



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:39 AM UTC

PDB ID : 8XMT / pdb_00008xmt
EMDB ID : EMD-38488
Title : Cryo-EM structure of SARS-CoV-2 Omicron EG.5.1 spike protein(6P), RBD-closed state
Authors : Li, L.J.; Gu, Y.H.; Shi, K.Y.; Qi, J.X.; Gao, G.F.
Deposited on : 2023-12-28
Resolution : 3.31 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:

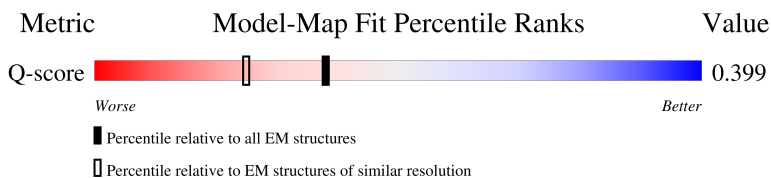
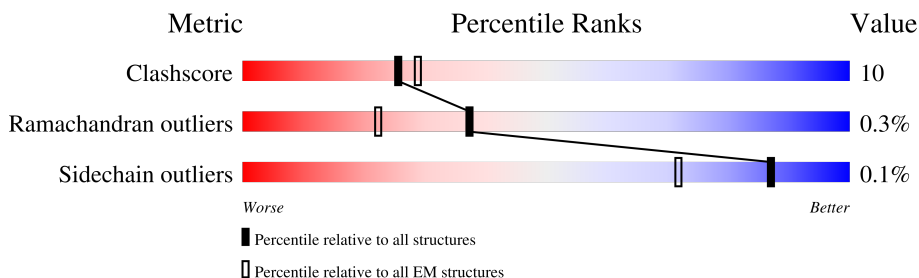
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.31 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	14550 (2.81 - 3.81)

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

Mol	Chain	Length	Quality of chain
1	A	1227	
1	B	1227	
1	C	1227	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0
			7978	5104	1331	1507	36		
1	B	1009	Total	C	N	O	S	0	0
			7903	5057	1317	1493	36		
1	C	1017	Total	C	N	O	S	0	0
			7958	5094	1328	1500	36		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	52	HIS	GLN	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	456	LEU	PHE	variant	UNP P0DTC2
A	460	LYS	ASN	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	PRO	PHE	variant	UNP P0DTC2
A	490	SER	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	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	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	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	TYR	-	expression tag	UNP P0DTC2
A	1211	ILE	-	expression tag	UNP P0DTC2
A	1212	PRO	-	expression tag	UNP P0DTC2
A	1213	GLU	-	expression tag	UNP P0DTC2
A	1214	ALA	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	ASP	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLN	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1221	TYR	-	expression tag	UNP P0DTC2
A	1222	VAL	-	expression tag	UNP P0DTC2
A	1223	ARG	-	expression tag	UNP P0DTC2
A	1224	LYS	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	TRP	-	expression tag	UNP P0DTC2
A	1229	VAL	-	expression tag	UNP P0DTC2
A	1230	LEU	-	expression tag	UNP P0DTC2
A	1231	LEU	-	expression tag	UNP P0DTC2
A	1232	SER	-	expression tag	UNP P0DTC2
A	1233	THR	-	expression tag	UNP P0DTC2
A	1234	PHE	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	ALA	-	expression tag	UNP P0DTC2
A	1237	HIS	-	expression tag	UNP P0DTC2
A	1238	HIS	-	expression tag	UNP P0DTC2
A	1239	HIS	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	52	HIS	GLN	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	456	LEU	PHE	variant	UNP P0DTC2
B	460	LYS	ASN	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	PRO	PHE	variant	UNP P0DTC2
B	490	SER	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	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	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	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	TYR	-	expression tag	UNP P0DTC2
B	1211	ILE	-	expression tag	UNP P0DTC2
B	1212	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1213	GLU	-	expression tag	UNP P0DTC2
B	1214	ALA	-	expression tag	UNP P0DTC2
B	1215	PRO	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	ASP	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLN	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	TYR	-	expression tag	UNP P0DTC2
B	1222	VAL	-	expression tag	UNP P0DTC2
B	1223	ARG	-	expression tag	UNP P0DTC2
B	1224	LYS	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	TRP	-	expression tag	UNP P0DTC2
B	1229	VAL	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	LEU	-	expression tag	UNP P0DTC2
B	1232	SER	-	expression tag	UNP P0DTC2
B	1233	THR	-	expression tag	UNP P0DTC2
B	1234	PHE	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	ALA	-	expression tag	UNP P0DTC2
B	1237	HIS	-	expression tag	UNP P0DTC2
B	1238	HIS	-	expression tag	UNP P0DTC2
B	1239	HIS	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	52	HIS	GLN	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2

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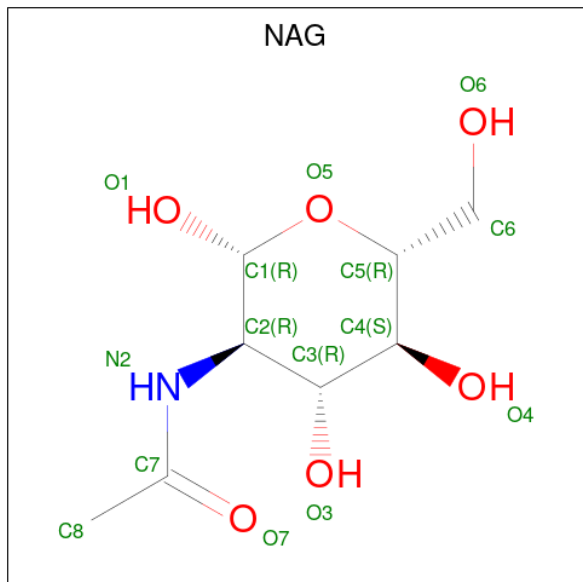
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	456	LEU	PHE	variant	UNP P0DTC2
C	460	LYS	ASN	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	PRO	PHE	variant	UNP P0DTC2
C	490	SER	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	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	TYR	-	expression tag	UNP P0DTC2
C	1211	ILE	-	expression tag	UNP P0DTC2
C	1212	PRO	-	expression tag	UNP P0DTC2
C	1213	GLU	-	expression tag	UNP P0DTC2
C	1214	ALA	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	ASP	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLN	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	TYR	-	expression tag	UNP P0DTC2
