



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:53 AM UTC

PDB ID : 7YVP / pdb_00007yvp
EMDB ID : EMD-34135
Title : Omicron BA.4/5 SARS-CoV-2 S in complex with TH272/281 Fab
Authors : Guo, Y.; Zhang, G.; Liang, J.; Liu, F.; Rao, Z.
Deposited on : 2022-08-19
Resolution : 3.80 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:

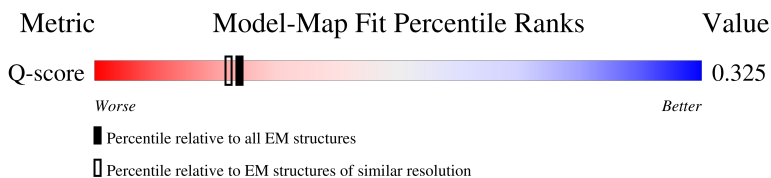
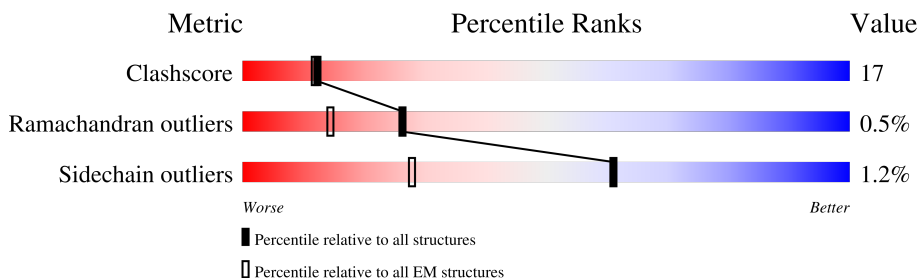
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB 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 3.80 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	10198 (3.30 - 4.30)

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	I	119	66% 47% 52%
1	L	119	50% 51% 48%
2	J	109	72% 48% 50%
2	M	109	55% 46% 52%

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Mol	Chain	Length	Quality of chain
3	H	109	51% 45% 53% ..
3	O	109	23% 49% 49% .
4	K	118	50% 48% 51% .
4	P	118	17% 53% 47%
5	A	1288	57% 21% 20% .
5	B	1288	58% 18% 23% .
5	C	1288	58% 21% 20% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30177 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 TH272 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	118	Total	C	N	O	S	0	0
			914	588	145	178	3		
1	L	118	Total	C	N	O	S	0	0
			914	588	145	178	3		

- Molecule 2 is a protein called TH272 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	108	Total	C	N	O	S	0	0
			796	498	129	166	3		
2	M	108	Total	C	N	O	S	0	0
			796	498	129	166	3		

- Molecule 3 is a protein called TH281 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	109	Total	C	N	O	S	0	0
			821	513	139	166	3		
3	H	109	Total	C	N	O	S	0	0
			821	513	139	166	3		

- Molecule 4 is a protein called TH281 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	118	Total	C	N	O	S	0	0
			870	548	146	171	5		
4	K	118	Total	C	N	O	S	0	0
			870	548	146	171	5		

- Molecule 5 is a protein called Spike glycoprotein.

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

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2

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

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

- Molecule 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	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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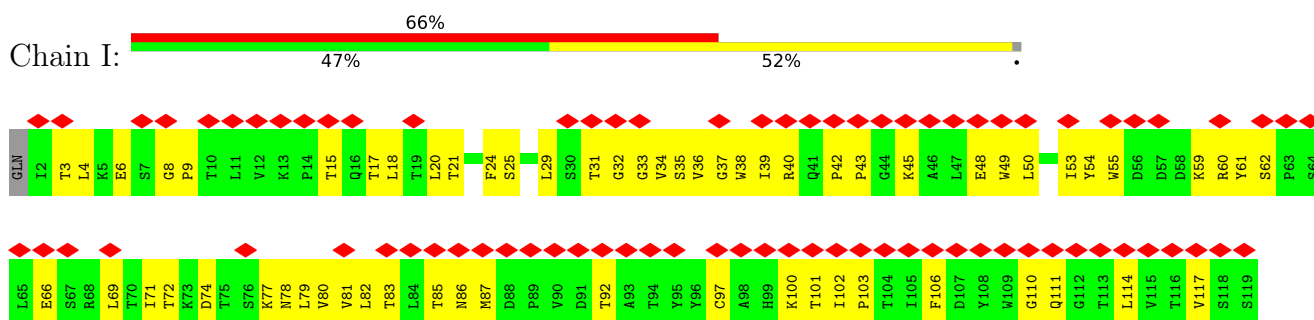
Continued from previous page...

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	

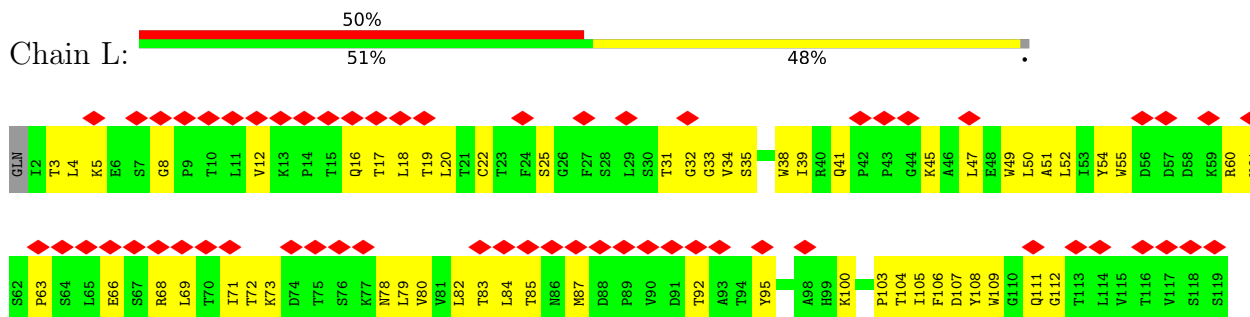
3 Residue-property plots

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.

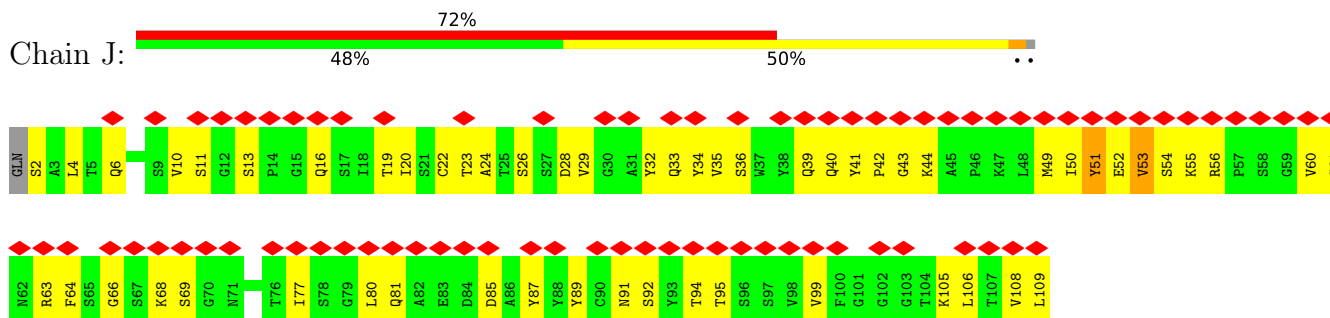
- Molecule 1: TH272 Fab heavy chain



- Molecule 1: TH272 Fab heavy chain

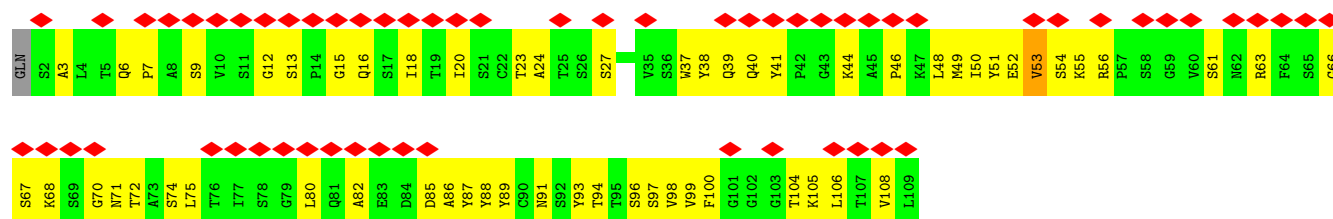


- Molecule 2: TH272 Fab light chain



- Molecule 2: TH272 Fab light chain

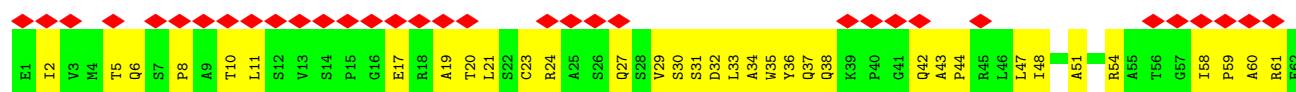
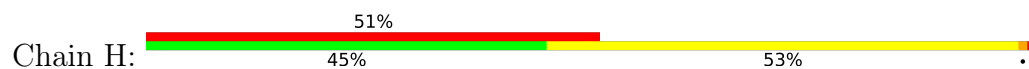




• Molecule 3: TH281 Fab light chain



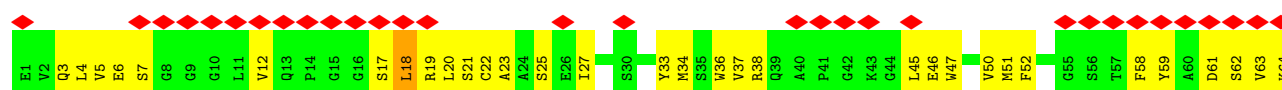
• Molecule 3: TH281 Fab light chain



• Molecule 4: TH281 Fab heavy chain



• Molecule 4: TH281 Fab heavy chain





GLN	PRO	LYS	S1003	ALA	THR	F541	L461	F374	G261	S172	W83
PHE	GLU	TYR	L1004	GLY	LYS	N542	K462	F375	A262	Q173	L84
GLU	ALA	PHE	F543	PHE	SER	F543	P463	A376	A263	L176	P85
LYS	PRO	LYS	T1006	ILE	HIS	N544	F464	C379	A264	MET	F86
GLY	ARG	ASN	Y1007	LYS	GLY	G545	R465	S383	ASP	ASP	N87
GLY	ASP	HIS	V1008	GLN	SER	L546	R466	Y269	LEU	LEU	D88
SER	GLY	THR	E1017	TYR	ALA	F559	I468	S383	GLU	GLU	G89
HIS	GLN	SER	I1018	GLY	SER	L560	T470	K386	GLY	GLY	E96
HIS	ALA	PRO	R1019	ASP	SER	Q563	E471	L387	LYS	LYS	N99
HIS	TYR	ASP	A1020	CYS	VAL	Q564	I472	N388	GLN	GLN	G103
HIS	VAL	VAL	S1021	LEU	ALA	F565	Y473	T284	GLY	GLY	W104
HIS	ARG	ASP	L1049	GLY	SER	R577	K478	E288	ASN	ASN	G103
HIS	LYS	LEU	P1057	ASP	Q690	E583	P479	F392	PHE	PHE	W104
HIS	ASP	GLY	L1057	ILE	Y695	E584	N481	Y396	K187	K187	I105
HIS	GLY	ASP	P1057	ALA	T696	I584	V486	S399	N188	N188	F106
HIS	GLY	ASP	K1073	ALA	M697	V896	G482	Y396	G107	G107	T108
HIS	TRP	SER	N1074	ARG	S698	T602	V483	S399	L189	L189	
HIS	VAL	ILE	F1075	ASP	I712	N603	A484	R403	M196	M196	
HIS	PHE	ASN	T1076	LEU	A713	G617	G485	G404	Y200	Y200	K113
HIS	LEU	ALA	A1077	ILE	I742	T618	A485	N405	F201	F201	T114
HIS	THR	ALA	P1079	CYS	I742	E619	G485	N405	K206	K206	Q115
HIS	PHE	ALA	K1086	ALA	C743	V619	G485	N410	H207	H207	L117
HIS	LEU	VAL	GLY	GLN	G744	C617	G485	I410	T208	T208	L118
HIS	SER	ASN	ILE	LYS	S755	T618	G485	I417	P209	P209	I119
HIS	GLY	ILE	GLN	LYS	S755	E619	G485	N417	I210	I210	V126
HIS	LEU	GLN	LYS	GLY	S755	V620	G485	I418	ASN	ASN	V127
HIS	GLU	LYS	E1092	ALA	S755	PRO	G485	I419	LEU	LEU	I128
HIS	VAL	ILE	S1097	ARG	L754	VAL	G485	D420	GLY	GLY	K129
HIS	PHE	ASP	Y1102	ASP	S758	ALA	G485	N422	ARG	ARG	V130
HIS	GLN	ARG	F1103	ASP	Q762	ILE	G485	N423	D215	D215	C131
HIS	GLY	LEU	V1104	ASP	I770	HIS	G485	K424	G219	G219	F140
HIS	PRO	ASN	I1115	ASP	I770	ALA	G485	L425	F220	F220	L141
HIS	GLY	VAL	D1118	ASP	Q774	GLN	G485	C432	S221	S221	D142
HIS	TRP	ALA	N1119	THR	D776	LEU	G485	I433	P230	P230	VAL
HIS	SER	LYS	N1125	THR	K776	THR	G485	I434	I231	I231	TYR
HIS	PRO	LEU	C1126	THR	N777	PRO	G485	A435	I235	I235	HIS
HIS	GLN	ASN	D1127	TRP	N777	TRP	G485	W436	T236	T236	LYS
HIS	PHE	GLU	N1128	VAL	E780	ARG	G485	N439	R237	R237	ASN
HIS	GLU	GLY	V1129	TYR	V781	VAL	G485	N439	F238	F238	LYS
HIS	LYS	ILE	V1129	SER	N801	TYR	G485	N439	Q239	Q239	TRP
HIS	GLY	ASP	I1130	THR	Q804	THR	G485	N439	L241	L241	MET
HIS	GLY	LEU	G1131	GLY	S813	GLY	G485	N439	L242	L242	GLU
HIS	SER	GLN	I1132	SER	S813	SER	G485	N439	A243	A243	SER
HIS	GLY	GLY	V1133	GLY	R814	N641	G485	N439	L244	L244	GLU
HIS	GLY	LEU	N1134	GLY	R815	M657	G485	N439	F157	F157	VAL
HIS	GLY	GLY	N1135	GLY	S816	S658	G485	N439	R158	R158	VAL
HIS	GLY	LYS	T993	LYS	D820	S659	G485	N439	S247	S247	V159
HIS	SER	TYR	D994	GLY	D820	Y660	G485	N439	L249	L249	N165
HIS	GLY	GLY	R995	GLY	V826	E661	G485	N439	S255	S255	C166
HIS	SER	GLY	T998	LYS	T827	C662	G485	N439	W258	W258	Y170
HIS	TRP	GLY	G999	GLY	T827	D663	G485	N439			V171
HIS	SER	GLY	R1000	GLY	L228		G485	N439			
HIS	TYR	ILE	L1001	ALA	ALA	T676	G485	N439			
HIS	PRO	ILE	Q1002	ASP	ASP		G485	N439			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70980	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	1.207	Depositor
Minimum map value	-0.473	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.20	0/937	0.56	0/1284
1	L	0.20	0/937	0.56	0/1284
2	J	0.22	0/813	0.73	1/1106 (0.1%)
2	M	0.18	0/813	0.62	0/1106
3	H	0.22	0/840	0.67	0/1144
3	O	0.20	0/840	0.56	0/1144
4	K	0.20	0/886	0.55	0/1203
4	P	0.18	0/886	0.54	0/1203
5	A	0.42	0/7912	0.60	4/10810 (0.0%)
5	B	0.40	0/7589	0.59	1/10370 (0.0%)
5	C	0.41	0/7905	0.60	2/10801 (0.0%)
All	All	0.37	0/30358	0.60	8/41455 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1
3	O	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	326	ILE	CA-C-N	6.42	133.53	121.97
5	C	326	ILE	C-N-CA	6.42	133.53	121.97
5	A	519	HIS	CA-C-N	-5.69	101.44	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	519	HIS	C-N-CA	-5.69	101.44	121.59
2	J	51	TYR	N-CA-C	-5.37	101.20	109.52
5	B	432	CYS	CA-CB-SG	5.20	126.37	114.40
5	A	336	CYS	CB-CA-C	-5.14	100.05	110.17
5	A	538	CYS	CA-CB-SG	5.11	126.16	114.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	95	PRO	Peptide
3	O	95	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	914	0	911	57	0
1	L	914	0	911	49	0
2	J	796	0	766	44	0
2	M	796	0	766	48	0
3	H	821	0	788	55	0
3	O	821	0	788	59	0
4	K	870	0	836	59	0
4	P	870	0	836	52	0
5	A	7725	0	7317	232	0
5	B	7413	0	7008	168	0
5	C	7719	0	7310	217	0
6	A	168	0	156	15	0
6	B	168	0	156	14	0
6	C	182	0	169	8	0
All	All	30177	0	28718	999	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 17.

