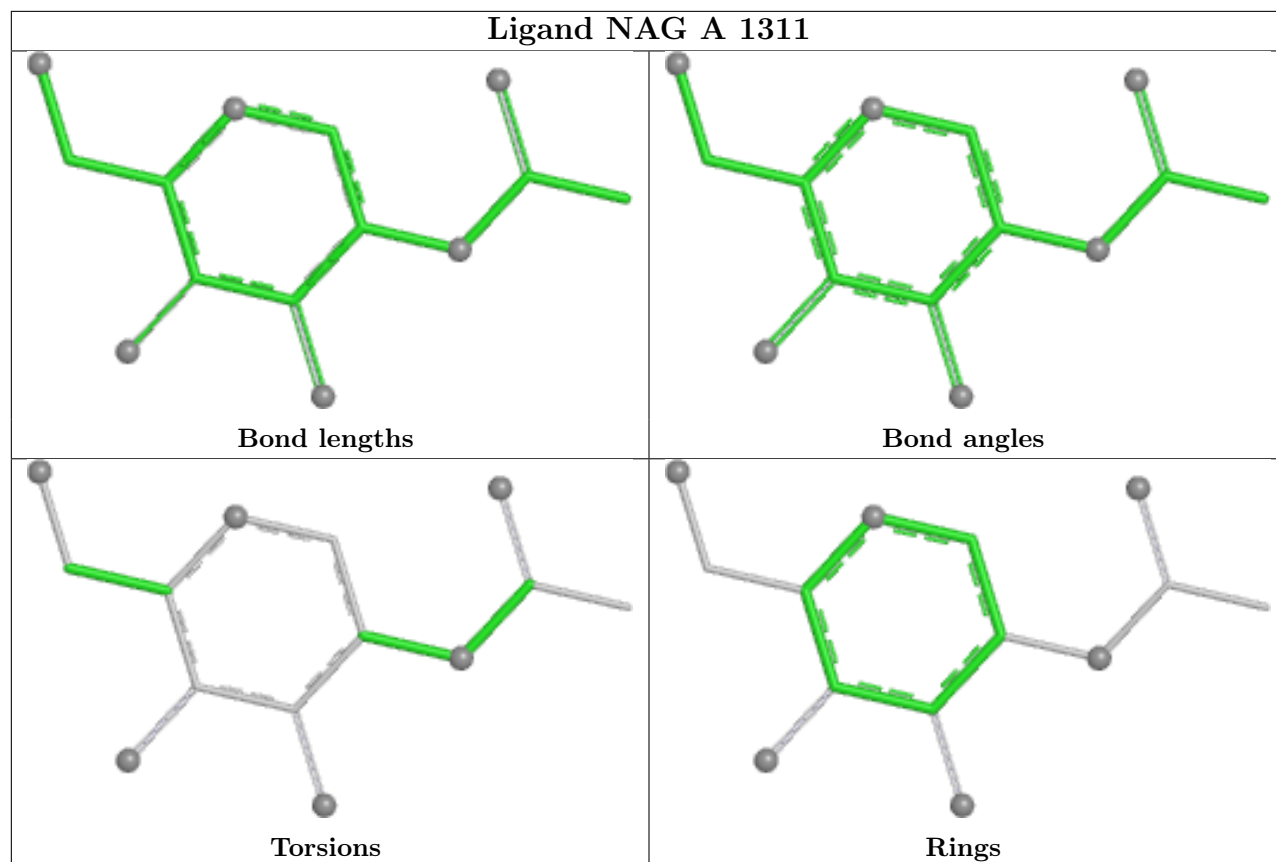
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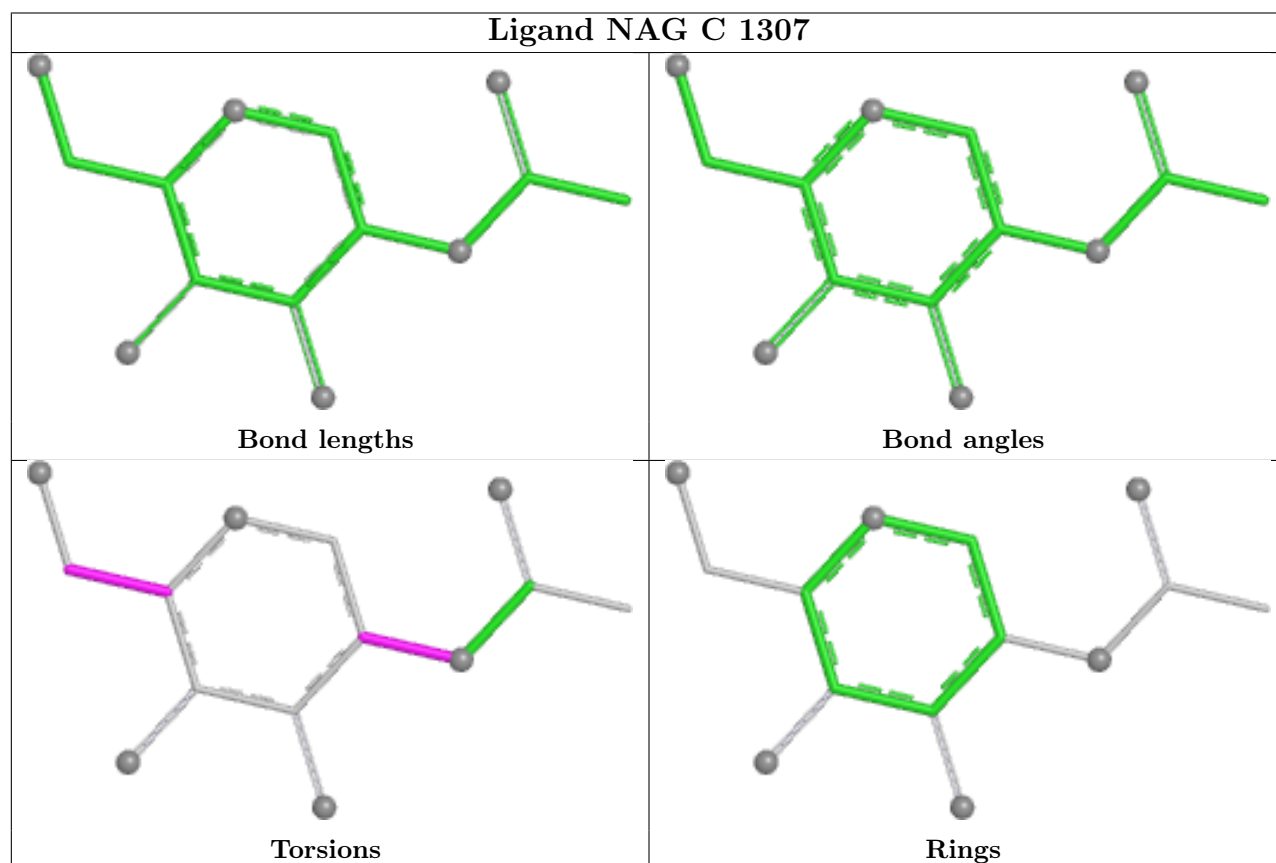
Ligand NAG A 1301