C	1222	VAL	-	expression tag	UNP P0DTC2
C	1223	ARG	-	expression tag	UNP P0DTC2
C	1224	LYS	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	TRP	-	expression tag	UNP P0DTC2
C	1229	VAL	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	LEU	-	expression tag	UNP P0DTC2
C	1232	SER	-	expression tag	UNP P0DTC2
C	1233	THR	-	expression tag	UNP P0DTC2
C	1234	PHE	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	ALA	-	expression tag	UNP P0DTC2
C	1237	HIS	-	expression tag	UNP P0DTC2
C	1238	HIS	-	expression tag	UNP P0DTC2
C	1239	HIS	-	expression tag	UNP P0DTC2
C	1240	HIS	-	expression tag	UNP P0DTC2
C	1241	HIS	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2

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



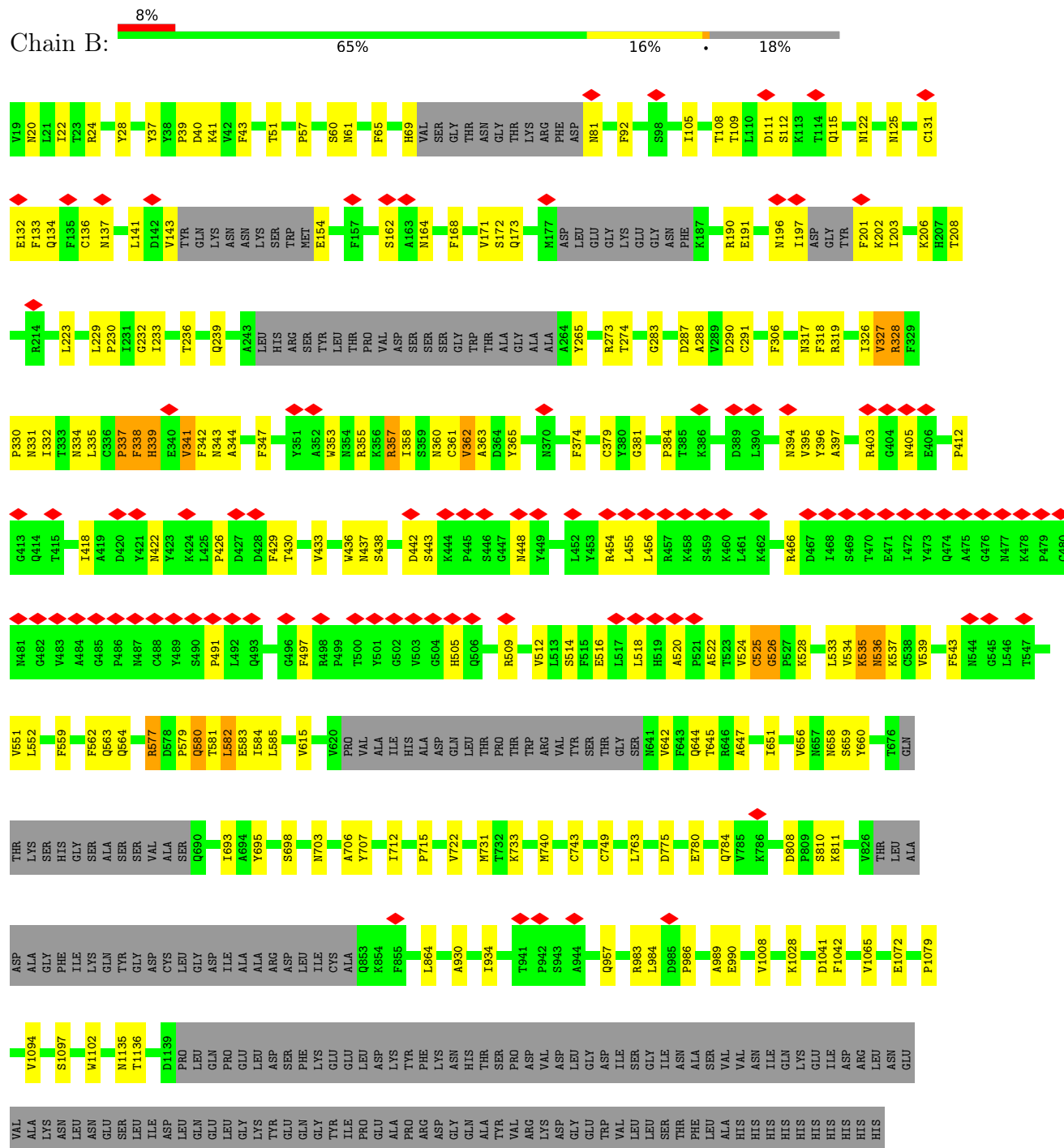
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2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

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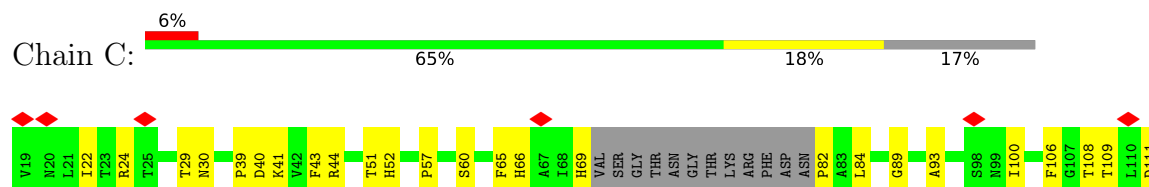
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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C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

• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



HIS	L18	L203	N282	N439	L552	C662	I805	A930	Q1106	LYS
HIS	N125	Y204	G283	K440	T553	P665	R815	I934	E1111	GLU
HIS	V130	H207	I285	L441	E554	I666	R820	Q935	P1112	ILE
HIS	C131	I210	T286	D442	F559	C671	L821	P942	T1116	ASP
	E132	N211	D287	S443	L560	Q675	L822	L945	T1117	LEU
	F135	L212	F306	N448	Q563	T676	V826	V963	D1118	ASN
	C136	L213	T307	R454	R567	GLN	THR	L966	V1122	GLY
	N137	R214	K310	L455	T573	THR	ALA	L985	S1123	ASN
	D138	F220	S316	L456	D578	LYS	ASP	N978	T1132	ASN
	L141	A222	N317	R457	T581	HIS	ALA	I980	M1135	GLU
ASP	VAL	L223	F318	K458	L585	GLY	LYS	L981	T1136	LEU
VAL	P225	E224	R319	L461	L699	SER	ALA	S982	D1139	ILE
TRP	L226	P226	S325	D467	C617	ALA	SER	R983	PRO	ASP
LYS	V227	E225	R328	I472	T598	VAL	THR	L984	LEU	GLN
ASN	L228	P227	F347	Y473	P600	ALA	ASP	D985	GLN	LEU
ASN	L229	A228	R347	Q474	G601	S989	ASP	E988	PRO	GLY
LYS	P230	G232	N353	A475	T602	L699	GLY	A989	LEU	GLY
LYS	L231	I233	R355	G476	C617	S711	ASP	Q992	ASP	TYR
SER	L234	N235	F374	N477	V820	T712	ILE	I997	SER	GLN
TRP	GLU	T236	N389	K478	PRO	A713	ALA	T998	LYS	GLY
S155			D389	P479	VAL	I713	ARG	G999	GLU	TYR
A163			L390	C480	ALA	T724	ASP	R1000	LEU	ILE
N164			Y396	N481	ILE	I726	LEU	Q1002	LEU	PRO
P174			R446	G482	HIS	I726	CYS	S1003	ILE	ALA
N177			Y401	V483	ALA	K733	A852	L1004	TYR	PRO
ASP			I402	A484	ASP	M740	Q853	V1008	PHE	ARG
LEU			R403	G485	GLN	Y741	K854	Q1011	LYS	ASP
GLU			G404	P486	LEU	I742	F855	L1012	ASN	GLY
GLY			M405	N487	THR	C743	P862	K1028	HIS	GLN
LYS			G413	C488	THR	G744	L878	R1029	THR	VAL
GLU			Q414	Y489	TRP	L753	S884	S1030	ASP	ARG
ASN			T415	P491	ARG	L754	T887	F1042	LEU	LYS
LYS			I418	G502	VAL	Q755	Q895	V1061	ASP	ASP
ASN			Y421	P507	THR	Y756	L895	F1062	GLY	GLY
LYS			N422	V512	GLY	F759	A903	L1063	ILE	THR
L189			A260	L513	N641	L763	Y904	C1082	ALA	PHE
E191			G261	S514	F643	K764	Q913	R1091	ALA	LEU
F192			A262	F515	Q644	R765	N914	S1097	VAL	LEU
V193			A263	L518	T645	I770	V915	W1102	VAL	ALA
F194			A264	H519	C649	A771	L916	T1105	ASN	VAL
K196			Y265	A520	I651	Y789	Y917		ILE	HIS
N196			Y266	P521	E654	P792	I923		GLN	HIS
I197			L270	N532						HIS
D198			R273	L533						
G199			T274	V534						
Y200			V433	K535						
F201			W436	N540						
K202			E281							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145930	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)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.129	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	413.696, 413.696, 413.696	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/8167	0.32	0/11116
1	B	0.27	0/8087	0.48	5/11004 (0.0%)
1	C	0.16	0/8147	0.34	1/11088 (0.0%)
All	All	0.20	0/24401	0.39	6/33208 (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
1	B	0	4
1	C	0	1
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	582	LEU	N-CA-C	-6.26	105.92	112.93
1	B	525	CYS	CB-CA-C	-5.84	102.93	111.23
1	C	231	ILE	N-CA-C	-5.68	107.28	112.96
1	B	580	GLN	N-CA-C	-5.51	99.07	110.80
1	B	341	VAL	N-CA-C	-5.32	106.24	111.77
1	B	337	PRO	N-CA-C	-5.15	105.44	113.78

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	ARG	Sidechain
1	B	355	ARG	Sidechain
1	B	357	ARG	Sidechain
1	B	577	ARG	Sidechain
1	C	273	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7978	0	7800	122	0
1	B	7903	0	7743	240	0
1	C	7958	0	7791	184	0
2	A	154	0	143	2	0
2	B	112	0	104	2	0
2	C	112	0	104	0	0
All	All	24217	0	23685	495	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 10.