All (999) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:6:GLN:HB3	2:M:104:THR:HG23	1.50	0.93
4:K:61:ASP:HA	4:K:64:LYS:HD2	1.51	0.92
5:B:379:CYS:HA	5:B:432:CYS:HB3	1.50	0.92
5:B:365:TYR:HB2	5:B:388:ASN:HD22	1.33	0.91
3:H:31:SER:HB2	3:H:51:ALA:HB2	1.54	0.89
2:J:36:SER:HB3	2:J:51:TYR:HD1	1.39	0.87
3:O:47:LEU:HA	3:O:58:ILE:HG13	1.58	0.86
3:O:2:ILE:HB	3:O:90:GLN:HE22	1.41	0.85
5:A:657:ASN:HD21	6:A:1305:NAG:H2	1.44	0.83
5:C:376:ALA:HB3	5:C:435:ALA:HB3	1.60	0.82
4:K:85:LEU:HD12	4:K:89:ASP:HB3	1.62	0.82
3:H:2:ILE:HB	3:H:90:GLN:HE22	1.45	0.81
3:H:42:GLN:NE2	3:H:43:ALA:O	2.14	0.81
2:M:12:GLY:HA3	2:M:18:ILE:HD11	1.61	0.81
5:A:353:TRP:HZ3	5:A:355:ARG:HD3	1.45	0.81
5:C:335:LEU:HD23	5:C:336:CYS:H	1.44	0.80
4:K:22:CYS:HB3	4:K:78:LEU:HB3	1.62	0.80
5:A:1098:ASN:ND2	6:A:1309:NAG:O7	2.14	0.79
3:H:47:LEU:HA	3:H:58:ILE:HG13	1.63	0.78
5:B:1017:GLU:OE2	5:C:1019:ARG:NH1	2.17	0.78
5:C:353:TRP:HZ3	5:C:355:ARG:HD3	1.47	0.77
5:C:34:ARG:NH2	5:C:219:GLY:O	2.17	0.77
5:C:472:ILE:HD11	5:C:488:CYS:HB3	1.64	0.77
2:J:85:ASP:HB2	2:J:108:VAL:HG12	1.66	0.76
5:C:353:TRP:O	5:C:466:ARG:NH2	2.18	0.76
3:O:6:GLN:HE21	3:O:104:THR:HG23	1.49	0.76
5:A:1134:ASN:ND2	6:A:1308:NAG:O7	2.19	0.76
5:A:34:ARG:NH2	5:A:219:GLY:O	2.19	0.75
2:J:36:SER:HB3	2:J:51:TYR:CD1	2.22	0.75
1:L:12:VAL:HG23	1:L:16:GLN:HE21	1.51	0.75
5:C:329:PHE:H	5:C:531:THR:HG23	1.51	0.75
5:A:391:CYS:HA	5:A:525:CYS:HB3	1.68	0.74
5:B:503:VAL:HA	5:B:506:GLN:HE21	1.52	0.74
3:H:6:GLN:HG2	3:H:23:CYS:HB2	1.69	0.73
2:J:94:THR:HG22	2:J:95:THR:H	1.53	0.73
1:L:68:ARG:NH1	1:L:85:THR:O	2.21	0.73
5:B:34:ARG:NH2	5:B:219:GLY:O	2.22	0.73
5:C:68:ILE:HG13	5:C:69:HIS:H	1.54	0.73
4:P:66:ARG:NH1	4:P:89:ASP:OD2	2.17	0.72
5:B:328:ARG:NH2	5:B:531:THR:O	2.22	0.72
5:C:280:ASN:ND2	5:C:284:THR:OG1	2.21	0.72
2:J:49:MET:HG2	2:J:50:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:972:ALA:HA	5:C:995:ARG:HH21	1.55	0.72
4:K:38:ARG:NH2	4:K:89:ASP:OD2	2.22	0.71
1:I:25:SER:HA	5:A:444:LYS:HD2	1.72	0.71
5:C:328:ARG:HD3	5:C:542:ASN:HB3	1.71	0.71
5:A:337:PRO:HG2	5:A:358:ILE:HG12	1.73	0.71
5:B:656:VAL:HG22	5:B:658:SER:H	1.55	0.70
1:I:92:THR:HG22	1:I:117:VAL:HB	1.73	0.70
5:C:379:CYS:HA	5:C:432:CYS:HB3	1.73	0.70
1:L:95:TYR:O	1:L:112:GLY:HA2	1.91	0.70
5:A:431:GLY:HA2	5:A:515:PHE:CD2	2.26	0.70
5:B:68:ILE:HG13	5:B:69:HIS:H	1.55	0.70
5:C:106:PHE:CD1	5:C:238:PHE:HB2	2.27	0.70
5:A:334:ASN:HB2	5:A:361:CYS:HA	1.73	0.70
1:I:49:TRP:HH2	1:I:60:ARG:HG2	1.57	0.70
5:B:382:VAL:HG22	5:C:983:ARG:HB2	1.72	0.70
2:J:56:ARG:NH2	2:J:61:SER:O	2.19	0.69
5:B:81:ASN:O	5:B:239:GLN:NE2	2.17	0.69
5:C:1134:ASN:ND2	6:C:1306:NAG:O7	2.26	0.69
5:B:350:VAL:HA	5:B:400:PHE:HB2	1.73	0.69
5:A:353:TRP:O	5:A:466:ARG:NH2	2.23	0.69
3:H:6:GLN:NE2	3:H:104:THR:OG1	2.26	0.69
5:A:603:ASN:HD21	6:A:1306:NAG:H4	1.58	0.69
1:L:69:LEU:HA	1:L:83:THR:O	1.93	0.69
5:C:448:ASN:OD1	5:C:450:ASN:ND2	2.26	0.69
1:L:17:THR:HG23	1:L:85:THR:HG22	1.74	0.68
4:P:13:GLN:HG2	4:P:14:PRO:HD2	1.75	0.68
4:P:17:SER:HA	4:P:83:ASN:HA	1.74	0.68
5:C:326:ILE:O	5:C:328:ARG:N	2.23	0.68
1:I:17:THR:HA	1:I:85:THR:HA	1.76	0.68
3:H:94:TRP:O	3:H:97:GLY:N	2.27	0.68
5:A:353:TRP:CZ3	5:A:355:ARG:HD3	2.29	0.68
5:B:282:ASN:ND2	6:B:1312:NAG:O7	2.26	0.68
1:I:42:PRO:HB2	1:I:45:LYS:HD3	1.75	0.68
4:P:36:TRP:HE1	4:P:78:LEU:HG	1.58	0.68
5:A:457:ARG:HG2	5:A:458:LYS:H	1.59	0.68
5:C:328:ARG:HD3	5:C:542:ASN:CG	2.19	0.68
1:L:41:GLN:NE2	2:M:89:TYR:OH	2.27	0.68
5:B:106:PHE:HD1	5:B:238:PHE:HB2	1.58	0.67
5:B:972:ALA:HA	5:B:995:ARG:HH21	1.59	0.67
4:K:47:TRP:HZ2	4:K:50:VAL:HG12	1.60	0.67
5:A:657:ASN:ND2	6:A:1305:NAG:O7	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:85:ASP:HB3	2:M:108:VAL:HG22	1.76	0.67
4:K:17:SER:OG	4:K:81:GLN:NE2	2.28	0.67
5:C:742:ILE:O	5:C:1000:ARG:NH2	2.27	0.67
5:A:131:CYS:HA	5:A:166:CYS:HA	1.75	0.67
1:L:39:ILE:HD13	1:L:49:TRP:HA	1.76	0.67
4:P:82:MET:HE1	4:P:114:VAL:HG11	1.77	0.66
5:C:886:TRP:HH2	5:C:904:TYR:HB3	1.60	0.66
5:B:419:ALA:HA	5:B:423:TYR:O	1.95	0.66
5:A:480:CYS:HB3	5:A:483:VAL:HG13	1.78	0.66
5:B:519:HIS:NE2	5:C:41:LYS:HD2	2.11	0.66
1:I:61:TYR:HB2	1:I:66:GLU:HG2	1.78	0.66
5:C:104:TRP:HB2	5:C:119:ILE:HD11	1.78	0.66
5:B:106:PHE:CD1	5:B:238:PHE:HB2	2.31	0.66
3:H:94:TRP:CD1	3:H:95:PRO:HD3	2.30	0.66
5:B:280:ASN:ND2	5:B:284:THR:OG1	2.29	0.65
4:P:47:TRP:HZ2	4:P:50:VAL:HG12	1.62	0.65
5:B:247:SER:HG	5:B:258:TRP:CG	2.13	0.65
5:A:308:VAL:HG22	5:A:602:THR:HG23	1.77	0.65
5:C:454:ARG:HG3	5:C:491:PRO:HB2	1.77	0.65
5:B:64:TRP:HE1	5:B:264:ALA:HB1	1.61	0.65
3:H:2:ILE:O	3:H:99:THR:HG21	1.97	0.65
1:I:74:ASP:HB3	1:I:79:LEU:HD21	1.78	0.65
1:L:18:LEU:HB2	1:L:87:MET:HE1	1.78	0.65
5:A:327:VAL:HG22	5:A:531:THR:HG23	1.78	0.65
2:M:20:ILE:HD11	2:M:104:THR:HG21	1.79	0.65
5:B:1076:THR:O	5:B:1097:SER:OG	2.15	0.65
2:J:6:GLN:HE22	2:J:89:TYR:HA	1.61	0.64
5:C:64:TRP:HE1	5:C:264:ALA:HB1	1.62	0.64
5:B:1097:SER:HB3	5:B:1102:TRP:CD2	2.32	0.64
4:P:105:THR:OG1	4:P:108:TRP:NE1	2.30	0.64
5:A:379:CYS:HA	5:A:432:CYS:HB3	1.79	0.64
5:C:319:ARG:O	5:C:321:GLN:NE2	2.30	0.64
1:I:40:ARG:NE	1:I:48:GLU:OE2	2.30	0.64
2:J:53:VAL:HG11	2:J:68:LYS:HG2	1.79	0.64
1:L:3:THR:HG1	1:L:25:SER:HG	1.43	0.64
5:C:457:ARG:HG2	5:C:458:LYS:H	1.63	0.64
5:B:104:TRP:HB2	5:B:119:ILE:HD11	1.80	0.64
5:C:280:ASN:OD1	5:C:284:THR:N	2.23	0.64
5:A:379:CYS:HA	5:A:432:CYS:CB	2.27	0.64
5:B:364:ASP:HB3	5:B:367:VAL:HG12	1.79	0.64
3:O:96:PRO:HG3	4:P:50:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:10:VAL:HG21	2:J:20:ILE:HD12	1.80	0.63
5:A:280:ASN:ND2	5:A:284:THR:OG1	2.31	0.63
5:A:546:LEU:HD22	5:A:565:PHE:HE1	1.62	0.63
1:I:21:THR:HG21	2:J:23:THR:HG21	1.80	0.63
1:L:100:LYS:HE2	1:L:106:PHE:HE1	1.64	0.63
5:C:117:LEU:HD13	5:C:235:ILE:HD11	1.81	0.63
5:C:328:ARG:HD3	5:C:542:ASN:CB	2.29	0.63
1:L:38:TRP:HB3	1:L:50:LEU:HD12	1.81	0.62
5:A:326:ILE:HD13	5:A:534:VAL:HG12	1.80	0.62
5:B:961:THR:HA	5:B:964:LYS:HD2	1.79	0.62
5:C:379:CYS:HA	5:C:432:CYS:CB	2.29	0.62
3:H:108:ILE:HG22	3:H:109:LYS:HG2	1.80	0.62
5:B:657:ASN:HD21	6:B:1301:NAG:H2	1.63	0.62
5:A:1089:PHE:HE2	5:B:917:TYR:HD2	1.46	0.62
5:A:68:ILE:HG12	5:A:69:HIS:ND1	2.15	0.62
5:A:353:TRP:CE2	5:A:466:ARG:HB2	2.35	0.62
5:A:424:LYS:HB3	5:A:461:LEU:HG	1.82	0.62
5:B:725:GLU:OE2	5:B:1028:LYS:NZ	2.26	0.62
1:L:107:ASP:HA	2:M:48:LEU:HD23	1.82	0.62
5:B:906:PHE:CD2	5:B:916:LEU:HB2	2.35	0.62
3:H:77:SER:O	3:H:79:GLN:NE2	2.33	0.62
5:A:81:ASN:ND2	5:A:265:TYR:OH	2.27	0.61
5:A:709:ASN:HD21	6:A:1311:NAG:H2	1.65	0.61
3:H:91:TYR:HE2	4:K:101:VAL:HA	1.64	0.61
3:H:61:ARG:HH11	3:H:78:LEU:HA	1.64	0.61
5:A:64:TRP:HE1	5:A:264:ALA:HB1	1.65	0.61
5:B:363:ALA:N	5:B:525:CYS:O	2.31	0.61
5:A:400:PHE:HE2	5:A:402:ILE:HD11	1.65	0.61
2:M:15:GLY:N	2:M:80:LEU:O	2.34	0.61
5:C:419:ALA:O	5:C:424:LYS:HB2	2.00	0.61
5:C:480:CYS:HB2	5:C:483:VAL:HG13	1.83	0.61
3:H:94:TRP:CG	3:H:95:PRO:HD3	2.36	0.61
1:I:15:THR:HA	1:I:86:ASN:HA	1.83	0.60
3:O:66:GLY:HA3	3:O:71:PHE:HA	1.83	0.60
5:C:30:ASN:HA	5:C:61:ASN:HA	1.83	0.60
5:C:977:LEU:HD21	5:C:1000:ARG:HH22	1.65	0.60
2:M:94:THR:HG22	2:M:97:SER:O	2.00	0.60
5:A:106:PHE:CD1	5:A:238:PHE:HB2	2.35	0.60
5:A:971:GLY:O	5:A:995:ARG:NH2	2.34	0.60
5:C:128:ILE:HD13	5:C:170:TYR:HD1	1.67	0.60
1:I:6:GLU:OE1	1:I:111:GLN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:712:ILE:HD11	5:B:896:ILE:HG13	1.84	0.60
2:J:35:VAL:HG22	2:J:92:SER:OG	2.02	0.60
5:C:1097:SER:HB3	5:C:1102:TRP:CD2	2.36	0.60
5:A:67:ALA:HB3	5:A:263:ALA:HB3	1.82	0.60
5:A:603:ASN:ND2	6:A:1306:NAG:H4	2.17	0.60
5:A:1097:SER:HB2	5:A:1102:TRP:CD2	2.36	0.60
5:C:372:ALA:HB1	5:C:373:PRO:HD2	1.84	0.60
4:P:82:MET:HB3	4:P:85:LEU:HD21	1.83	0.60
5:A:68:ILE:HG23	5:A:69:HIS:H	1.65	0.60
5:A:402:ILE:HG22	5:A:403:ARG:H	1.67	0.60
5:C:247:SER:HG	5:C:258:TRP:CD1	2.19	0.60
1:L:106:PHE:O	1:L:109:TRP:NE1	2.34	0.60
5:A:361:CYS:N	5:A:523:THR:O	2.27	0.60
5:A:486:VAL:HG13	5:A:487:ASN:H	1.66	0.60
5:B:335:LEU:HD23	5:B:362:VAL:HB	1.82	0.60
2:J:77:ILE:HD12	2:J:80:LEU:HD21	1.84	0.60
3:H:61:ARG:NH1	3:H:78:LEU:HA	2.17	0.59
3:H:2:ILE:HB	3:H:90:GLN:NE2	2.16	0.59
1:I:38:TRP:HB3	1:I:50:LEU:HD23	1.84	0.59
2:M:93:TYR:HA	2:M:98:VAL:HA	1.84	0.59
2:J:53:VAL:HG22	2:J:66:GLY:HA3	1.83	0.59
5:A:327:VAL:N	5:A:531:THR:OG1	2.28	0.59
4:K:63:VAL:HG12	4:K:66:ARG:HH11	1.67	0.59
1:L:69:LEU:HD12	1:L:82:LEU:HD11	1.83	0.59
5:C:486:VAL:HG13	5:C:487:ASN:H	1.67	0.59
3:H:78:LEU:HB3	3:H:108:ILE:HD11	1.83	0.59
5:A:70:VAL:HG21	5:A:255:SER:HA	1.84	0.59
5:C:316:SER:OG	5:C:317:ASN:N	2.36	0.59
4:K:17:SER:C	4:K:18:LEU:HD12	2.28	0.59
5:B:379:CYS:CA	5:B:432:CYS:HB3	2.26	0.59
2:M:38:TYR:HE2	2:M:91:ASN:HB3	1.68	0.58
1:L:105:ILE:O	2:M:38:TYR:OH	2.11	0.58
5:A:316:SER:OG	5:A:317:ASN:N	2.33	0.58
5:B:316:SER:OG	5:B:317:ASN:N	2.36	0.58
4:K:19:ARG:HH12	4:K:70:SER:HB3	1.68	0.58
1:I:39:ILE:HD11	1:I:106:PHE:CD2	2.38	0.58
5:A:365:TYR:HD2	5:A:388:ASN:HA	1.66	0.58
5:A:657:ASN:HD21	6:A:1305:NAG:C2	2.15	0.58
3:H:6:GLN:HA	3:H:23:CYS:HA	1.86	0.58
5:B:70:VAL:HG13	5:B:80:ASP:HA	1.83	0.58
4:K:38:ARG:NE	4:K:46:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:6:GLN:HE22	2:M:89:TYR:HA	1.69	0.58
5:B:108:THR:OG1	5:B:234:ASN:O	2.21	0.58
5:A:351:TYR:HB3	5:A:422:ASN:HB2	1.86	0.57
1:L:73:LYS:HB3	1:L:80:VAL:HG23	1.85	0.57
5:A:372:ALA:HB1	5:A:373:PRO:HD2	1.86	0.57
5:A:726:ILE:HG13	5:A:1061:VAL:HG12	1.86	0.57
5:B:30:ASN:HA	5:B:61:ASN:HA	1.86	0.57
5:C:106:PHE:HD1	5:C:238:PHE:HB2	1.67	0.57
5:C:336:CYS:HB2	5:C:337:PRO:HD2	1.85	0.57
2:J:2:SER:HB3	5:A:499:PRO:O	2.04	0.57
1:L:12:VAL:HG21	1:L:87:MET:HE3	1.85	0.57
5:A:197:ILE:HG13	5:A:198:ASP:N	2.19	0.57
5:A:483:VAL:HG22	5:A:484:ALA:H	1.68	0.57
5:B:420:ASP:OD2	5:B:460:ASN:ND2	2.37	0.57
5:A:438:SER:OG	5:A:509:ARG:HG3	2.05	0.57
5:A:455:LEU:N	5:A:491:PRO:O	2.30	0.57
5:C:308:VAL:N	5:C:602:THR:OG1	2.34	0.57
4:P:14:PRO:HD3	4:P:117:SER:HB3	1.87	0.57
5:C:1125:ASN:ND2	5:C:1127:ASP:OD1	2.38	0.57
3:O:34:ALA:HA	3:O:49:TYR:HA	1.86	0.57
5:B:762:GLN:HG3	5:B:765:ARG:HH22	1.70	0.57
1:L:54:TYR:HE2	1:L:60:ARG:HE	1.52	0.56
5:B:326:ILE:HD13	5:B:534:VAL:HG22	1.86	0.56
5:C:353:TRP:CE2	5:C:466:ARG:HB2	2.40	0.56
1:L:32:GLY:HA2	1:L:55:TRP:CE2	2.39	0.56
4:P:22:CYS:HB3	4:P:78:LEU:HB3	1.87	0.56
4:P:37:VAL:HG23	4:P:94:TYR:HB2	1.85	0.56
5:B:1097:SER:HB3	5:B:1102:TRP:CE2	2.39	0.56
5:C:542:ASN:HA	5:C:546:LEU:O	2.04	0.56
5:A:438:SER:OG	5:A:438:SER:O	2.24	0.56
5:B:729:VAL:HG23	5:B:1059:GLY:HA2	1.86	0.56
5:C:1076:THR:O	5:C:1097:SER:OG	2.24	0.56
1:I:33:GLY:H	1:I:55:TRP:NE1	2.03	0.56
5:C:419:ALA:HA	5:C:423:TYR:O	2.05	0.56
5:A:1054:GLN:HB2	5:A:1061:VAL:HG23	1.87	0.56
5:B:335:LEU:HD21	5:B:364:ASP:HB2	1.87	0.56
1:L:31:THR:O	1:L:34:VAL:HG22	2.06	0.56
5:C:70:VAL:HG21	5:C:255:SER:HA	1.87	0.56
5:C:367:VAL:O	5:C:370:ASN:ND2	2.38	0.56
5:C:776:LYS:NZ	5:C:780:GLU:OE1	2.39	0.56
2:M:40:GLN:OE1	2:M:46:PRO:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:112:SER:O	6:B:1311:NAG:H2	2.05	0.56
5:C:483:VAL:HG22	5:C:484:ALA:H	1.71	0.56
4:K:12:VAL:HG21	4:K:18:LEU:HD11	1.88	0.56
2:J:60:VAL:HG12	2:J:61:SER:H	1.70	0.56
5:A:417:ASN:ND2	4:K:33:TYR:OH	2.38	0.56
1:L:104:THR:HG22	1:L:107:ASP:HB3	1.87	0.56
3:O:32:ASP:HB2	3:O:92:ASN:ND2	2.21	0.56
5:B:327:VAL:HG12	5:B:542:ASN:HB3	1.87	0.56
5:C:131:CYS:HB3	5:C:166:CYS:CA	2.36	0.56
5:A:917:TYR:HB3	5:C:1129:VAL:HG23	1.88	0.55
5:B:383:SER:OG	5:B:386:LYS:NZ	2.32	0.55
5:C:108:THR:HG22	5:C:114:THR:HG21	1.87	0.55
3:O:63:SER:HB2	3:O:74:THR:OG1	2.06	0.55
1:I:77:LYS:HB3	1:I:79:LEU:HD22	1.86	0.55
5:C:455:LEU:N	5:C:491:PRO:O	2.28	0.55
2:M:88:TYR:O	2:M:104:THR:OG1	2.24	0.55
4:P:99:LEU:HB2	4:P:103:GLY:O	2.06	0.55
5:C:480:CYS:N	5:C:488:CYS:SG	2.78	0.55
5:A:497:PHE:CD2	5:A:507:PRO:HB3	2.42	0.55
3:H:6:GLN:HB2	3:H:102:GLN:HE21	1.72	0.55
3:H:61:ARG:NH2	3:H:82:ASP:OD2	2.34	0.55
5:C:461:LEU:HD23	5:C:461:LEU:H	1.71	0.55
4:K:17:SER:HA	4:K:83:ASN:HA	1.87	0.55
5:B:131:CYS:HB3	5:B:166:CYS:CA	2.37	0.55
5:B:453:TYR:HB3	5:B:495:TYR:CZ	2.42	0.55
5:C:439:ASN:HA	5:C:507:PRO:HG2	1.89	0.55
3:O:10:THR:HG23	3:O:105:LYS:HB2	1.89	0.55
3:O:94:TRP:HB3	3:O:95:PRO:HD3	1.90	0.55
5:A:444:LYS:O	5:A:498:ARG:HA	2.07	0.55
5:A:456:PHE:HB2	5:A:491:PRO:HA	1.89	0.55
5:B:280:ASN:OD1	5:B:284:THR:N	2.29	0.55
5:B:190:ARG:HH21	5:B:207:HIS:CD2	2.25	0.54
4:K:99:LEU:HB2	4:K:103:GLY:O	2.06	0.54
5:A:559:PHE:HB3	5:A:577:ARG:NH1	2.22	0.54
5:A:603:ASN:OD1	6:A:1306:NAG:H2	2.07	0.54
5:C:347:PHE:CE2	5:C:399:SER:HB3	2.42	0.54
5:A:896:ILE:HG13	5:C:712:ILE:HD11	1.89	0.54
4:K:66:ARG:HG3	4:K:67:PHE:CD1	2.43	0.54
1:L:19:THR:HG23	1:L:83:THR:HG22	1.89	0.54
5:B:386:LYS:HE2	5:C:982:SER:O	2.07	0.54
2:J:36:SER:OG	2:J:91:ASN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2:ILE:HG12	3:O:27:GLN:HB2	1.90	0.54
5:A:663:ASP:N	5:A:663:ASP:OD1	2.40	0.54
5:C:70:VAL:HG13	5:C:80:ASP:HA	1.88	0.54
5:C:118:LEU:N	5:C:129:LYS:O	2.34	0.54
4:K:20:LEU:O	4:K:80:LEU:N	2.29	0.54
4:K:38:ARG:HD2	4:K:93:TYR:CZ	2.42	0.54
1:I:100:LYS:HB2	1:I:106:PHE:CE1	2.42	0.54
5:A:433:VAL:HG22	5:A:512:VAL:HG22	1.89	0.54
1:I:77:LYS:HE2	5:A:499:PRO:HG2	1.90	0.54
5:A:417:ASN:HD21	5:A:455:LEU:HD12	1.73	0.54
5:C:1002:GLN:O	5:C:1006:THR:HG23	2.08	0.54
4:K:63:VAL:HA	4:K:66:ARG:HE	1.72	0.54
4:K:5:VAL:HA	4:K:110:GLN:OE1	2.08	0.53
4:K:19:ARG:NH1	4:K:70:SER:HB3	2.23	0.53
1:I:53:ILE:HG22	1:I:59:LYS:HD3	1.90	0.53
5:A:140:PHE:HB2	5:A:249:LEU:HD11	1.89	0.53
3:H:37:GLN:HB2	3:H:47:LEU:HD11	1.90	0.53
1:I:62:SER:O	1:I:66:GLU:HG3	2.08	0.53
5:A:298:GLU:O	5:A:302:THR:HG23	2.08	0.53
5:B:663:ASP:OD1	5:B:663:ASP:N	2.40	0.53
1:I:24:PHE:CE1	1:I:78:ASN:HB3	2.44	0.53
1:L:61:TYR:CE1	1:L:71:ILE:HG22	2.43	0.53
2:M:9:SER:OG	2:M:105:LYS:HB2	2.09	0.53
5:A:470:THR:HG22	5:A:492:LEU:HD22	1.89	0.53
5:A:1094:VAL:HG23	5:A:1096:VAL:HG23	1.91	0.53
5:B:1118:ASP:OD1	5:B:1119:ASN:N	2.41	0.53
3:O:43:ALA:HB1	4:P:108:TRP:HB2	1.90	0.53
2:J:22:CYS:SG	2:J:32:TYR:OH	2.67	0.53
2:J:39:GLN:NE2	2:J:49:MET:SD	2.82	0.53
5:A:555:SER:OG	5:A:584:ILE:HB	2.09	0.53
5:A:735:SER:OG	5:A:861:LEU:HD21	2.08	0.53
2:J:87:TYR:CZ	2:J:105:LYS:HD2	2.44	0.53
1:L:39:ILE:HG21	1:L:47:LEU:HD23	1.90	0.53
5:C:106:PHE:O	5:C:116:SER:OG	2.27	0.53
4:P:22:CYS:O	4:P:78:LEU:N	2.30	0.53
4:P:97:ARG:HD2	4:P:97:ARG:O	2.09	0.53
5:A:133:PHE:HA	5:A:163:ALA:O	2.09	0.53
4:K:68:THR:HG23	4:K:81:GLN:HB3	1.89	0.53
2:J:33:GLN:N	2:J:33:GLN:OE1	2.42	0.53
5:A:353:TRP:CD1	5:A:353:TRP:H	2.27	0.53
5:B:70:VAL:HG11	5:B:255:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:316:SER:O	5:C:595:VAL:HG12	2.09	0.53
1:I:61:TYR:CE1	1:I:71:ILE:HG22	2.44	0.53
3:O:62:PHE:CD1	3:O:75:ILE:HD13	2.44	0.52
5:A:422:ASN:OD1	5:A:422:ASN:N	2.42	0.52
1:I:24:PHE:HZ	1:I:29:LEU:HG	1.74	0.52
1:I:69:LEU:HA	1:I:83:THR:O	2.09	0.52
2:J:24:ALA:HB1	2:J:29:VAL:HG11	1.91	0.52
5:A:330:PRO:HD3	5:A:544:ASN:HD21	1.74	0.52
5:C:497:PHE:CE2	5:C:507:PRO:HB3	2.44	0.52
1:L:22:CYS:HB3	1:L:80:VAL:HG12	1.90	0.52
1:I:36:VAL:HG11	1:I:80:VAL:HG21	1.91	0.52
5:A:417:ASN:O	5:A:421:TYR:HB2	2.10	0.52
5:C:479:PRO:HG2	5:C:481:ASN:OD1	2.09	0.52
3:H:19:ALA:HB2	3:H:78:LEU:HD11	1.90	0.52
3:O:61:ARG:NH2	3:O:79:GLN:HG2	2.25	0.52
5:B:1134:ASN:ND2	6:B:1305:NAG:O7	2.42	0.52
5:C:113:LYS:HA	6:C:1312:NAG:H81	1.91	0.52
1:I:35:SER:OG	1:I:54:TYR:HA	2.09	0.52
3:O:61:ARG:O	3:O:75:ILE:HD12	2.09	0.52
4:P:90:THR:HG22	4:P:115:THR:HA	1.90	0.52
5:B:295:PRO:O	5:B:299:THR:HG23	2.10	0.52
5:B:764:LYS:O	5:B:768:THR:HG23	2.10	0.52
5:C:31:SER:N	5:C:60:SER:O	2.28	0.52
5:C:546:LEU:HD22	5:C:565:PHE:HE1	1.73	0.52
5:A:334:ASN:O	5:A:361:CYS:HB2	2.10	0.52
5:B:68:ILE:HG13	5:B:69:HIS:N	2.24	0.52
5:B:335:LEU:HA	5:B:362:VAL:HB	1.92	0.52
5:A:81:ASN:O	5:A:239:GLN:NE2	2.27	0.52
5:A:1019:ARG:NH1	5:C:1017:GLU:OE2	2.43	0.52
3:H:2:ILE:HG12	3:H:27:GLN:HG2	1.91	0.52
6:B:1312:NAG:C7	6:B:1312:NAG:HO3	2.22	0.52
5:A:189:LEU:HB2	5:A:210:ILE:HD11	1.92	0.52
5:A:440:LYS:HB2	5:A:441:LEU:HD12	1.92	0.52
5:A:459:SER:OG	5:A:460:ASN:N	2.43	0.52
5:A:467:ASP:N	5:A:467:ASP:OD1	2.43	0.52
5:A:906:PHE:CD2	5:A:916:LEU:HB2	2.44	0.52
5:B:905:ARG:NH2	5:B:1049:LEU:O	2.43	0.52
1:L:111:GLN:OE1	1:L:111:GLN:N	2.44	0.51
3:O:46:LEU:HG	3:O:55:ALA:HB2	1.92	0.51
4:P:78:LEU:HD23	4:P:95:CYS:SG	2.50	0.51
5:A:334:ASN:OD1	5:A:334:ASN:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:419:ALA:HA	5:A:423:TYR:O	2.10	0.51
5:B:330:PRO:HD3	5:B:579:PRO:HB2	1.92	0.51
5:C:196:ASN:ND2	5:C:201:PHE:HB2	2.25	0.51
5:C:446:GLY:O	5:C:498:ARG:NH1	2.43	0.51
1:L:5:LYS:HA	1:L:111:GLN:OE1	2.10	0.51
4:P:67:PHE:HB3	4:P:80:LEU:HD21	1.92	0.51
5:B:712:ILE:HG13	5:B:1077:THR:HG21	1.92	0.51
4:K:34:MET:HE1	4:K:97:ARG:HB2	1.92	0.51
4:K:51:MET:SD	4:K:69:ILE:HG12	2.51	0.51
1:L:41:GLN:NE2	1:L:45:LYS:O	2.32	0.51
5:C:353:TRP:CZ2	5:C:466:ARG:HB2	2.45	0.51
5:C:357:ARG:HG3	5:C:396:TYR:HE1	1.75	0.51
5:C:804:GLN:O	5:C:816:SER:OG	2.29	0.51
5:C:117:LEU:HD21	5:C:119:ILE:HG23	1.92	0.51
5:C:663:ASP:OD1	5:C:663:ASP:N	2.42	0.51
1:L:72:THR:HG22	1:L:73:LYS:H	1.75	0.51
4:K:19:ARG:HE	4:K:79:TYR:HB3	1.76	0.51
2:M:61:SER:OG	2:M:63:ARG:HG2	2.10	0.51
5:A:96:GLU:OE1	5:A:98:SER:N	2.34	0.51
5:A:281:GLU:OE1	5:A:281:GLU:N	2.41	0.51
5:A:334:ASN:ND2	5:A:362:VAL:HG13	2.25	0.51
5:C:443:SER:OG	5:C:497:PHE:HB3	2.11	0.51
2:M:13:SER:O	2:M:16:GLN:HG2	2.10	0.51
3:O:78:LEU:HD21	3:O:106:LEU:HD11	1.92	0.51
5:A:396:TYR:HB2	5:A:514:SER:OG	2.09	0.51
5:B:979:ASP:OD2	5:B:983:ARG:NE	2.44	0.51
4:K:20:LEU:N	4:K:80:LEU:O	2.28	0.51
5:B:126:VAL:HG23	5:B:174:PRO:HA	1.92	0.51
2:M:82:ALA:HA	2:M:108:VAL:HG21	1.91	0.51
5:B:365:TYR:HB2	5:B:388:ASN:ND2	2.16	0.51
1:I:71:ILE:HG13	1:I:81:VAL:O	2.11	0.50
5:B:344:ALA:HB1	5:B:346:ARG:HG2	1.91	0.50
5:A:342:PHE:HE2	5:A:368:LEU:HG	1.76	0.50
5:C:81:ASN:O	5:C:239:GLN:NE2	2.39	0.50
5:C:335:LEU:CD2	5:C:336:CYS:H	2.18	0.50
5:B:439:ASN:HA	5:B:507:PRO:HG2	1.93	0.50
5:C:758:SER:O	5:C:762:GLN:HG3	2.11	0.50
2:J:28:ASP:OD2	3:H:67:SER:HB2	2.11	0.50
2:M:49:MET:HG3	2:M:50:ILE:H	1.76	0.50
5:A:490:PHE:CD1	5:A:491:PRO:HD2	2.47	0.50
5:B:36:VAL:HG11	5:B:220:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:377:PHE:HB3	5:B:434:ILE:HG22	1.92	0.50
5:A:546:LEU:HD22	5:A:565:PHE:CE1	2.45	0.50
5:C:200:TYR:CD2	5:C:230:PRO:HA	2.47	0.50
1:I:31:THR:O	1:I:34:VAL:HG12	2.12	0.50
1:L:35:SER:HB3	1:L:100:LYS:HG3	1.93	0.50
3:O:78:LEU:HB3	3:O:108:ILE:HD11	1.94	0.50
5:A:172:SER:OG	5:A:173:GLN:N	2.45	0.50
5:A:330:PRO:HD3	5:A:544:ASN:ND2	2.27	0.50
5:B:353:TRP:NE1	5:B:423:TYR:HD2	2.10	0.50
5:B:1075:PHE:HB3	5:B:1096:VAL:HG13	1.92	0.50
5:A:368:LEU:HB3	5:A:374:PHE:CE2	2.47	0.50
5:C:977:LEU:HD21	5:C:1000:ARG:NH2	2.27	0.50
5:C:998:THR:O	5:C:1002:GLN:HG2	2.12	0.50
5:B:34:ARG:NH2	5:B:217:PRO:O	2.45	0.50
4:K:7:SER:OG	4:K:21:SER:HB3	2.12	0.50
2:M:55:LYS:HD3	2:M:56:ARG:N	2.27	0.49
5:A:355:ARG:NH1	5:A:396:TYR:HD2	2.10	0.49
1:I:20:LEU:N	1:I:82:LEU:O	2.39	0.49
1:I:25:SER:HA	5:A:444:LYS:CD	2.41	0.49
3:O:63:SER:N	3:O:74:THR:O	2.40	0.49
5:A:247:SER:HA	5:A:258:TRP:CE2	2.47	0.49
5:A:393:THR:HG23	5:A:521:PRO:HD2	1.94	0.49
5:B:391:CYS:HB3	5:B:522:ALA:HB1	1.93	0.49
3:H:21:LEU:HD13	3:H:104:THR:HG21	1.92	0.49
3:H:63:SER:N	3:H:74:THR:O	2.45	0.49
2:M:51:TYR:HD1	2:M:52:GLU:HG3	1.77	0.49
3:O:33:LEU:HD22	3:O:71:PHE:CG	2.47	0.49
4:P:4:LEU:HD23	4:P:22:CYS:SG	2.53	0.49
5:A:1104:VAL:HG23	5:A:1115:ILE:HG12	1.93	0.49
5:B:70:VAL:HG21	5:B:255:SER:HA	1.95	0.49
5:B:364:ASP:O	5:B:368:LEU:HG	2.12	0.49
1:L:100:LYS:HE2	1:L:106:PHE:CE1	2.46	0.49
3:O:91:TYR:HE2	4:P:101:VAL:HG22	1.77	0.49
5:B:1125:ASN:ND2	5:B:1127:ASP:OD1	2.46	0.49
5:C:905:ARG:NH2	5:C:1049:LEU:O	2.46	0.49
5:C:546:LEU:HD22	5:C:565:PHE:CE1	2.47	0.49
3:H:94:TRP:HA	3:H:94:TRP:CE3	2.47	0.49
3:O:48:ILE:HG12	3:O:54:ARG:HG2	1.94	0.49
5:A:1097:SER:HB2	5:A:1102:TRP:CE3	2.47	0.49
5:B:377:PHE:C	5:B:378:LYS:HD3	2.36	0.49
5:C:660:TYR:HB2	5:C:695:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:36:TYR:O	3:H:86:TYR:HA	2.13	0.49
3:O:33:LEU:HD22	3:O:71:PHE:CD2	2.47	0.49
5:A:330:PRO:O	5:A:332:ILE:N	2.40	0.49
5:A:816:SER:OG	5:A:817:PRO:HD2	2.12	0.49
5:B:116:SER:OG	5:B:117:LEU:N	2.46	0.49
5:B:331:ASN:OD1	5:B:331:ASN:N	2.46	0.49
5:B:732:THR:OG1	5:B:955:ASN:OD1	2.27	0.49
5:C:662:CYS:HB2	5:C:697:MET:HG2	1.95	0.49
1:I:85:THR:HG23	1:I:86:ASN:ND2	2.28	0.49
5:B:393:THR:OG1	5:B:394:ASN:N	2.44	0.49
5:C:84:LEU:HB2	5:C:238:PHE:CE1	2.48	0.49
5:B:233:ILE:HG23	5:B:235:ILE:HG13	1.95	0.49
3:H:91:TYR:HB3	3:H:98:TYR:CD1	2.48	0.49
4:K:63:VAL:HA	4:K:66:ARG:NE	2.28	0.49
1:L:5:LYS:HG3	1:L:111:GLN:NE2	2.28	0.49
5:A:567:ARG:HD3	5:A:571:ASP:HA	1.94	0.49
5:B:657:ASN:ND2	6:B:1301:NAG:H2	2.26	0.49
5:C:338:PHE:HA	5:C:341:VAL:HG12	1.95	0.49
5:C:454:ARG:NH1	5:C:469:SER:O	2.38	0.49
3:H:29:VAL:HG13	3:H:92:ASN:HD21	1.77	0.49
4:K:61:ASP:OD1	4:K:62:SER:N	2.45	0.49
3:O:91:TYR:HB3	3:O:98:TYR:HE1	1.77	0.48
4:P:16:GLY:O	4:P:84:SER:N	2.46	0.48
5:A:167:THR:O	5:C:357:ARG:NH2	2.46	0.48
5:A:329:PHE:HA	5:A:544:ASN:HD21	1.78	0.48
5:A:330:PRO:HA	5:A:579:PRO:O	2.13	0.48
5:B:578:ASP:OD2	5:B:583:GLU:HB3	2.13	0.48
5:C:126:VAL:O	5:C:171:VAL:HA	2.13	0.48
1:L:4:LEU:HD11	1:L:108:TYR:HB3	1.95	0.48
5:A:424:LYS:O	5:A:463:PRO:HA	2.13	0.48
5:A:486:VAL:HG13	5:A:487:ASN:N	2.28	0.48
4:P:70:SER:O	4:P:78:LEU:HD12	2.13	0.48
3:H:10:THR:O	3:H:11:LEU:HD12	2.14	0.48
1:I:18:LEU:HB3	1:I:87:MET:HE2	1.96	0.48
3:O:8:PRO:HD2	3:O:21:LEU:HG	1.96	0.48
5:B:738:CYS:SG	5:B:739:THR:N	2.87	0.48
5:C:1104:VAL:HG23	5:C:1115:ILE:HG12	1.95	0.48
3:O:36:TYR:OH	4:P:104:ALA:HB1	2.13	0.48
5:C:189:LEU:HB2	5:C:210:ILE:HD11	1.95	0.48
1:I:87:MET:HB3	1:I:117:VAL:HG11	1.95	0.48
3:O:35:TRP:CE2	3:O:88:CYS:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:328:ARG:HG2	5:A:579:PRO:HD2	1.94	0.48
5:B:580:GLN:O	6:B:1302:NAG:H5	2.13	0.48
2:J:56:ARG:NH1	2:J:64:PHE:HB2	2.28	0.48
5:B:133:PHE:HA	5:B:163:ALA:O	2.13	0.48
5:C:353:TRP:CD1	5:C:353:TRP:H	2.30	0.48
1:I:9:PRO:HB3	2:J:69:SER:O	2.14	0.48
3:O:15:PRO:HG3	3:O:108:ILE:HG21	1.94	0.48
5:A:657:ASN:ND2	6:A:1305:NAG:H2	2.23	0.48
5:C:375:PHE:HB3	5:C:436:TRP:HA	1.95	0.48
5:C:502:GLY:O	5:C:506:GLN:HG3	2.13	0.48
4:K:19:ARG:HH11	4:K:79:TYR:HB2	1.78	0.48
1:I:77:LYS:HB3	1:I:79:LEU:CD2	2.44	0.48
2:M:48:LEU:HD12	2:M:48:LEU:O	2.14	0.48
5:A:165:ASN:ND2	6:A:1302:NAG:H4	2.29	0.48
5:C:1097:SER:HB3	5:C:1102:TRP:CE2	2.48	0.48
5:A:197:ILE:HG13	5:A:198:ASP:H	1.79	0.47
5:A:473:TYR:HB3	5:A:489:TYR:O	2.14	0.47
5:B:709:ASN:HD21	6:B:1308:NAG:H2	1.79	0.47
5:C:88:ASP:N	5:C:88:ASP:OD1	2.46	0.47
2:M:67:SER:HB2	2:M:74:SER:OG	2.14	0.47
5:A:129:LYS:HB3	5:A:131:CYS:SG	2.54	0.47
5:B:332:ILE:O	5:B:333:THR:O	2.32	0.47
5:B:1045:LYS:O	5:B:1066:THR:HG21	2.14	0.47
4:K:97:ARG:HD2	4:K:97:ARG:O	2.13	0.47
5:B:134:GLN:O	5:B:162:SER:N	2.46	0.47
6:B:1308:NAG:O4	6:C:1301:NAG:H5	2.14	0.47
5:C:444:LYS:O	5:C:498:ARG:HA	2.14	0.47
5:C:813:SER:OG	5:C:815:ARG:HG3	2.14	0.47
1:I:4:LEU:HA	1:I:24:PHE:HA	1.96	0.47
2:J:35:VAL:HA	2:J:91:ASN:O	2.15	0.47
5:C:36:VAL:HG21	5:C:220:PHE:CZ	2.50	0.47
3:H:34:ALA:HA	3:H:48:ILE:O	2.14	0.47
5:B:453:TYR:O	5:B:493:GLN:N	2.44	0.47
5:C:1000:ARG:O	5:C:1003:SER:OG	2.26	0.47
3:H:33:LEU:HD22	3:H:71:PHE:CD2	2.49	0.47
2:M:24:ALA:HB3	2:M:71:ASN:ND2	2.29	0.47
5:A:347:PHE:CE1	5:A:509:ARG:HD3	2.50	0.47
5:B:67:ALA:HB3	5:B:263:ALA:HB3	1.95	0.47
3:H:59:PRO:HB2	3:H:61:ARG:HG2	1.95	0.47
2:M:23:THR:HA	2:M:72:THR:HB	1.95	0.47
5:A:37:TYR:HB3	5:A:223:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:365:TYR:CD2	5:A:388:ASN:HA	2.49	0.47
5:A:502:GLY:O	5:A:506:GLN:HG3	2.15	0.47
5:A:538:CYS:HA	5:A:550:GLY:O	2.14	0.47
5:A:1140:PRO:O	5:A:1143:PRO:HD2	2.14	0.47
5:B:712:ILE:HD11	5:C:896:ILE:HG13	1.96	0.47
5:C:329:PHE:H	5:C:531:THR:CG2	2.22	0.47
4:K:106:ASP:O	4:K:108:TRP:HD1	1.98	0.47
3:O:6:GLN:NE2	3:O:104:THR:HG23	2.25	0.47
3:H:63:SER:HB2	3:H:74:THR:OG1	2.14	0.47
3:O:8:PRO:O	3:O:104:THR:HG22	2.15	0.47
5:A:316:SER:O	5:A:595:VAL:HG12	2.14	0.47
5:B:353:TRP:CE2	5:B:423:TYR:HD2	2.33	0.47
5:C:106:PHE:CD2	5:C:117:LEU:HD22	2.50	0.47
5:C:971:GLY:O	5:C:995:ARG:NH2	2.48	0.47
1:L:52:LEU:O	1:L:60:ARG:N	2.37	0.47
2:M:80:LEU:HD21	2:M:108:VAL:HG12	1.96	0.47
5:A:196:ASN:ND2	5:A:201:PHE:HB2	2.30	0.47
5:B:1089:PHE:HE2	5:C:917:TYR:HD2	1.61	0.47
5:B:1104:VAL:HG23	5:B:1115:ILE:HG12	1.96	0.47
2:M:87:TYR:CE2	2:M:105:LYS:HG2	2.49	0.46
4:P:22:CYS:O	4:P:77:THR:OG1	2.15	0.46
5:A:395:VAL:HG23	5:A:524:VAL:HG11	1.97	0.46
5:A:461:LEU:HD23	5:A:461:LEU:H	1.80	0.46
5:A:645:THR:OG1	5:A:648:GLY:O	2.24	0.46
5:A:1074:ASN:HD21	6:A:1307:NAG:C7	2.27	0.46
5:B:715:PRO:HA	5:B:1072:GLU:HA	1.96	0.46
1:I:6:GLU:OE2	1:I:97:CYS:N	2.30	0.46
4:P:31:ARG:O	5:C:473:TYR:OH	2.27	0.46
5:C:1086:LYS:HA	5:C:1125:ASN:HA	1.95	0.46
2:J:63:ARG:NH2	2:J:81:GLN:OE1	2.49	0.46
5:A:530:SER:O	5:A:531:THR:C	2.58	0.46
5:B:38:TYR:CE1	5:B:285:ILE:HG13	2.50	0.46
5:C:659:SER:OG	5:C:698:SER:HB3	2.15	0.46
5:C:776:LYS:O	5:C:780:GLU:HG3	2.16	0.46
2:J:10:VAL:O	2:J:106:LEU:HA	2.15	0.46
5:A:353:TRP:CZ2	5:A:466:ARG:HB2	2.50	0.46
5:A:886:TRP:HD1	5:A:1035:GLY:HA2	1.79	0.46
5:C:103:GLY:HA3	5:C:241:LEU:HD12	1.98	0.46
5:C:369:TYR:HA	5:C:374:PHE:CE2	2.51	0.46
5:C:422:ASN:OD1	5:C:422:ASN:N	2.48	0.46
4:K:12:VAL:HG21	4:K:18:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:69:ILE:HG13	4:K:79:TYR:O	2.16	0.46
5:A:356:LYS:O	5:A:396:TYR:HA	2.16	0.46
5:A:395:VAL:HG22	5:A:515:PHE:CD1	2.50	0.46
5:B:738:CYS:HB3	5:B:760:CYS:HB2	1.80	0.46
5:B:886:TRP:CD1	5:B:1035:GLY:HA2	2.50	0.46
5:C:330:PRO:HB3	5:C:544:ASN:ND2	2.29	0.46
2:M:39:GLN:HE21	2:M:86:ALA:HB1	1.79	0.46
2:M:41:TYR:HB3	2:M:44:LYS:HG3	1.97	0.46
4:P:63:VAL:HB	4:P:67:PHE:CD2	2.50	0.46
5:C:67:ALA:HB3	5:C:263:ALA:HB3	1.96	0.46
2:M:3:ALA:CB	2:M:99:VAL:HG11	2.45	0.46
3:O:38:GLN:O	3:O:85:VAL:HG12	2.16	0.46
5:A:405:ASN:OD1	5:A:405:ASN:N	2.47	0.46
5:C:108:THR:HA	5:C:236:THR:HB	1.98	0.46
5:C:391:CYS:HA	5:C:525:CYS:HB3	1.97	0.46
5:C:1018:ILE:O	5:C:1021:SER:OG	2.26	0.46
5:C:1102:TRP:HB2	5:C:1135:ASN:ND2	2.31	0.46
5:A:70:VAL:HG22	5:A:80:ASP:HA	1.97	0.46
5:A:86:PHE:CZ	5:A:89:GLY:HA2	2.50	0.46
5:A:393:THR:HA	5:A:521:PRO:HD2	1.98	0.46
4:K:78:LEU:HD23	4:K:95:CYS:SG	2.56	0.46
2:J:92:SER:O	2:J:99:VAL:HG12	2.16	0.46
5:B:452:ARG:HB3	5:B:492:LEU:HG	1.97	0.46
5:B:816:SER:OG	5:B:817:PRO:HD2	2.15	0.46
5:C:231:ILE:H	5:C:231:ILE:HD12	1.81	0.46
5:C:467:ASP:N	5:C:467:ASP:OD1	2.48	0.46
4:K:18:LEU:N	4:K:82:MET:O	2.47	0.46
4:P:37:VAL:HG12	4:P:47:TRP:HA	1.98	0.46
5:A:104:TRP:HB3	5:A:106:PHE:CE1	2.51	0.46
5:C:470:THR:HB	5:C:490:PHE:CZ	2.51	0.46
5:A:282:ASN:HB2	6:A:1303:NAG:H82	1.97	0.45
5:A:395:VAL:HG22	5:A:515:PHE:HD1	1.81	0.45
5:B:361:CYS:O	5:B:524:VAL:HA	2.16	0.45
5:B:461:LEU:HD21	5:B:465:GLU:O	2.16	0.45
5:C:396:TYR:HB2	5:C:514:SER:OG	2.16	0.45
5:C:906:PHE:CD2	5:C:916:LEU:HB2	2.51	0.45
4:K:6:GLU:HA	4:K:21:SER:O	2.16	0.45
4:P:30:SER:HB3	4:P:73:ASN:CB	2.46	0.45
5:B:350:VAL:HB	5:B:401:VAL:O	2.16	0.45
4:K:68:THR:CG2	4:K:81:GLN:HB3	2.46	0.45
2:J:33:GLN:HG2	2:J:34:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:331:ASN:ND2	6:B:1302:NAG:H2	2.32	0.45
5:C:85:PRO:O	5:C:269:TYR:OH	2.31	0.45
5:C:86:PHE:CZ	5:C:89:GLY:HA2	2.51	0.45
2:J:4:LEU:HD12	2:J:24:ALA:HA	1.98	0.45
1:L:4:LEU:C	1:L:5:LYS:HD3	2.41	0.45
5:A:402:ILE:HD13	5:A:418:ILE:HD12	1.98	0.45
5:C:410:ILE:HD12	5:C:433:VAL:HG21	1.98	0.45
5:C:444:LYS:HE3	5:C:448:ASN:ND2	2.32	0.45
3:O:29:VAL:HG13	3:O:92:ASN:OD1	2.16	0.45
3:O:85:VAL:HA	3:O:104:THR:O	2.16	0.45
5:B:89:GLY:HA3	5:B:270:LEU:HD12	1.98	0.45
3:H:38:GLN:HA	3:H:44:PRO:HA	1.98	0.45
3:O:37:GLN:HB2	3:O:47:LEU:HD11	1.97	0.45
5:A:974:SER:HB2	5:A:983:ARG:NH1	2.32	0.45
5:B:115:GLN:HA	5:B:132:GLU:CB	2.46	0.45
5:B:231:ILE:HG22	5:B:233:ILE:H	1.82	0.45
5:B:406:GLU:HA	5:B:409:GLN:HG3	1.98	0.45
5:B:858:LEU:H	5:B:858:LEU:HG	1.55	0.45
1:I:74:ASP:HB3	1:I:79:LEU:CD2	2.45	0.45
2:M:18:ILE:HD12	2:M:80:LEU:HD22	1.99	0.45
2:M:94:THR:HG23	2:M:96:SER:H	1.81	0.45
3:O:48:ILE:HG12	3:O:54:ARG:HA	1.98	0.45
5:A:200:TYR:CD2	5:A:230:PRO:HA	2.51	0.45
5:B:200:TYR:CD2	5:B:230:PRO:HA	2.51	0.45
5:B:326:ILE:HG21	5:B:534:VAL:HG22	1.98	0.45
5:C:403:ARG:HD2	5:C:405:ASN:OD1	2.16	0.45
3:H:20:THR:HG23	3:H:74:THR:HG22	1.99	0.45
4:K:4:LEU:HA	4:K:23:ALA:O	2.16	0.45
1:I:59:LYS:NZ	1:I:72:THR:HA	2.32	0.45
1:L:8:GLY:HA3	1:L:20:LEU:HD23	1.99	0.45
3:O:78:LEU:HD23	3:O:106:LEU:HD21	1.99	0.45
6:A:1304:NAG:O6	6:A:1311:NAG:O6	2.18	0.45
5:C:420:ASP:OD1	5:C:460:ASN:ND2	2.50	0.45
5:C:456:PHE:HB3	5:C:473:TYR:CD1	2.52	0.45
4:K:33:TYR:HE1	4:K:52:PHE:CE1	2.35	0.45
2:J:26:SER:OG	5:A:500:THR:HG21	2.17	0.45
2:J:40:GLN:HB2	2:J:87:TYR:HB2	1.99	0.45
5:A:314:GLN:CD	5:A:314:GLN:H	2.24	0.45
5:B:616:ASN:OD1	5:B:617:CYS:N	2.50	0.45
5:C:140:PHE:CE1	5:C:159:VAL:HA	2.52	0.45
5:C:361:CYS:SG	5:C:524:VAL:HG23	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:364:ASP:OD1	5:C:367:VAL:HG23	2.17	0.45
3:H:5:THR:HG23	3:H:24:ARG:HB3	1.99	0.45
1:I:3:THR:CG2	1:I:25:SER:HB2	2.47	0.44
5:A:401:VAL:HA	5:A:508:TYR:O	2.17	0.44
5:C:559:PHE:HB3	5:C:577:ARG:NH1	2.32	0.44
5:C:560:LEU:N	5:C:563:GLN:OE1	2.44	0.44
4:K:18:LEU:HD22	4:K:82:MET:HE3	1.98	0.44
1:L:63:PRO:O	1:L:66:GLU:HG2	2.16	0.44
1:L:68:ARG:O	1:L:69:LEU:HD23	2.17	0.44
2:M:52:GLU:O	2:M:55:LYS:N	2.30	0.44
3:O:2:ILE:HB	3:O:90:GLN:NE2	2.19	0.44
5:A:353:TRP:NE1	5:A:466:ARG:HB2	2.32	0.44
5:B:534:VAL:HG21	5:B:539:VAL:HG21	2.00	0.44
5:C:776:LYS:HG2	5:C:780:GLU:OE1	2.18	0.44
5:C:886:TRP:HZ3	5:C:904:TYR:HD2	1.64	0.44
3:H:63:SER:O	3:H:74:THR:N	2.44	0.44
3:O:36:TYR:HE2	3:O:89:GLN:HB3	1.81	0.44
5:A:426:PRO:HG3	5:A:463:PRO:HB3	1.98	0.44
5:B:324:GLU:HB3	5:B:539:VAL:HG23	2.00	0.44
5:B:906:PHE:HD2	5:B:916:LEU:HB2	1.81	0.44
5:C:444:LYS:HG3	5:C:448:ASN:CG	2.42	0.44
5:C:583:GLU:OE2	5:C:584:ILE:N	2.47	0.44
5:C:880:GLY:O	5:C:884:SER:OG	2.34	0.44
1:I:69:LEU:HD12	1:I:69:LEU:O	2.18	0.44
4:P:29:VAL:HG12	4:P:76:ASN:HA	1.98	0.44
5:B:709:ASN:HD21	6:B:1308:NAG:H4	1.81	0.44
5:C:141:LEU:HG	5:C:243:ALA:HA	1.99	0.44
4:K:20:LEU:HB2	4:K:80:LEU:HB3	2.00	0.44
1:L:105:ILE:HD12	1:L:105:ILE:H	1.82	0.44
5:A:958:ALA:O	5:A:961:THR:HG22	2.18	0.44
5:A:357:ARG:NE	5:A:359:SER:OG	2.41	0.44
5:A:498:ARG:NH2	5:A:501:TYR:OH	2.50	0.44
5:A:660:TYR:HB2	5:A:695:TYR:CZ	2.52	0.44
5:A:979:ASP:HA	5:A:982:SER:OG	2.18	0.44
5:C:81:ASN:OD1	5:C:82:PRO:HD2	2.17	0.44
1:I:24:PHE:CZ	1:I:78:ASN:HB3	2.53	0.44
2:J:53:VAL:CG1	2:J:68:LYS:HG2	2.46	0.44
3:O:24:ARG:HE	3:O:24:ARG:HB2	1.63	0.44
5:A:906:PHE:HD1	5:A:906:PHE:HA	1.64	0.44
5:B:353:TRP:HB3	5:B:400:PHE:HB3	1.99	0.44
2:M:7:PRO:O	2:M:104:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:20:ILE:HD12	2:M:106:LEU:HD21	2.00	0.44
3:O:36:TYR:HE2	3:O:89:GLN:CB	2.30	0.44
5:A:36:VAL:HG11	5:A:220:PHE:CZ	2.53	0.44
5:B:119:ILE:HG22	5:B:128:ILE:HG23	2.00	0.44
5:B:968:SER:HB3	5:B:970:PHE:CE2	2.53	0.44
5:C:353:TRP:CZ3	5:C:355:ARG:HD3	2.39	0.44
2:J:43:GLY:O	2:J:44:LYS:HD3	2.18	0.44
2:M:37:TRP:HB2	2:M:50:ILE:CG1	2.47	0.44
5:A:31:SER:N	5:A:60:SER:O	2.37	0.44
5:A:410:ILE:HG22	5:A:433:VAL:HG21	2.00	0.44
5:B:189:LEU:HB2	5:B:210:ILE:HD11	2.00	0.44
5:B:353:TRP:CE2	5:B:423:TYR:CD2	3.05	0.44
2:J:19:THR:O	2:J:20:ILE:HD13	2.18	0.43
3:O:30:SER:O	3:O:67:SER:OG	2.27	0.43
3:O:91:TYR:CE2	4:P:101:VAL:HA	2.53	0.43
3:O:96:PRO:CG	4:P:50:VAL:HG11	2.47	0.43
4:P:4:LEU:HA	4:P:23:ALA:O	2.17	0.43
4:P:72:ASP:HB2	4:P:77:THR:CG2	2.48	0.43
5:A:666:ILE:HB	5:A:670:ILE:O	2.18	0.43
5:B:335:LEU:CD2	5:B:364:ASP:HB2	2.47	0.43
5:C:801:ASN:HD21	6:C:1310:NAG:C2	2.31	0.43
2:J:50:ILE:HG23	2:J:55:LYS:O	2.18	0.43
5:A:342:PHE:CE2	5:A:368:LEU:HG	2.53	0.43
5:A:501:TYR:HB3	5:A:505:HIS:HB2	2.00	0.43
5:A:748:GLU:O	5:A:752:LEU:HG	2.18	0.43
5:B:552:LEU:HA	5:B:586:ASP:O	2.19	0.43
5:B:860:VAL:O	5:B:861:LEU:C	2.61	0.43
5:C:68:ILE:HG13	5:C:69:HIS:N	2.27	0.43
5:C:480:CYS:HB2	5:C:483:VAL:CG1	2.48	0.43
5:C:487:ASN:HA	5:C:489:TYR:CE2	2.54	0.43
5:C:815:ARG:NH2	5:C:820:ASP:OD1	2.52	0.43
3:H:29:VAL:HB	3:H:71:PHE:CZ	2.53	0.43
4:K:116:VAL:HG22	4:K:117:SER:H	1.83	0.43
1:I:34:VAL:O	1:I:55:TRP:HB3	2.18	0.43
2:M:50:ILE:HG22	2:M:56:ARG:HG3	2.00	0.43
3:O:10:THR:HA	3:O:105:LYS:O	2.18	0.43
3:O:62:PHE:CE1	3:O:75:ILE:HD13	2.53	0.43
5:B:374:PHE:N	5:B:374:PHE:CD1	2.84	0.43
1:I:101:THR:HG22	1:I:102:ILE:H	1.83	0.43
4:P:17:SER:OG	4:P:18:LEU:N	2.51	0.43
5:A:327:VAL:O	5:A:531:THR:OG1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:764:LYS:O	5:A:768:THR:HG23	2.18	0.43
3:H:93:ASN:O	3:H:94:TRP:C	2.62	0.43
3:H:94:TRP:HA	3:H:94:TRP:HE3	1.82	0.43
4:K:22:CYS:HB2	4:K:36:TRP:CZ2	2.53	0.43
4:K:47:TRP:HZ2	4:K:50:VAL:CG1	2.29	0.43
1:I:53:ILE:HD11	1:I:80:VAL:HG22	2.01	0.43
1:L:18:LEU:CB	1:L:87:MET:HE1	2.48	0.43
1:L:51:ALA:HA	1:L:61:TYR:HA	1.99	0.43
4:P:34:MET:O	4:P:50:VAL:HG23	2.19	0.43
5:A:660:TYR:HB2	5:A:695:TYR:CE2	2.54	0.43
4:K:19:ARG:HA	4:K:81:GLN:HA	1.99	0.43
5:A:88:ASP:N	5:A:88:ASP:OD1	2.51	0.43
5:A:442:ASP:O	5:A:448:ASN:ND2	2.40	0.43
5:C:196:ASN:HB2	5:C:201:PHE:HD1	1.82	0.43
1:I:85:THR:HG23	1:I:86:ASN:CG	2.44	0.43
2:M:52:GLU:O	2:M:54:SER:N	2.52	0.43
5:A:115:GLN:HA	5:A:132:GLU:CB	2.49	0.43
5:A:474:GLN:HA	5:A:479:PRO:HB3	2.01	0.43
5:A:584:ILE:C	5:A:585:LEU:HD22	2.43	0.43
5:B:374:PHE:CE1	5:B:436:TRP:HZ2	2.36	0.43
5:C:119:ILE:O	5:C:119:ILE:HG13	2.19	0.43
5:C:119:ILE:HG22	5:C:128:ILE:HG23	2.01	0.43
5:C:172:SER:OG	5:C:173:GLN:N	2.51	0.43
5:C:383:SER:HB3	5:C:386:LYS:HG2	2.01	0.43
5:C:461:LEU:HD12	5:C:465:GLU:O	2.18	0.43
5:C:826:VAL:CG1	5:C:1057:PRO:HG2	2.49	0.43
5:C:1005:GLN:O	5:C:1008:VAL:HG12	2.19	0.43
1:I:35:SER:HB2	1:I:100:LYS:O	2.19	0.43
3:O:54:ARG:NE	3:O:60:ALA:HA	2.33	0.43
5:A:497:PHE:CE2	5:A:507:PRO:HB3	2.54	0.43
5:B:81:ASN:OD1	5:B:82:PRO:HD2	2.18	0.43
5:B:676:THR:H	5:B:690:GLN:N	2.17	0.43
5:C:130:VAL:O	5:C:130:VAL:HG13	2.18	0.43
5:C:676:THR:HA	5:C:690:GLN:N	2.34	0.43
5:C:886:TRP:CZ3	5:C:904:TYR:HD2	2.37	0.43
2:J:51:TYR:CD2	2:J:52:GLU:HG2	2.54	0.43
1:L:87:MET:HE2	1:L:87:MET:HB2	1.87	0.43
4:P:59:TYR:HB2	4:P:64:LYS:HZ3	1.83	0.43
5:B:196:ASN:HA	5:B:200:TYR:O	2.19	0.43
5:B:338:PHE:HA	5:B:341:VAL:HG12	2.00	0.43
5:B:777:ASN:O	5:B:780:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:417:ASN:O	5:C:421:TYR:HB2	2.19	0.43
4:K:21:SER:HA	4:K:79:TYR:HA	1.99	0.43
1:I:61:TYR:CZ	1:I:71:ILE:HG22	2.54	0.42
2:J:41:TYR:HB3	2:J:42:PRO:HD2	2.01	0.42
5:A:96:GLU:OE1	5:A:99:ASN:N	2.52	0.42
5:B:331:ASN:HD21	6:B:1302:NAG:H2	1.83	0.42
5:B:401:VAL:HA	5:B:508:TYR:O	2.19	0.42
3:H:32:ASP:HB2	3:H:92:ASN:OD1	2.19	0.42
1:I:53:ILE:HG13	1:I:53:ILE:O	2.19	0.42
2:M:68:LYS:HD3	2:M:70:GLY:H	1.84	0.42
4:P:17:SER:OG	4:P:81:GLN:NE2	2.53	0.42
4:P:90:THR:HA	4:P:114:VAL:O	2.19	0.42
5:A:340:GLU:OE2	5:A:340:GLU:N	2.53	0.42
5:A:403:ARG:HD3	5:A:505:HIS:HA	2.00	0.42
5:B:176:LEU:O	5:B:190:ARG:NH2	2.50	0.42
5:B:357:ARG:NH2	5:C:230:PRO:HG2	2.34	0.42
5:B:546:LEU:HD22	5:B:565:PHE:HE1	1.84	0.42
5:B:906:PHE:CE2	5:B:916:LEU:HB2	2.53	0.42
4:K:25:SER:C	4:K:27:ILE:H	2.27	0.42
5:A:355:ARG:HH11	5:A:396:TYR:HD2	1.67	0.42
5:A:389:ASP:OD1	5:A:389:ASP:N	2.43	0.42
5:B:391:CYS:HA	5:B:525:CYS:HB3	2.01	0.42
5:C:326:ILE:HD11	5:C:541:PHE:CB	2.48	0.42
3:H:17:GLU:OE1	3:H:17:GLU:N	2.52	0.42
2:J:13:SER:O	2:J:16:GLN:HG3	2.20	0.42
3:O:2:ILE:O	3:O:99:THR:HG21	2.19	0.42
5:A:426:PRO:HD2	5:A:429:PHE:HB2	2.00	0.42
5:B:934:ILE:HD13	5:B:934:ILE:HA	1.92	0.42
1:I:43:PRO:O	1:I:45:LYS:HD2	2.19	0.42
5:B:126:VAL:O	5:B:171:VAL:HA	2.19	0.42
5:C:280:ASN:OD1	5:C:283:GLY:N	2.53	0.42
5:C:410:ILE:HG13	5:C:410:ILE:O	2.18	0.42
5:C:770:ILE:O	5:C:774:GLN:HG2	2.20	0.42
3:H:24:ARG:HE	3:H:24:ARG:HB2	1.51	0.42
1:L:5:LYS:HE2	1:L:5:LYS:HB2	1.94	0.42
4:P:4:LEU:HG	4:P:24:ALA:HB2	2.02	0.42
5:A:396:TYR:O	5:A:513:LEU:HA	2.19	0.42
5:A:760:CYS:HA	5:A:763:LEU:HG	2.00	0.42
5:A:1077:THR:OG1	5:A:1078:ALA:N	2.50	0.42
5:A:616:ASN:OD1	5:A:616:ASN:C	2.62	0.42
5:A:1102:TRP:HB2	5:A:1135:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:231:ILE:HG22	5:B:233:ILE:HG22	2.00	0.42
5:B:404:GLY:N	5:B:504:GLY:O	2.52	0.42
5:C:521:PRO:O	5:C:522:ALA:C	2.62	0.42
5:C:603:ASN:CG	6:C:1304:NAG:H2	2.44	0.42
1:I:83:THR:HG21	2:J:19:THR:OG1	2.19	0.42
2:J:11:SER:OG	2:J:109:LEU:HD22	2.19	0.42
3:O:34:ALA:HA	3:O:48:ILE:O	2.19	0.42
5:A:118:LEU:C	5:A:118:LEU:HD23	2.45	0.42
5:A:118:LEU:HD21	5:A:120:VAL:HG23	2.02	0.42
5:B:855:PHE:HB3	5:B:858:LEU:HD12	2.01	0.42
3:H:8:PRO:HG2	3:H:11:LEU:CD1	2.49	0.42
3:H:35:TRP:CE2	3:H:88:CYS:HB3	2.55	0.42
4:K:3:GLN:O	4:K:4:LEU:HD12	2.19	0.42
5:A:333:THR:O	5:A:335:LEU:HD22	2.20	0.42
5:A:483:VAL:HG22	5:A:484:ALA:N	2.34	0.42
5:A:991:VAL:HA	5:A:994:ASP:OD1	2.20	0.42
5:C:141:LEU:HD21	5:C:244:LEU:CB	2.49	0.42
5:C:298:GLU:O	5:C:302:THR:HG23	2.20	0.42
5:C:328:ARG:NH2	5:C:545:GLY:H	2.18	0.42
3:H:36:TYR:HE1	4:K:105:THR:O	2.03	0.42
1:L:18:LEU:HD22	1:L:84:LEU:HD21	2.02	0.42
3:O:6:GLN:HG2	3:O:23:CYS:CB	2.50	0.42
3:O:90:GLN:HE21	3:O:99:THR:HB	1.85	0.42
4:P:47:TRP:HE1	4:P:50:VAL:HB	1.84	0.42
4:P:51:MET:SD	4:P:57:THR:HB	2.60	0.42
5:A:430:THR:O	5:A:515:PHE:N	2.40	0.42
5:B:906:PHE:HD1	5:B:906:PHE:HA	1.68	0.42
5:C:189:LEU:HB3	5:C:208:THR:OG1	2.20	0.42
5:C:617:CYS:C	5:C:619:GLU:N	2.77	0.42
5:C:777:ASN:O	5:C:781:VAL:HG12	2.20	0.42
4:K:66:ARG:HG3	4:K:67:PHE:CE1	2.54	0.42
3:O:91:TYR:CE2	4:P:101:VAL:HG22	2.53	0.41
5:A:394:ASN:OD1	5:A:394:ASN:N	2.53	0.41
5:A:532:ASN:OD1	5:A:533:LEU:N	2.53	0.41
5:A:1049:LEU:HA	5:A:1049:LEU:HD23	1.90	0.41
5:A:1125:ASN:ND2	5:A:1127:ASP:OD1	2.52	0.41
5:B:118:LEU:C	5:B:118:LEU:HD23	2.44	0.41
5:B:204:TYR:HA	5:B:224:GLU:O	2.20	0.41
5:C:405:ASN:OD1	5:C:405:ASN:N	2.53	0.41
5:C:534:VAL:HG11	5:C:539:VAL:HG21	2.01	0.41
5:C:1079:PRO:HD2	5:C:1131:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:GLY:HA3	1:I:20:LEU:HD23	2.01	0.41
3:O:91:TYR:HB3	3:O:98:TYR:CE1	2.54	0.41
4:P:13:GLN:HG2	4:P:14:PRO:CD	2.48	0.41
5:A:234:ASN:ND2	6:A:1301:NAG:O5	2.54	0.41
5:B:116:SER:O	5:B:130:VAL:HG23	2.19	0.41
5:B:720:ILE:HG21	5:B:720:ILE:HD13	1.81	0.41
5:C:141:LEU:H	5:C:249:LEU:HD13	1.85	0.41
5:C:206:LYS:HE3	5:C:221:SER:OG	2.20	0.41
5:A:390:LEU:HG	5:A:391:CYS:N	2.35	0.41
5:A:1140:PRO:C	5:A:1143:PRO:HD2	2.45	0.41
5:C:392:PHE:CD2	5:C:515:PHE:HB3	2.55	0.41
5:C:657:ASN:OD1	6:C:1303:NAG:H2	2.20	0.41
3:H:96:PRO:HG3	4:K:58:PHE:CG	2.55	0.41
1:I:49:TRP:NE1	1:I:106:PHE:HZ	2.17	0.41
4:P:37:VAL:HG21	4:P:108:TRP:CZ3	2.56	0.41
5:A:521:PRO:O	5:A:522:ALA:C	2.63	0.41
5:B:196:ASN:ND2	5:B:201:PHE:HB2	2.35	0.41
5:C:1049:LEU:HA	5:C:1049:LEU:HD23	1.88	0.41
4:K:90:THR:HG22	4:K:115:THR:HA	2.00	0.41
2:M:3:ALA:HB1	2:M:99:VAL:HG11	2.02	0.41
3:O:11:LEU:N	3:O:105:LYS:O	2.53	0.41
4:P:32:ASN:O	4:P:34:MET:HE2	2.21	0.41
5:A:391:CYS:HA	5:A:525:CYS:CB	2.43	0.41
5:A:431:GLY:HA3	5:A:513:LEU:O	2.19	0.41
5:C:1118:ASP:OD2	5:C:1119:ASN:N	2.53	0.41
1:I:37:GLY:HA3	1:I:106:PHE:CE1	2.55	0.41
1:L:104:THR:CG2	1:L:107:ASP:HB3	2.51	0.41
2:M:27:SER:OG	3:O:70:GLU:HG3	2.20	0.41
4:P:27:ILE:HD11	4:P:32:ASN:HD21	1.86	0.41
4:P:84:SER:O	4:P:84:SER:OG	2.33	0.41
5:A:359:SER:HA	5:A:524:VAL:HB	2.02	0.41
5:A:444:LYS:C	5:A:499:PRO:HD3	2.45	0.41
5:A:720:ILE:HG21	5:A:720:ILE:HD13	1.81	0.41
5:B:801:ASN:HD21	6:B:1309:NAG:C2	2.34	0.41
5:C:38:TYR:OH	5:C:284:THR:HA	2.21	0.41
3:H:95:PRO:HB3	4:K:52:PHE:HZ	1.84	0.41
2:M:37:TRP:HB2	2:M:50:ILE:HG13	2.03	0.41
5:A:563:GLN:O	5:A:577:ARG:NE	2.47	0.41
5:A:735:SER:OG	5:A:861:LEU:HD11	2.20	0.41
5:A:1077:THR:OG1	5:B:900:MET:HE1	2.20	0.41
5:C:36:VAL:HG21	5:C:220:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:498:ARG:NH2	5:C:501:TYR:OH	2.53	0.41
3:H:8:PRO:HG2	3:H:11:LEU:HD12	2.02	0.41
4:K:74:SER:O	4:K:75:LYS:HD2	2.20	0.41
1:I:4:LEU:HB2	1:I:110:GLY:HA2	2.02	0.41
2:M:99:VAL:HG12	2:M:100:PHE:N	2.36	0.41
3:O:36:TYR:OH	4:P:105:THR:HG22	2.21	0.41
3:O:63:SER:HB2	3:O:74:THR:HG1	1.83	0.41
5:A:713:ALA:HB3	5:B:894:LEU:HB3	2.03	0.41
5:A:813:SER:OG	5:A:815:ARG:HG3	2.21	0.41
5:A:965:GLN:HG2	5:A:970:PHE:HZ	1.85	0.41
5:B:666:ILE:HD11	5:B:672:ALA:HB2	2.03	0.41
5:C:96:GLU:OE1	5:C:99:ASN:N	2.54	0.41
5:C:388:ASN:OD1	5:C:527:PRO:HD3	2.20	0.41
5:C:713:ALA:HA	5:C:1073:LYS:O	2.21	0.41
5:C:762:GLN:HG3	5:C:762:GLN:H	1.62	0.41
5:C:906:PHE:HD1	5:C:906:PHE:HA	1.73	0.41
5:C:989:ALA:O	5:C:993:ILE:HG12	2.20	0.41
3:H:85:VAL:HG12	3:H:105:LYS:HD2	2.01	0.41
4:K:59:TYR:CE2	4:K:69:ILE:HG22	2.55	0.41
1:I:9:PRO:CG	2:J:69:SER:HB2	2.51	0.41
1:I:59:LYS:HZ2	1:I:72:THR:HA	1.86	0.41
1:L:5:LYS:O	1:L:22:CYS:HA	2.20	0.41
4:P:3:GLN:O	4:P:4:LEU:HD12	2.21	0.41
5:A:175:PHE:O	5:A:176:LEU:HD23	2.21	0.41
5:A:364:ASP:O	5:A:367:VAL:HG12	2.21	0.41
5:A:524:VAL:O	5:A:525:CYS:HB3	2.21	0.41
5:A:738:CYS:HB3	5:A:760:CYS:HB2	1.51	0.41
5:A:763:LEU:HD12	5:A:764:LYS:N	2.36	0.41
5:B:762:GLN:HG3	5:B:765:ARG:NH2	2.35	0.41
5:B:1129:VAL:HG23	5:B:1132:ILE:HB	2.02	0.41
5:C:335:LEU:HD21	5:C:338:PHE:CD2	2.56	0.41
5:C:347:PHE:CE1	5:C:509:ARG:HD3	2.56	0.41
4:K:70:SER:O	4:K:79:TYR:N	2.51	0.41
3:O:93:ASN:O	3:O:94:TRP:C	2.64	0.41
5:A:713:ALA:HA	5:A:1073:LYS:O	2.20	0.41
5:A:1129:VAL:HG13	5:A:1132:ILE:HB	2.03	0.41
5:B:168:PHE:CZ	5:B:170:TYR:HB2	2.56	0.41
5:B:197:ILE:HG13	5:B:198:ASP:N	2.35	0.41
5:B:580:GLN:C	6:B:1302:NAG:H5	2.46	0.41
5:B:986:PRO:O	5:B:990:GLU:HG3	2.21	0.41
5:C:118:LEU:HB2	5:C:129:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:336:CYS:HB2	5:C:337:PRO:CD	2.51	0.41
3:H:17:GLU:O	3:H:78:LEU:HD12	2.20	0.41
1:I:32:GLY:HA2	1:I:55:TRP:CD2	2.55	0.40
2:J:53:VAL:HG13	2:J:54:SER:N	2.36	0.40
3:O:29:VAL:O	3:O:30:SER:C	2.64	0.40
5:A:240:THR:HG22	5:A:241:LEU:N	2.36	0.40
5:A:334:ASN:HB2	5:A:361:CYS:CA	2.48	0.40
5:B:425:LEU:HD23	5:B:426:PRO:O	2.21	0.40
5:B:457:ARG:HD2	5:B:457:ARG:HA	1.77	0.40
5:C:743:CYS:O	5:C:744:GLY:C	2.64	0.40
3:H:54:ARG:NE	3:H:60:ALA:HA	2.36	0.40
2:J:87:TYR:OH	2:J:105:LYS:HD2	2.22	0.40
1:L:78:ASN:O	1:L:79:LEU:HD23	2.20	0.40
1:L:92:THR:O	1:L:92:THR:HG23	2.21	0.40
2:M:24:ALA:HB3	2:M:71:ASN:HD21	1.86	0.40
3:O:27:GLN:O	3:O:69:THR:HG22	2.21	0.40
5:A:168:PHE:CZ	5:A:170:TYR:HB2	2.56	0.40
5:A:189:LEU:HB3	5:A:208:THR:OG1	2.21	0.40
5:A:330:PRO:C	5:A:332:ILE:N	2.79	0.40
5:A:409:GLN:OE1	5:A:418:ILE:HG12	2.21	0.40
5:A:437:ASN:HB2	5:A:508:TYR:CE2	2.56	0.40
5:B:131:CYS:HA	5:B:166:CYS:HA	2.02	0.40
5:C:165:ASN:OD1	6:C:1312:NAG:H62	2.22	0.40
5:C:1077:THR:OG1	5:C:1078:ALA:N	2.54	0.40
5:C:1092:GLU:OE2	5:C:1092:GLU:N	2.54	0.40
4:K:17:SER:OG	4:K:18:LEU:N	2.54	0.40
2:M:49:MET:HE1	2:M:75:LEU:HD21	2.03	0.40
2:M:53:VAL:HG13	2:M:54:SER:N	2.37	0.40
2:M:66:GLY:HA2	2:M:75:LEU:HA	2.02	0.40
5:A:906:PHE:HD2	5:A:916:LEU:HB2	1.86	0.40
5:B:806:LEU:HD23	5:B:806:LEU:HA	1.89	0.40
5:C:328:ARG:HH22	5:C:544:ASN:CA	2.34	0.40
5:C:347:PHE:CD1	5:C:509:ARG:HD3	2.56	0.40
5:C:417:ASN:HD21	5:C:455:LEU:HD12	1.86	0.40
5:C:1074:ASN:OD1	6:C:1305:NAG:H82	2.21	0.40
4:K:37:VAL:HG11	4:K:45:LEU:HD23	2.03	0.40
2:M:49:MET:HE3	2:M:49:MET:HB2	1.74	0.40
4:P:39:GLN:N	4:P:92:VAL:O	2.46	0.40
5:A:363:ALA:HB2	5:A:524:VAL:HG23	2.03	0.40
5:A:365:TYR:HB2	5:A:388:ASN:HA	2.03	0.40
5:C:426:PRO:HG3	5:C:463:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:750:SER:O	5:C:754:LEU:HD23	2.21	0.40
5:C:1129:VAL:HG13	5:C:1132:ILE:HB	2.03	0.40
1:L:33:GLY:H	1:L:55:TRP:NE1	2.19	0.40
4:P:70:SER:O	4:P:79:TYR:N	2.49	0.40
5:A:96:GLU:CD	5:A:99:ASN:H	2.29	0.40
5:A:141:LEU:HD21	5:A:244:LEU:CB	2.52	0.40
5:A:449:TYR:HA	5:A:494:SER:OG	2.21	0.40
5:A:855:PHE:HD1	5:A:858:LEU:HD12	1.85	0.40
5:A:900:MET:HE1	5:C:1077:THR:OG1	2.22	0.40
5:B:730:SER:OG	5:B:731:MET:N	2.53	0.40
5:B:826:VAL:HG11	5:B:1057:PRO:HG2	2.04	0.40
5:C:439:ASN:HB2	5:C:507:PRO:HD2	2.04	0.40
5:C:1102:TRP:HB2	5:C:1135:ASN:HD22	1.86	0.40
3:H:91:TYR:HB3	3:H:98:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	116/119 (98%)	109 (94%)	6 (5%)	1 (1%)	14	45
1	L	116/119 (98%)	105 (90%)	10 (9%)	1 (1%)	14	45
2	J	106/109 (97%)	98 (92%)	7 (7%)	1 (1%)	14	45
2	M	106/109 (97%)	100 (94%)	5 (5%)	1 (1%)	14	45
3	H	107/109 (98%)	101 (94%)	4 (4%)	2 (2%)	6	32
3	O	107/109 (98%)	100 (94%)	5 (5%)	2 (2%)	6	32
4	K	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
4	P	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
5	A	1008/1288 (78%)	947 (94%)	56 (6%)	5 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	965/1288 (75%)	914 (95%)	49 (5%)	2 (0%)	43	73
5	C	1008/1288 (78%)	952 (94%)	52 (5%)	4 (0%)	30	62
All	All	3871/4774 (81%)	3641 (94%)	211 (6%)	19 (0%)	26	57