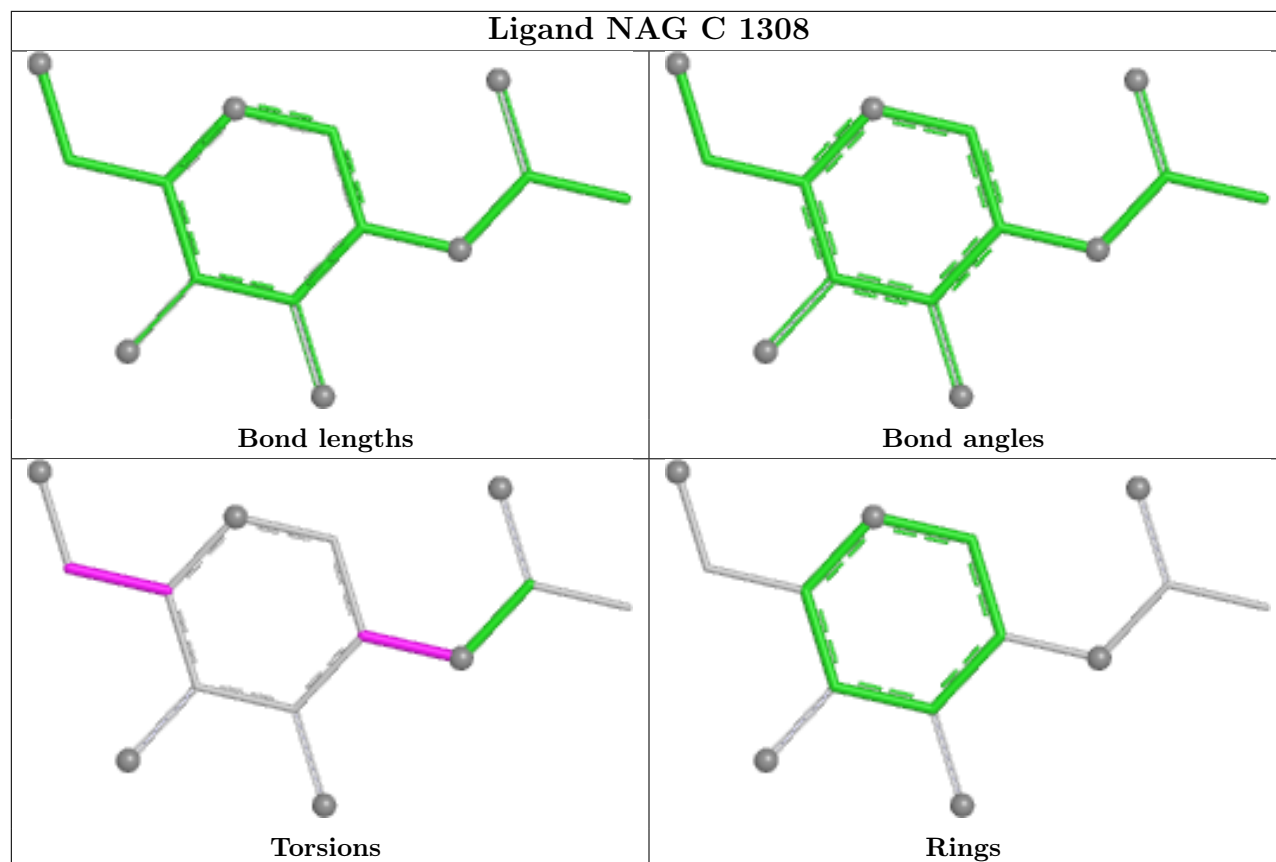
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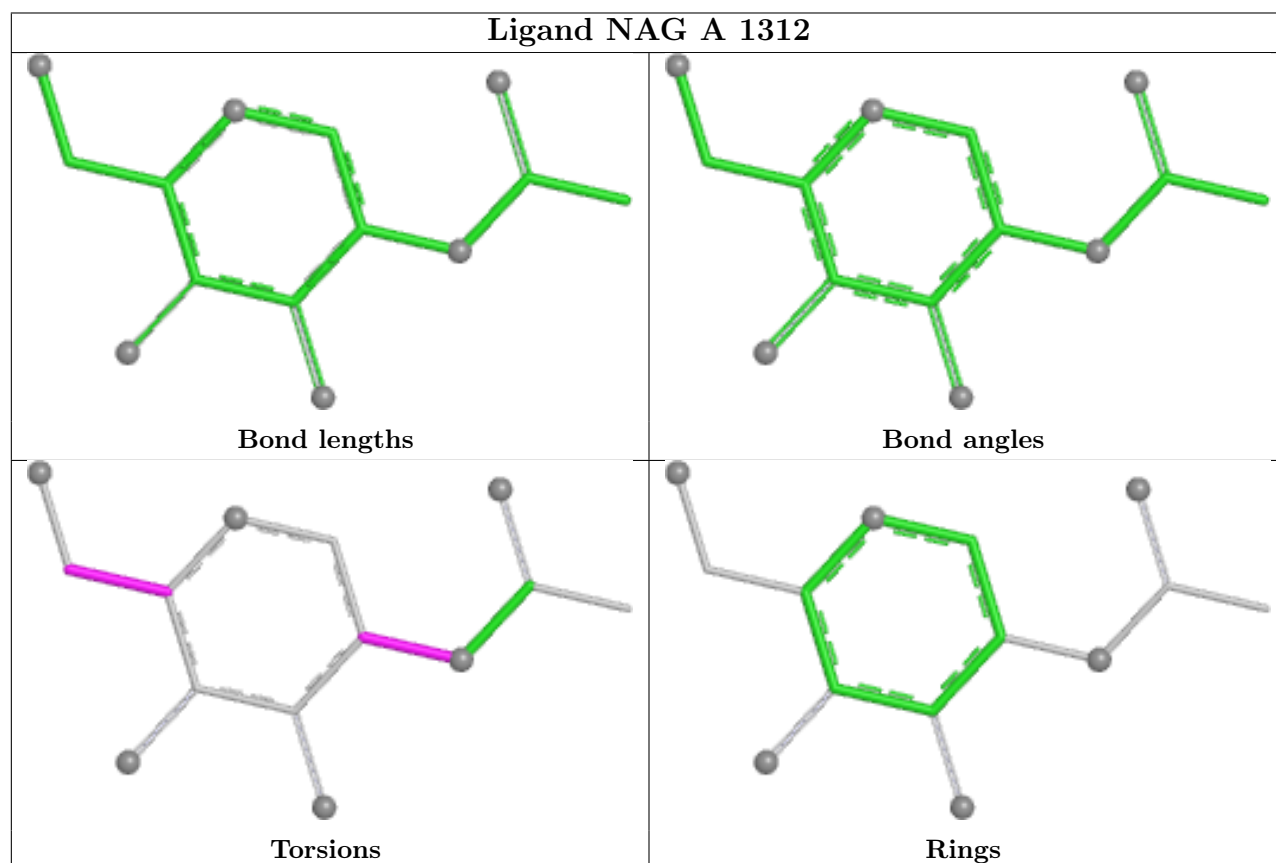
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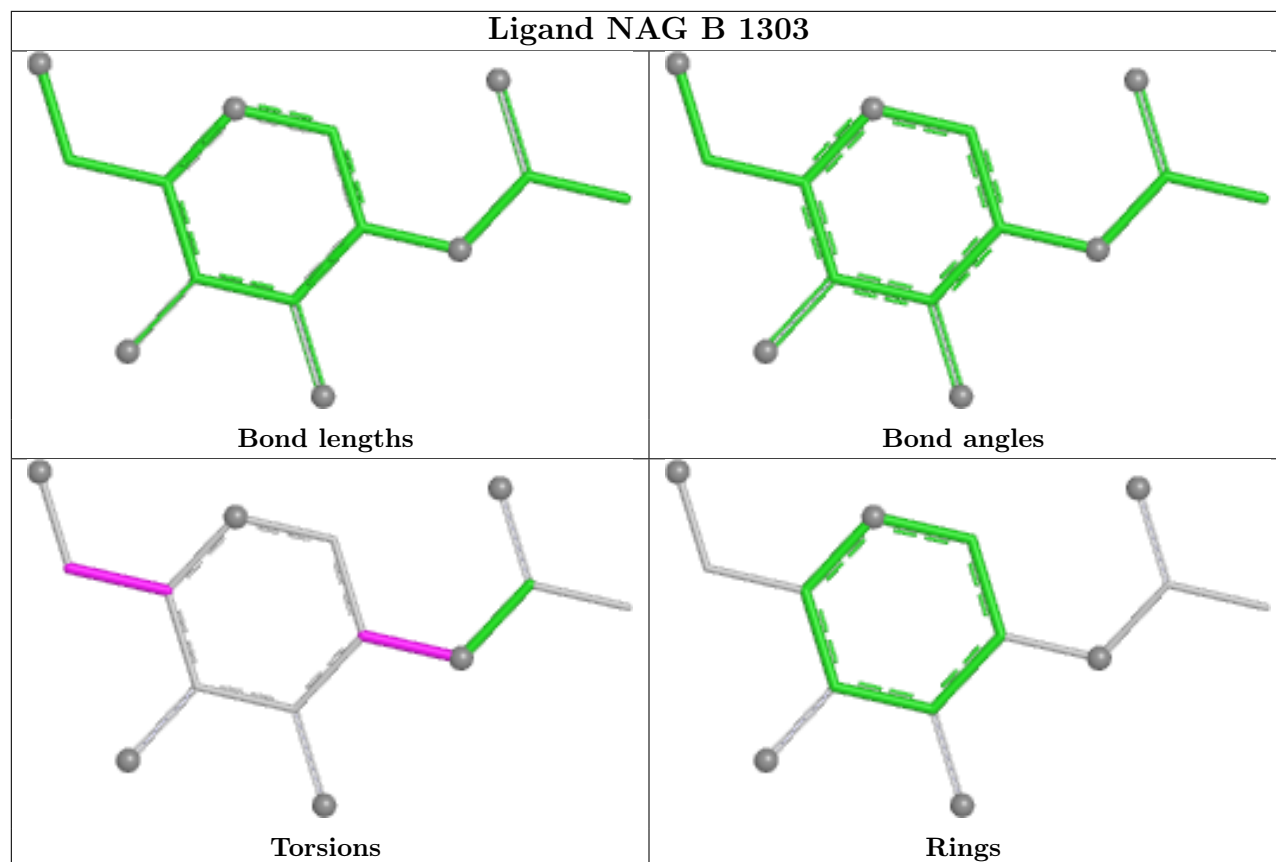
Ligand NAG C 1308