All (495) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:PHE:CE1	1:C:222:ALA:HB1	1.69	1.26
1:B:535:LYS:NZ	1:B:585:LEU:HD21	1.50	1.26
1:B:342:PHE:HA	1:B:509:ARG:NH2	1.57	1.19
1:B:563:GLN:HG2	1:C:41:LYS:HD3	1.34	1.09
1:B:562:PHE:CZ	1:C:222:ALA:HB1	1.87	1.08
1:B:347:PHE:CZ	1:B:509:ARG:HD2	1.90	1.07
1:B:342:PHE:HA	1:B:509:ARG:HH22	0.94	1.06
1:B:559:PHE:HB2	1:B:584:ILE:HD11	1.36	1.04
1:B:562:PHE:CZ	1:C:222:ALA:CB	2.40	1.04
1:B:535:LYS:HZ2	1:B:585:LEU:HD21	0.90	1.04
1:B:534:VAL:CG1	1:B:537:LYS:HD2	1.88	1.04
1:C:756:TYR:CE2	1:C:997:ILE:HG21	1.96	0.99
1:B:535:LYS:NZ	1:B:585:LEU:CD2	2.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:GLN:HB2	1:C:41:LYS:HB3	1.46	0.96
1:B:361:CYS:SG	1:B:362:VAL:N	2.38	0.95
1:B:563:GLN:CG	1:C:41:LYS:HD3	1.97	0.92
1:B:396:TYR:HE2	1:B:516:GLU:OE1	1.52	0.92
1:B:347:PHE:CE2	1:B:509:ARG:HD2	2.04	0.91
1:B:559:PHE:HB2	1:B:584:ILE:CD1	2.01	0.91
1:B:395:VAL:HG21	1:B:524:VAL:HG11	1.52	0.90
1:B:533:LEU:HD11	1:B:552:LEU:HD13	1.55	0.88
1:B:535:LYS:HZ2	1:B:585:LEU:CD2	1.82	0.88
1:C:41:LYS:NZ	1:C:226:LEU:HD13	1.89	0.87
1:B:536:ASN:O	1:B:537:LYS:HG3	1.73	0.87
1:B:342:PHE:CA	1:B:509:ARG:NH2	2.38	0.86
1:B:436:TRP:CZ2	1:B:509:ARG:HD3	2.11	0.86
1:B:562:PHE:HZ	1:C:222:ALA:HB2	1.41	0.85
1:B:563:GLN:CB	1:C:41:LYS:HB3	2.05	0.85
1:C:756:TYR:HE2	1:C:997:ILE:HG21	1.37	0.85
1:B:342:PHE:CA	1:B:509:ARG:HH22	1.85	0.84
1:B:562:PHE:HE1	1:C:222:ALA:HB1	1.40	0.84
1:C:231:ILE:HD12	1:C:233:ILE:H	1.43	0.84
1:B:533:LEU:HD21	1:B:535:LYS:NZ	1.93	0.83
1:B:533:LEU:HD23	1:B:535:LYS:HE2	1.59	0.83
1:B:347:PHE:CZ	1:B:509:ARG:CD	2.62	0.83
1:B:562:PHE:HZ	1:C:222:ALA:CB	1.88	0.82
1:B:563:GLN:CG	1:C:41:LYS:HB3	2.10	0.81
1:B:396:TYR:CE2	1:B:516:GLU:OE1	2.35	0.79
1:B:341:VAL:HG23	1:B:342:PHE:CE2	2.18	0.79
1:C:226:LEU:HG	1:C:227:VAL:H	1.46	0.78
1:B:436:TRP:CE3	1:B:437:ASN:O	2.37	0.78
1:B:564:GLN:CB	1:B:577:ARG:HB2	2.15	0.77
1:C:226:LEU:HG	1:C:227:VAL:N	2.00	0.77
1:B:436:TRP:HE3	1:B:437:ASN:O	1.67	0.76
1:C:41:LYS:HZ1	1:C:226:LEU:HD13	1.50	0.75
1:B:535:LYS:HZ3	1:B:585:LEU:CD2	1.98	0.75
1:B:394:ASN:ND2	1:B:396:TYR:CZ	2.55	0.74
1:B:341:VAL:HG23	1:B:342:PHE:CD2	2.23	0.73
1:B:455:LEU:HD12	1:B:456:LEU:HG	1.71	0.73
1:B:533:LEU:HD11	1:B:552:LEU:CD1	2.17	0.73
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.20	0.72
1:B:534:VAL:HG13	1:B:537:LYS:HD2	1.71	0.72
1:B:65:PHE:HB2	1:B:265:TYR:HD2	1.55	0.72
1:B:125:ASN:ND2	1:B:172:SER:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:ND2	1:A:172:SER:O	2.24	0.71
1:A:420:ASP:HB2	1:A:460:LYS:HD2	1.72	0.70
1:C:753:LEU:HD12	1:C:756:TYR:HD2	1.57	0.70
1:B:564:GLN:HB3	1:B:577:ARG:HB2	1.73	0.70
1:A:106:PHE:HB3	1:A:235:ILE:HD11	1.73	0.69
1:B:518:LEU:HD12	1:B:520:ALA:H	1.58	0.69
1:C:770:ILE:HD13	1:C:1011:GLN:HG3	1.75	0.68
1:B:196:ASN:HA	1:B:201:PHE:HA	1.74	0.68
1:B:563:GLN:HG3	1:C:41:LYS:CB	2.23	0.68
1:C:454:ARG:HG3	1:C:491:PRO:HB2	1.75	0.68
1:B:534:VAL:HG11	1:B:537:LYS:HD2	1.73	0.68
1:B:563:GLN:HG3	1:C:41:LYS:HB3	1.75	0.68
1:C:455:LEU:HD12	1:C:456:LEU:HG	1.76	0.67
1:C:192:PHE:HB3	1:C:203:ILE:HD11	1.75	0.67
1:A:455:LEU:HD12	1:A:456:LEU:HG	1.75	0.67
1:B:533:LEU:CD2	1:B:535:LYS:HZ1	2.08	0.67
1:C:22:ILE:HD13	1:C:69:HIS:HA	1.77	0.67
1:B:443:SER:HA	1:B:448:ASN:HD21	1.60	0.66
1:B:658:ASN:ND2	1:B:660:TYR:OH	2.27	0.66
1:B:707:TYR:HB3	1:C:792:PRO:HG2	1.75	0.66
1:B:582:LEU:N	1:B:582:LEU:HD12	2.09	0.66
1:A:231:ILE:HD12	1:A:233:ILE:HG12	1.77	0.66
1:B:134:GLN:NE2	1:B:162:SER:OG	2.29	0.66
1:B:533:LEU:CD2	1:B:535:LYS:NZ	2.58	0.66
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.78	0.66
1:B:930:ALA:O	1:B:934:ILE:HG12	1.96	0.66
1:C:226:LEU:CG	1:C:227:VAL:H	2.09	0.66
1:B:564:GLN:HB2	1:B:577:ARG:H	1.61	0.65
1:B:436:TRP:HZ2	1:B:509:ARG:HD3	1.62	0.65
1:B:563:GLN:CG	1:C:41:LYS:CD	2.75	0.65
1:B:436:TRP:HE1	1:B:509:ARG:HH11	1.45	0.65
1:C:642:VAL:HG12	1:C:651:ILE:HG12	1.79	0.65
1:A:930:ALA:O	1:A:934:ILE:HG12	1.96	0.64
1:A:642:VAL:HG12	1:A:651:ILE:HG22	1.78	0.64
1:B:533:LEU:CD2	1:B:535:LYS:HE2	2.26	0.64
1:B:564:GLN:HB2	1:B:577:ARG:HB2	1.79	0.64
1:A:393:THR:HA	1:A:522:ALA:HA	1.79	0.63
1:B:395:VAL:CG2	1:B:524:VAL:HG11	2.26	0.63
1:C:29:THR:OG1	1:C:214:ARG:NH2	2.26	0.63