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	53	VAL
2	M	53	VAL
3	O	30	SER
5	B	333	THR
5	C	327	VAL
3	H	94	TRP
5	A	525	CYS
5	A	526	GLY
5	A	529	LYS
5	B	528	LYS
5	C	333	THR
3	O	96	PRO
5	A	331	ASN
5	C	527	PRO
3	H	30	SER
1	I	103	PRO
1	L	103	PRO
5	C	332	ILE
5	A	330	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	105/107 (98%)	104 (99%)	1 (1%)	68	74
1	L	105/107 (98%)	105 (100%)	0	100	100
2	J	89/90 (99%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	89/90 (99%)	89 (100%)	0	100	100
3	H	89/90 (99%)	88 (99%)	1 (1%)	65	73
3	O	89/90 (99%)	89 (100%)	0	100	100
4	K	90/95 (95%)	89 (99%)	1 (1%)	65	73
4	P	90/95 (95%)	90 (100%)	0	100	100
5	A	811/1113 (73%)	795 (98%)	16 (2%)	48	65
5	B	776/1113 (70%)	763 (98%)	13 (2%)	53	67
5	C	810/1113 (73%)	804 (99%)	6 (1%)	76	77
All	All	3143/4103 (77%)	3105 (99%)	38 (1%)	61	72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	114	LEU
5	A	118	LEU
5	A	327	VAL
5	A	331	ASN
5	A	333	THR
5	A	334	ASN
5	A	335	LEU
5	A	336	CYS
5	A	488	CYS
5	A	538	CYS
5	A	617	CYS
5	A	649	CYS
5	A	858	LEU
5	A	859	THR
5	A	860	VAL
5	A	861	LEU
5	A	906	PHE
5	B	118	LEU
5	B	131	CYS
5	B	166	CYS
5	B	331	ASN
5	B	398	ASP
5	B	432	CYS
5	B	518	LEU
5	B	617	CYS
5	B	649	CYS

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Mol	Chain	Res	Type
5	B	858	LEU
5	B	859	THR
5	B	861	LEU
5	B	906	PHE
5	C	131	CYS
5	C	166	CYS
5	C	327	VAL
5	C	336	CYS
5	C	538	CYS
5	C	617	CYS
3	H	95	PRO
4	K	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	78	ASN
1	I	86	ASN
1	I	111	GLN
2	J	6	GLN
1	L	16	GLN
1	L	41	GLN
2	M	6	GLN
2	M	39	GLN
3	O	90	GLN
4	P	39	GLN
4	P	81	GLN
5	A	49	HIS
5	A	450	ASN
5	A	460	ASN
5	A	536	ASN
5	A	657	ASN
5	A	709	ASN
5	A	914	ASN
5	A	949	GLN
5	A	1054	GLN
5	A	1134	ASN
5	B	66	HIS
5	B	207	HIS
5	B	234	ASN
5	B	282	ASN
5	B	388	ASN

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Mol	Chain	Res	Type
5	B	437	ASN
5	B	506	GLN
5	B	536	ASN
5	B	657	ASN
5	B	709	ASN
5	B	751	ASN
5	B	774	GLN
5	B	801	ASN
5	B	954	HIS
5	B	1005	GLN
5	B	1098	ASN
5	B	1134	ASN
5	C	370	ASN
5	C	417	ASN
5	C	448	ASN
5	C	450	ASN
5	C	542	ASN
5	C	544	ASN
5	C	751	ASN
5	C	774	GLN
5	C	801	ASN
5	C	957	GLN
5	C	1005	GLN
5	C	1134	ASN
3	H	6	GLN
3	H	27	GLN
3	H	42	GLN
3	H	90	GLN
3	H	102	GLN
4	K	81	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	C	1310	-	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	B	1303	-	14,14,15	0.37	0	17,19,21	0.54	0
6	NAG	B	1305	-	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	B	1306	-	14,14,15	0.32	0	17,19,21	0.52	0
6	NAG	C	1312	-	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	C	1313	-	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	B	1312	-	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	C	1303	-	14,14,15	0.20	0	17,19,21	0.44	0
6	NAG	B	1304	-	14,14,15	0.34	0	17,19,21	0.50	0
6	NAG	B	1307	-	14,14,15	0.27	0	17,19,21	0.60	0
6	NAG	C	1308	-	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	A	1305	-	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	A	1310	-	14,14,15	0.30	0	17,19,21	0.59	0
6	NAG	A	1303	-	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	A	1311	-	14,14,15	0.20	0	17,19,21	0.56	0
6	NAG	A	1301	-	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	A	1307	-	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	C	1304	-	14,14,15	0.36	0	17,19,21	0.53	0
6	NAG	C	1311	-	14,14,15	0.20	0	17,19,21	0.46	0
6	NAG	C	1302	-	14,14,15	0.28	0	17,19,21	0.60	0
6	NAG	C	1307	-	14,14,15	0.30	0	17,19,21	0.56	0
6	NAG	C	1306	-	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	A	1308	-	14,14,15	0.29	0	17,19,21	0.45	0
6	NAG	C	1301	-	14,14,15	0.16	0	17,19,21	0.53	0
6	NAG	C	1309	-	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	A	1312	-	14,14,15	0.21	0	17,19,21	0.37	0
6	NAG	B	1301	-	14,14,15	0.21	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1308	-	14,14,15	0.22	0	17,19,21	0.47	0
6	NAG	B	1310	-	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	B	1302	-	14,14,15	0.19	0	17,19,21	0.43	0
6	NAG	B	1311	-	14,14,15	0.19	0	17,19,21	0.48	0
6	NAG	A	1306	-	14,14,15	0.34	0	17,19,21	0.58	0
6	NAG	A	1302	-	14,14,15	0.26	0	17,19,21	0.45	0
6	NAG	B	1309	-	14,14,15	0.21	0	17,19,21	0.38	0
6	NAG	C	1305	-	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	A	1304	-	14,14,15	0.34	0	17,19,21	0.50	0
6	NAG	A	1309	-	14,14,15	0.24	0	17,19,21	0.52	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	C	1310	-	-	1/6/23/26	0/1/1/1
6	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1305	-	-	1/6/23/26	0/1/1/1
6	NAG	B	1306	-	-	1/6/23/26	0/1/1/1
6	NAG	C	1312	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1313	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1312	-	-	3/6/23/26	0/1/1/1
6	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	-	-	4/6/23/26	0/1/1/1
6	NAG	C	1308	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1305	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1310	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1303	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1311	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1311	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	-	-	4/6/23/26	0/1/1/1
6	NAG	C	1307	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1308	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1309	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1312	-	-	1/6/23/26	0/1/1/1
6	NAG	B	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1308	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1310	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1311	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1306	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1302	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1309	-	-	1/6/23/26	0/1/1/1
6	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1309	-	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (75) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
6	B	1304	NAG	C4-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	B	1312	NAG	O5-C5-C6-O6
6	C	1312	NAG	O5-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	C	1313	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	A	1308	NAG	C4-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	C	1311	NAG	O5-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	A	1310	NAG	O5-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	A	1311	NAG	C4-C5-C6-O6
6	C	1307	NAG	C4-C5-C6-O6
6	B	1307	NAG	C4-C5-C6-O6
6	C	1302	NAG	O5-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	B	1309	NAG	O5-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	A	1309	NAG	O5-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	A	1312	NAG	O5-C5-C6-O6
6	A	1304	NAG	C3-C2-N2-C7
6	C	1302	NAG	C3-C2-N2-C7
6	C	1309	NAG	C3-C2-N2-C7
6	B	1306	NAG	O5-C5-C6-O6
6	C	1310	NAG	O5-C5-C6-O6
6	A	1311	NAG	O5-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	A	1304	NAG	C1-C2-N2-C7
6	C	1309	NAG	C1-C2-N2-C7
6	A	1307	NAG	O5-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1306	NAG	O5-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	B	1312	NAG	C4-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	A	1310	NAG	C3-C2-N2-C7
6	B	1307	NAG	C3-C2-N2-C7
6	C	1308	NAG	C3-C2-N2-C7
6	C	1311	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	A	1303	NAG	C1-C2-N2-C7
6	A	1310	NAG	C1-C2-N2-C7
6	B	1307	NAG	C1-C2-N2-C7
6	C	1308	NAG	C1-C2-N2-C7
6	B	1312	NAG	C3-C2-N2-C7
6	A	1301	NAG	O5-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6

There are no ring outliers.