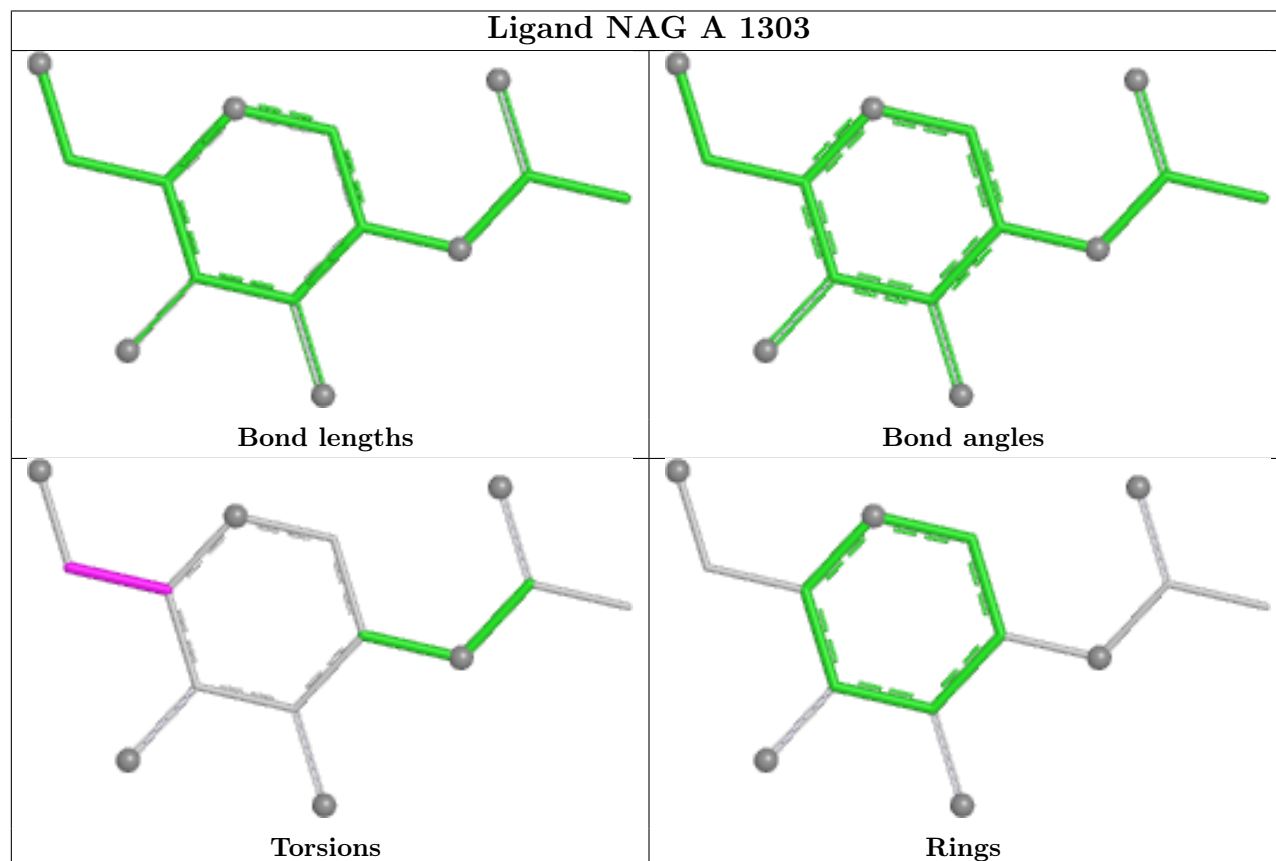
Ligand NAG A 1312

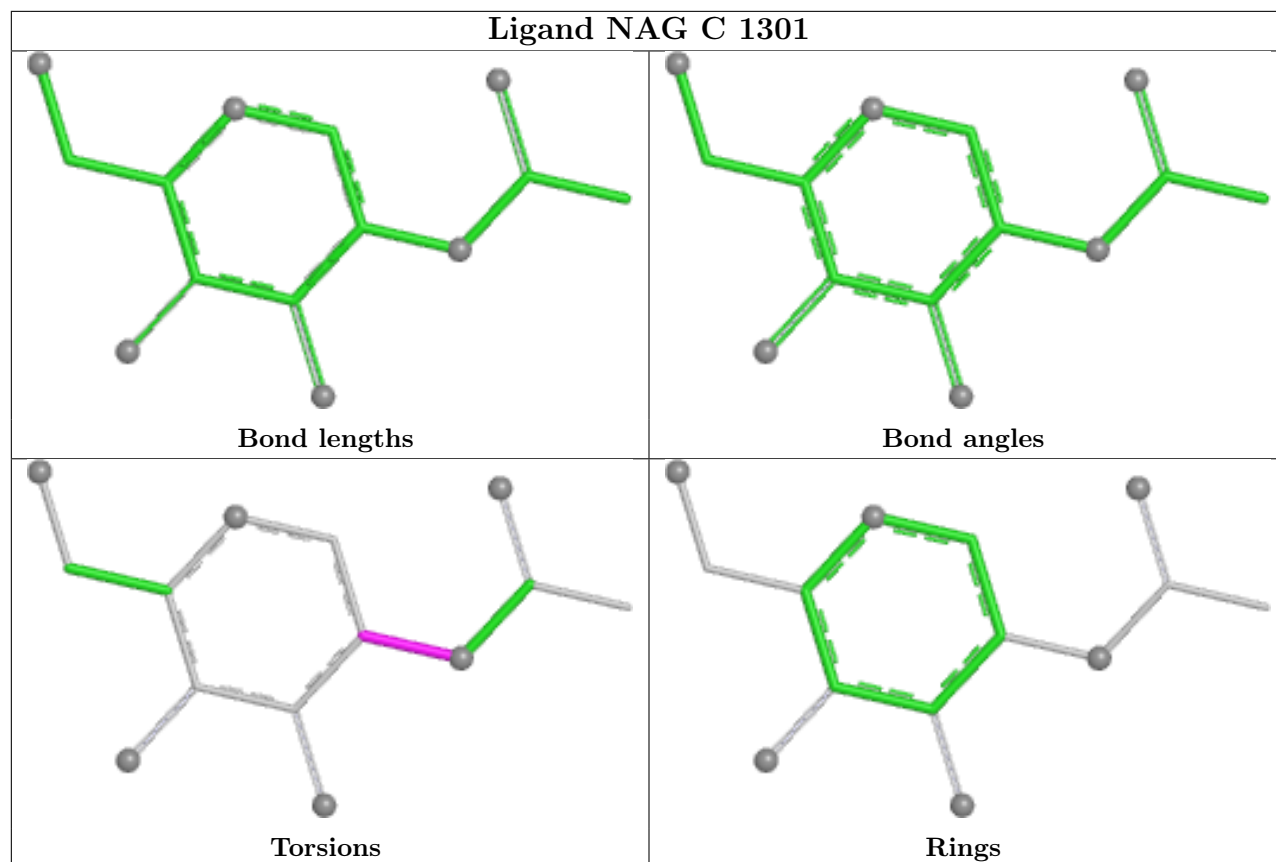


Ligand NAG B 1303



Ligand NAG A 1303





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

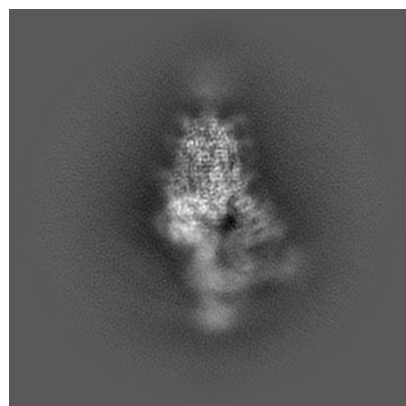
6 Map visualisation [i](#)