1:A:319:ARG:HH22	1:B:740:MET:HB2	1.64	0.63
1:A:132:GLU:O	1:A:164:ASN:ND2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.80	0.63
1:C:644:GLN:NE2	1:C:645:THR:O	2.30	0.63
1:B:533:LEU:CD2	1:B:535:LYS:CE	2.77	0.62
1:B:361:CYS:SG	1:B:363:ALA:N	2.72	0.62
1:C:1122:VAL:HG23	1:C:1123:SER:H	1.64	0.62
1:A:1122:VAL:HG23	1:A:1123:SER:H	1.63	0.62
1:C:196:ASN:ND2	1:C:200:TYR:O	2.28	0.62
1:B:330:PRO:HA	1:B:579:PRO:HB2	1.81	0.62
1:C:1082:CYS:HB2	1:C:1132:ILE:HG12	1.82	0.62
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.82	0.62
1:B:347:PHE:CZ	1:B:509:ARG:NE	2.67	0.62
1:B:536:ASN:O	1:B:537:LYS:CG	2.48	0.62
1:B:780:GLU:O	1:B:784:GLN:NE2	2.33	0.62
1:B:562:PHE:CE1	1:C:222:ALA:CB	2.60	0.62
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.82	0.61
1:B:581:THR:OG1	1:B:583:GLU:HG3	2.00	0.61
1:A:96:GLU:HB3	1:A:100:ILE:HD13	1.82	0.61
1:C:742:ILE:HD13	1:C:1001:LEU:HD22	1.81	0.61
1:B:518:LEU:HD21	1:C:200:TYR:OH	2.00	0.61
1:A:96:GLU:OE2	1:A:264:ALA:N	2.29	0.61
1:B:582:LEU:N	1:B:582:LEU:CD1	2.64	0.61
1:A:34:ARG:NH2	1:A:191:GLU:OE2	2.34	0.60
1:B:326:ILE:HD12	1:B:539:VAL:HG21	1.83	0.60
1:B:347:PHE:CE2	1:B:509:ARG:CD	2.82	0.60
1:B:535:LYS:O	1:B:536:ASN:C	2.43	0.60
1:A:329:PHE:O	1:A:580:GLN:NE2	2.35	0.60
1:A:96:GLU:O	1:A:190:ARG:NH1	2.35	0.60
1:A:454:ARG:HG3	1:A:491:PRO:HB2	1.82	0.60
1:B:206:LYS:HB3	1:B:223:LEU:HB3	1.83	0.60
1:B:357:ARG:HE	1:C:229:LEU:HG	1.66	0.60
1:B:535:LYS:O	1:B:537:LYS:N	2.35	0.60
1:B:394:ASN:ND2	1:B:396:TYR:OH	2.35	0.59
1:B:456:LEU:HB2	1:B:491:PRO:HB3	1.83	0.59
1:C:231:ILE:HD12	1:C:233:ILE:N	2.14	0.59
1:C:641:ASN:ND2	1:C:654:GLU:OE1	2.35	0.59
1:C:1116:THR:OG1	1:C:1118:ASP:OD1	2.20	0.59
1:B:337:PRO:O	1:B:338:PHE:C	2.46	0.59
1:C:770:ILE:HD11	1:C:1012:LEU:HD12	1.84	0.59
1:B:559:PHE:CG	1:B:584:ILE:HD13	2.38	0.58
1:C:108:THR:OG1	1:C:234:ASN:O	2.21	0.58
1:C:980:ILE:HG23	1:C:984:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASN:O	1:B:344:ALA:C	2.45	0.58
1:A:442:ASP:O	1:A:448:ASN:ND2	2.24	0.58
1:A:456:LEU:HB2	1:A:491:PRO:HB3	1.85	0.58
1:A:740:MET:HE1	1:C:319:ARG:HD2	1.86	0.58
1:B:201:PHE:HB3	1:B:232:GLY:HA2	1.86	0.58
1:C:41:LYS:HZ2	1:C:226:LEU:HD13	1.66	0.58
1:A:141:LEU:HB3	1:A:243:ALA:HA	1.85	0.57
1:B:403:ARG:HH12	1:B:405:ASN:HD21	1.52	0.57
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.39	0.57
1:B:197:ILE:O	1:B:201:PHE:N	2.37	0.57
1:C:194:PHE:CE1	1:C:203:ILE:HD13	2.39	0.57
1:C:65:PHE:HB2	1:C:265:TYR:HB2	1.86	0.57
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.38	0.57
1:B:559:PHE:CB	1:B:584:ILE:CD1	2.81	0.57
1:C:963:VAL:HA	1:C:966:LEU:HD12	1.86	0.57
1:A:106:PHE:HB3	1:A:235:ILE:CD1	2.33	0.56
1:B:358:ILE:HB	1:B:395:VAL:HB	1.87	0.56
1:B:533:LEU:HD21	1:B:535:LYS:CE	2.35	0.56
1:C:426:PRO:HG2	1:C:429:PHE:HB2	1.87	0.56
1:C:325:SER:HA	1:C:540:ASN:OD1	2.05	0.56
1:A:109:THR:HG22	1:A:109:THR:O	2.05	0.56
1:B:957:GLN:OE1	1:C:765:ARG:NH1	2.38	0.56
1:B:563:GLN:HG3	1:C:41:LYS:CD	2.36	0.56
1:C:742:ILE:HD11	1:C:1004:LEU:HD12	1.87	0.56
1:B:122:ASN:OD1	1:B:125:ASN:N	2.36	0.56
1:C:233:ILE:HG13	1:C:234:ASN:H	1.71	0.56
1:A:105:ILE:HB	1:A:241:LEU:HD11	1.87	0.56
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.38	0.56
1:A:887:THR:HB	1:A:894:LEU:HD12	1.87	0.56
1:B:131:CYS:HB2	1:B:133:PHE:CZ	2.41	0.56
1:C:141:LEU:HB3	1:C:243:ALA:HA	1.88	0.56
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.86	0.56
1:B:168:PHE:CE2	1:B:229:LEU:HD22	2.41	0.56
1:C:194:PHE:CD1	1:C:203:ILE:HD13	2.41	0.56
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.88	0.56
1:A:403:ARG:HH12	1:A:405:ASN:HD21	1.54	0.56
1:B:334:ASN:O	1:B:335:LEU:HD23	2.06	0.56
1:B:644:GLN:NE2	1:B:645:THR:O	2.39	0.56
1:B:319:ARG:HH21	1:C:740:MET:HB2	1.72	0.55
1:B:341:VAL:CG2	1:B:342:PHE:CE2	2.88	0.55
1:C:224:GLU:HB2	1:C:225:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PHE:HE2	1:B:615:VAL:HG11	1.70	0.55
1:B:327:VAL:HG11	1:B:528:LYS:HE2	1.89	0.55
1:A:562:PHE:CZ	1:B:41:LYS:HE2	2.42	0.55
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.88	0.54
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.22	0.54
1:A:195:LYS:HG2	1:A:202:LYS:HB2	1.89	0.54
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.42	0.54
1:B:28:TYR:CG	2:B:1308:NAG:H61	2.43	0.54