24 monomers are involved in 36 short contacts:

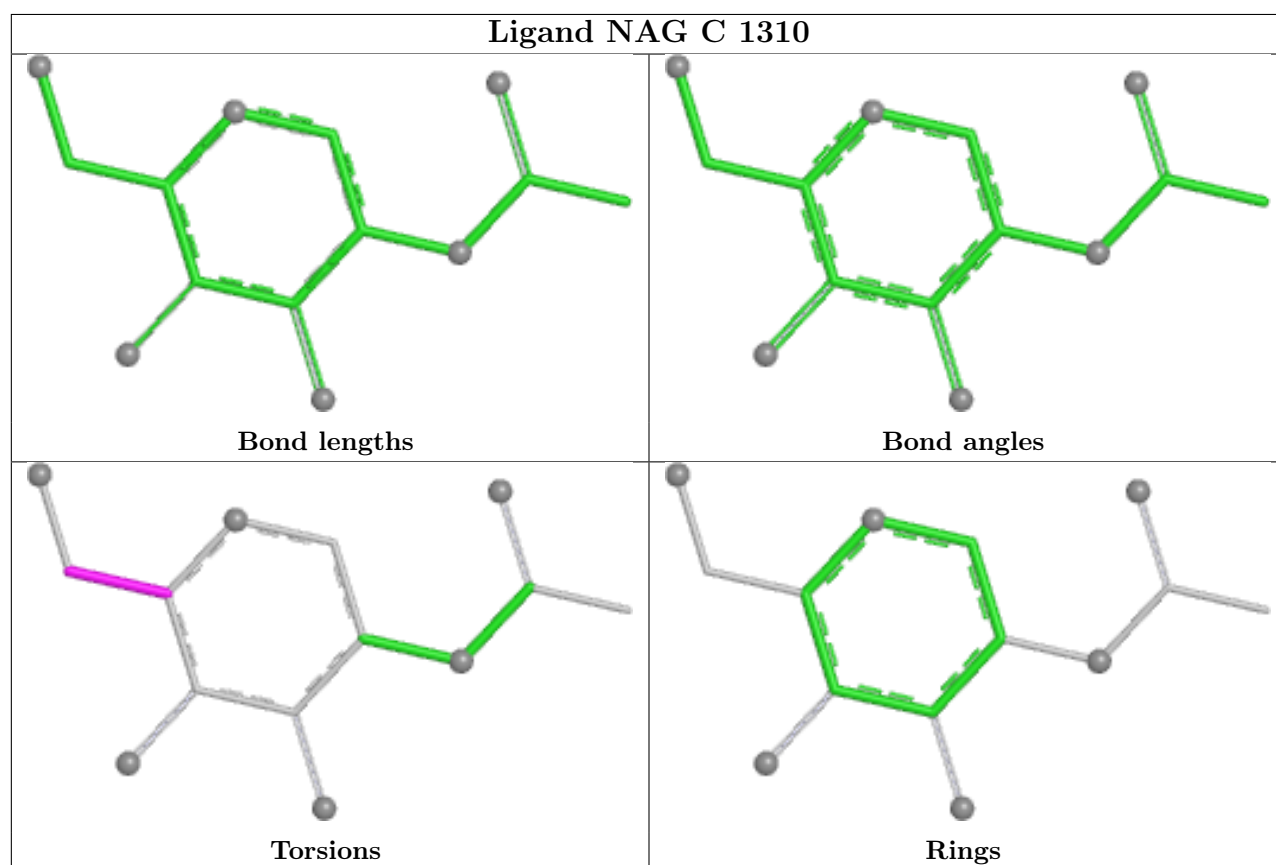
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1310	NAG	1	0
6	B	1305	NAG	1	0
6	C	1312	NAG	2	0
6	B	1312	NAG	2	0
6	C	1303	NAG	1	0
6	A	1305	NAG	4	0
6	A	1303	NAG	1	0
6	A	1311	NAG	2	0
6	A	1301	NAG	1	0
6	A	1307	NAG	1	0
6	C	1304	NAG	1	0
6	C	1306	NAG	1	0
6	A	1308	NAG	1	0
6	C	1301	NAG	1	0
6	B	1301	NAG	2	0
6	B	1308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

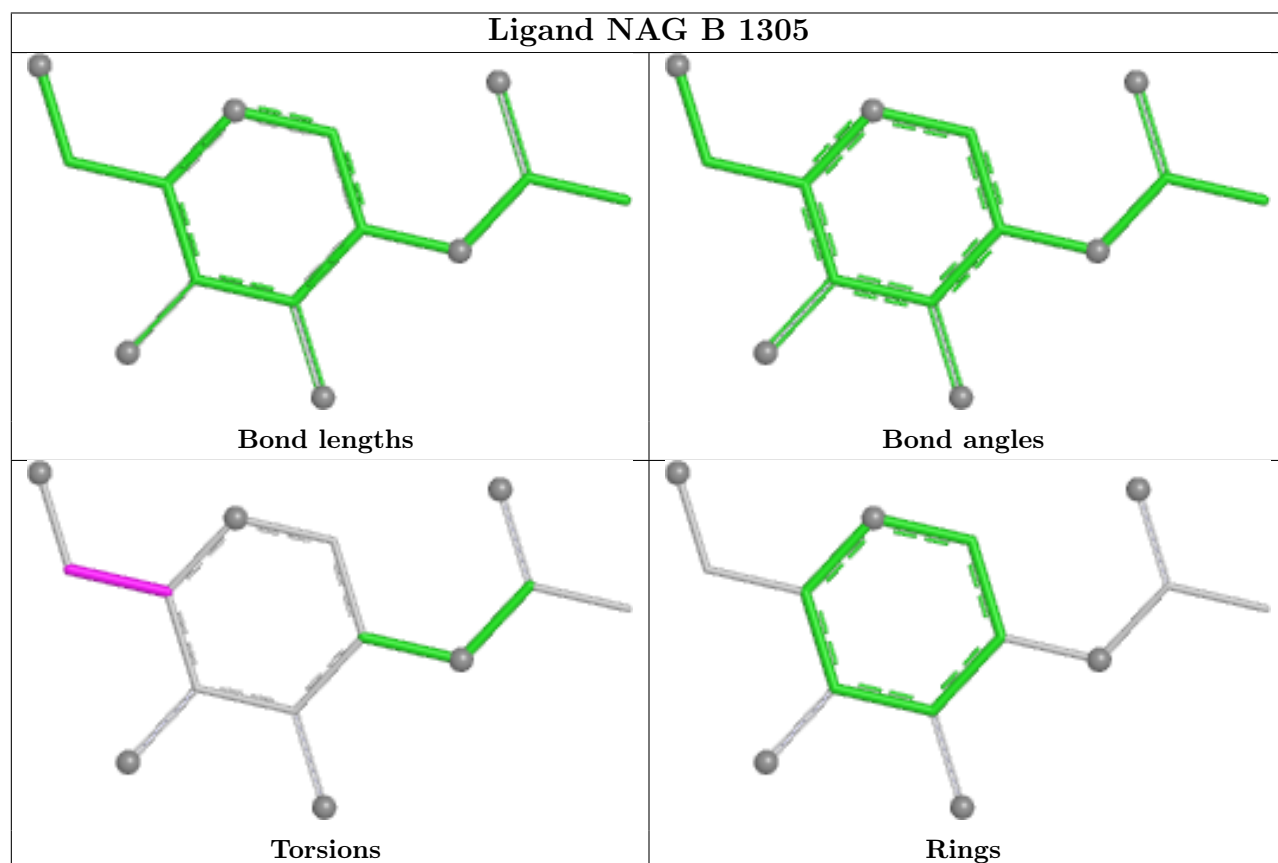
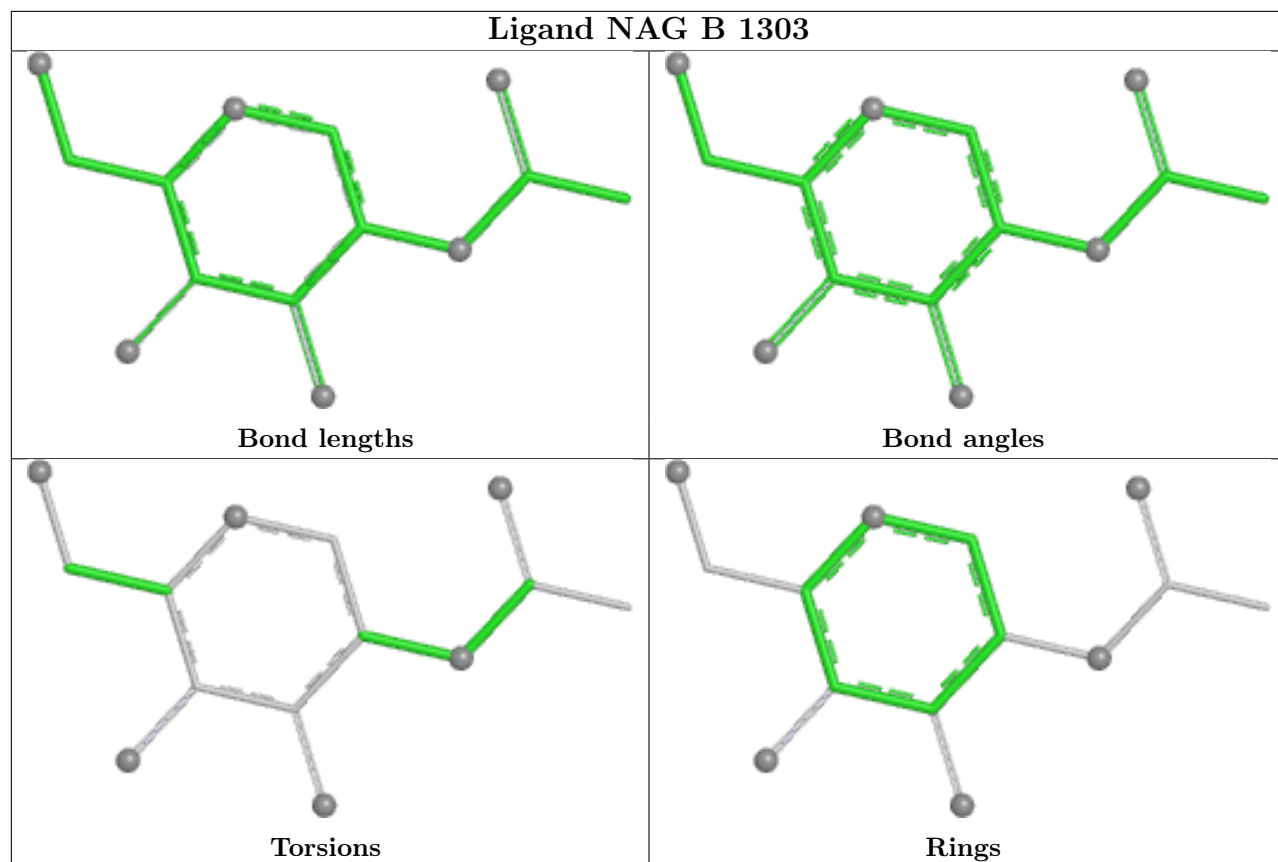
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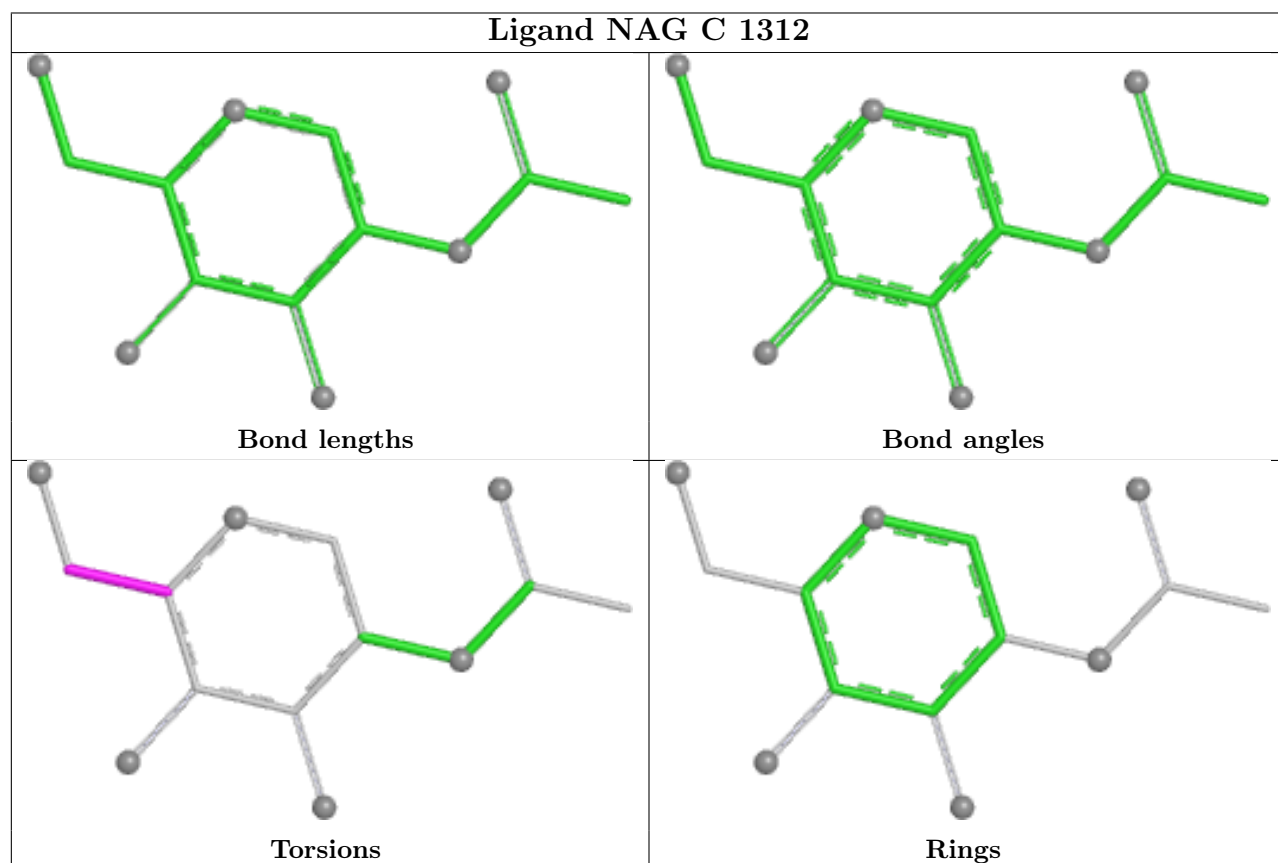
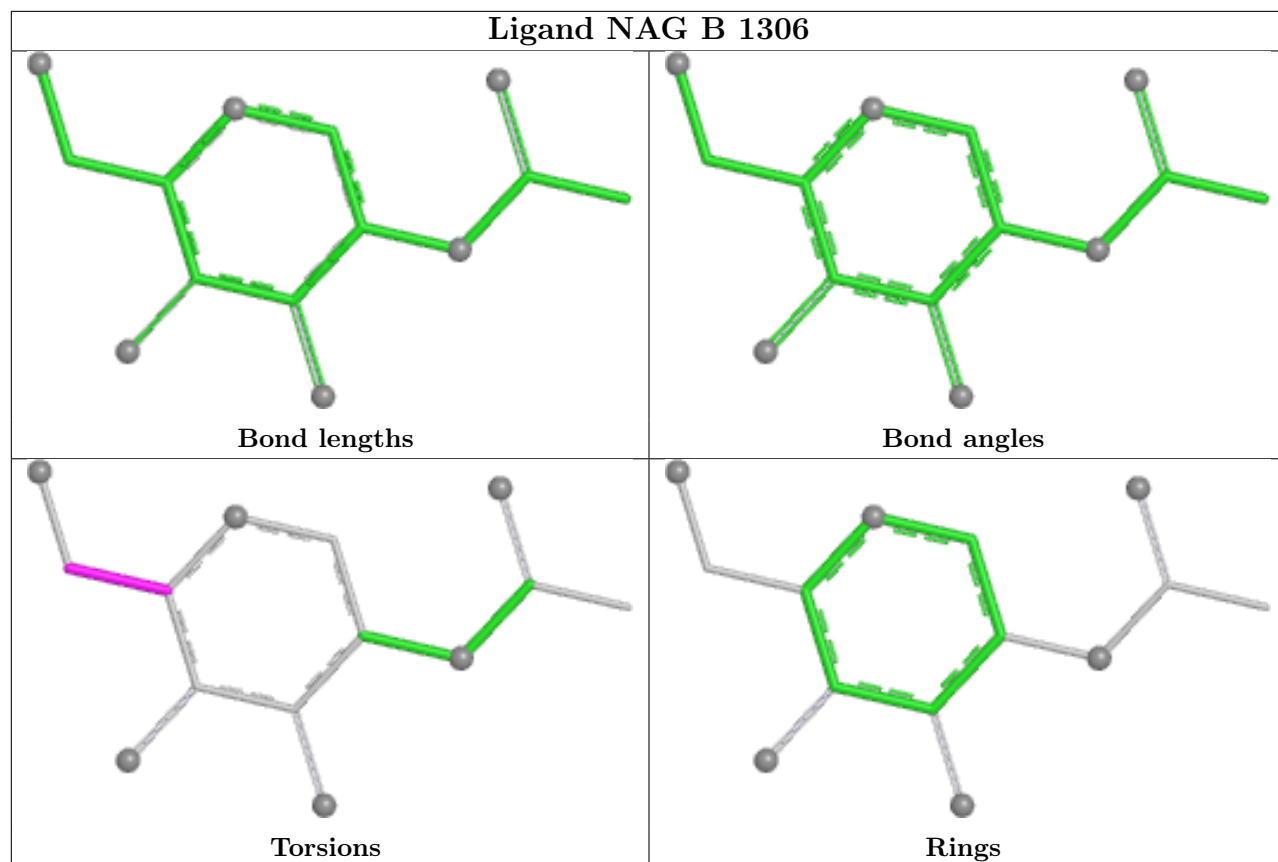
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1309	NAG	1	0
6	C	1305	NAG	1	0
6	A	1304	NAG	1	0
6	A	1309	NAG	1	0

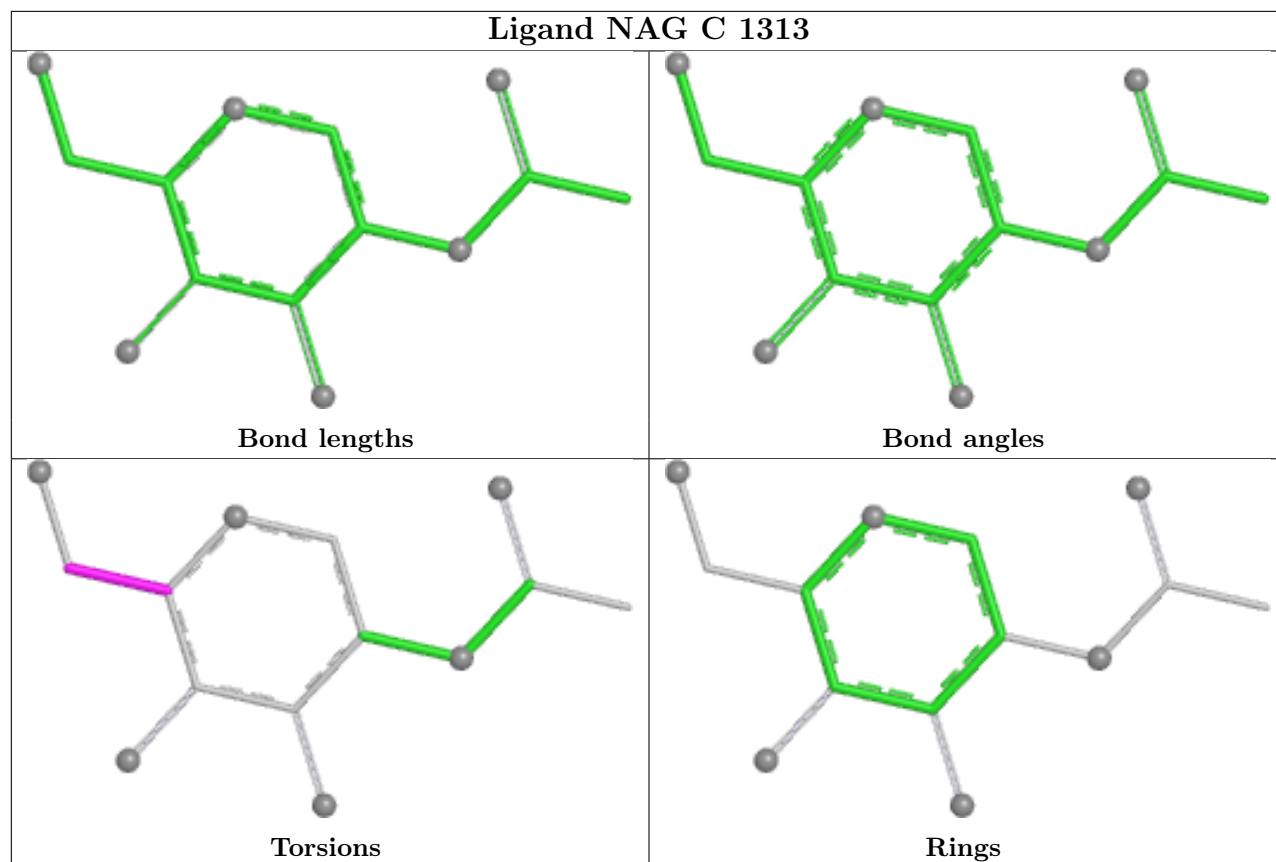
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



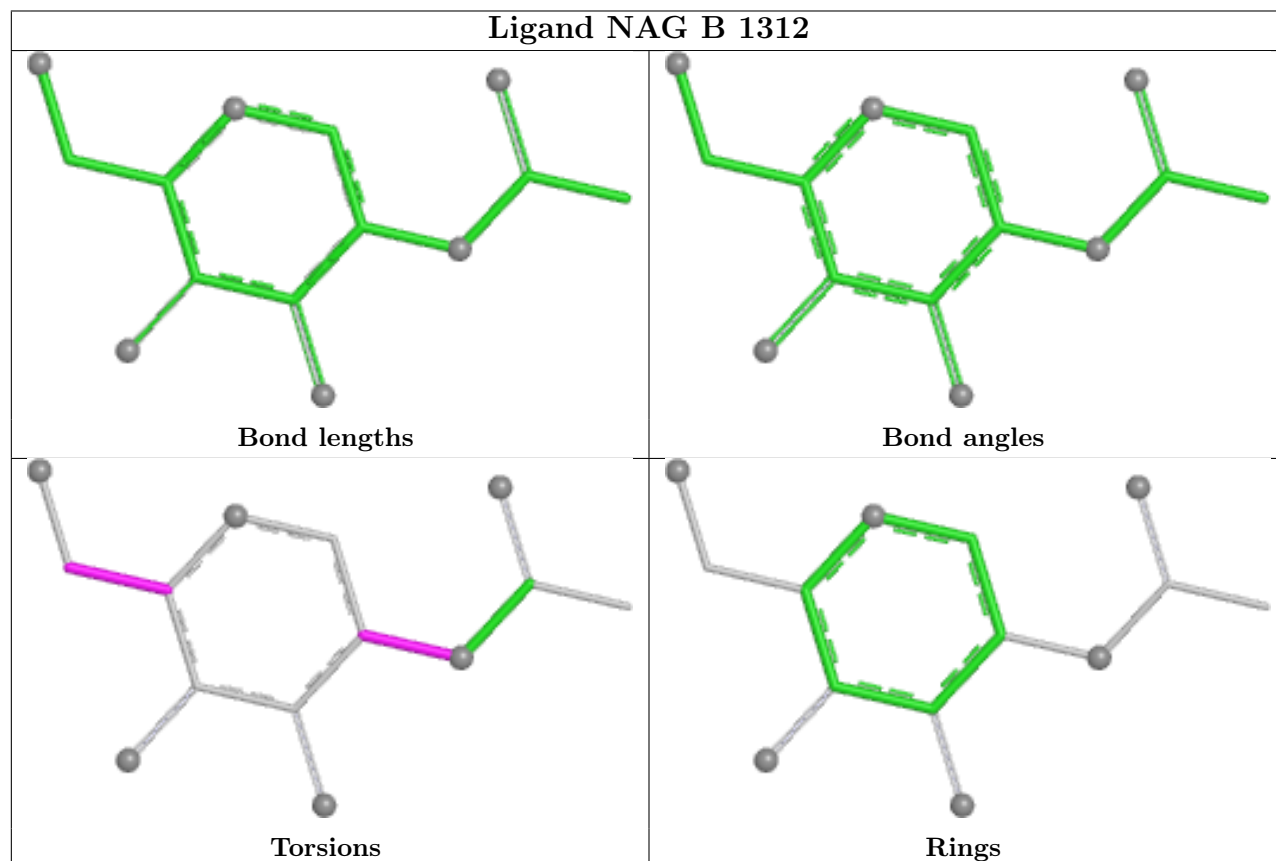


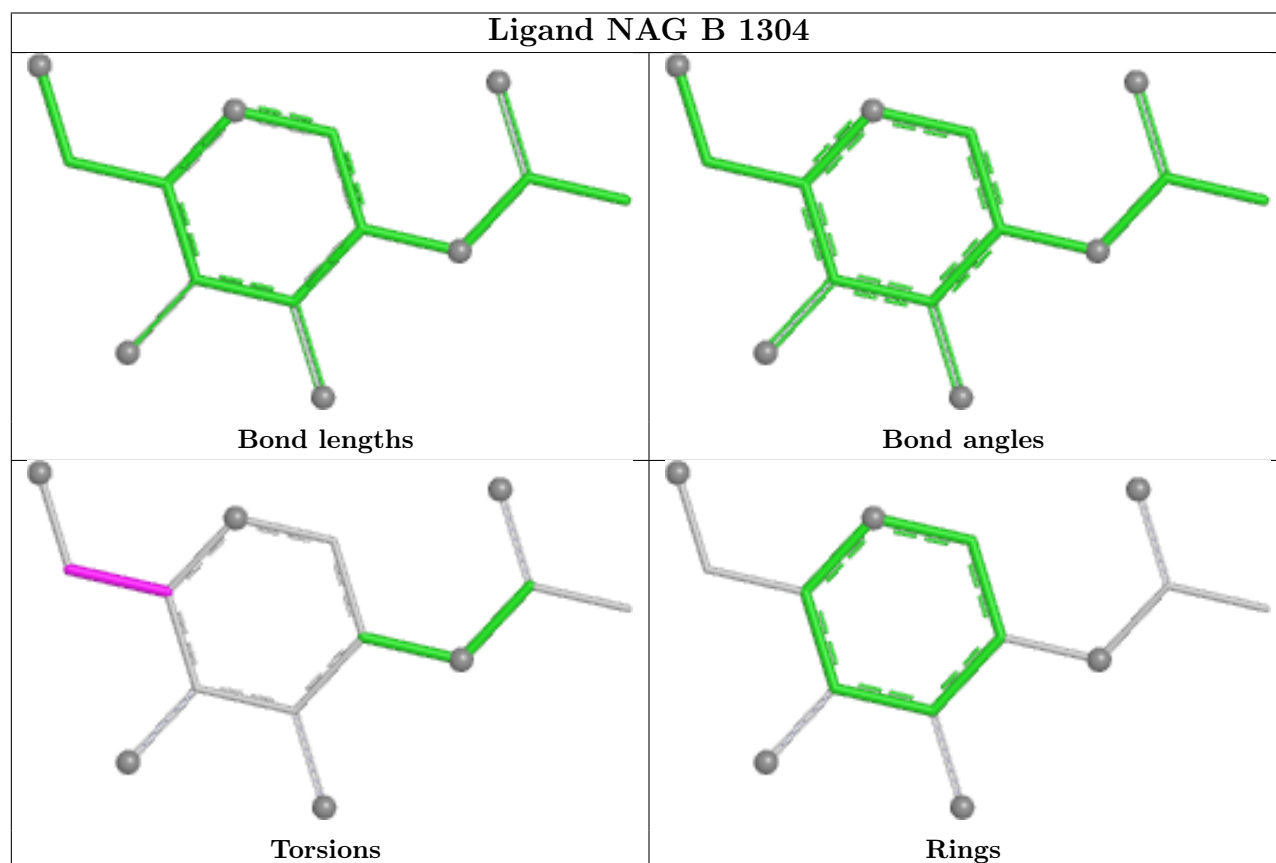
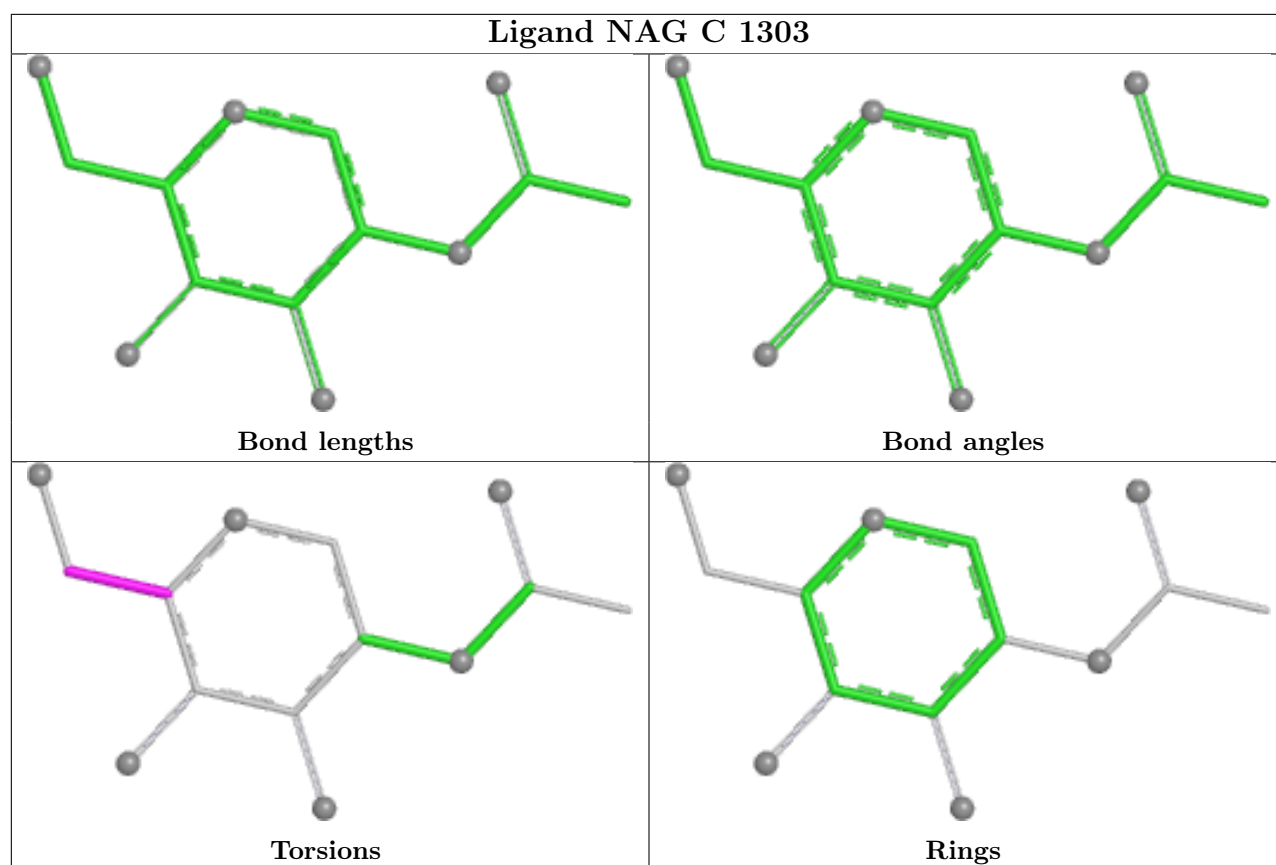