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

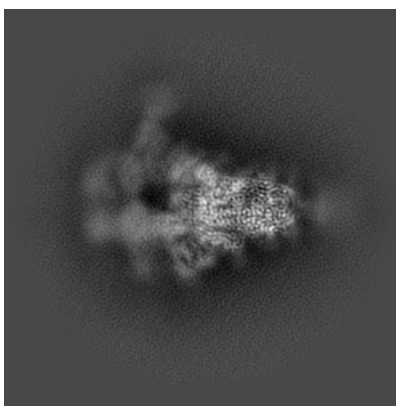
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

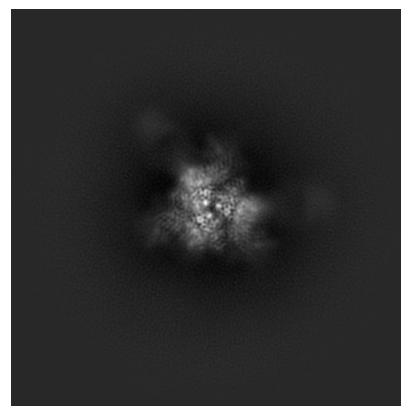
6.1.1 Primary map



X

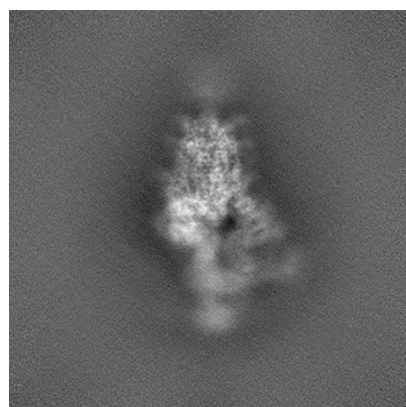


Y

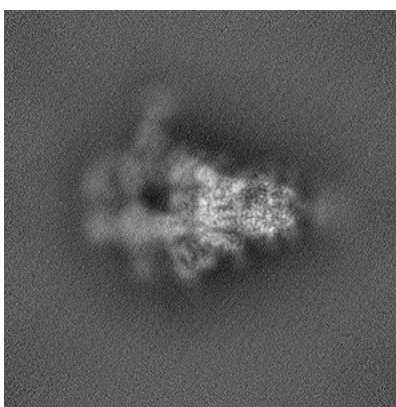


Z

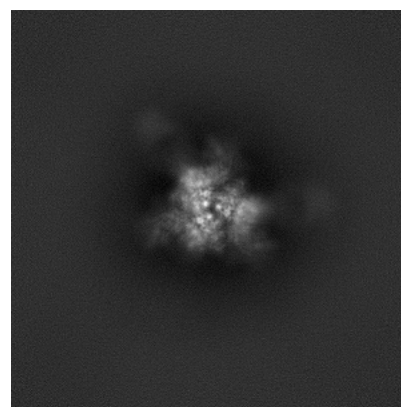
6.1.2 Raw map



X



Y

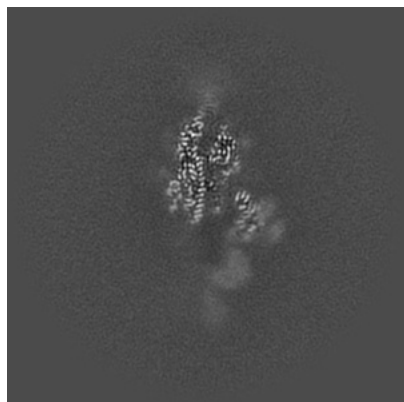


Z

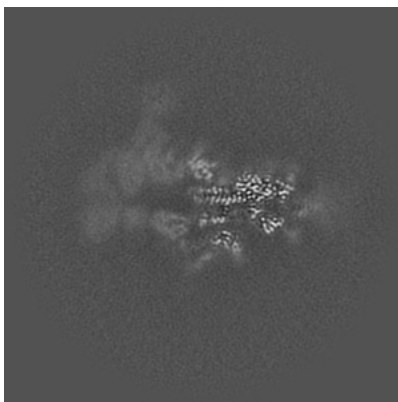
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

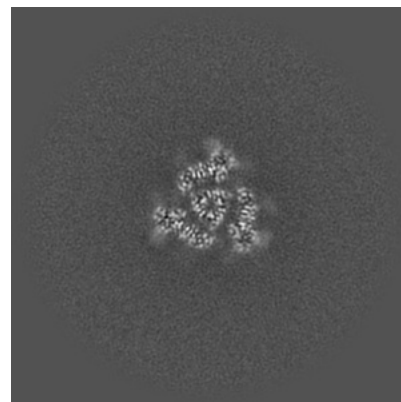
6.2.1 Primary map



X Index: 256

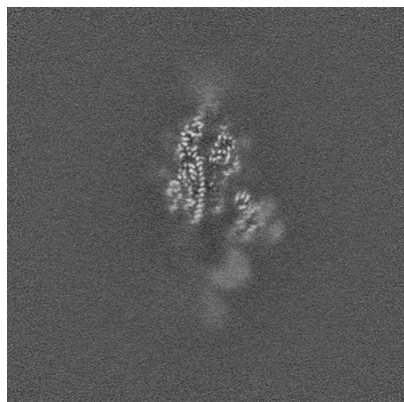


Y Index: 256



Z Index: 256

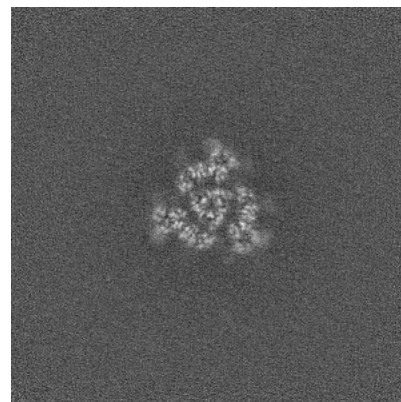
6.2.2 Raw map



X Index: 256



Y Index: 256

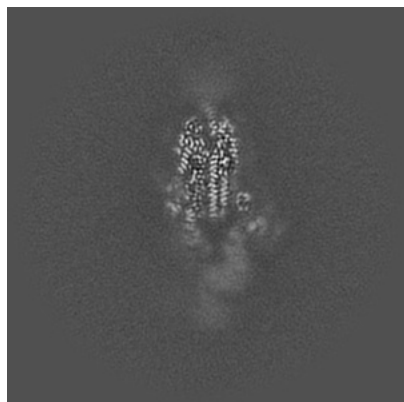


Z Index: 256

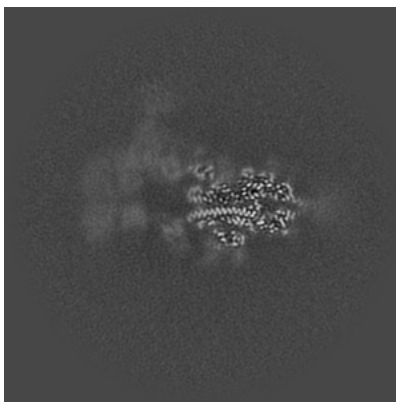
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