1:A:736:VAL:HG21	1:A:1004:LEU:HD11	1.89	0.54
1:C:316:SER:OG	1:C:317:ASN:N	2.40	0.54
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.88	0.54
1:C:578:ASP:HB3	1:C:581:THR:O	2.07	0.54
1:A:458:LYS:N	1:A:473:TYR:OH	2.41	0.54
1:B:357:ARG:HG2	1:B:396:TYR:CE1	2.43	0.54
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.89	0.54
1:B:274:THR:HG23	1:B:291:CYS:HB2	1.89	0.54
1:B:363:ALA:HB1	1:B:365:TYR:HE1	1.73	0.54
1:B:319:ARG:HE	1:C:740:MET:HE3	1.71	0.53
1:A:201:PHE:HB2	1:A:231:ILE:HG12	1.90	0.53
1:B:577:ARG:HG3	1:B:584:ILE:HG12	1.90	0.53
1:B:656:VAL:HG21	1:B:693:ILE:HD12	1.91	0.53
1:A:201:PHE:HD2	1:A:203:ILE:HD11	1.73	0.53
1:A:328:ARG:NH2	1:A:578:ASP:OD2	2.33	0.53
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.91	0.53
1:C:988:GLU:OE2	1:C:992:GLN:NE2	2.38	0.53
1:A:752:LEU:HD22	1:A:997:ILE:HD12	1.89	0.53
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.42	0.53
1:A:125:ASN:HD21	1:A:171:VAL:HG13	1.74	0.52
1:C:118:LEU:HD12	1:C:135:PHE:HE1	1.72	0.52
1:C:815:ARG:NH1	1:C:820:ASP:OD1	2.42	0.52
1:B:563:GLN:CG	1:C:41:LYS:CB	2.83	0.52
1:C:884:SER:OG	1:C:887:THR:OG1	2.27	0.52
1:B:22:ILE:HD13	1:B:69:HIS:HA	1.92	0.52
1:B:559:PHE:CD1	1:B:584:ILE:HD13	2.45	0.52
1:A:143:VAL:HG21	1:A:154:GLU:HG2	1.91	0.52
1:B:136:CYS:SG	1:B:137:ASN:N	2.82	0.52
1:A:124:THR:HG1	2:A:1301:NAG:HN2	1.56	0.52
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.91	0.52
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.91	0.52
1:B:581:THR:CB	1:B:583:GLU:HG3	2.40	0.52
1:A:448:ASN:HD21	1:A:497:PHE:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:THR:HG23	1:A:670:ILE:HD13	1.92	0.52
1:B:330:PRO:HB3	1:B:579:PRO:HB3	1.92	0.52
1:A:388:ASN:O	1:A:527:PRO:HD2	2.10	0.51
1:A:914:ASN:ND2	1:C:1123:SER:OG	2.43	0.51
1:B:24:ARG:NH2	1:B:81:ASN:O	2.44	0.51
1:B:448:ASN:HD22	1:B:497:PHE:HB2	1.74	0.51
1:B:533:LEU:HD23	1:B:535:LYS:CE	2.34	0.51
1:B:533:LEU:CD1	1:B:552:LEU:HD13	2.35	0.51
1:C:396:TYR:HB2	1:C:514:SER:HB3	1.91	0.51
1:B:331:ASN:OD1	1:B:331:ASN:O	2.29	0.51
1:C:1091:ARG:NH2	1:C:1118:ASP:O	2.38	0.51
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.45	0.51
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.92	0.51
1:C:280:ASN:HD21	1:C:282:ASN:HB2	1.76	0.51
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.46	0.51
1:A:675:GLN:HG3	1:A:677:GLN:HG3	1.92	0.50
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.25	0.50
1:C:821:LEU:HD22	1:C:935:GLN:HG3	1.91	0.50
1:A:22:ILE:HD13	1:A:69:HIS:HA	1.93	0.50
1:B:108:THR:HA	1:B:236:THR:HG22	1.93	0.50
1:A:458:LYS:HG2	1:A:473:TYR:OH	2.11	0.50
1:B:319:ARG:NE	1:C:740:MET:HE3	2.26	0.50
1:A:763:LEU:HG	1:A:1008:VAL:HG21	1.93	0.50
1:B:191:GLU:HB3	1:B:206:LYS:HB2	1.93	0.50
1:B:328:ARG:HB2	1:B:543:PHE:CE1	2.46	0.50
1:B:533:LEU:CD1	1:B:552:LEU:CD1	2.89	0.50
1:A:983:ARG:HA	1:C:390:LEU:HD11	1.94	0.50
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.76	0.50
1:C:220:PHE:CD2	1:C:285:ILE:O	2.65	0.50
1:C:978:ASN:HA	1:C:981:LEU:HD12	1.92	0.50
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.93	0.50
1:C:724:THR:HG22	1:C:1063:LEU:HD23	1.94	0.49
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.94	0.49
1:C:979:ASP:O	1:C:983:ARG:CB	2.60	0.49
1:A:469:SER:OG	1:A:471:GLU:OE1	2.23	0.49
1:A:562:PHE:CE2	1:B:41:LYS:HG2	2.47	0.49
1:A:864:LEU:HD13	1:C:665:PRO:HB3	1.95	0.49
1:B:168:PHE:HE2	1:B:229:LEU:HD22	1.76	0.49
1:B:326:ILE:HD11	1:B:534:VAL:HB	1.94	0.49
1:B:363:ALA:HB1	1:B:365:TYR:CE1	2.47	0.49
1:B:442:ASP:O	1:B:448:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:ALA:HA	1:C:862:PRO:HG2	1.94	0.49
1:B:712:ILE:HD13	1:B:1094:VAL:HG11	1.94	0.49
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.78	0.49
1:C:914:ASN:O	1:C:915:VAL:C	2.54	0.49
1:B:125:ASN:HD21	1:B:171:VAL:HG13	1.77	0.49
1:B:172:SER:OG	1:B:173:GLN:OE1	2.31	0.49
1:B:353:TRP:O	1:B:466:ARG:NH2	2.41	0.49
1:B:394:ASN:CG	1:B:396:TYR:CZ	2.89	0.49
1:C:328:ARG:HE	1:C:533:LEU:HB2	1.78	0.49
1:A:578:ASP:HB3	1:A:581:THR:O	2.13	0.49
1:C:307:THR:HA	1:C:602:THR:HG21	1.94	0.49
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.95	0.49
1:A:154:GLU:N	1:A:246:ARG:HH21	2.10	0.49
1:B:20:ASN:ND2	1:B:137:ASN:OD1	2.43	0.49