Ligand NAG C 1313

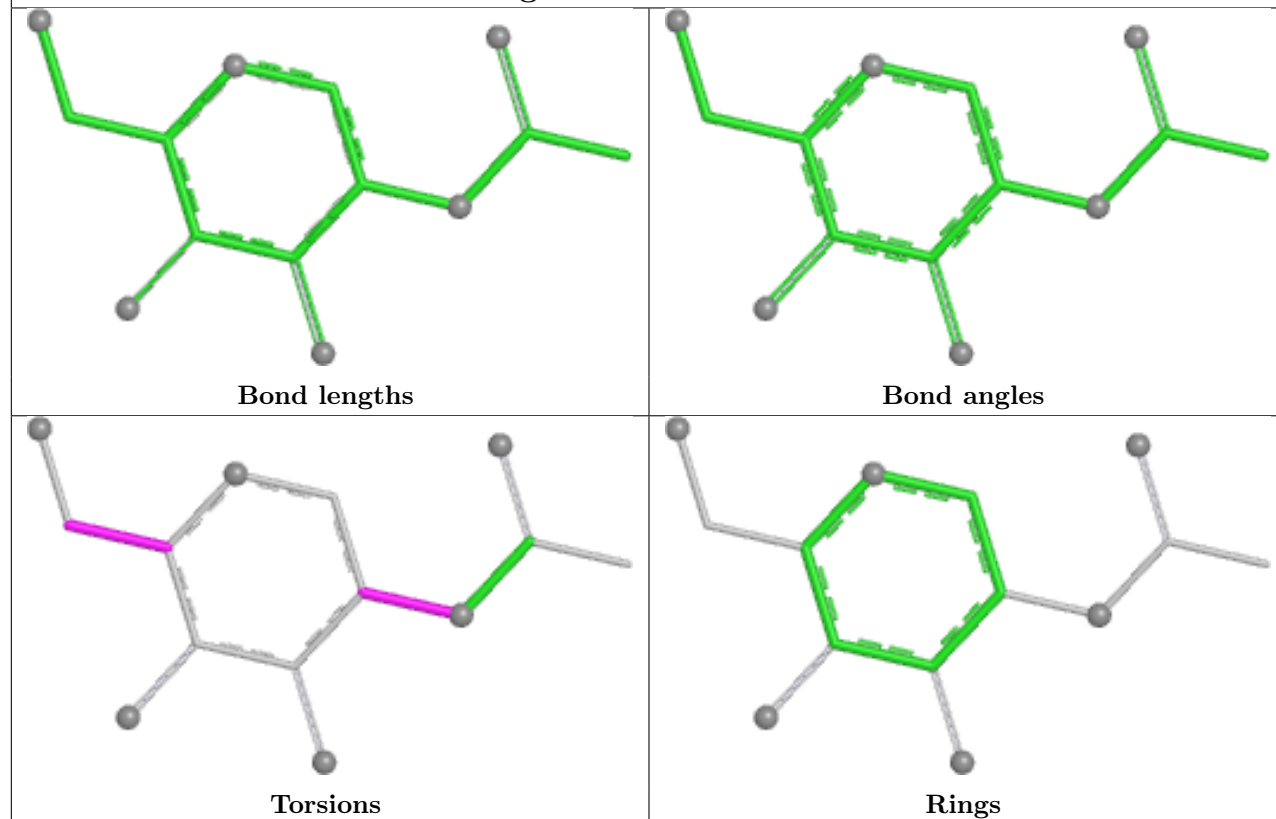


Ligand NAG B 1312

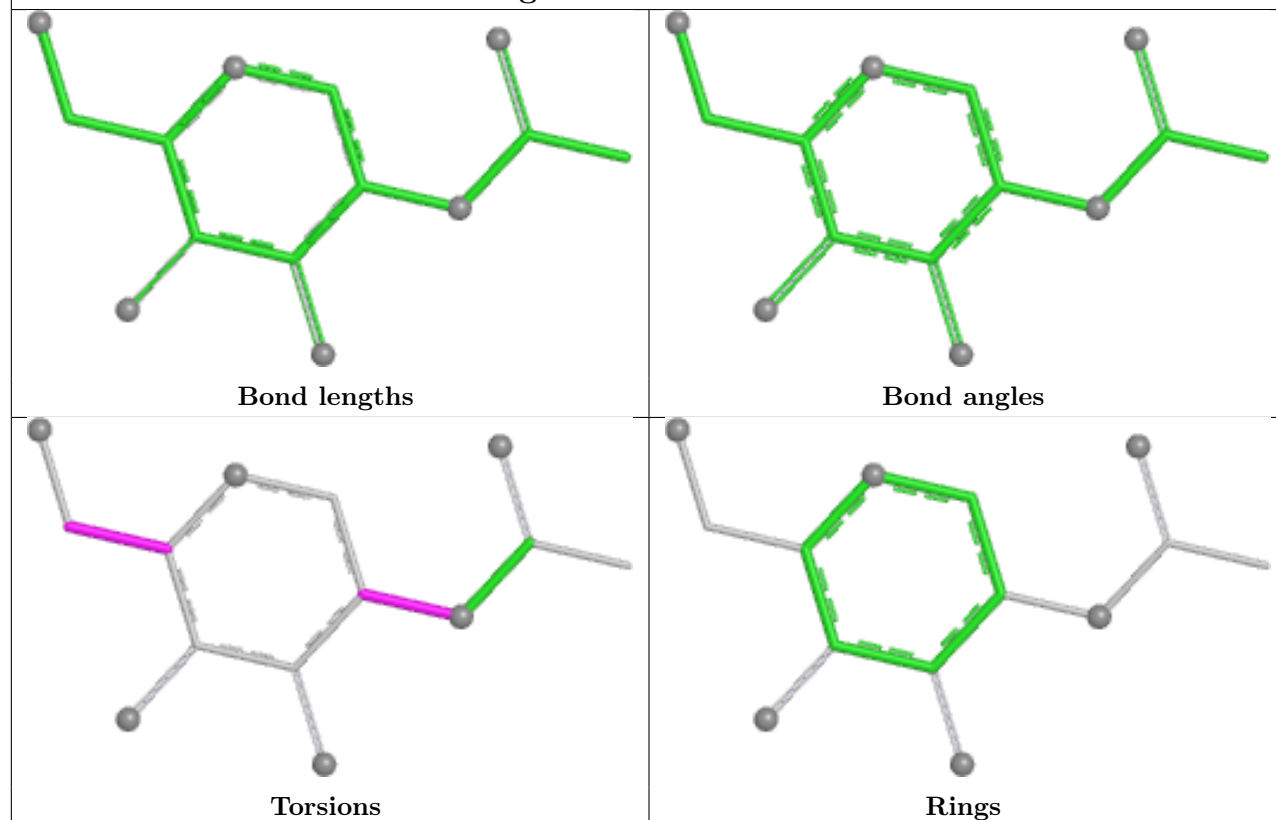


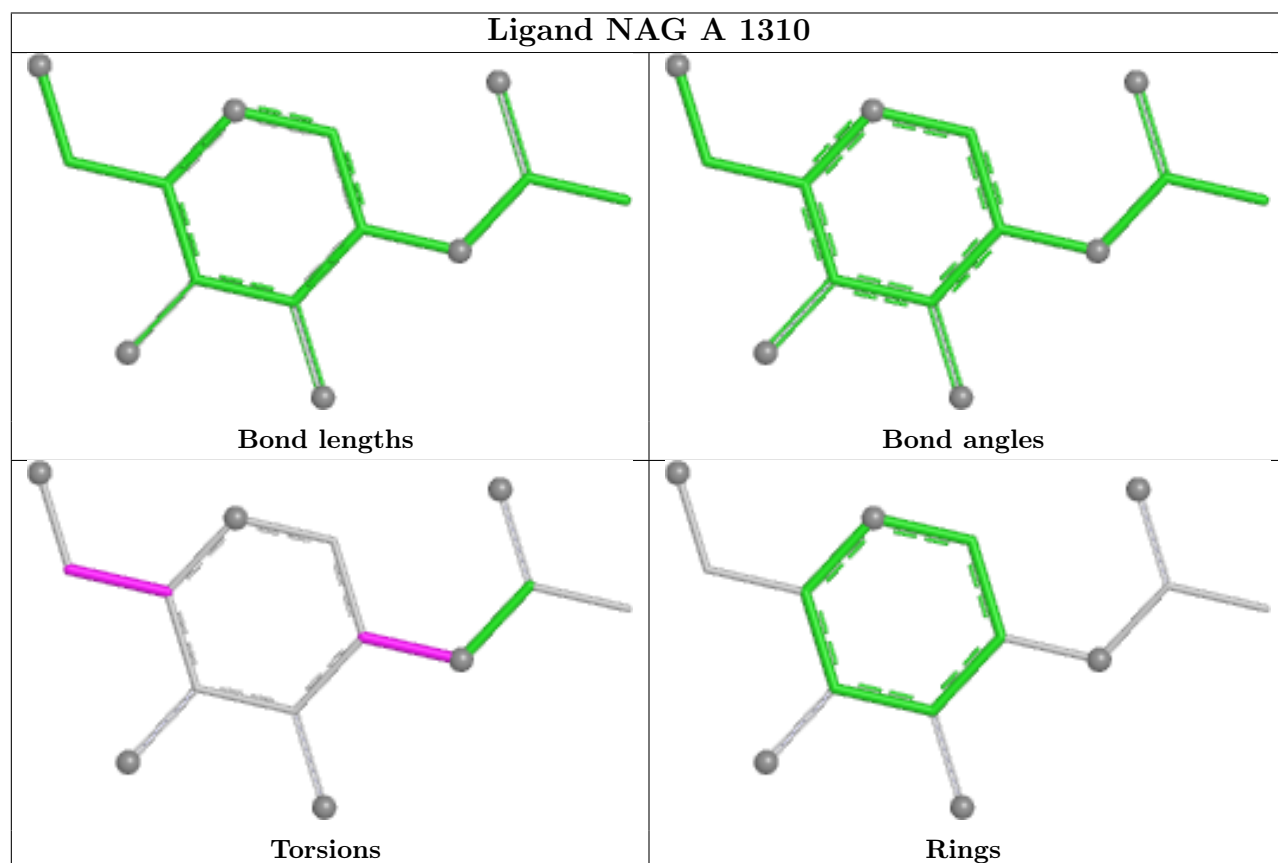
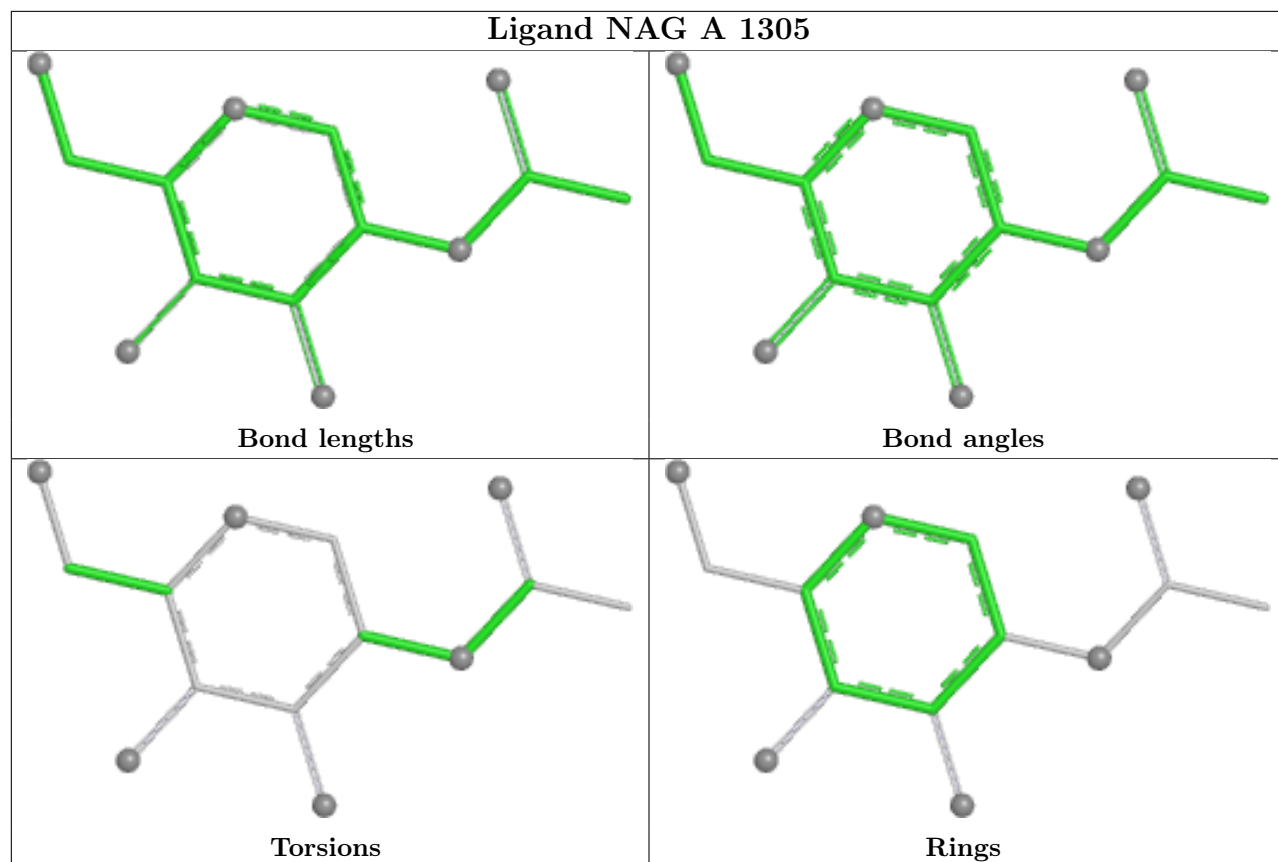


Ligand NAG B 1307

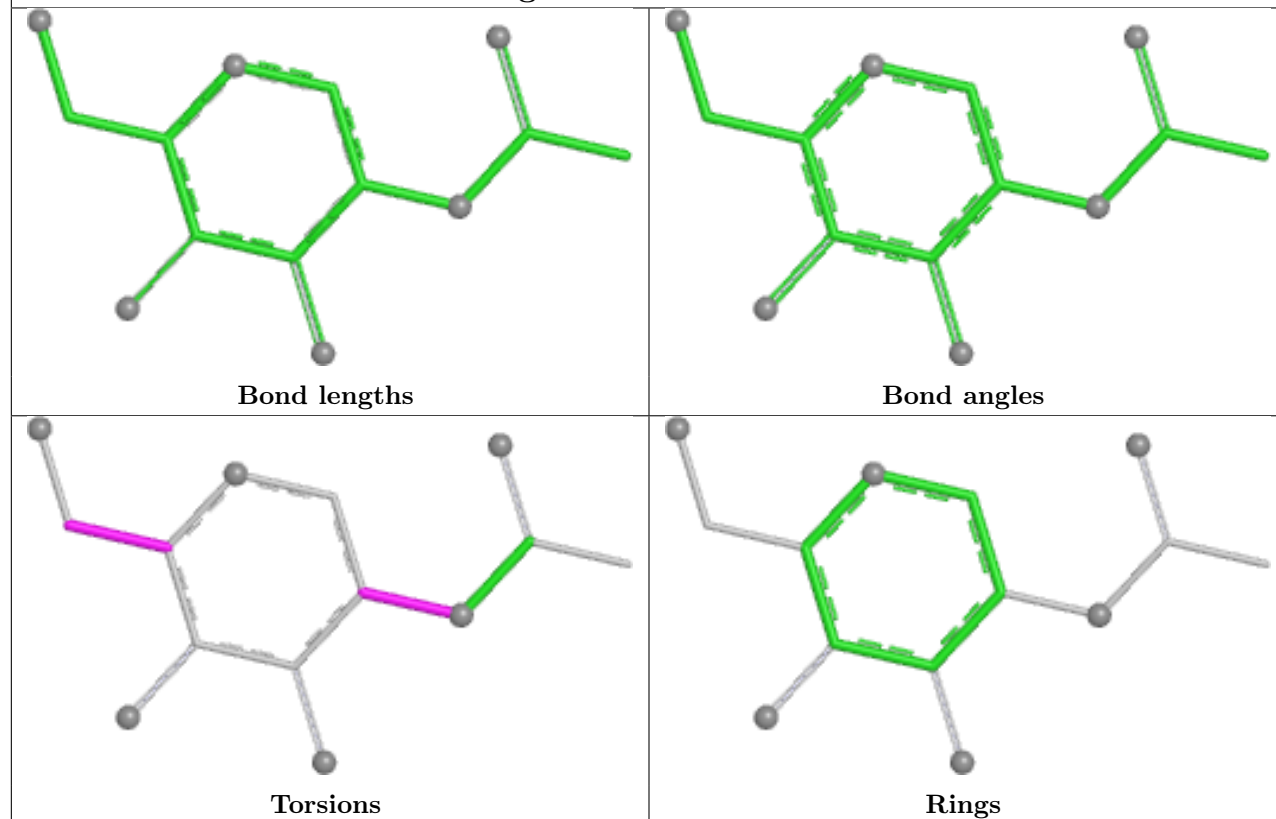


Ligand NAG C 1308

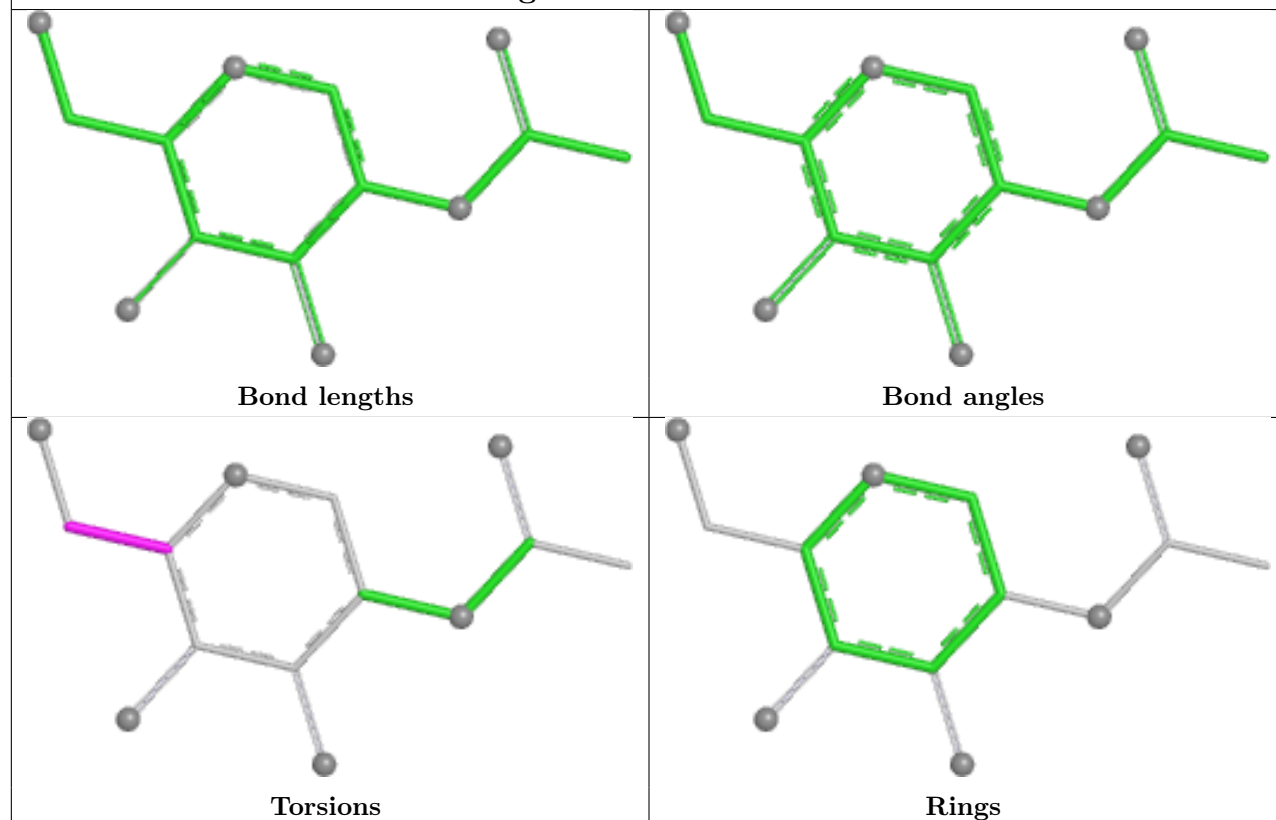


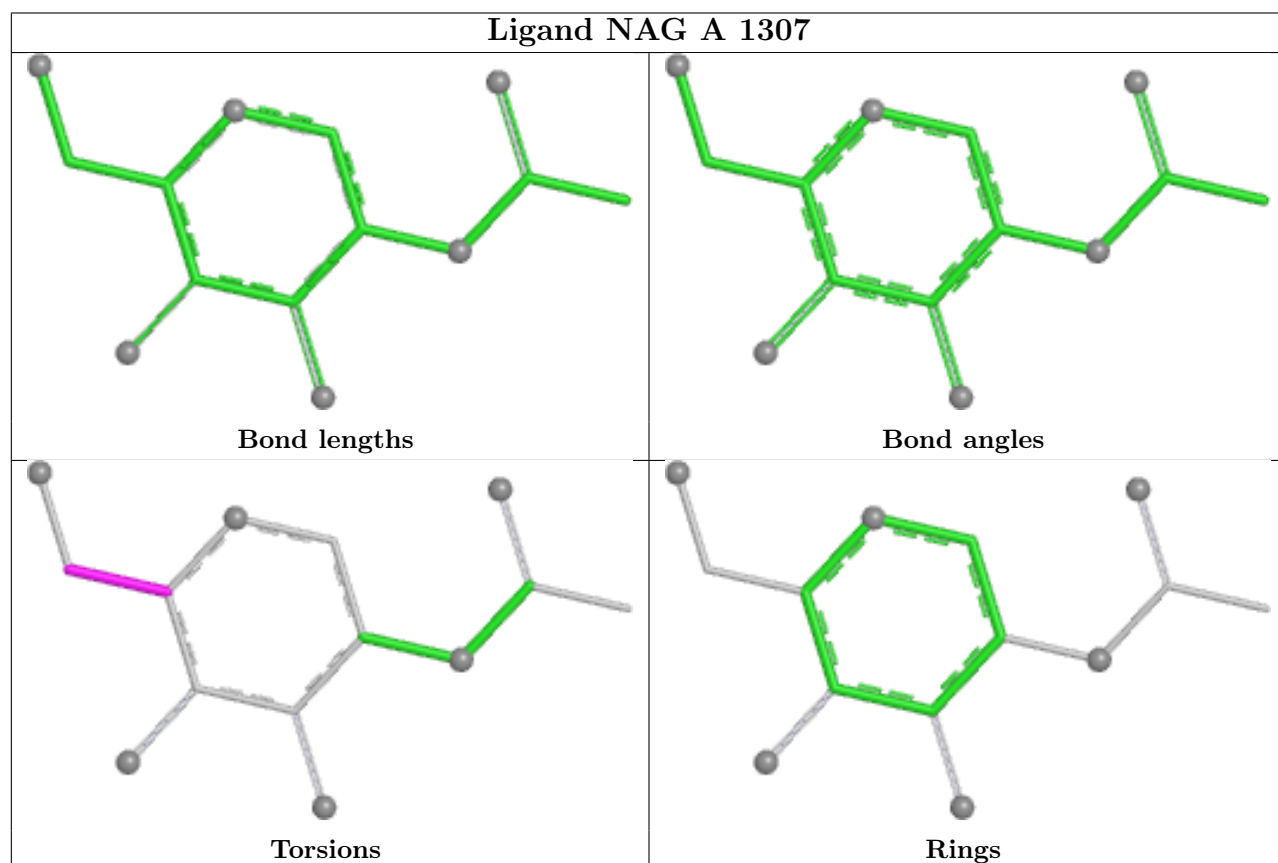
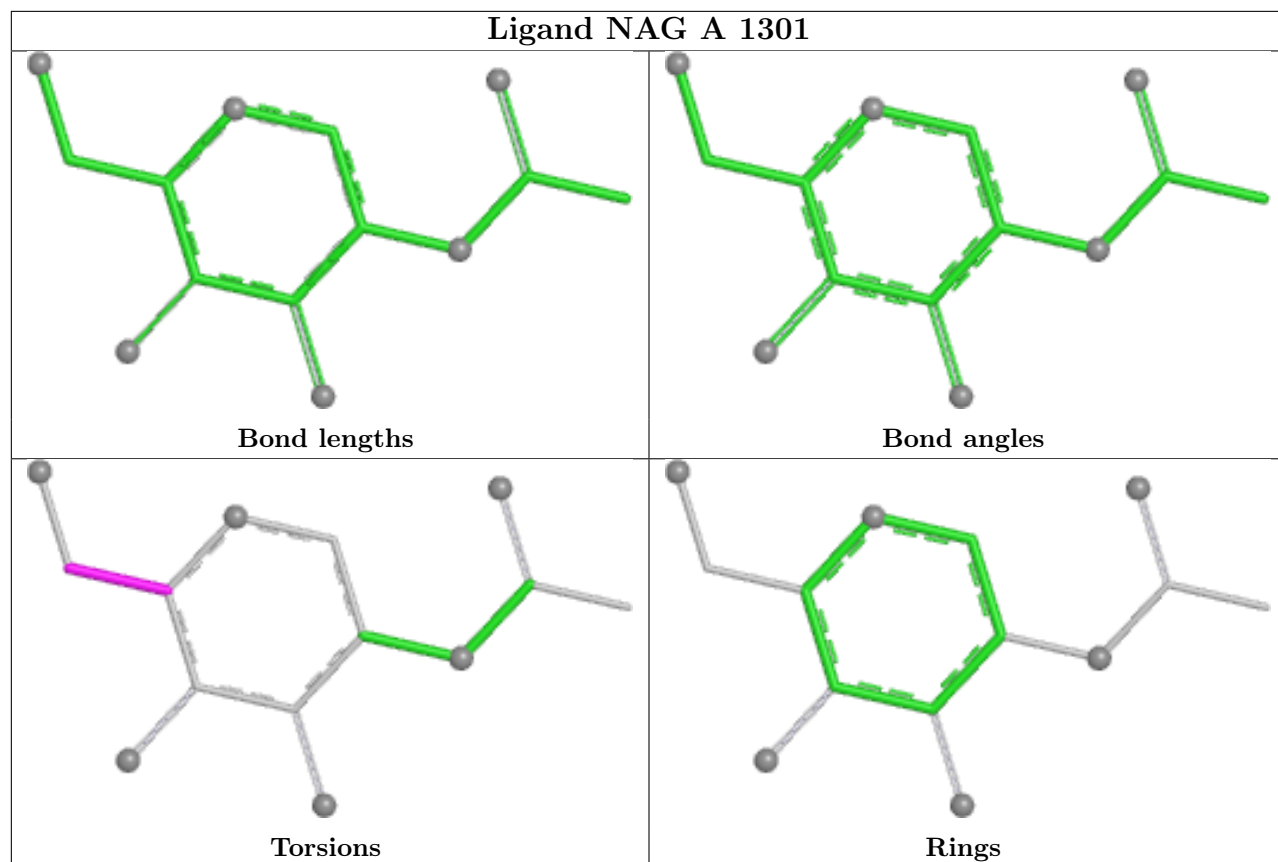


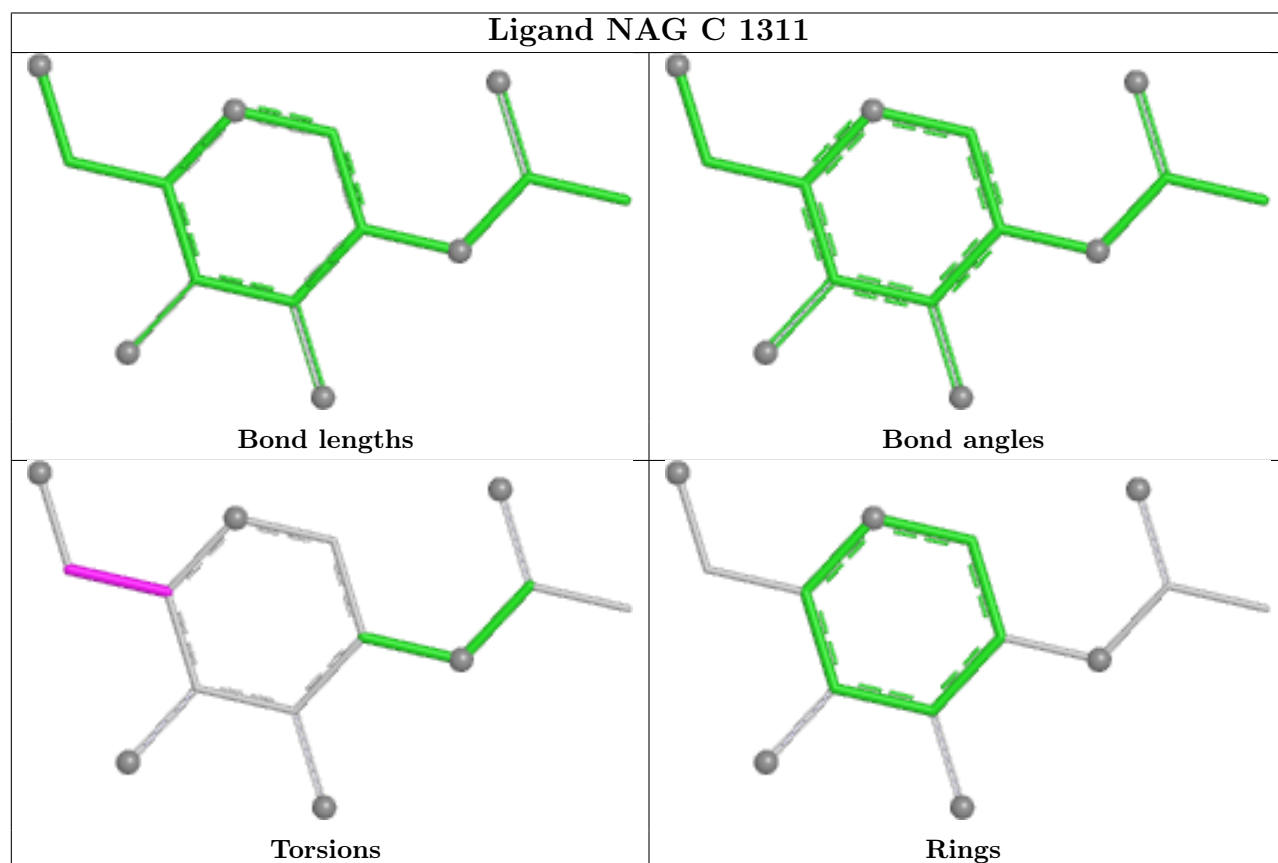
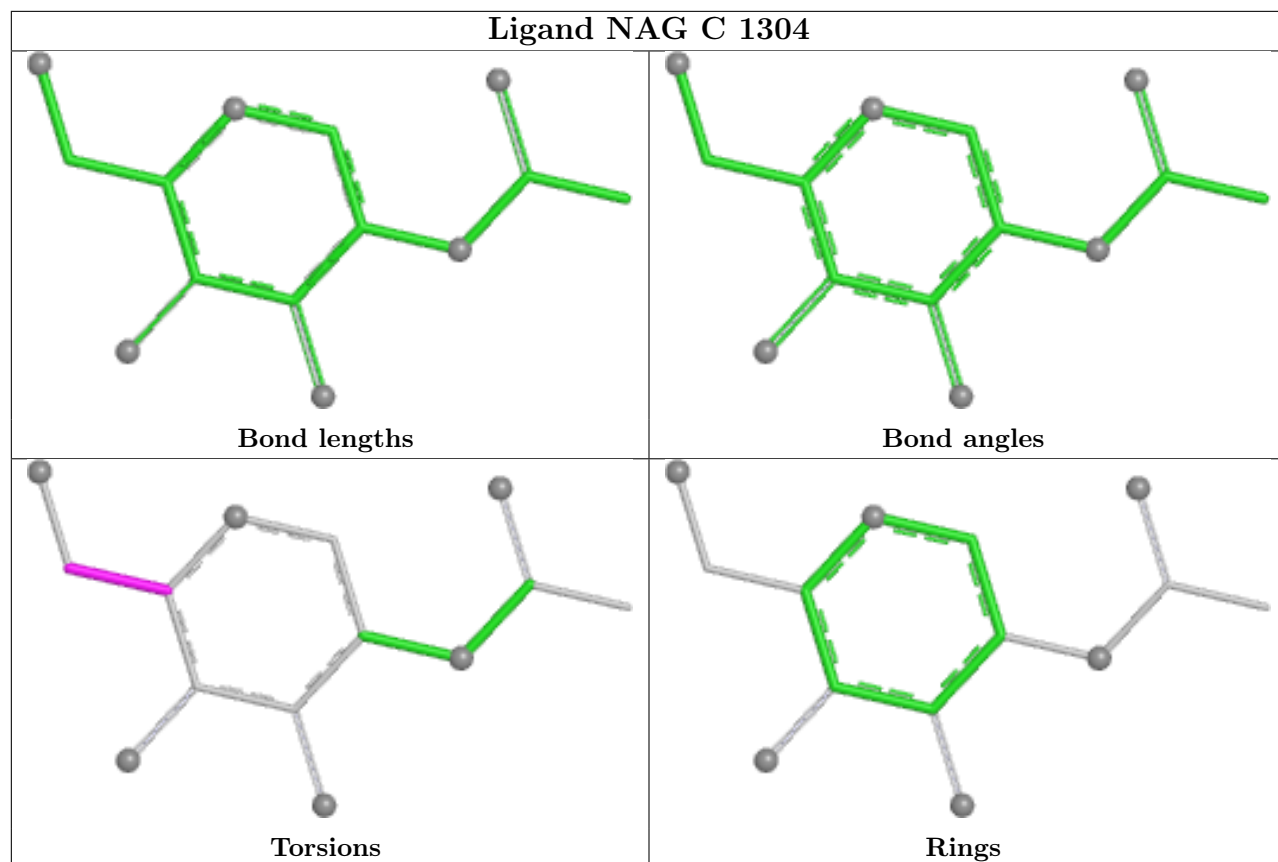
Ligand NAG A 1303