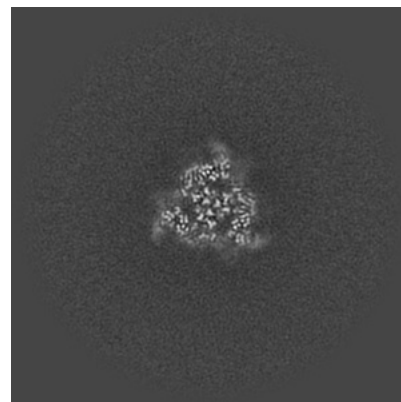
6.3.1 Primary map



X Index: 249

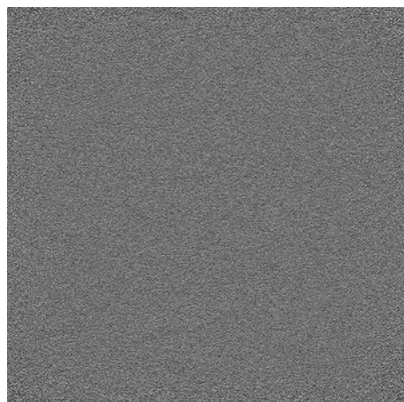


Y Index: 264

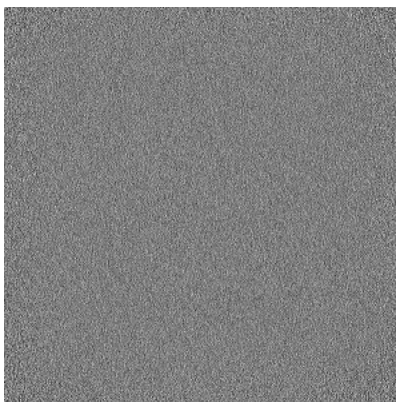


Z Index: 265

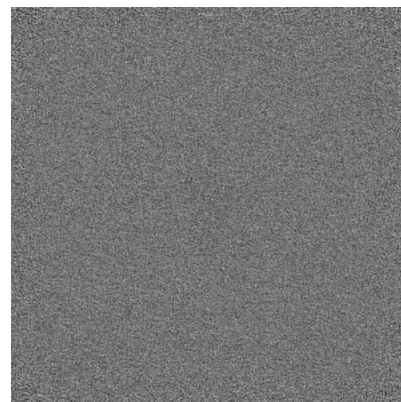
6.3.2 Raw map



X Index: 0



Y Index: 0

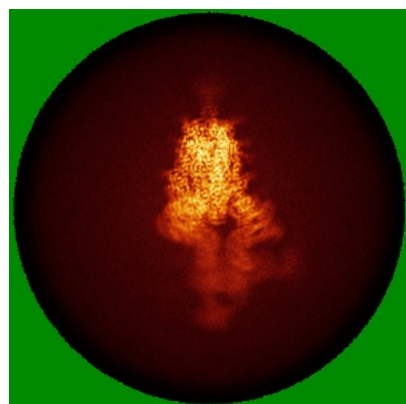


Z Index: 0

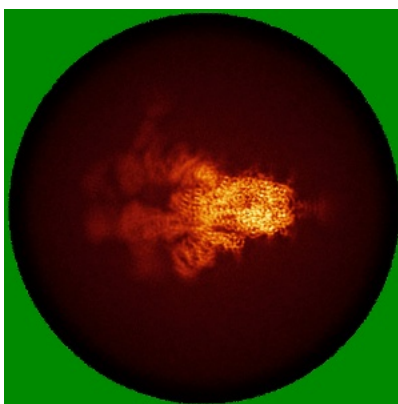
The images above show the largest variance slices of the map in three orthogonal directions.

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

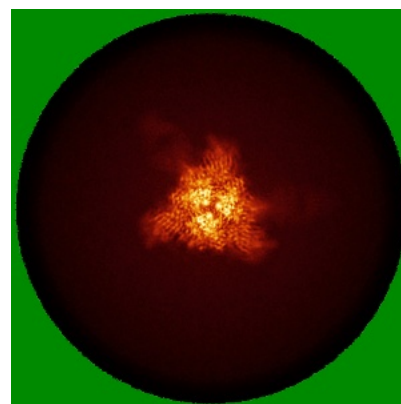
6.4.1 Primary map



X

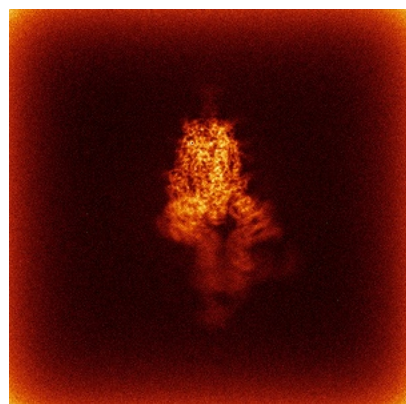


Y

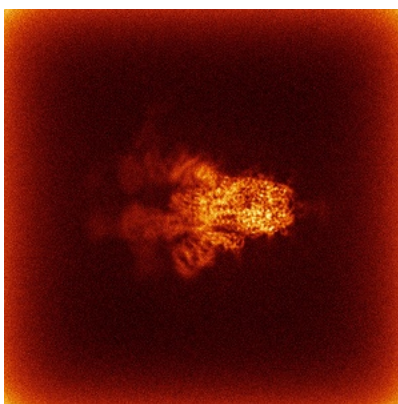


Z

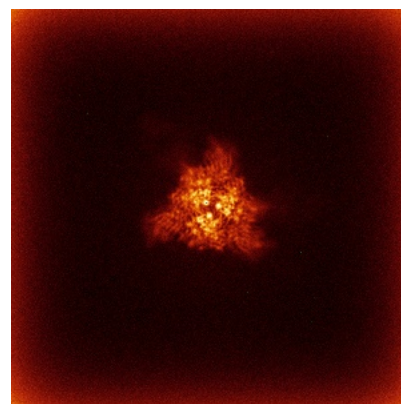
6.4.2 Raw map



X



Y

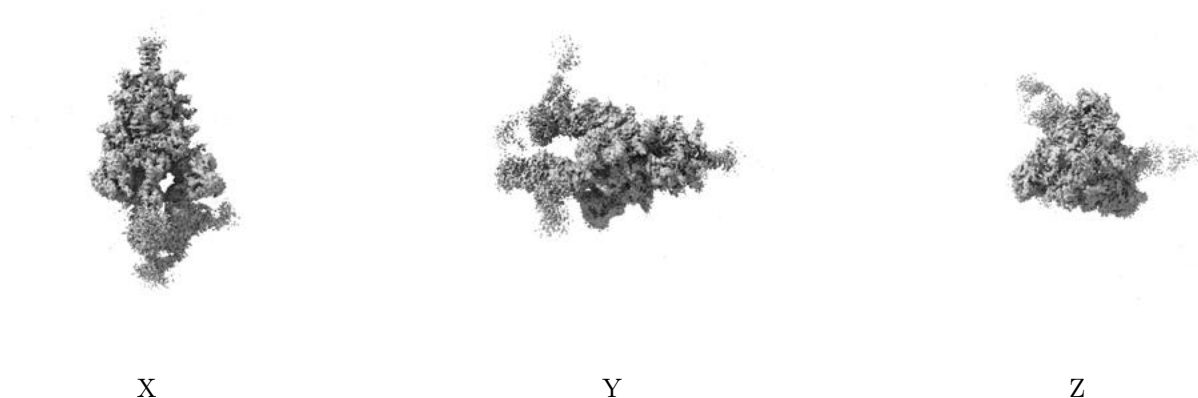


Z

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.

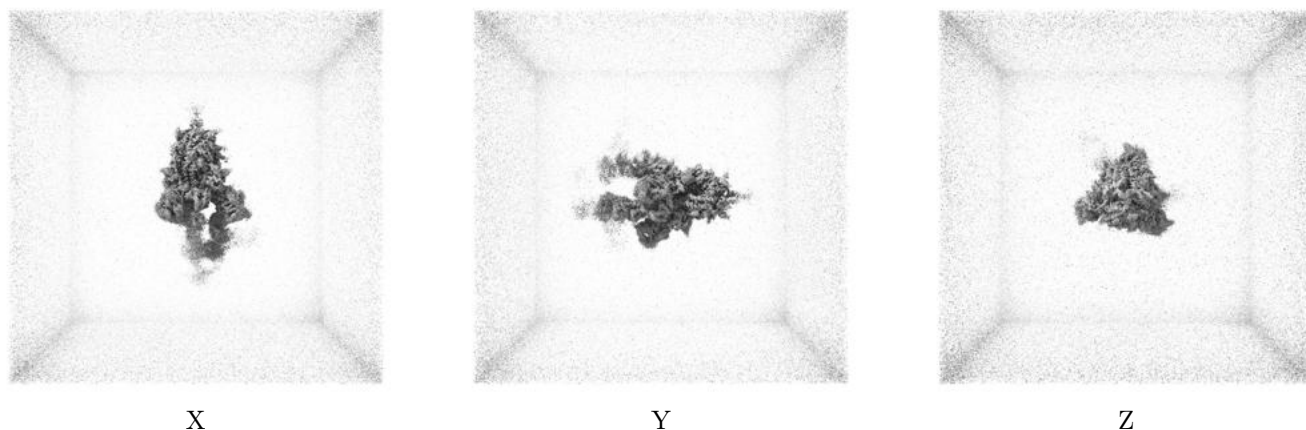
6.5 Orthogonal surface views [i](#)

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.