1:A:362:VAL:HG13	1:A:526:GLY:O	2.12	0.48
1:B:330:PRO:HA	1:B:579:PRO:CB	2.43	0.48
1:C:220:PHE:HD2	1:C:285:ILE:O	1.96	0.48
1:B:57:PRO:O	1:B:60:SER:OG	2.29	0.48
1:B:535:LYS:NZ	1:B:585:LEU:HD11	2.28	0.48
1:B:374:PHE:HD1	1:B:436:TRP:HB3	1.78	0.48
1:B:722:VAL:O	1:B:934:ILE:HD11	2.14	0.48
1:A:665:PRO:HB3	1:B:864:LEU:HD13	1.94	0.48
1:C:100:ILE:O	1:C:243:ALA:N	2.30	0.48
1:A:210:ILE:HD12	1:A:217:PRO:HD3	1.96	0.48
1:A:21:LEU:HD12	1:A:22:ILE:HG12	1.95	0.48
1:B:115:GLN:HB2	1:B:233:ILE:HG12	1.95	0.48
1:C:189:LEU:N	1:C:210:ILE:HD11	2.29	0.48
1:A:105:ILE:HG22	1:A:239:GLN:O	2.13	0.48
1:A:327:VAL:HG22	1:A:542:ASN:HB2	1.96	0.48
1:C:204:TYR:CE1	1:C:223:LEU:HD13	2.49	0.48
1:C:347:PHE:HB2	1:C:401:VAL:HG23	1.95	0.48
1:C:733:LYS:HG2	1:C:771:ALA:HA	1.96	0.48
1:B:581:THR:OG1	1:B:583:GLU:CG	2.62	0.47
1:C:374:PHE:HD1	1:C:436:TRP:HB3	1.79	0.47
1:A:466:ARG:HG2	1:A:468:ILE:HG23	1.96	0.47
1:C:204:TYR:CD1	1:C:223:LEU:HD13	2.48	0.47
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.48	0.47
1:B:208:THR:HG22	1:B:223:LEU:HG	1.97	0.47
1:B:358:ILE:N	1:B:395:VAL:O	2.34	0.47
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.79	0.47
1:B:564:GLN:HB2	1:B:577:ARG:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLU:HB2	1:B:223:LEU:HD22	1.97	0.47
1:C:57:PRO:HB2	1:C:60:SER:OG	2.14	0.47
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.44	0.47
1:C:29:THR:HG1	1:C:214:ARG:HH22	1.59	0.47
1:C:108:THR:HA	1:C:236:THR:HG22	1.96	0.47
1:C:189:LEU:HG	1:C:210:ILE:HG13	1.96	0.47
1:A:825:LYS:NZ	1:A:939:SER:HA	2.29	0.47
1:C:520:ALA:HB3	1:C:521:PRO:HD3	1.97	0.47
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.97	0.47
1:C:431:GLY:HA2	1:C:515:PHE:HD2	1.79	0.47
1:B:535:LYS:HZ3	1:B:585:LEU:CD1	2.27	0.47
1:B:337:PRO:O	1:B:339:HIS:N	2.48	0.47
1:C:560:LEU:HB2	1:C:563:GLN:HB2	1.95	0.47
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.98	0.46
1:A:873:TYR:CE1	1:C:699:LEU:HB3	2.50	0.46
1:B:334:ASN:O	1:B:335:LEU:HG	2.14	0.46
1:B:808:ASP:OD2	1:B:810:SER:OG	2.32	0.46
1:C:203:ILE:HG23	1:C:225:PRO:HG2	1.98	0.46
1:C:753:LEU:HD12	1:C:756:TYR:CD2	2.44	0.46
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.51	0.46
1:B:61:ASN:HB2	2:B:1308:NAG:H83	1.98	0.46
1:B:422:ASN:ND2	1:B:454:ARG:O	2.49	0.46
1:C:916:LEU:HD12	1:C:923:ILE:HD13	1.97	0.46
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.60	0.46
1:B:318:PHE:CE2	1:B:615:VAL:HG11	2.49	0.46
1:C:132:GLU:HB2	1:C:164:ASN:OD1	2.15	0.46
1:A:645:THR:HG22	1:A:647:ALA:H	1.80	0.46
1:C:24:ARG:HA	1:C:66:HIS:O	2.16	0.46
1:C:192:PHE:HA	1:C:204:TYR:O	2.16	0.46
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.47	0.46
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.46
1:B:203:ILE:HG22	1:B:229:LEU:HB2	1.99	0.45
1:B:287:ASP:OD1	1:B:288:ALA:N	2.49	0.45
1:C:193:VAL:O	1:C:203:ILE:HD12	2.17	0.45
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.49	0.45
1:A:422:ASN:ND2	1:A:454:ARG:O	2.47	0.45
1:C:287:ASP:HB3	1:C:306:PHE:HE2	1.81	0.45
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.99	0.45
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.52	0.45
1:B:984:LEU:HB3	1:B:989:ALA:HB2	1.98	0.45
1:C:822:LEU:HD23	1:C:945:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:HB2	1:B:584:ILE:HD13	1.95	0.45
1:C:1106:GLN:NE2	1:C:1111:GLU:OE2	2.50	0.45
1:C:202:LYS:HB3	1:C:204:TYR:CE1	2.52	0.45
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.99	0.45
1:B:337:PRO:HD2	1:B:358:ILE:HG23	1.99	0.45
1:B:422:ASN:OD1	1:B:454:ARG:N	2.42	0.45
1:C:999:GLY:O	1:C:1002:GLN:HG3	2.17	0.45
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.50	0.45
1:A:23:THR:O	1:A:68:ILE:N	2.35	0.44
1:A:986:PRO:O	1:A:990:GLU:HG2	2.16	0.44
1:B:202:LYS:HG2	1:B:230:PRO:HA	1.99	0.44
1:B:334:ASN:O	1:B:335:LEU:CD2	2.64	0.44
1:C:439:ASN:O	1:C:443:SER:HB2	2.18	0.44
1:C:753:LEU:HA	1:C:756:TYR:CD2	2.53	0.44
1:A:319:ARG:NH1	1:B:740:MET:SD	2.90	0.44
1:B:396:TYR:HB2	1:B:514:SER:HB3	2.00	0.44
1:C:567:ARG:HG2	1:C:573:THR:HA	2.00	0.44
1:A:131:CYS:HA	1:A:166:CYS:HA	1.99	0.44
1:A:741:TYR:CE1	1:A:966:LEU:HD13	2.53	0.44
1:A:741:TYR:CZ	1:A:966:LEU:HD13	2.53	0.44
1:A:752:LEU:HD11	1:A:994:ASP:OD1	2.18	0.44
1:B:287:ASP:HB3	1:B:306:PHE:HE2	1.83	0.44