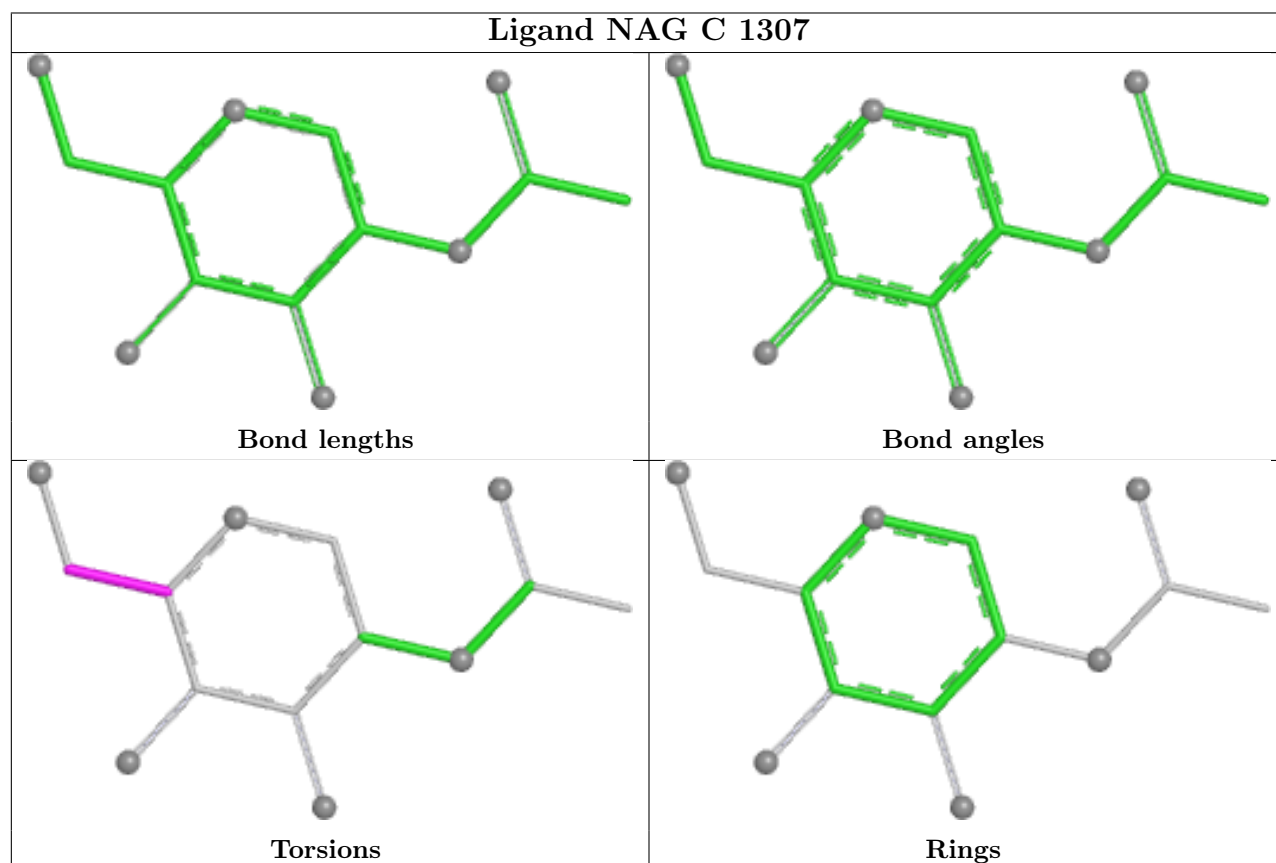
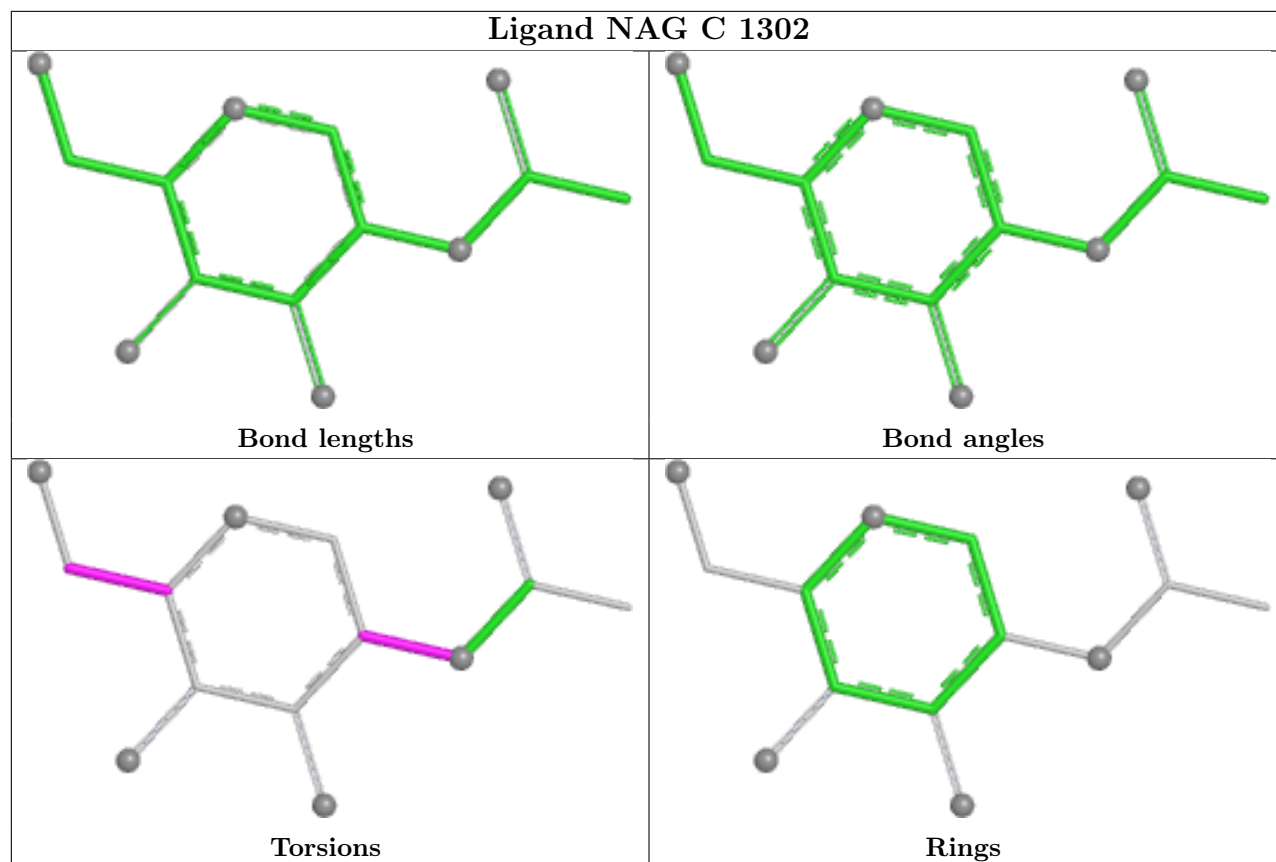


Ligand NAG A 1311

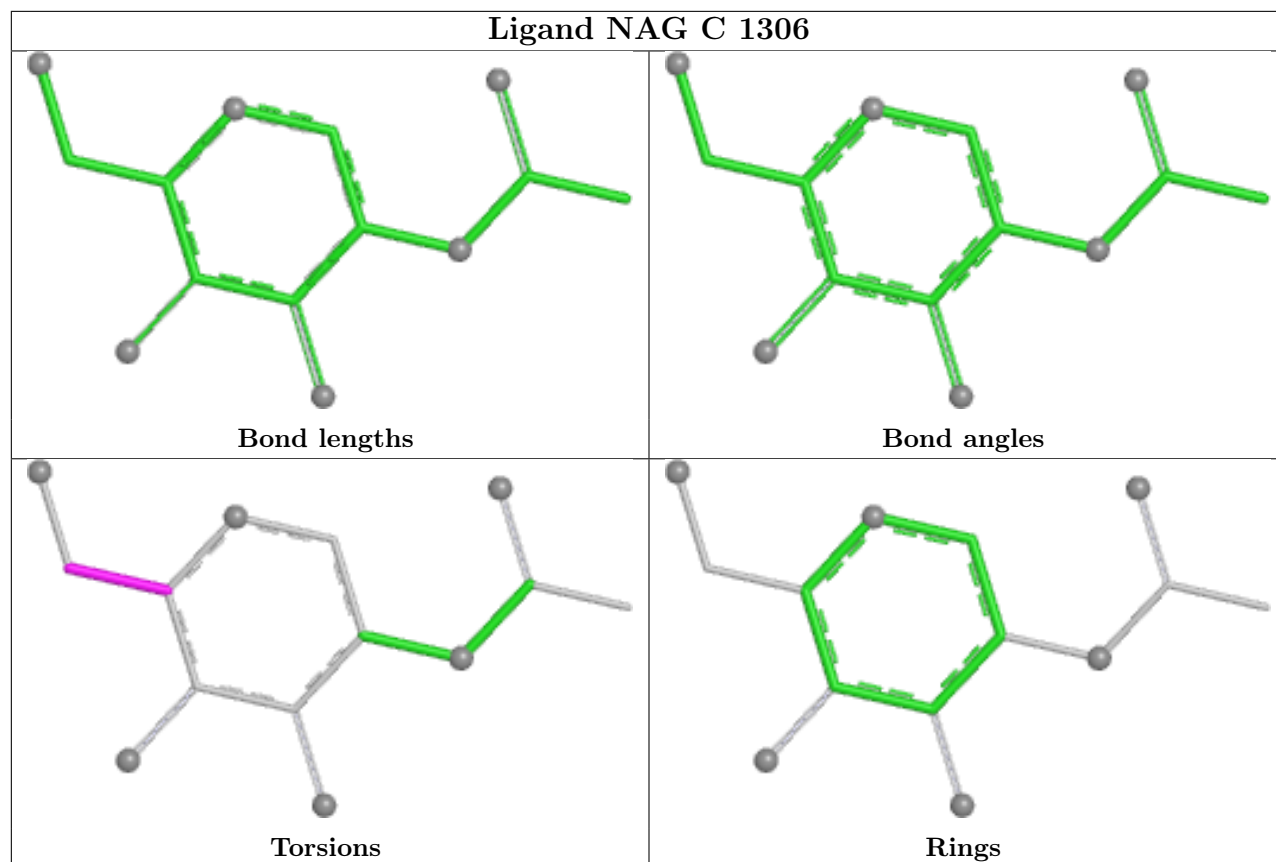




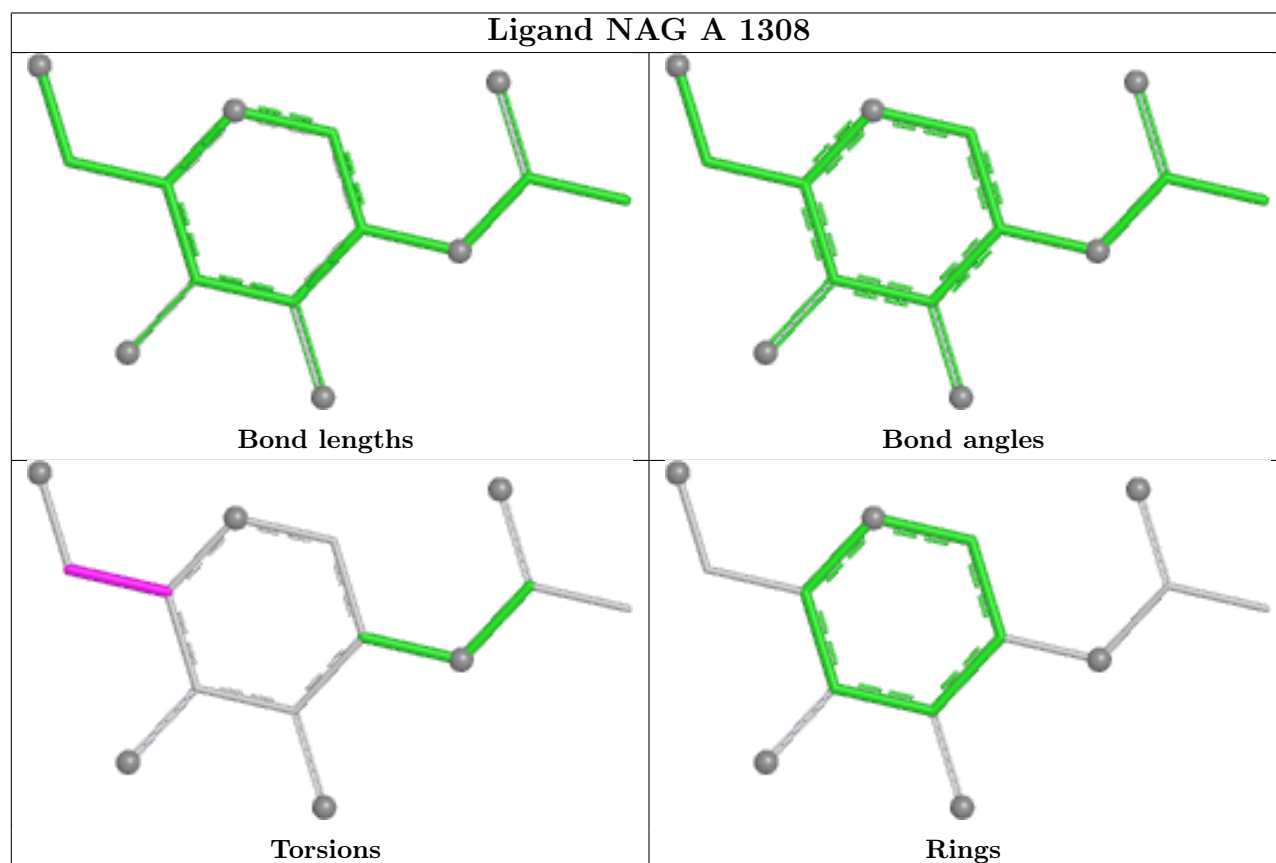


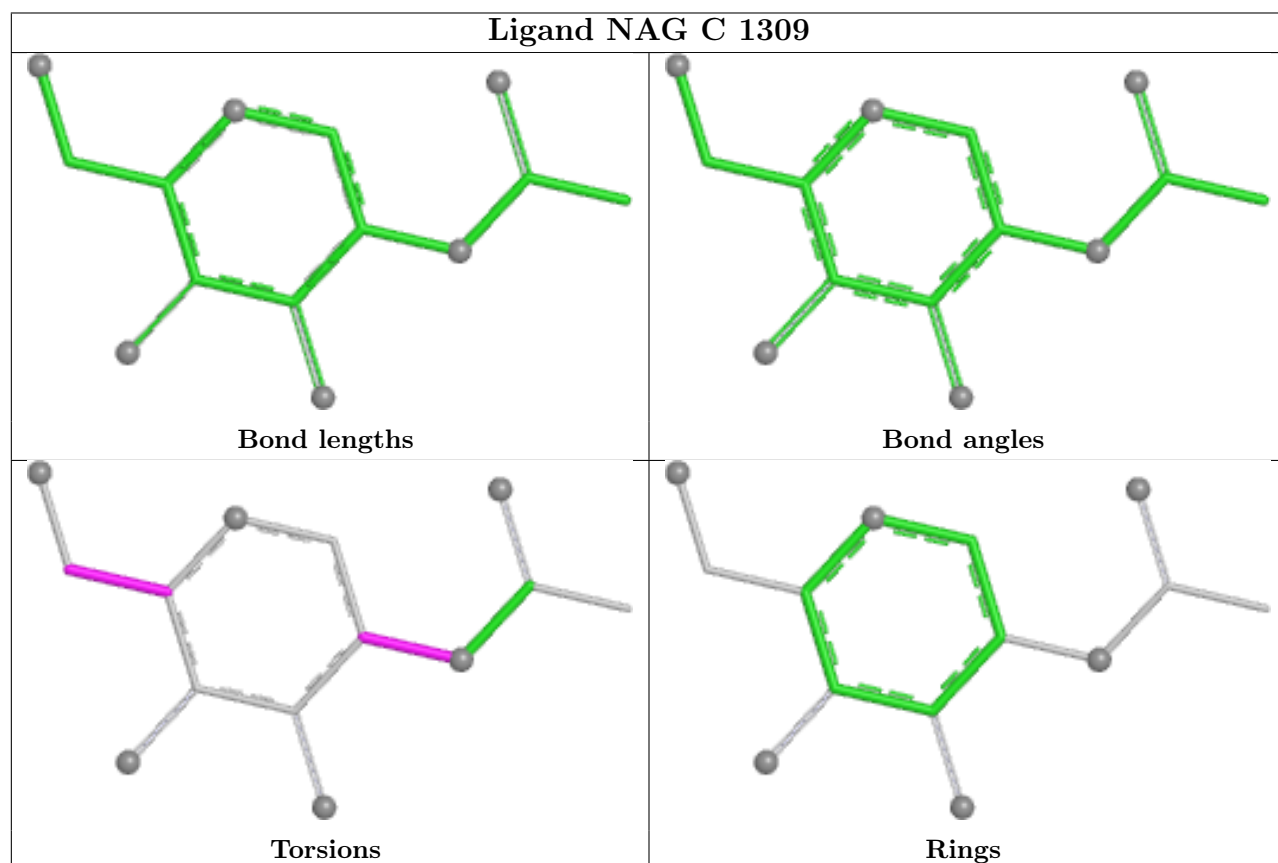
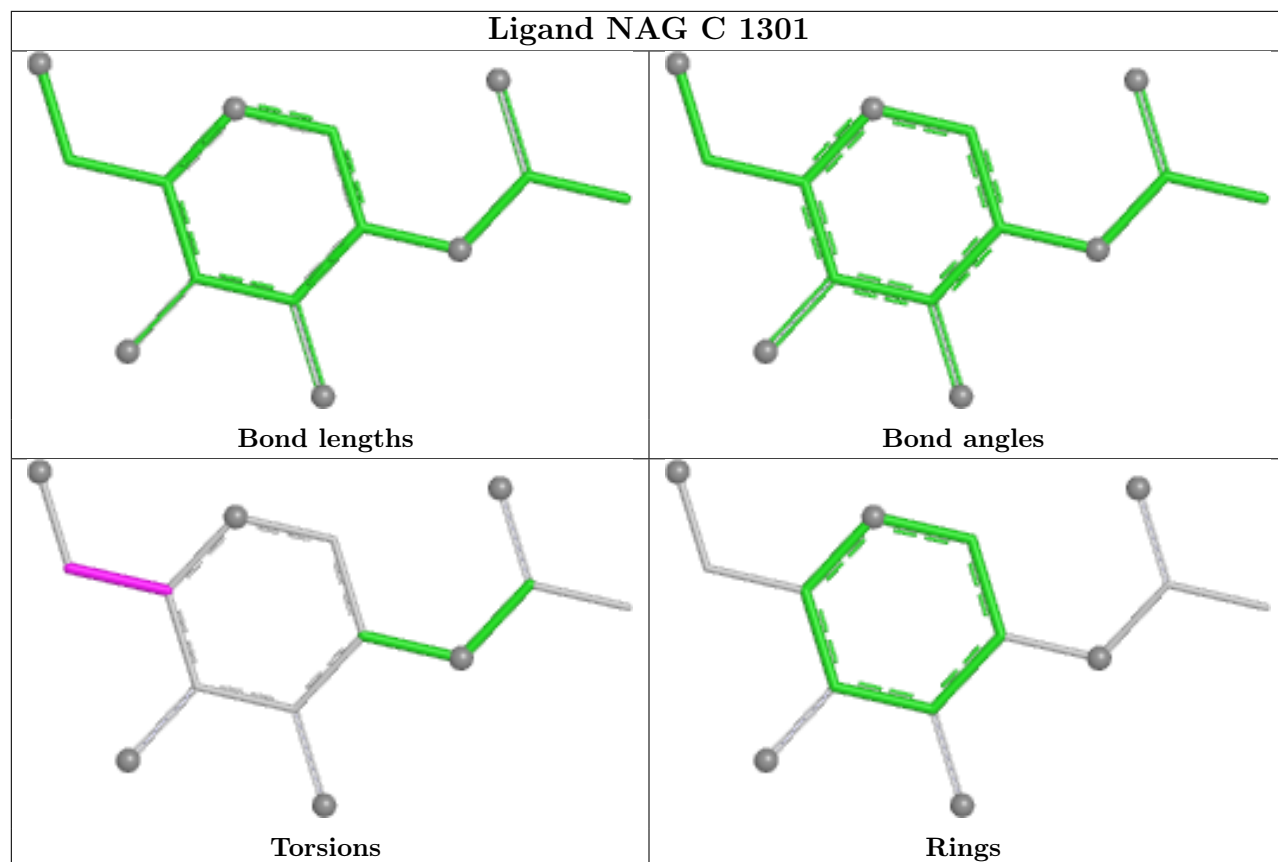


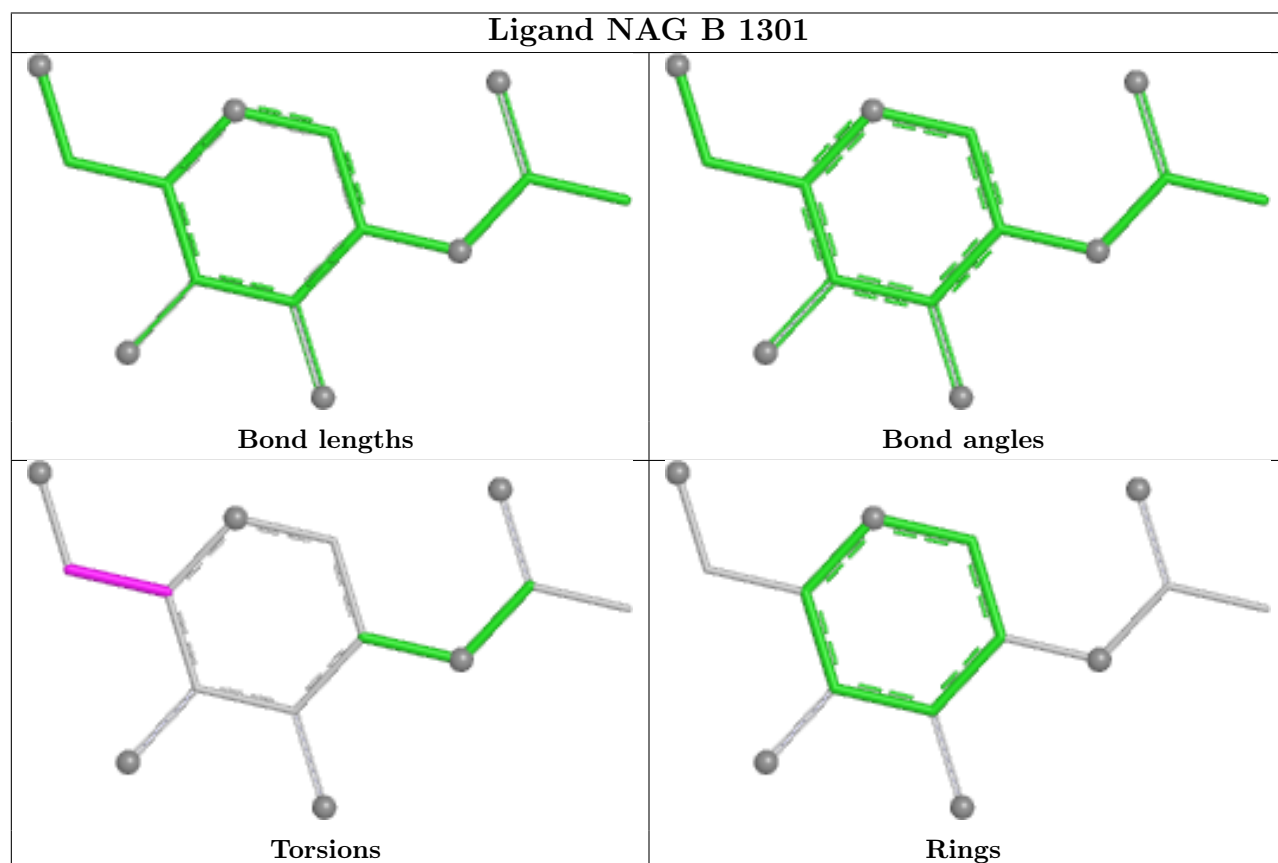
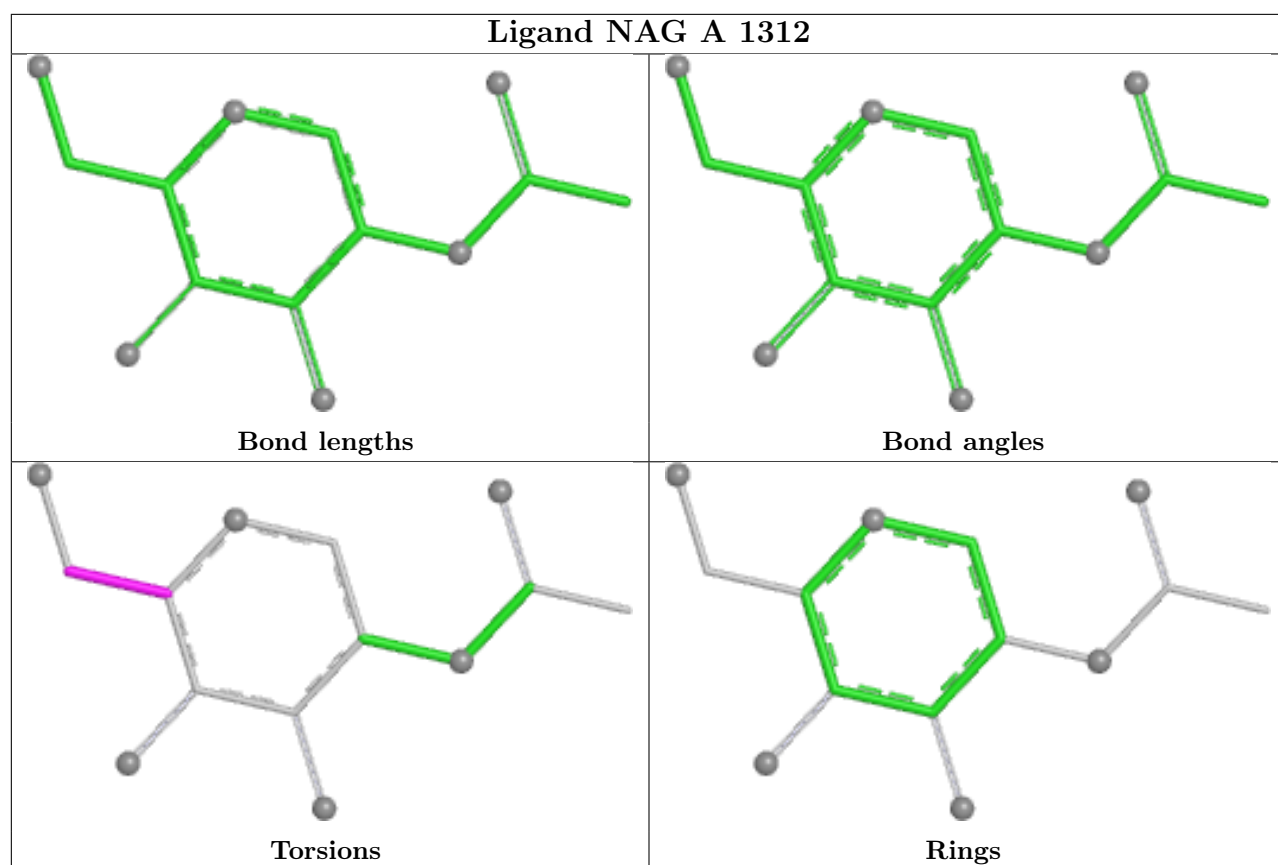
Ligand NAG C 1306

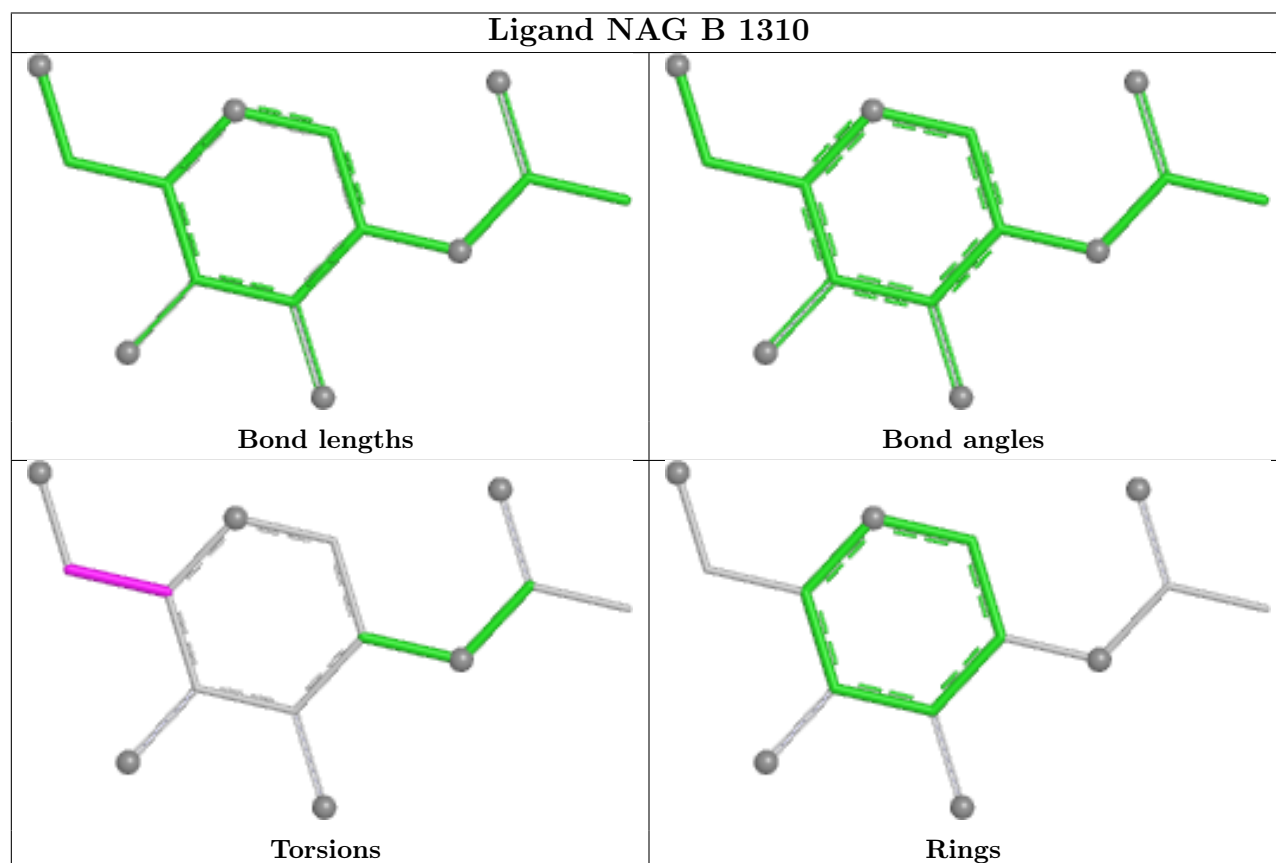
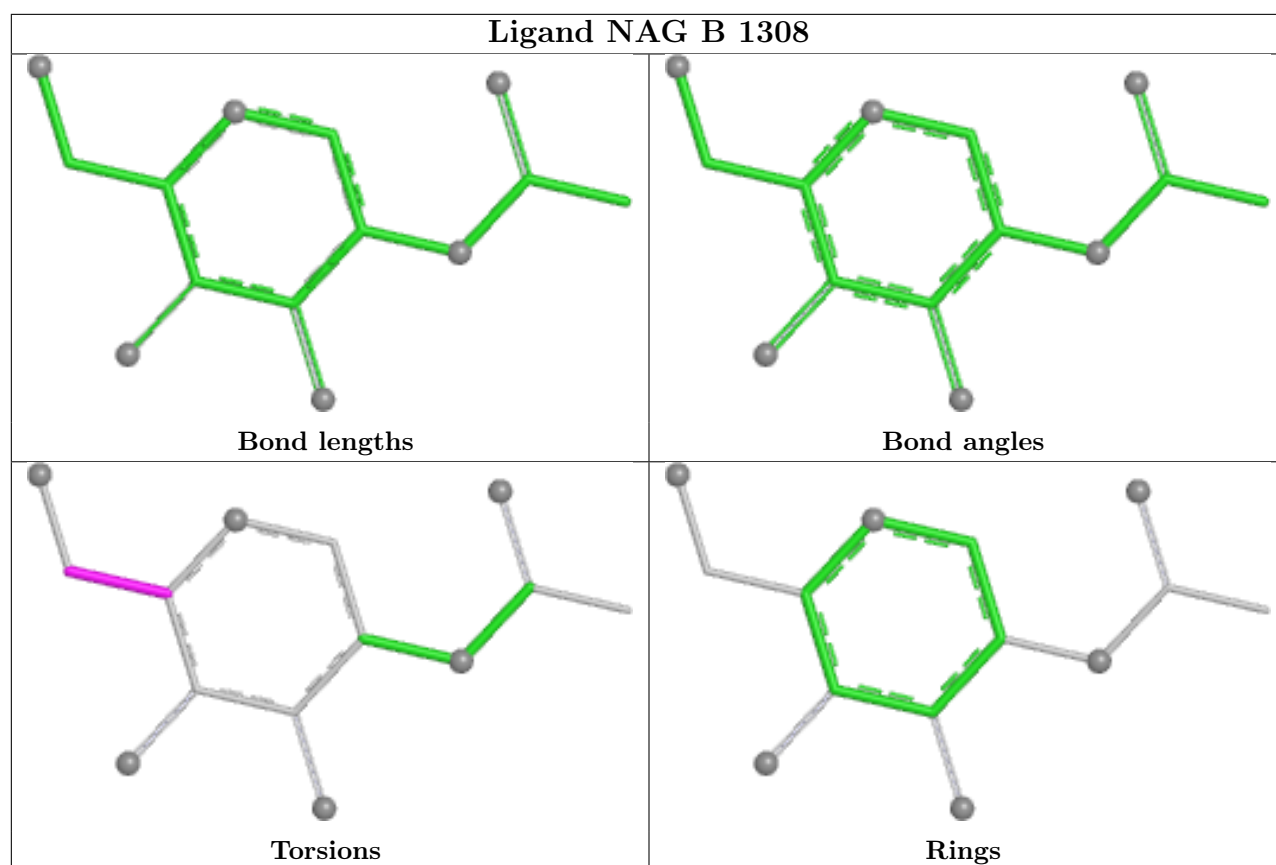