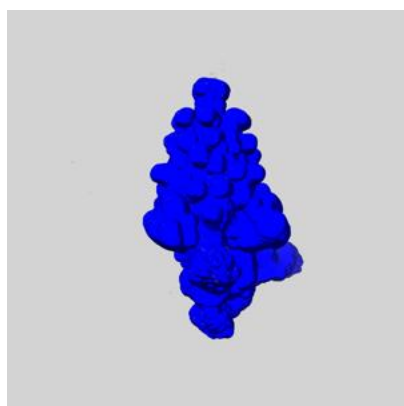
6.6 Mask visualisation [i](#)

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

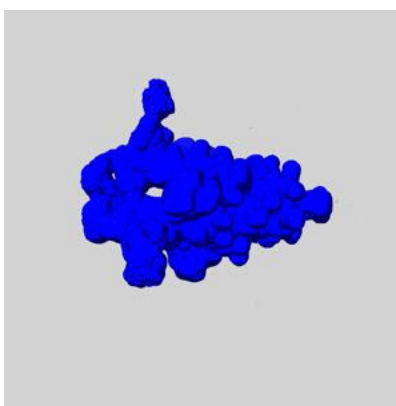
A mask typically either:

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

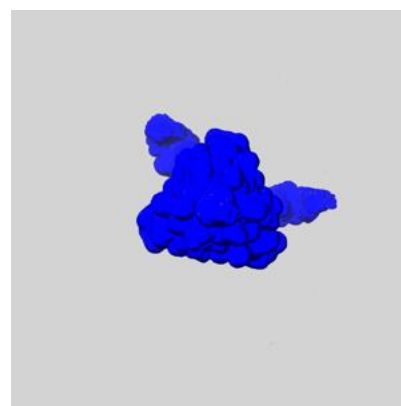
6.6.1 emd_34134_msk_1.map [i](#)



X



Y

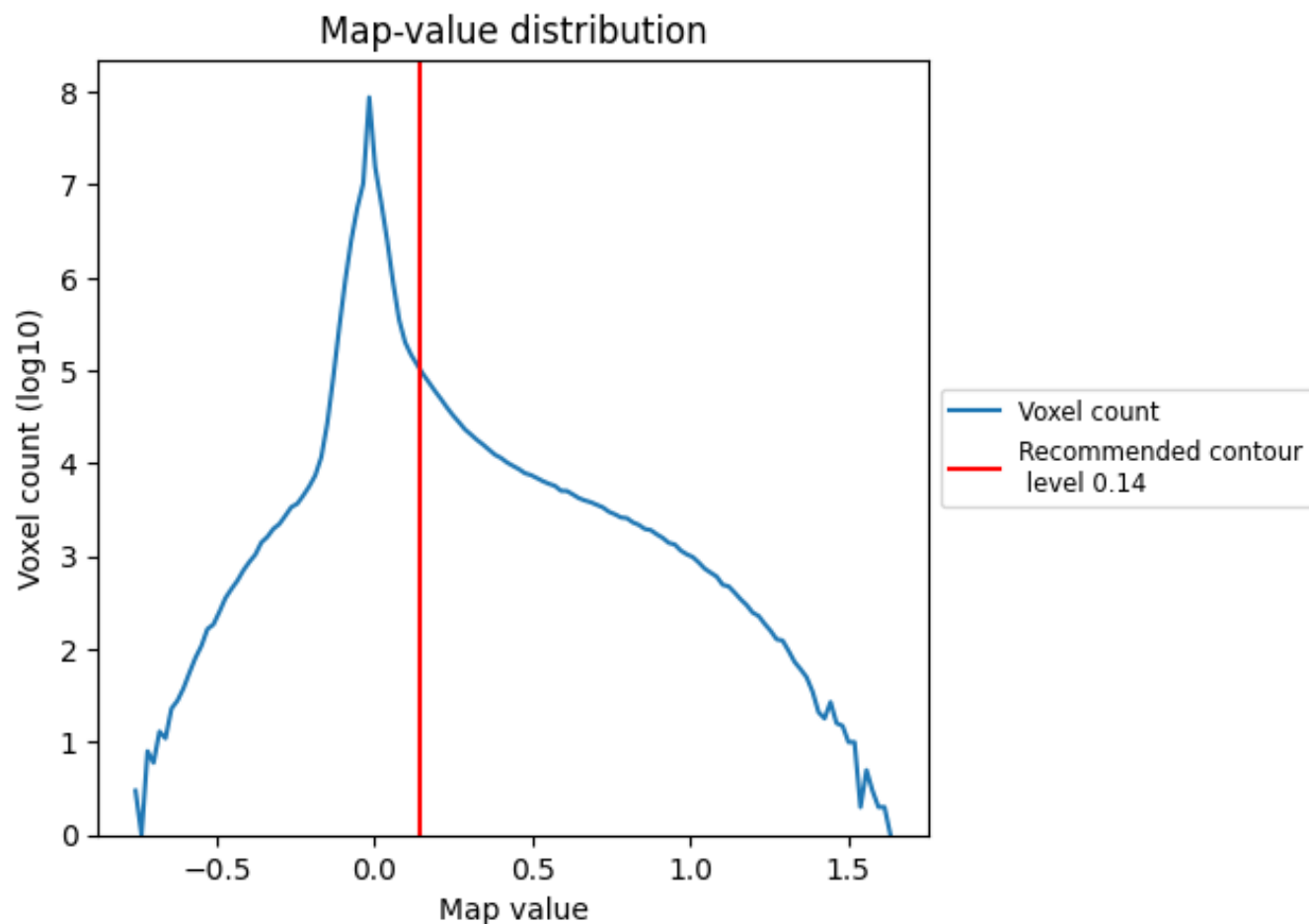


Z

7 Map analysis [i](#)

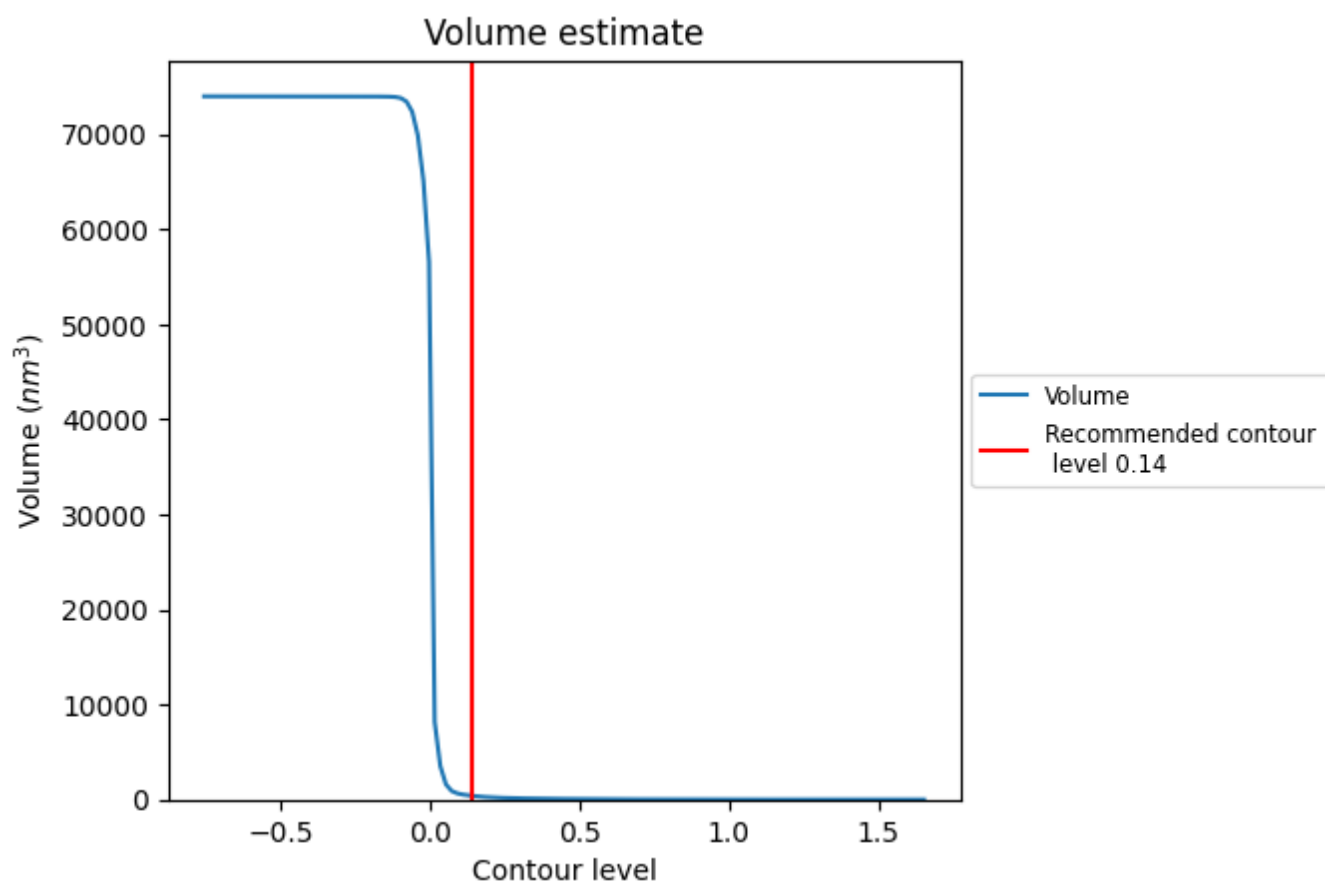
This section contains the results of statistical analysis of the map.