1:C:52:HIS:HD1	1:C:274:THR:HG1	1.65	0.44
1:C:197:ILE:HG23	1:C:198:ASP:H	1.83	0.44
1:C:229:LEU:N	1:C:230:PRO:HD3	2.33	0.44
1:B:112:SER:HB3	1:B:134:GLN:HB3	1.99	0.44
1:B:731:MET:HE3	1:B:731:MET:HB2	1.88	0.44
1:C:40:ASP:N	1:C:40:ASP:OD1	2.51	0.44
1:C:456:LEU:HB2	1:C:491:PRO:HB3	2.00	0.44
1:A:92:PHE:HZ	1:A:101:ILE:HD13	1.83	0.44
1:B:143:VAL:HG21	1:B:154:GLU:HG2	2.00	0.44
1:B:559:PHE:CB	1:B:584:ILE:HD13	2.47	0.44
1:C:310:LYS:HG3	1:C:600:PRO:HA	2.00	0.44
1:A:562:PHE:HZ	1:B:41:LYS:HE2	1.83	0.43
1:B:656:VAL:HG23	1:B:695:TYR:HB3	1.99	0.43
1:C:136:CYS:SG	1:C:137:ASN:N	2.91	0.43
1:C:560:LEU:HB2	1:C:563:GLN:CB	2.48	0.43
1:A:954:HIS:HB3	1:A:1014:ARG:HE	1.82	0.43
1:B:1079:PRO:HB3	1:C:917:TYR:CE1	2.53	0.43
1:C:197:ILE:HG23	1:C:198:ASP:N	2.33	0.43
1:A:804:GLN:OE1	1:A:817:PRO:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:HG2	1:C:273:ARG:HH21	1.84	0.43
1:C:461:LEU:HD21	1:C:467:ASP:HB2	2.00	0.43
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.34	0.43
1:B:986:PRO:O	1:B:990:GLU:HG2	2.18	0.43
1:A:330:PRO:HG2	1:A:332:ILE:HD11	2.00	0.43
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.53	0.43
1:B:111:ASP:HA	1:B:134:GLN:HA	1.99	0.43
1:B:319:ARG:NH1	1:C:744:GLY:O	2.52	0.43
1:B:1094:VAL:HG22	1:C:904:TYR:OH	2.19	0.43
1:C:403:ARG:HH12	1:C:405:ASN:HD21	1.65	0.43
1:B:105:ILE:N	1:B:239:GLN:O	2.39	0.43
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.52	0.43
1:B:363:ALA:O	1:B:526:GLY:HA2	2.17	0.43
1:B:403:ARG:HD2	1:B:505:HIS:HA	2.01	0.43
1:C:89:GLY:HA3	1:C:270:LEU:HD12	2.00	0.43
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.53	0.43
1:C:1118:ASP:OD1	1:C:1119:ASN:N	2.52	0.43
1:B:581:THR:C	1:B:583:GLU:H	2.27	0.43
1:A:41:LYS:HE2	1:A:225:PRO:HG2	2.01	0.42
1:A:773:GLU:O	1:A:774:GLN:C	2.61	0.42
1:A:1134:ASN:HD22	2:A:1307:NAG:H83	1.82	0.42
1:B:379:CYS:HB2	1:B:384:PRO:HG3	2.00	0.42
1:B:436:TRP:CZ3	1:B:438:SER:HA	2.54	0.42
1:C:1122:VAL:HG23	1:C:1123:SER:N	2.29	0.42
1:B:273:ARG:NH2	1:B:290:ASP:OD2	2.52	0.42
1:B:341:VAL:HB	1:B:397:ALA:HB1	2.02	0.42
1:C:439:ASN:HA	1:C:507:PRO:HG2	1.99	0.42
1:A:427:ASP:OD1	1:A:427:ASP:N	2.52	0.42
1:B:518:LEU:HD12	1:B:520:ALA:N	2.30	0.42
1:B:537:LYS:O	1:B:551:VAL:HG22	2.19	0.42
1:C:755:GLN:NE2	1:C:756:TYR:CE1	2.87	0.42
1:A:105:ILE:HD11	1:A:135:PHE:CE2	2.54	0.42
1:B:525:CYS:O	1:B:526:GLY:C	2.62	0.42
1:C:353:TRP:HZ3	1:C:355:ARG:HH11	1.66	0.42
1:B:436:TRP:CE2	1:B:509:ARG:HD3	2.53	0.42
1:B:522:ALA:C	1:B:524:VAL:H	2.27	0.42
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.69	0.42
1:A:40:ASP:OD1	1:A:40:ASP:N	2.53	0.42
1:A:41:LYS:HD2	1:C:563:GLN:HA	2.00	0.42
1:C:287:ASP:HB3	1:C:306:PHE:CE2	2.55	0.42
1:C:552:LEU:HD12	1:C:585:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:HB3	1:A:266:TYR:HB2	2.02	0.42
1:A:109:THR:O	1:A:109:THR:CG2	2.68	0.42
1:B:381:GLY:HA3	1:B:430:THR:HA	2.02	0.42
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.53	0.42
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.55	0.42
1:B:125:ASN:ND2	1:B:171:VAL:HG13	2.35	0.42
1:B:143:VAL:HG11	1:B:154:GLU:HG2	2.02	0.42
1:B:341:VAL:CG2	1:B:342:PHE:CD2	3.00	0.42
1:B:642:VAL:HG22	1:B:651:ILE:HG22	2.02	0.42
1:C:24:ARG:HH12	1:C:84:LEU:HG	1.85	0.42
1:C:30:ASN:O	1:C:214:ARG:NH2	2.51	0.42
1:A:394:ASN:HD22	1:A:394:ASN:HA	1.70	0.41
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.93	0.41
1:A:448:ASN:OD1	1:A:497:PHE:HB2	2.20	0.41
1:A:821:LEU:HD22	1:A:935:GLN:HG3	2.00	0.41
1:B:559:PHE:CE1	1:C:43:PHE:CD2	3.08	0.41
1:C:106:PHE:HB3	1:C:235:ILE:HD11	2.01	0.41
1:C:190:ARG:HG2	1:C:207:HIS:ND1	2.35	0.41
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.85	0.41
1:A:190:ARG:HG2	1:A:207:HIS:ND1	2.34	0.41
1:A:338:PHE:HE1	1:A:513:LEU:HD11	1.84	0.41
1:A:873:TYR:HE1	1:C:699:LEU:HB3	1.85	0.41
1:B:357:ARG:HG2	1:B:396:TYR:HE1	1.84	0.41
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.47	0.41
1:A:43:PHE:HB2	1:C:563:GLN:HG2	2.01	0.41
1:A:598:ILE:HB	1:A:609:ALA:HB3	2.02	0.41
1:B:703:ASN:O	1:C:789:TYR:HA	2.21	0.41
1:B:706:ALA:HB3	1:C:895:GLN:NE2	2.35	0.41
1:C:24:ARG:NH1	1:C:82:PRO:O	2.53	0.41
1:C:979:ASP:O	1:C:983:ARG:HB3	2.20	0.41
1:A:557:LYS:HB3	1:A:557:LYS:HE2	1.88	0.41
1:A:894:LEU:HD22	1:C:713:ALA:O	2.21	0.41