Ligand NAG A 1308

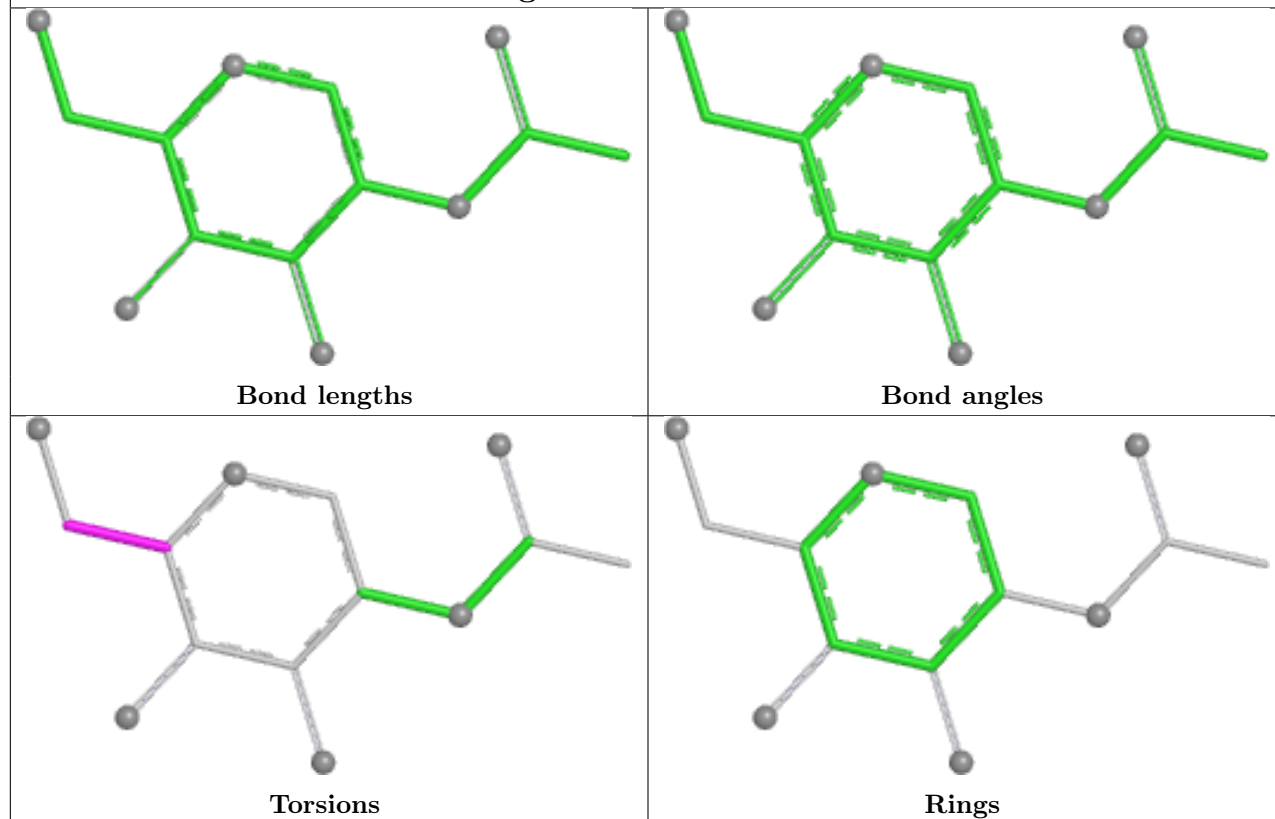




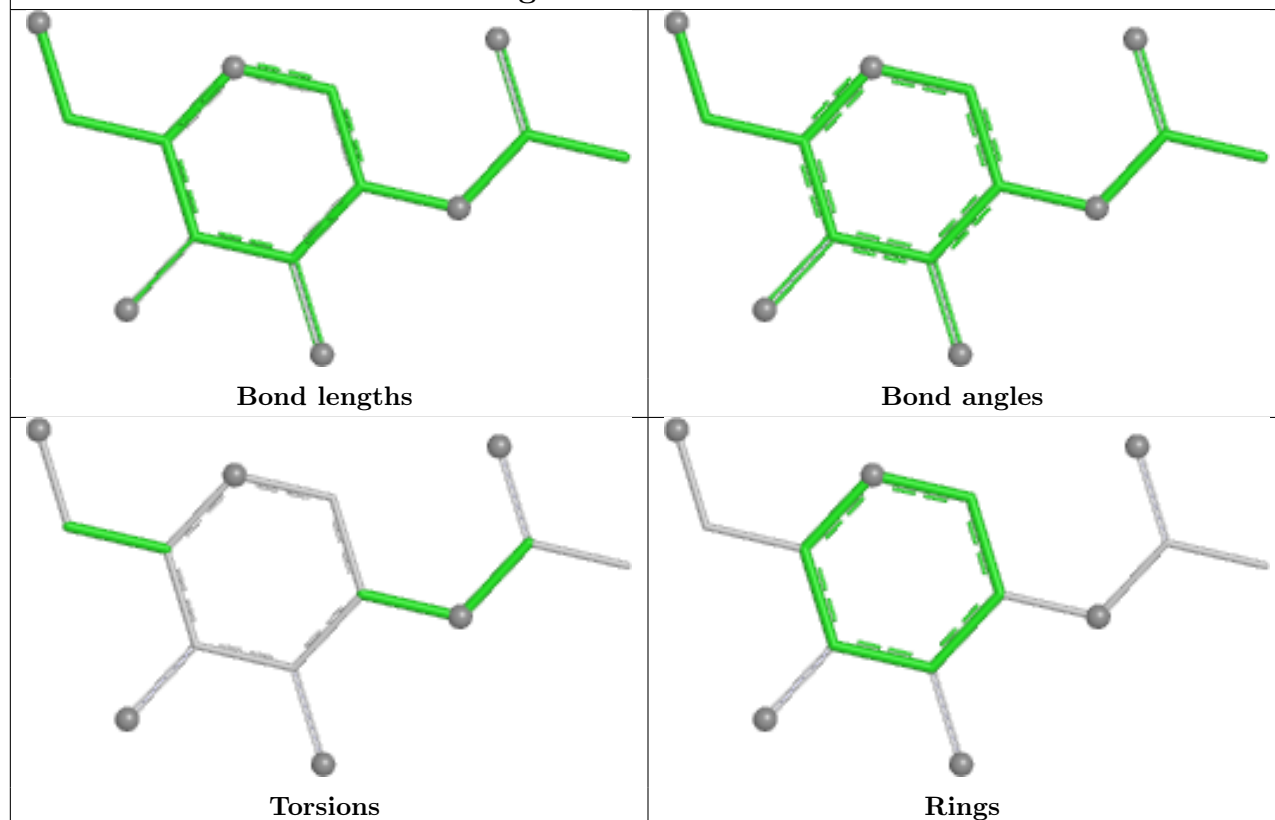




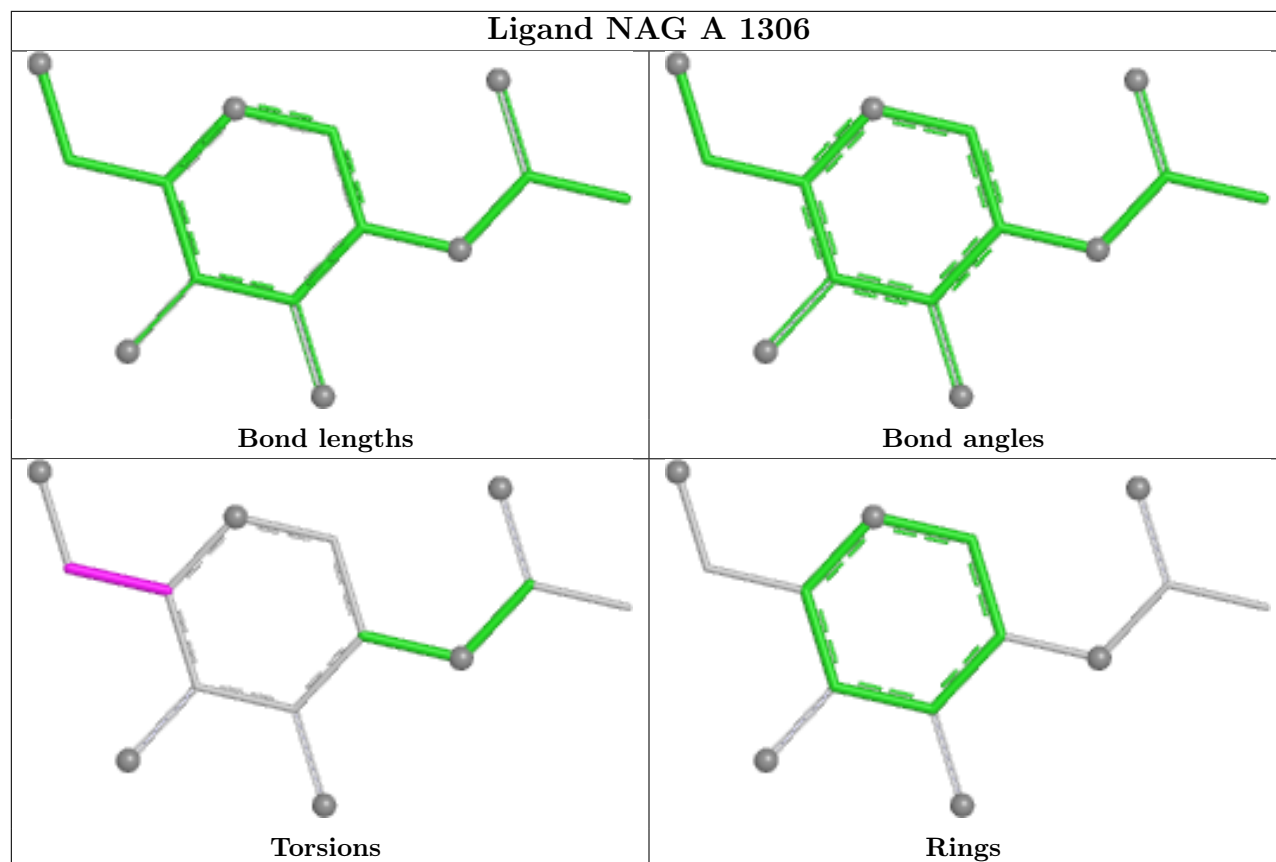
Ligand NAG B 1302



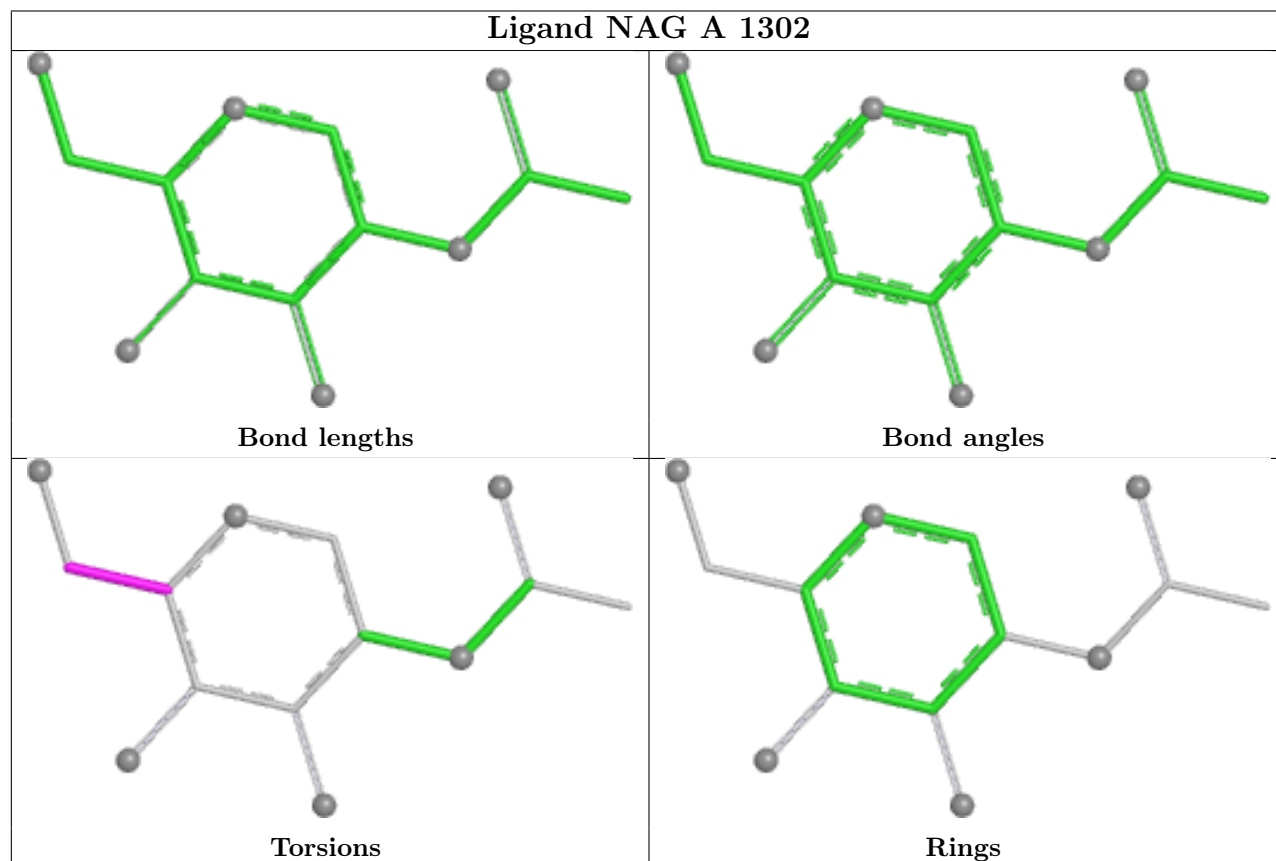
Ligand NAG B 1311



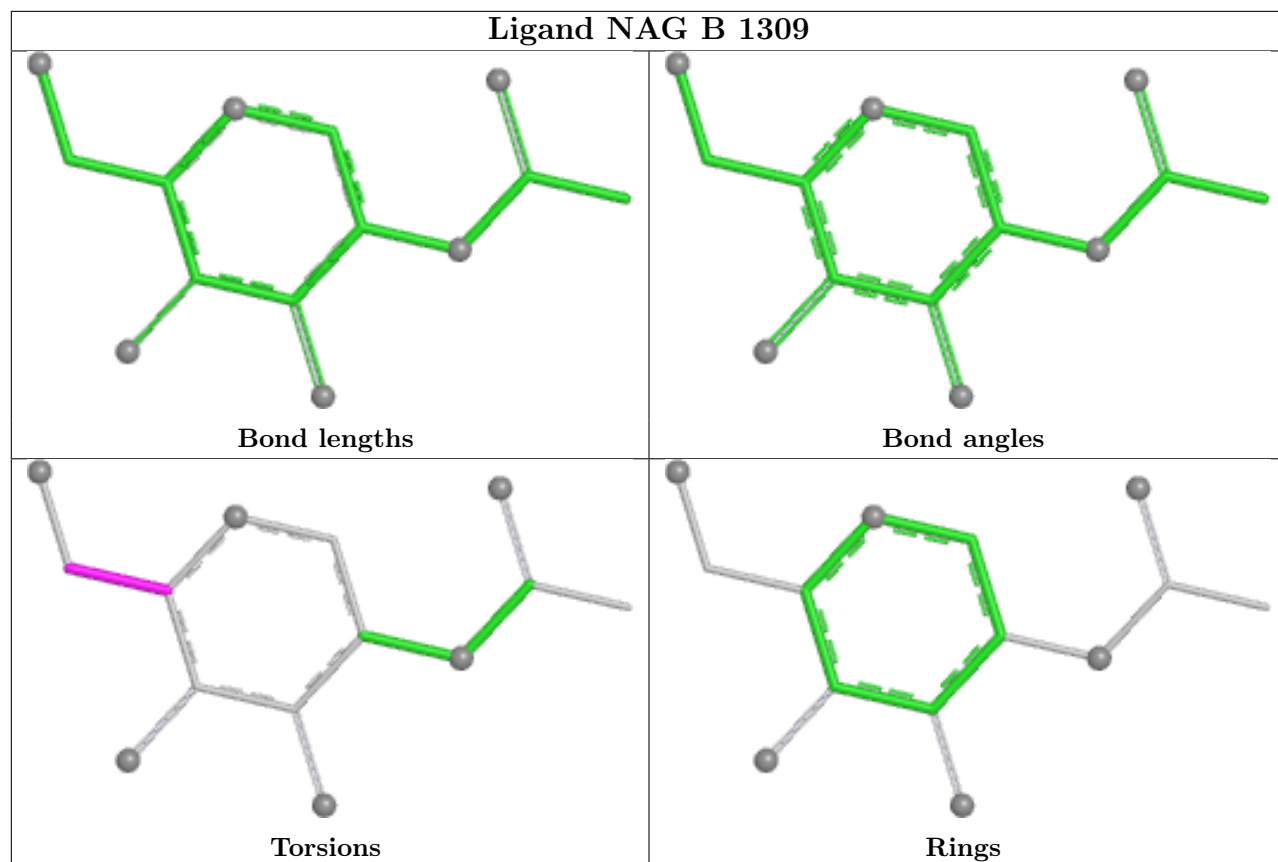
Ligand NAG A 1306



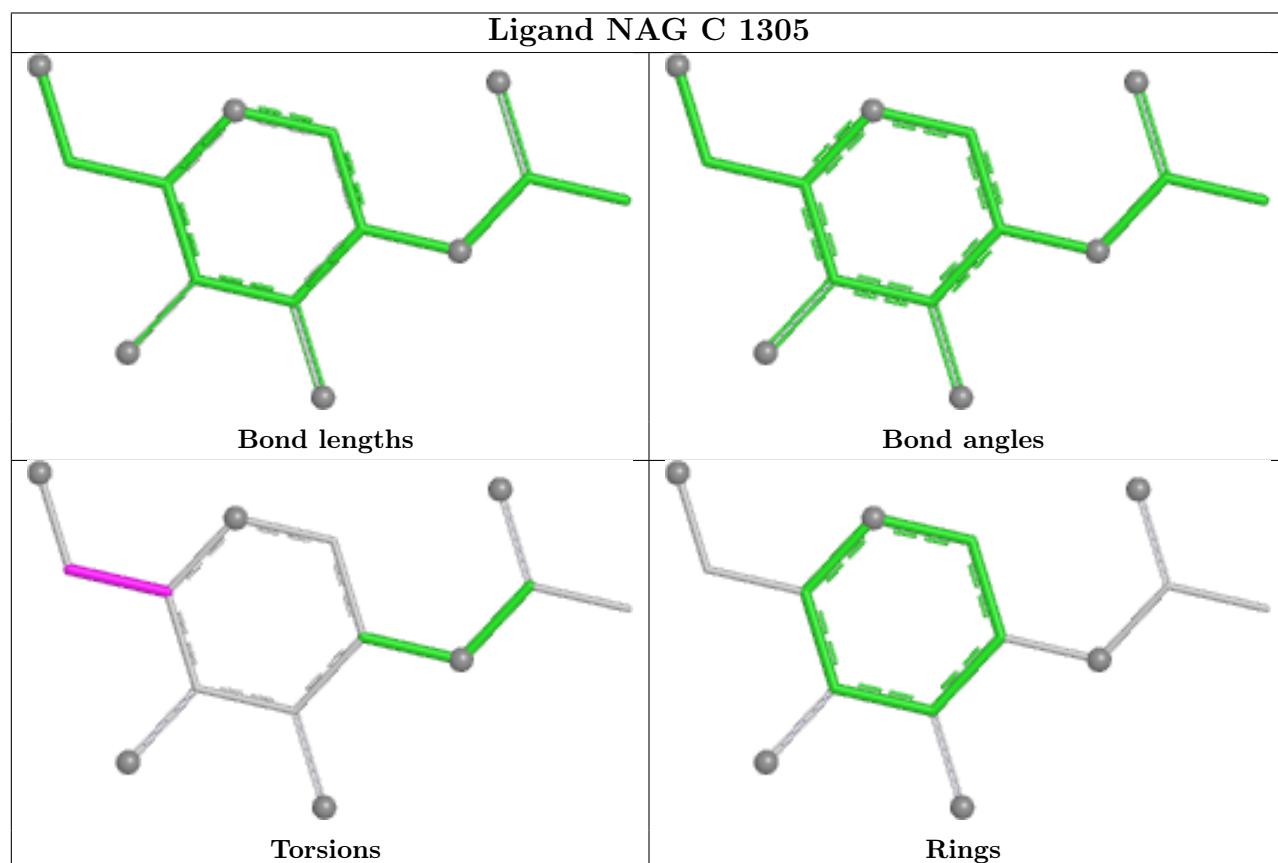
Ligand NAG A 1302



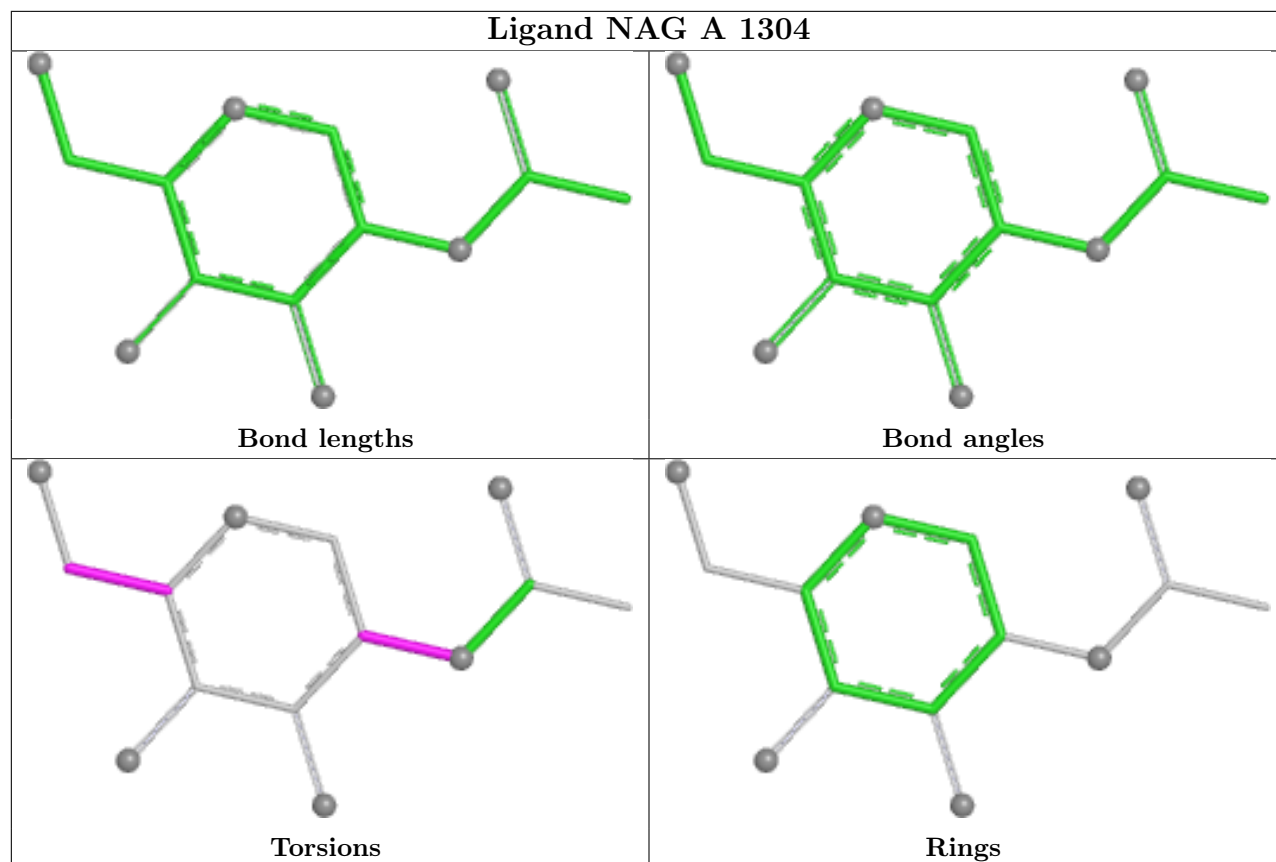
Ligand NAG B 1309



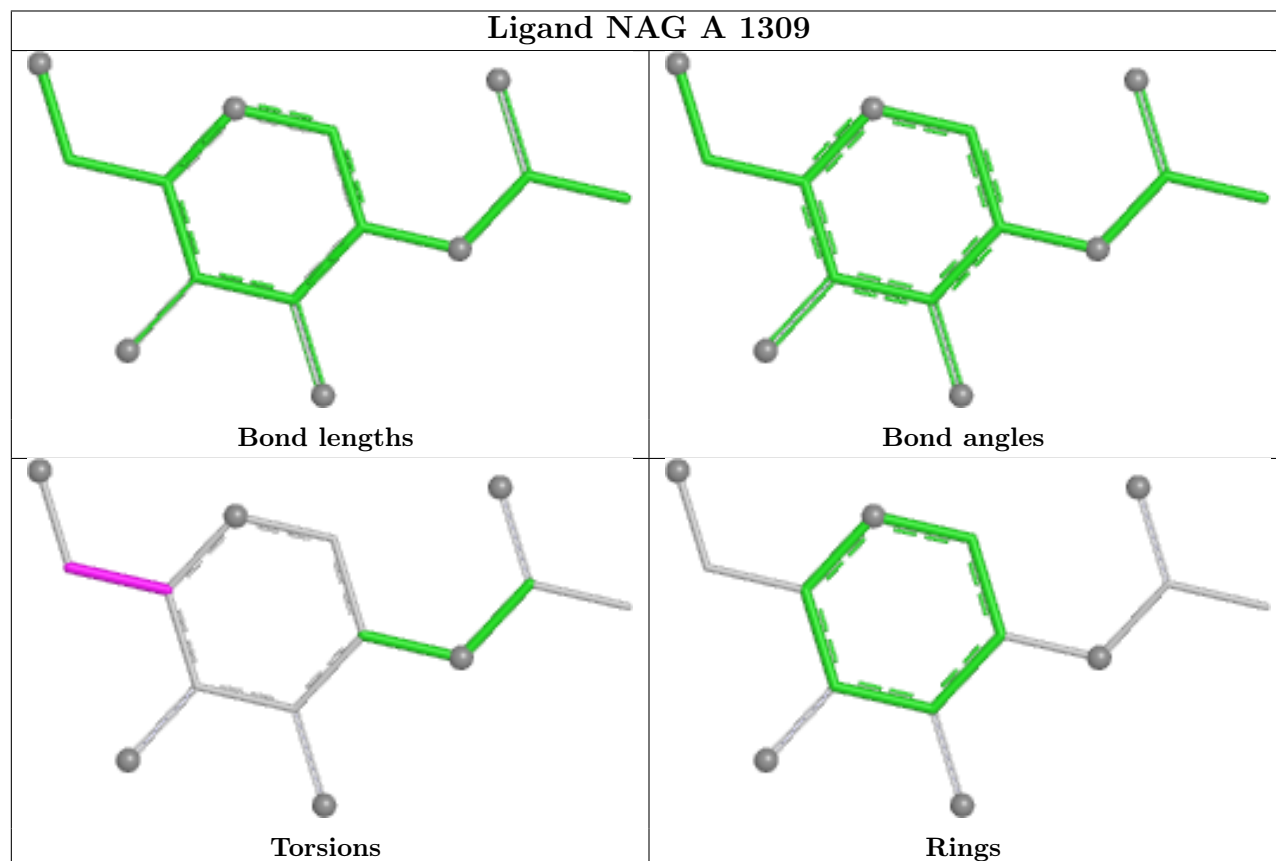
Ligand NAG C 1305



Ligand NAG A 1304



Ligand NAG A 1309



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

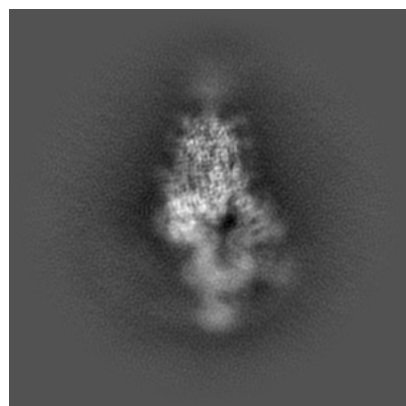
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34135. These allow visual inspection of the internal detail of the map and identification of artifacts.

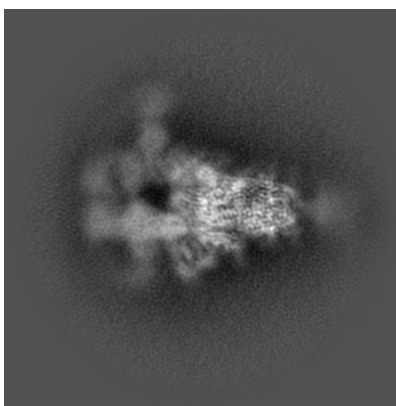
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

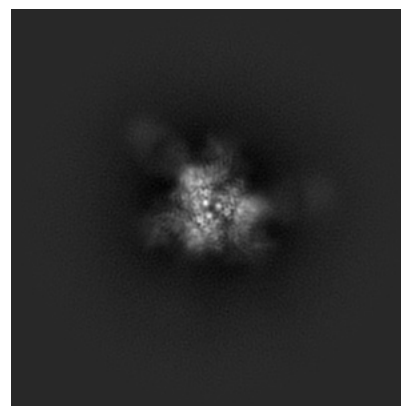
6.1.1 Primary map



X

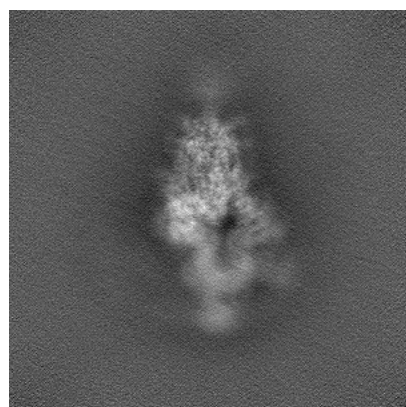


Y

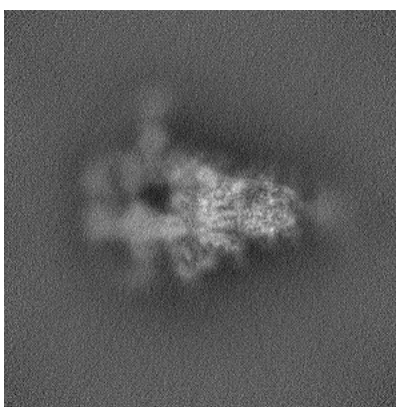


Z

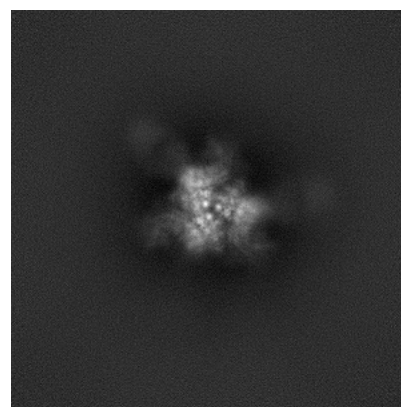
6.1.2 Raw map



X



Y

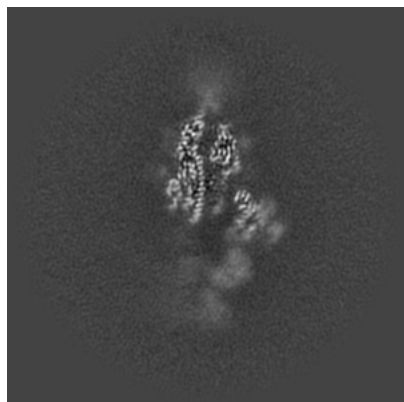


Z

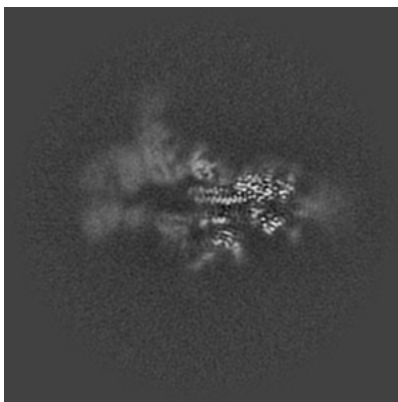
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

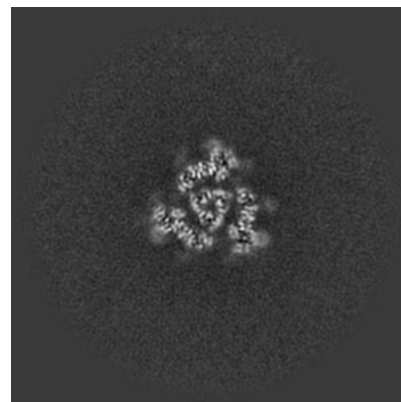
6.2.1 Primary map



X Index: 256

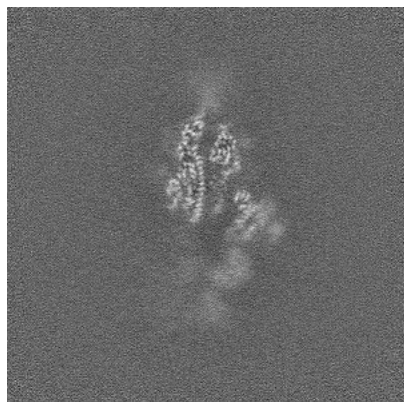


Y Index: 256



Z Index: 256

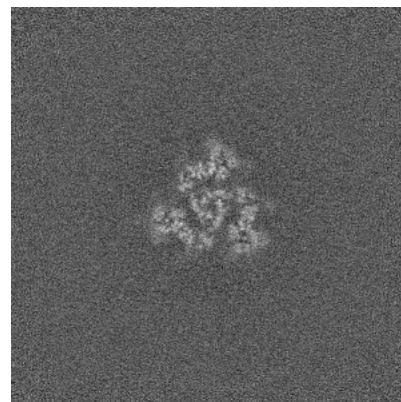
6.2.2 Raw map



X Index: 256



Y Index: 256

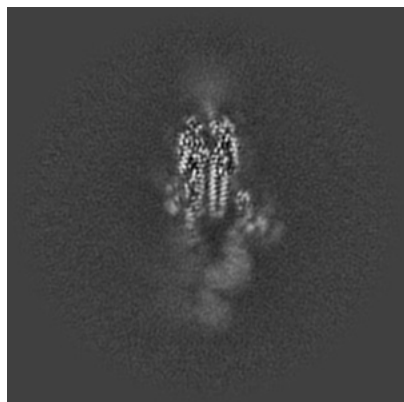


Z Index: 256

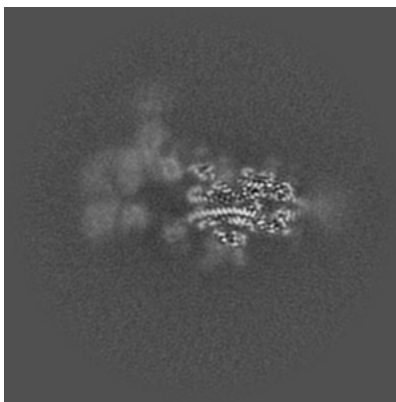
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

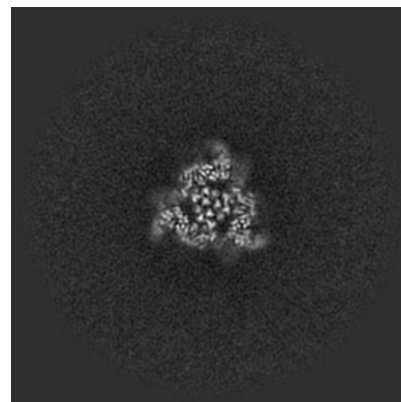
6.3.1 Primary map



X Index: 250

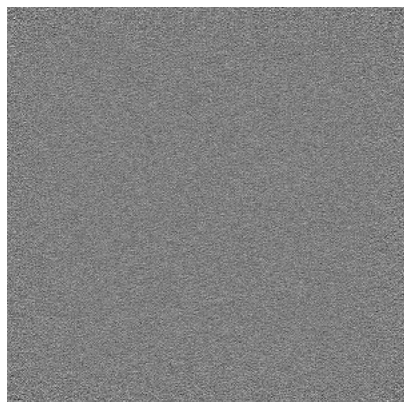


Y Index: 264

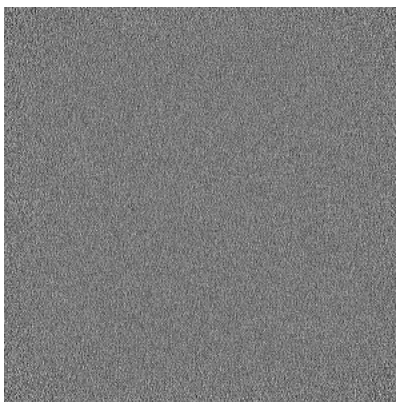


Z Index: 266

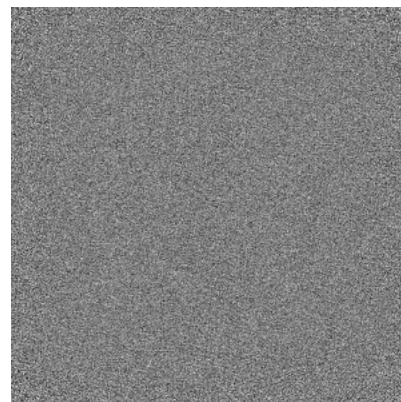
6.3.2 Raw map



X Index: 0



Y Index: 0

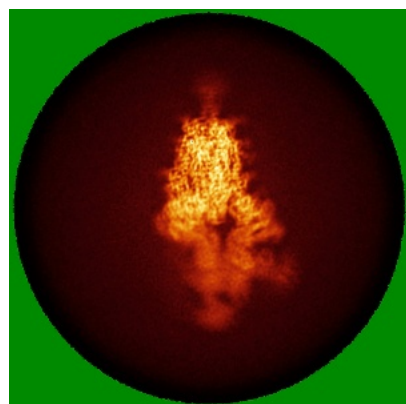


Z Index: 0

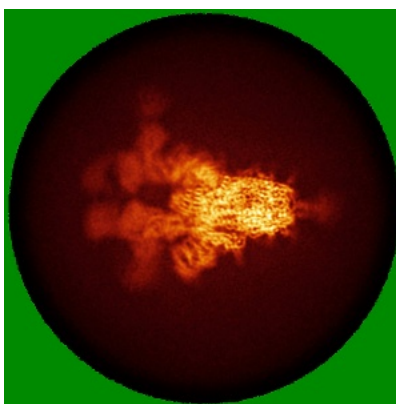
The images above show the largest variance slices of the map in three orthogonal directions.