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.

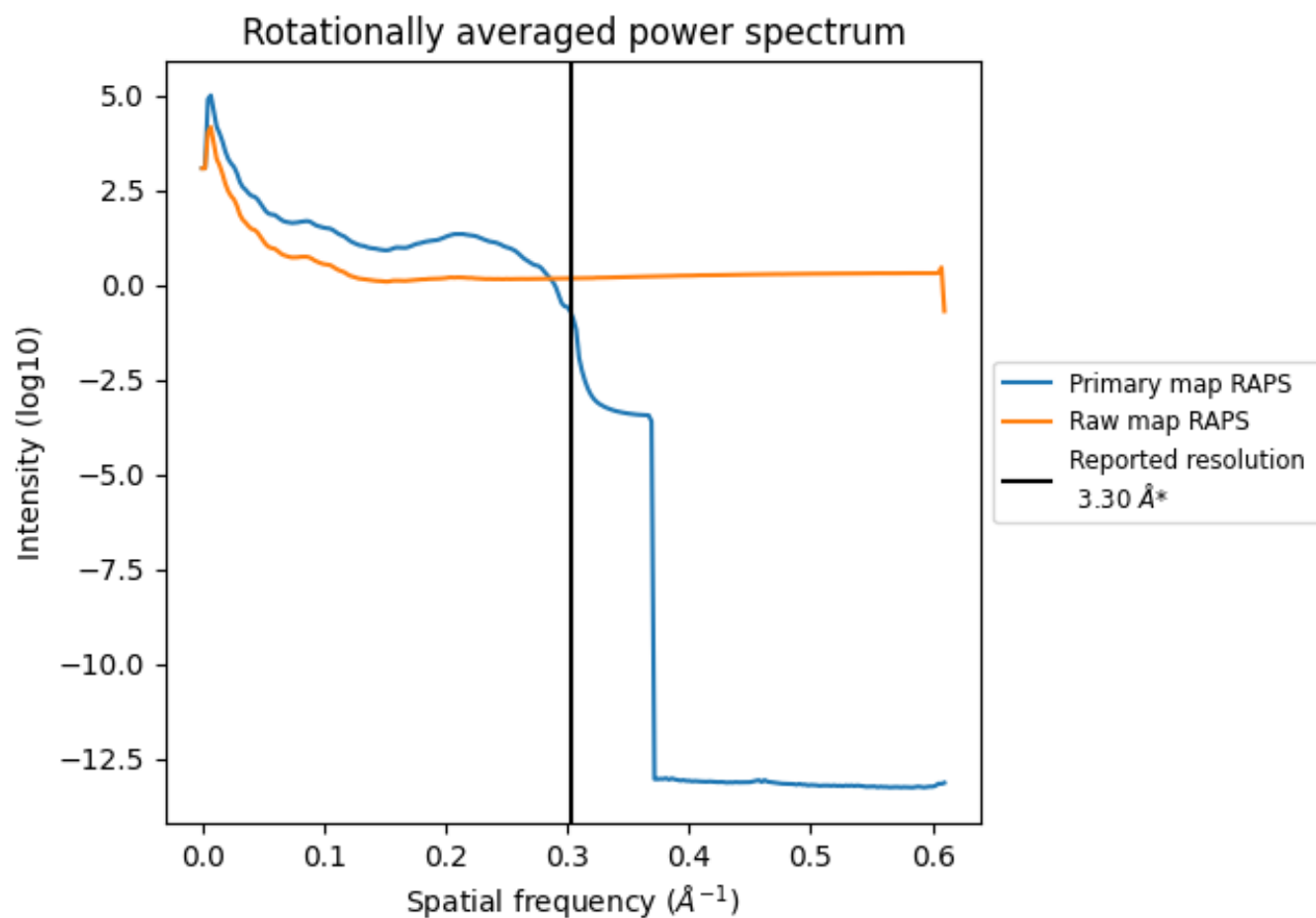
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 393 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 ⓘ

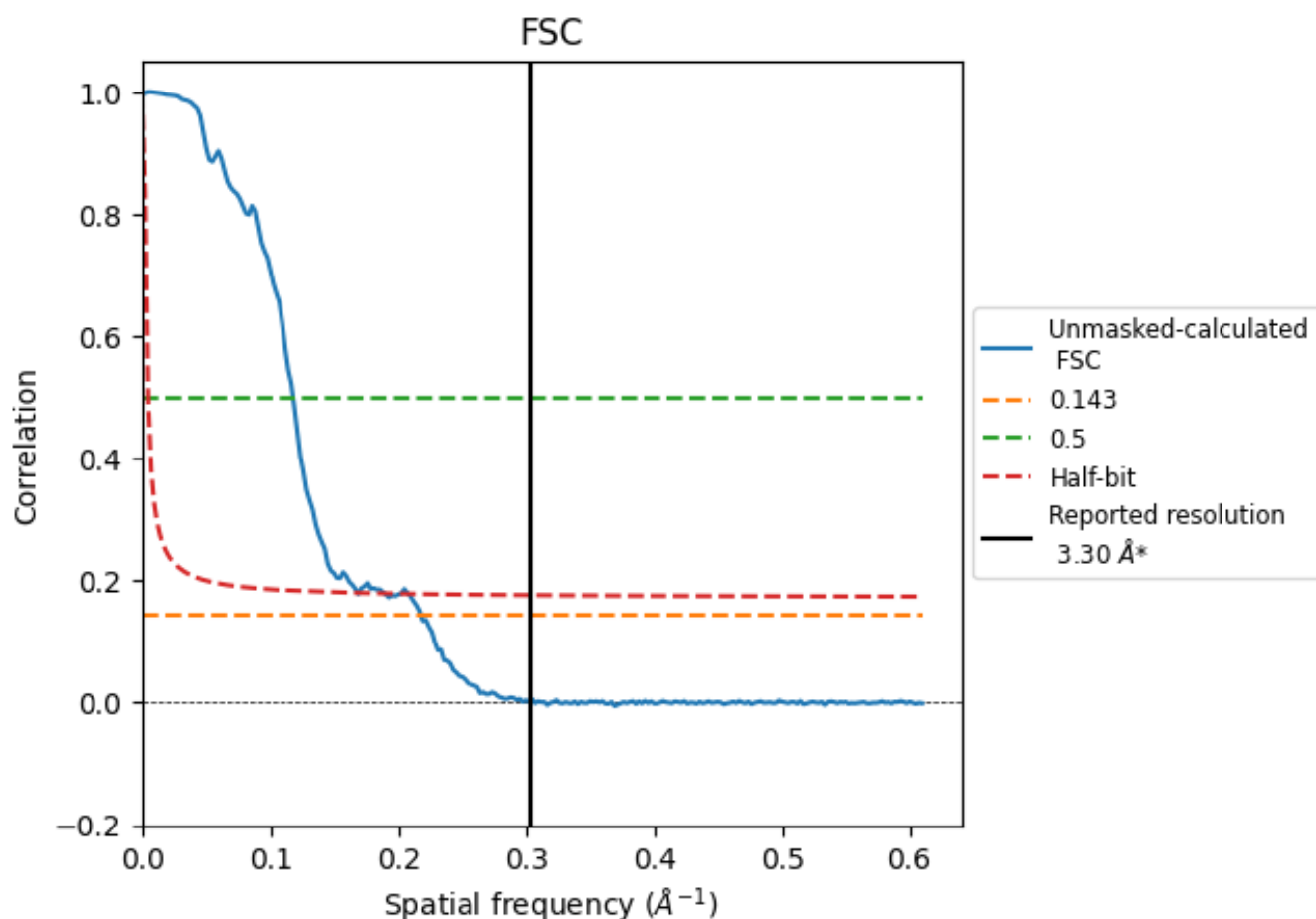


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
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 %