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

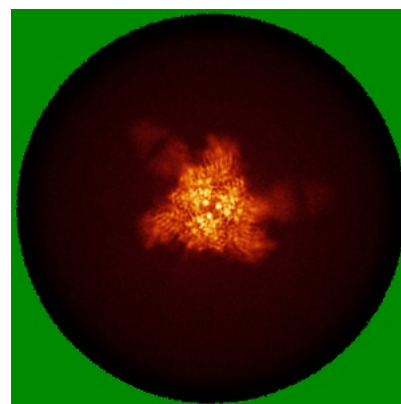
6.4.1 Primary map



X

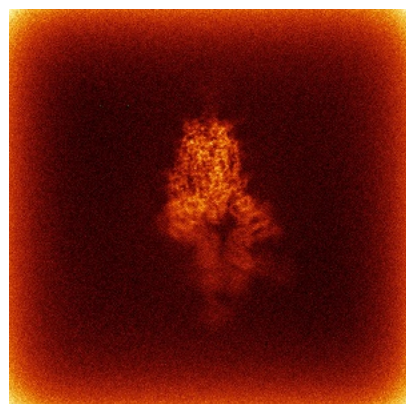


Y

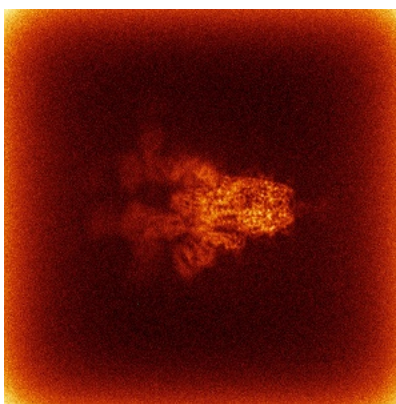


Z

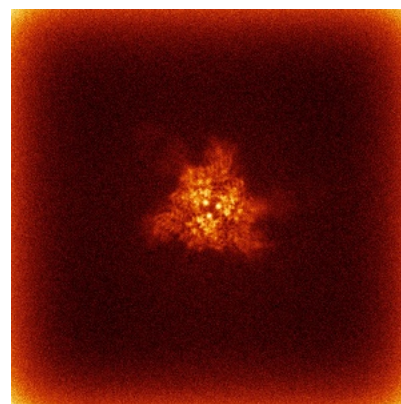
6.4.2 Raw map



X



Y

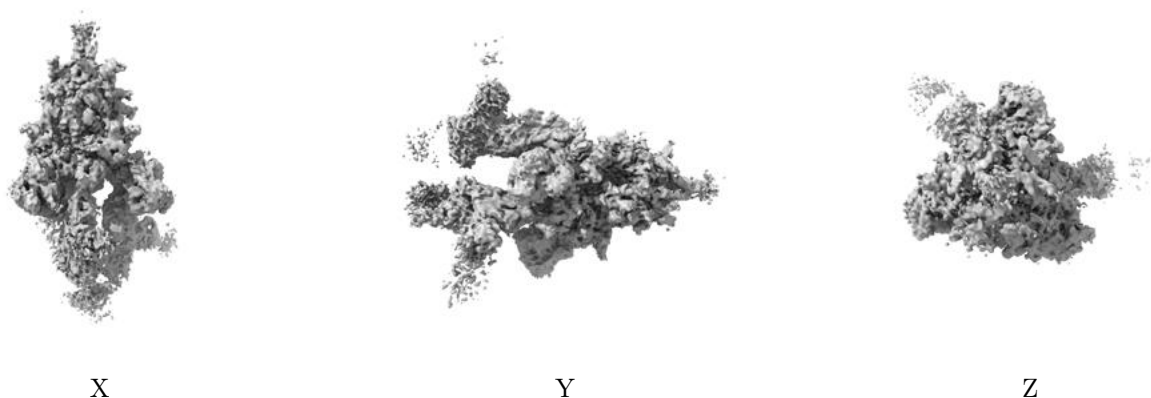


Z

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.

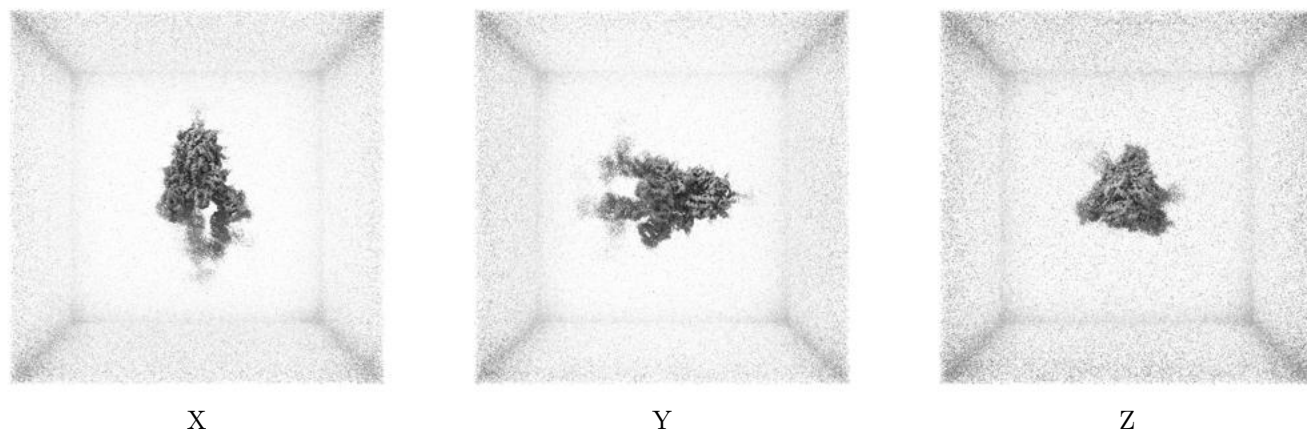
6.5 Orthogonal surface views [i](#)

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.

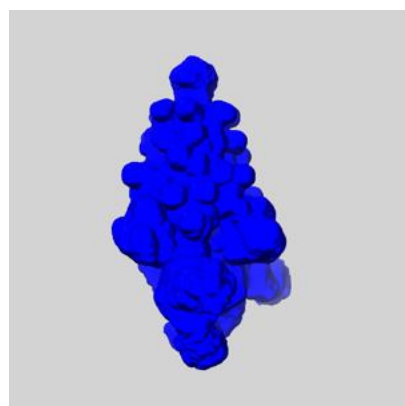
6.6 Mask visualisation [i](#)

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

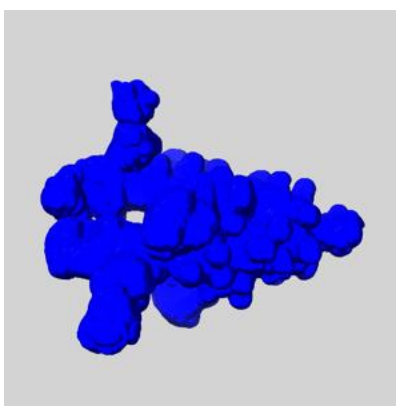
A mask typically either:

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

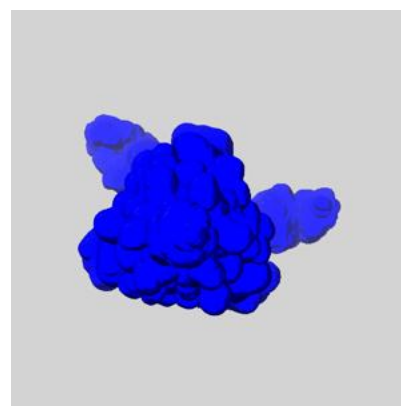
6.6.1 emd_34135_msk_1.map [i](#)



X



Y

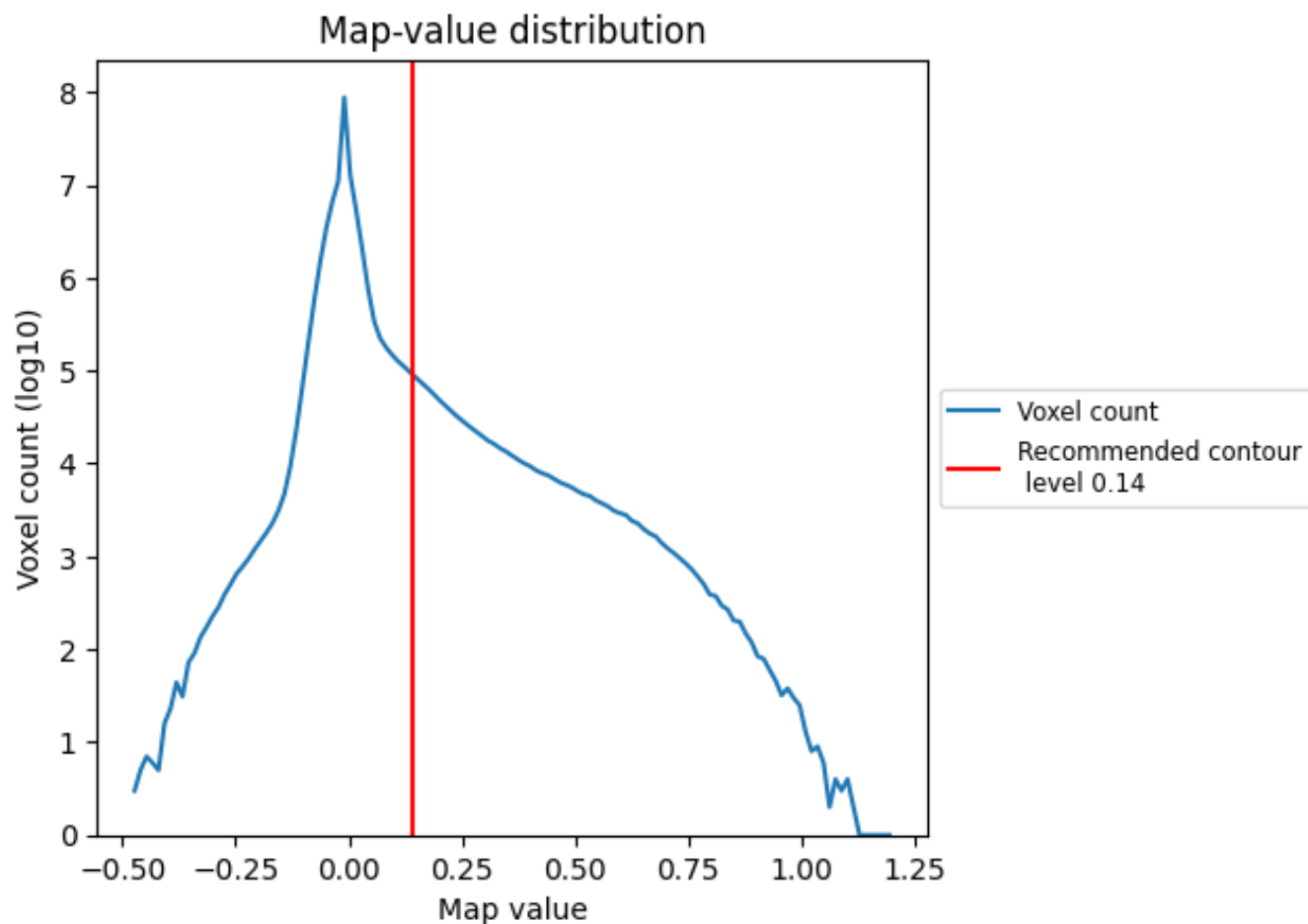


Z

7 Map analysis [i](#)

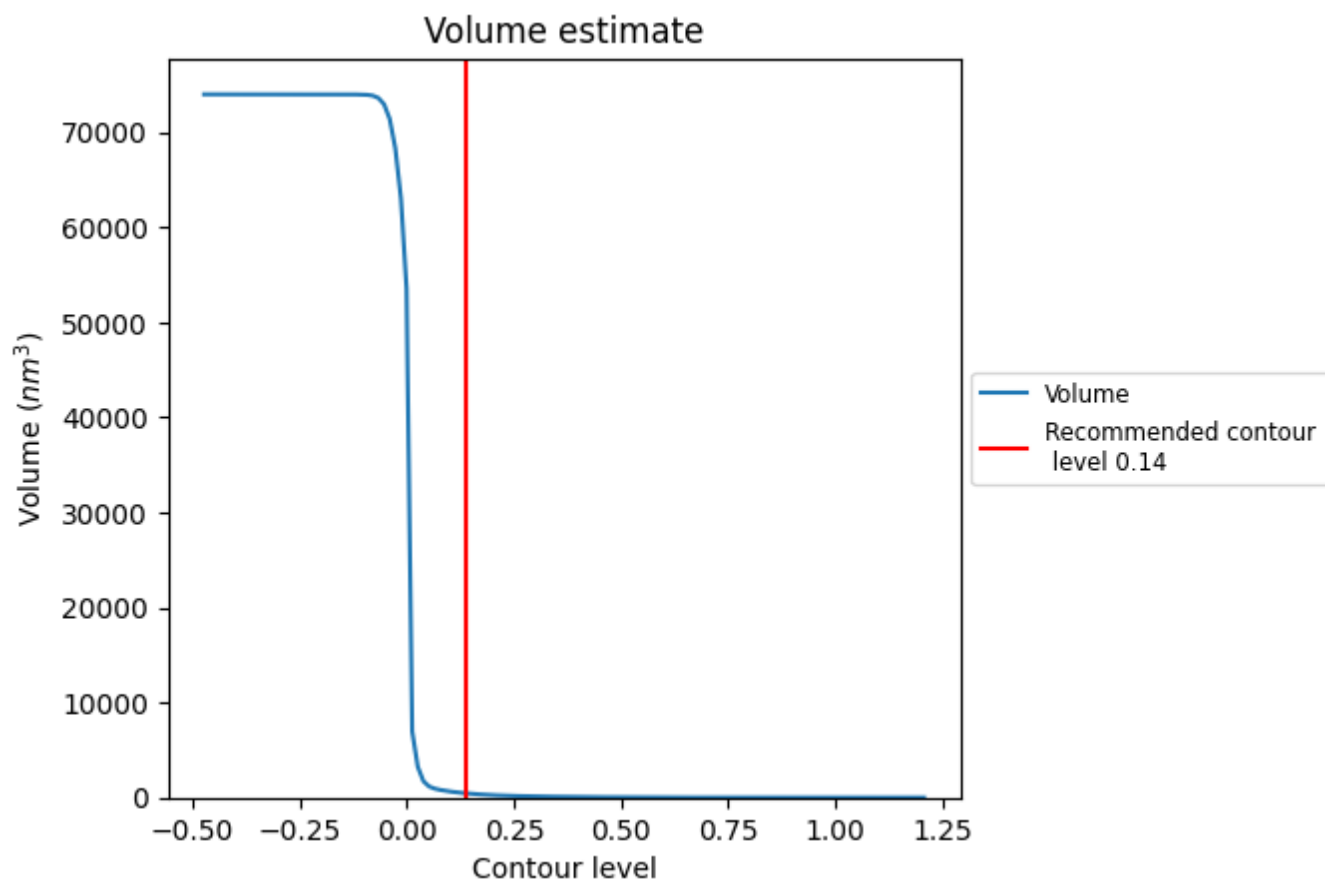
This section contains the results of statistical analysis of the map.

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.

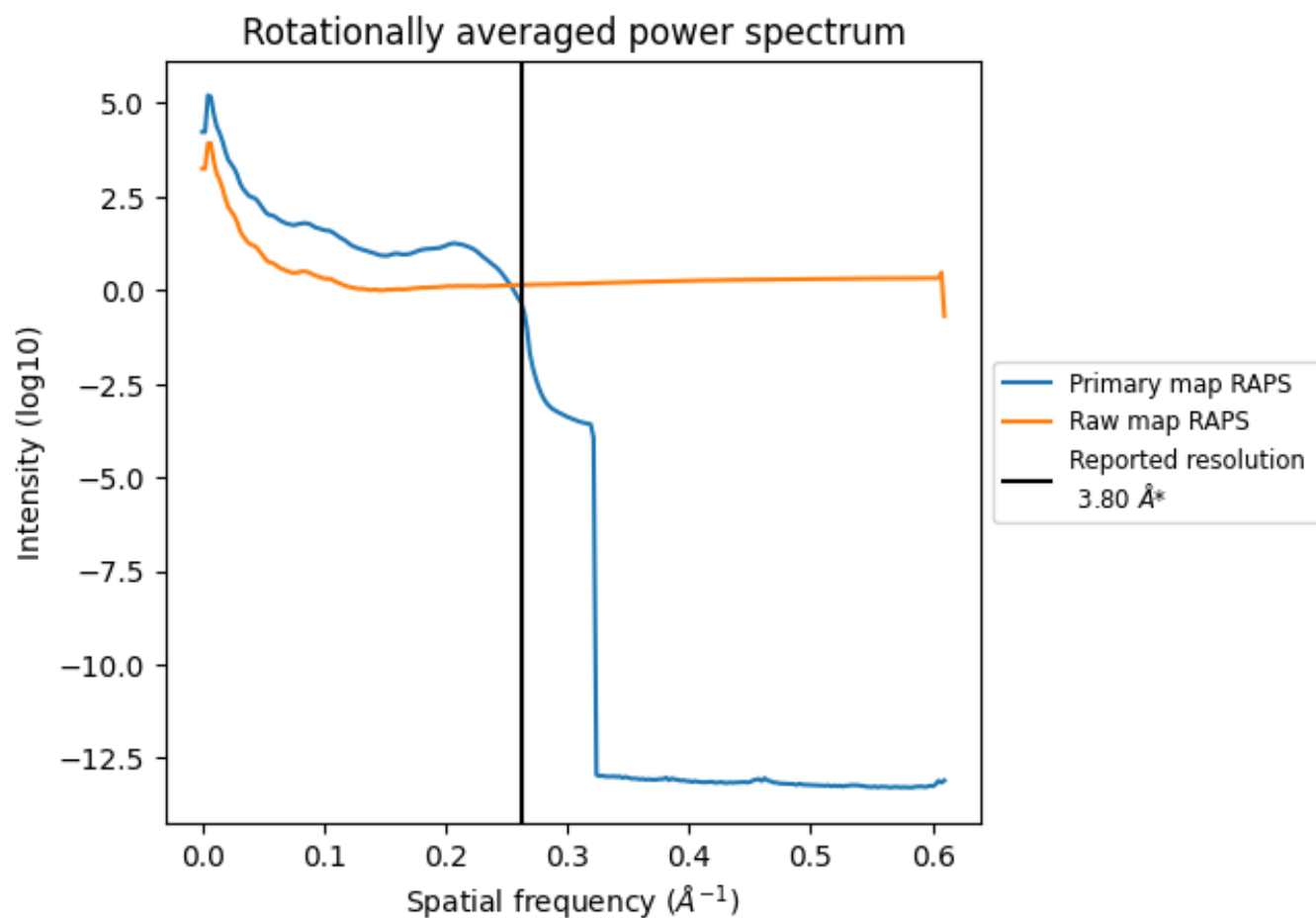
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm^3 ; this corresponds to an approximate mass of 397 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 ⓘ

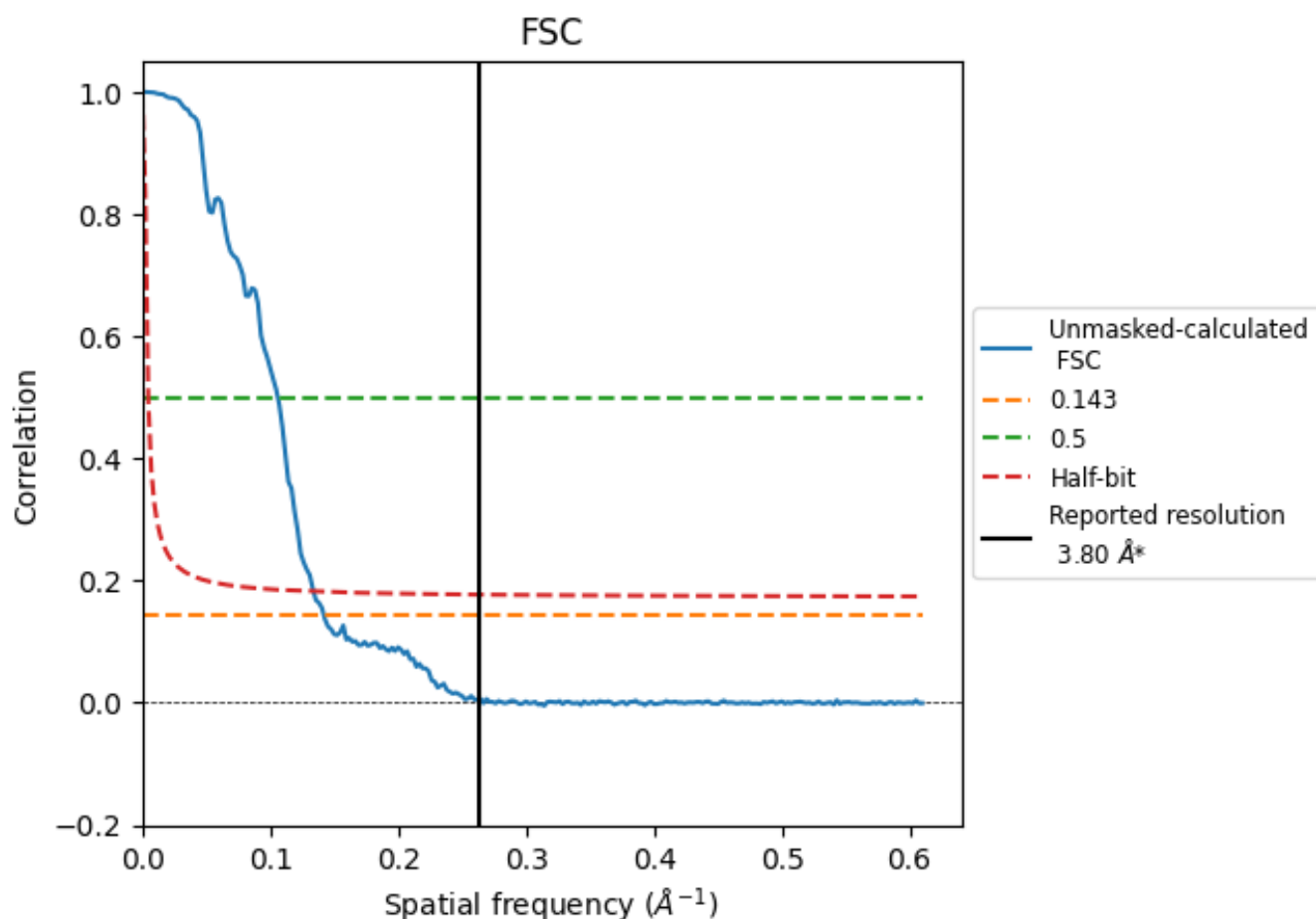


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

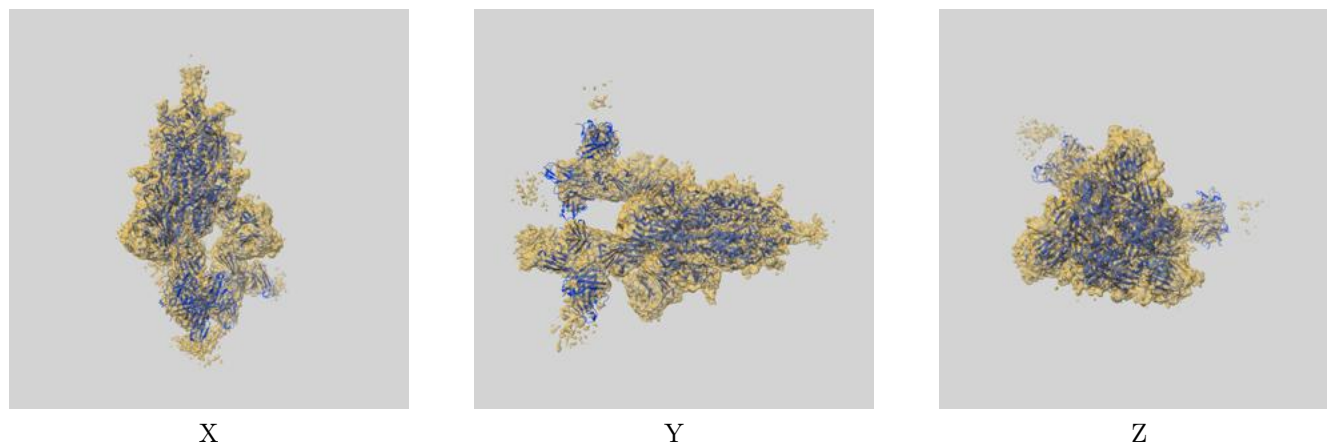
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.04	9.43	7.46

*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 7.04 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

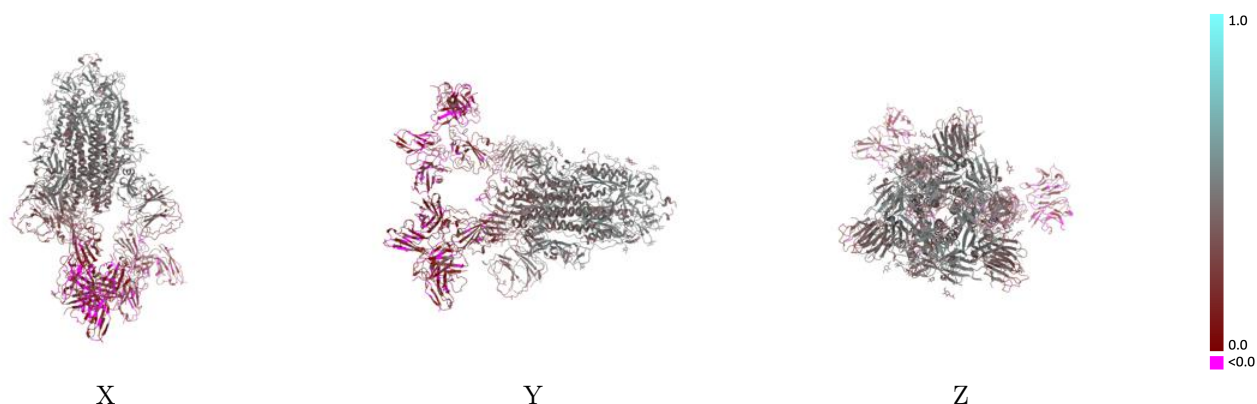
This section contains information regarding the fit between EMDB map EMD-34135 and PDB model 7YVP. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



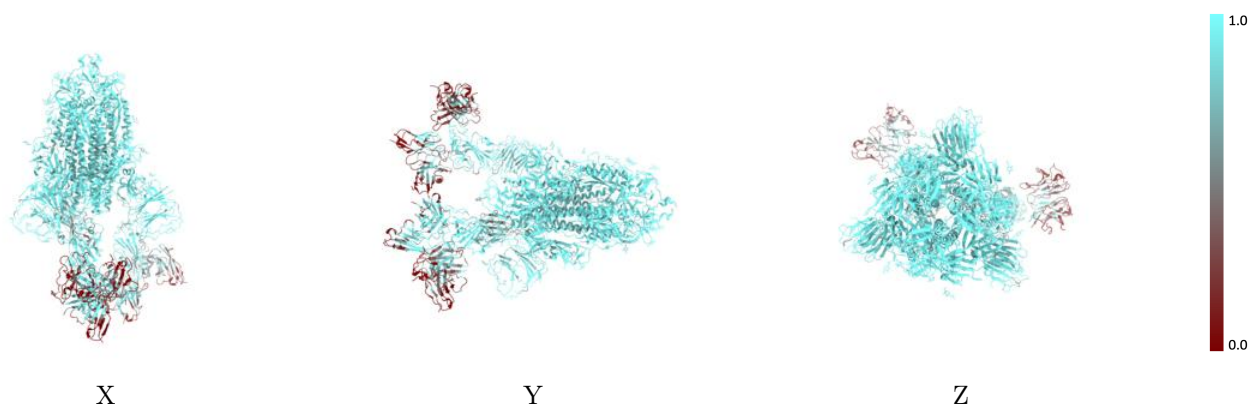
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



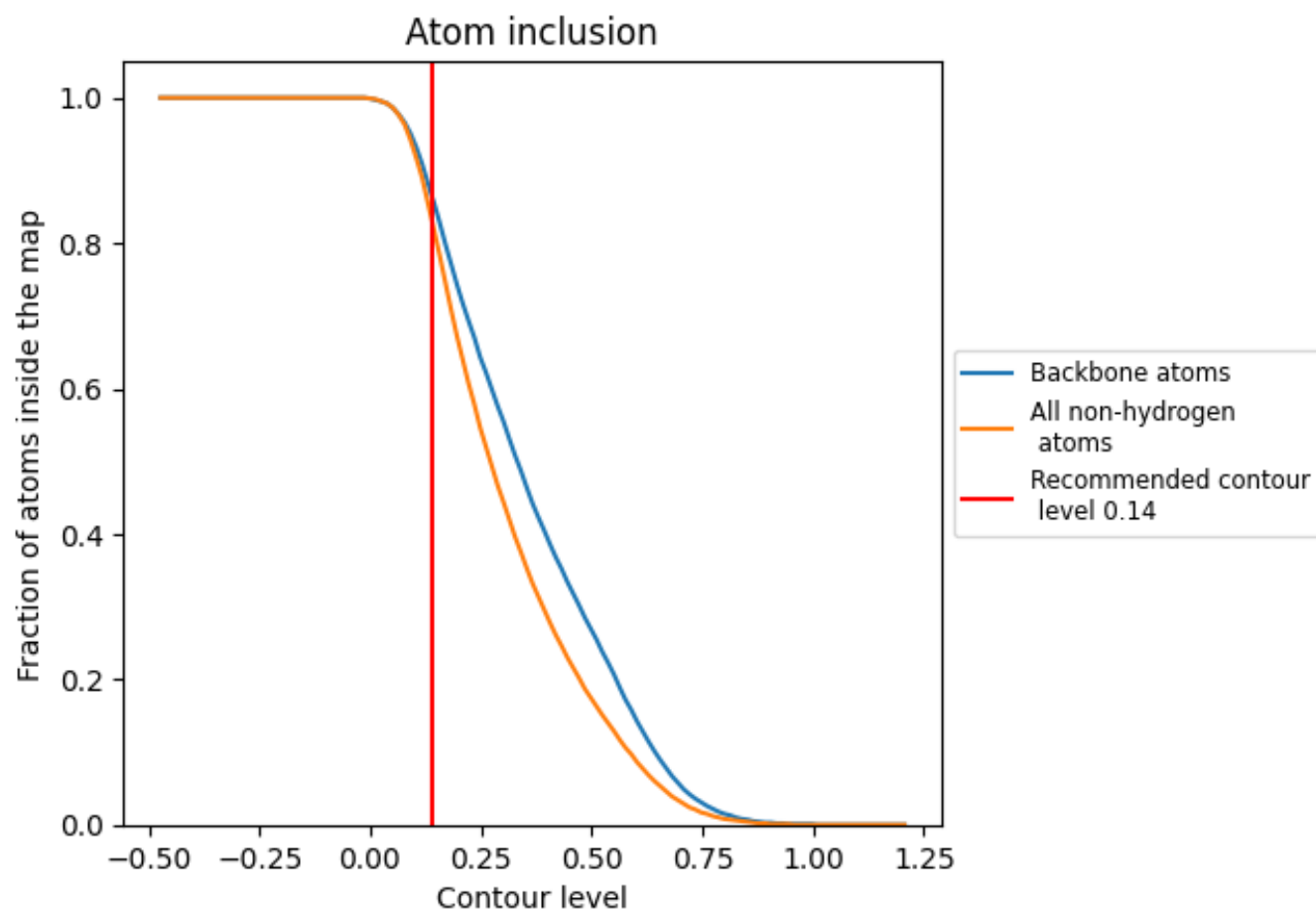
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 83% 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	0.8310	0.3250
A	0.9400	0.3780
B	0.9180	0.3870
C	0.9520	0.3850
H	0.4710	0.0680
I	0.2970	0.1000
J	0.2280	0.1100
K	0.4400	0.1140
L	0.4220	0.1510
M	0.3880	0.1650
O	0.7160	0.1500
P	0.7450	0.1480

1.0

0.0

<0.0