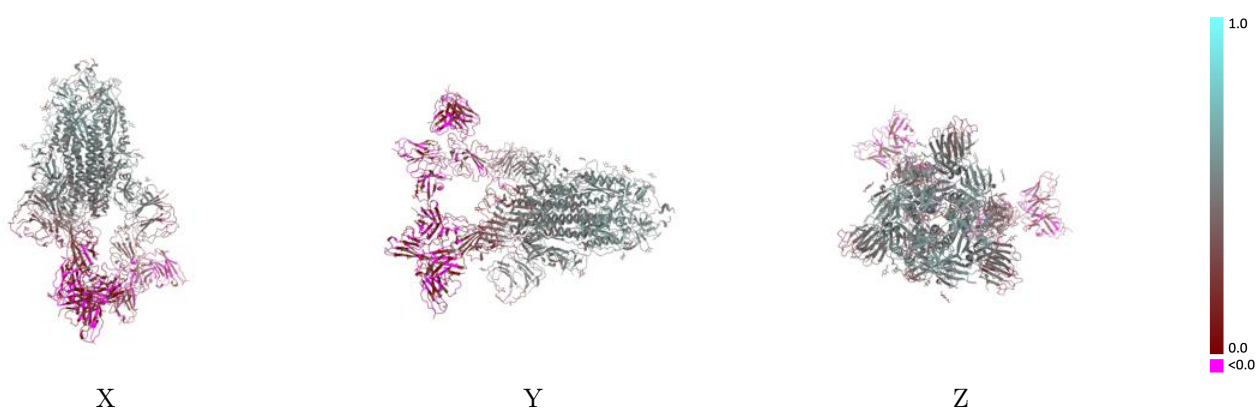
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD 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](#)

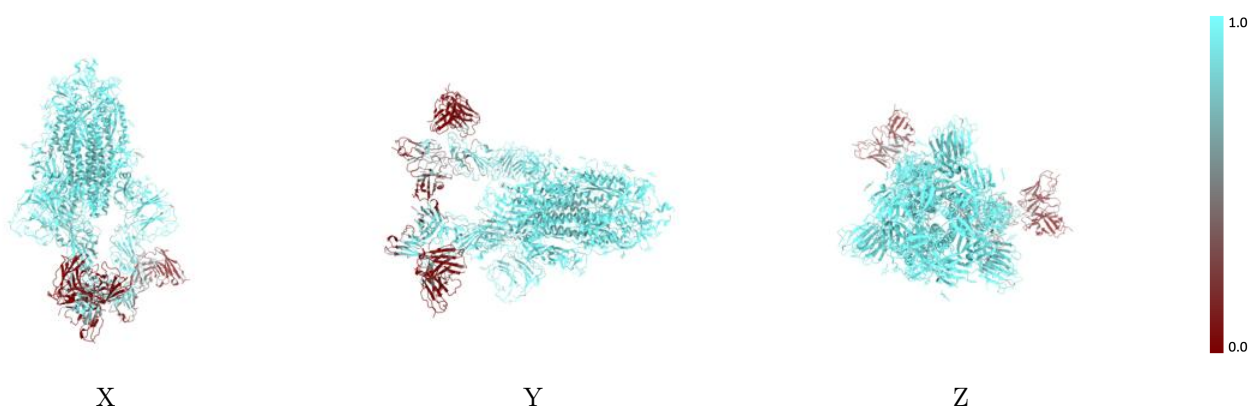
This section was not generated.

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



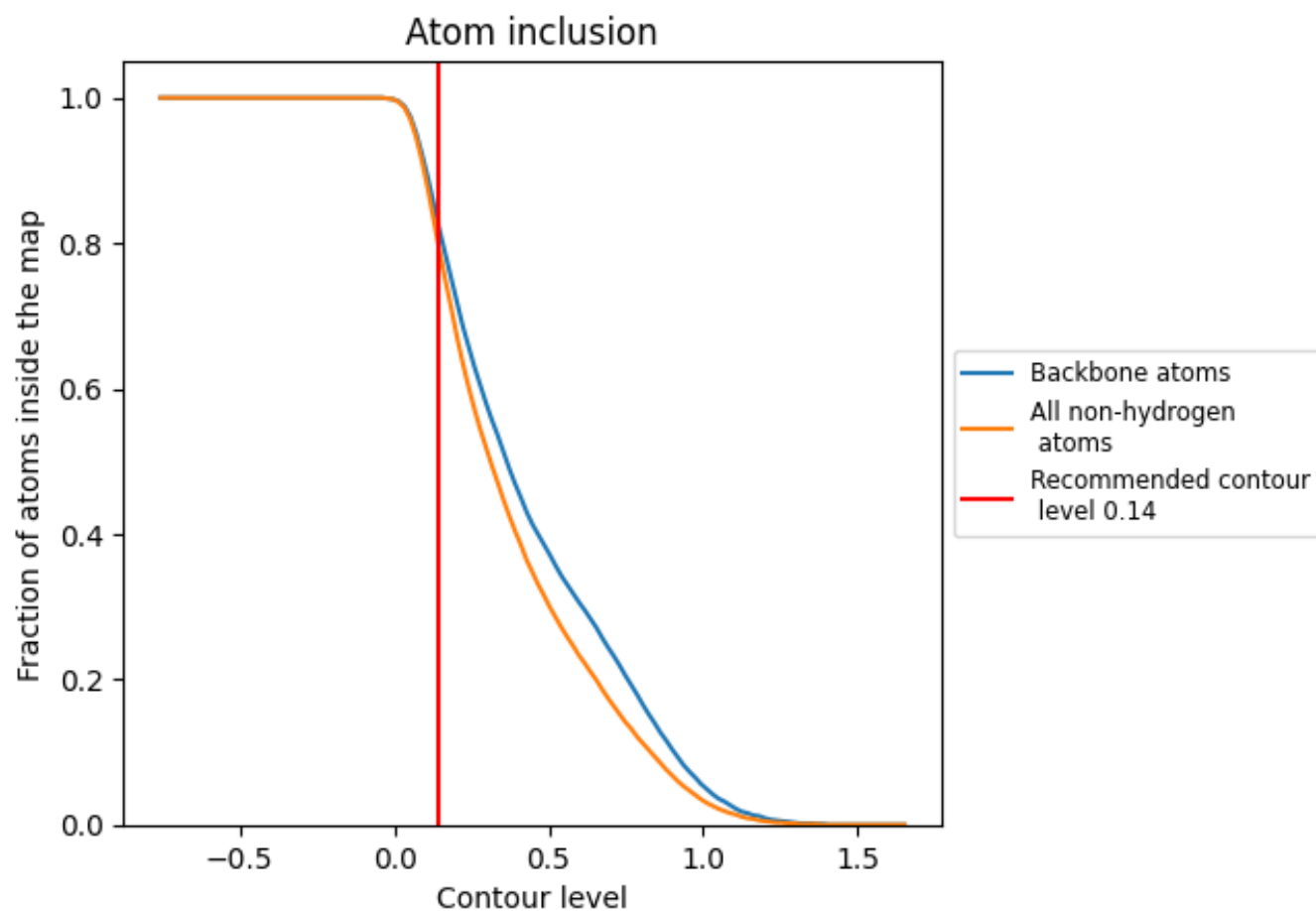
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8040	 0.3490
A	 0.9240	 0.4130
B	 0.9510	 0.4330
C	 0.9610	 0.4320
H	 0.4110	 0.0940
I	 0.3140	 0.0760
J	 0.6300	 0.0980
K	 0.7250	 0.0890
L	 0.0650	 0.0770
M	 0.0900	 0.0910
N	 0.1960	 0.0980
O	 0.1960	 0.0890