1:A:897:PRO:HD3	1:C:711:SER:O	2.19	0.41
1:A:914:ASN:OD1	1:A:915:VAL:N	2.54	0.41
1:A:1122:VAL:HG23	1:A:1123:SER:N	2.34	0.41
1:B:319:ARG:NH2	1:C:740:MET:CA	2.83	0.41
1:B:811:LYS:HE2	1:B:811:LYS:HB3	1.88	0.41
1:C:433:VAL:HG22	1:C:512:VAL:HG22	2.02	0.41
1:C:44:ARG:O	1:C:283:GLY:HA2	2.21	0.41
1:C:805:ILE:HD12	1:C:878:LEU:HD22	2.03	0.41
1:C:930:ALA:O	1:C:934:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HD11	1:B:983:ARG:HA	2.03	0.41
1:B:536:ASN:C	1:B:537:LYS:HG3	2.44	0.41
1:C:979:ASP:O	1:C:983:ARG:HB2	2.21	0.41
1:C:1102:TRP:CD1	1:C:1135:ASN:HD22	2.39	0.41
1:A:115:GLN:HG3	1:A:132:GLU:OE2	2.20	0.41
1:A:379:CYS:HB3	1:A:382:VAL:O	2.21	0.41
1:B:65:PHE:HB2	1:B:265:TYR:CD2	2.45	0.41
1:B:132:GLU:O	1:B:164:ASN:ND2	2.52	0.41
1:B:659:SER:HB3	1:B:698:SER:HB3	2.03	0.41
1:B:743:CYS:HB3	1:B:749:CYS:HB3	2.01	0.41
1:C:666:ILE:HG12	1:C:671:CYS:HA	2.02	0.41
1:A:89:GLY:HA3	1:A:270:LEU:HD12	2.03	0.41
1:B:40:ASP:N	1:B:40:ASP:OD1	2.52	0.41
1:B:317:ASN:OD1	1:B:317:ASN:C	2.64	0.41
1:C:598:ILE:HG12	1:C:666:ILE:HD12	2.02	0.41
1:A:733:LYS:HD2	1:A:771:ALA:HB1	2.03	0.40
1:B:334:ASN:O	1:B:335:LEU:CG	2.69	0.40
1:B:347:PHE:HZ	1:B:509:ARG:HD2	1.68	0.40
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.02	0.40
1:C:1004:LEU:HA	1:C:1004:LEU:HD23	1.86	0.40
1:B:37:TYR:HB2	1:B:206:LYS:HG2	2.03	0.40
1:B:319:ARG:NH2	1:C:740:MET:HB2	2.36	0.40
1:C:130:VAL:O	1:C:130:VAL:HG12	2.21	0.40
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.50	0.40
1:B:92:PHE:HB3	1:B:190:ARG:HB2	2.04	0.40
1:B:132:GLU:HB2	1:B:164:ASN:OD1	2.21	0.40
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	2.03	0.40
1:C:532:ASN:OD1	1:C:533:LEU:N	2.55	0.40
1:A:363:ALA:O	1:A:526:GLY:HA2	2.22	0.40
1:A:977:LEU:O	1:A:980:ILE:HG22	2.21	0.40
1:C:963:VAL:O	1:C:966:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1003/1227 (82%)	971 (97%)	31 (3%)	1 (0%)	48	76
1	B	991/1227 (81%)	934 (94%)	49 (5%)	8 (1%)	16	45
1	C	1001/1227 (82%)	961 (96%)	39 (4%)	1 (0%)	48	76
All	All	2995/3681 (81%)	2866 (96%)	119 (4%)	10 (0%)	37	66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	PHE
1	B	536	ASN
1	C	233	ILE
1	A	526	GLY
1	B	339	HIS
1	B	526	GLY
1	B	535	LYS
1	B	360	ASN
1	B	580	GLN
1	B	332	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	892/1070 (83%)	891 (100%)	1 (0%)	88	89
1	B	887/1070 (83%)	885 (100%)	2 (0%)	87	87
1	C	889/1070 (83%)	889 (100%)	0	100	100
All	All	2668/3210 (83%)	2665 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	LYS

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Mol	Chain	Res	Type
1	B	327	VAL
1	B	362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	334	ASN
1	A	1071	GLN
1	B	52	HIS
1	B	125	ASN
1	B	134	GLN
1	B	394	ASN
1	B	439	ASN
1	B	448	ASN
1	B	542	ASN
1	B	658	ASN
1	B	710	ASN
1	B	751	ASN
1	B	755	GLN
1	B	762	GLN
1	B	919	ASN
1	B	1002	GLN
1	B	1058	HIS
1	B	1088	HIS
1	B	1106	GLN
1	C	137	ASN
1	C	354	ASN
1	C	448	ASN
1	C	563	GLN
1	C	755	GLN
1	C	762	GLN
1	C	784	GLN
1	C	1071	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	A	1311	1	14,14,15	0.50	0	17,19,21	0.56	0
2	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.36	0
2	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	C	1304	1	14,14,15	0.31	0	17,19,21	0.63	0
2	NAG	B	1308	1	14,14,15	0.35	0	17,19,21	0.35	0
2	NAG	C	1307	1	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	C	1305	1	14,14,15	0.26	0	17,19,21	0.38	0
2	NAG	A	1303	1	14,14,15	0.16	0	17,19,21	0.45	0
2	NAG	C	1301	1	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.38	0
2	NAG	A	1307	1	14,14,15	0.17	0	17,19,21	0.51	0
2	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.39	0
2	NAG	A	1308	1	14,14,15	0.19	0	17,19,21	0.47	0
2	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.37	0
2	NAG	C	1306	1	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	A	1305	1	14,14,15	0.30	0	17,19,21	0.43	0
2	NAG	A	1310	1	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.45	0
2	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1309	1	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	A	1306	1	14,14,15	0.29	0	17,19,21	0.48	0
2	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	B	1301	1	14,14,15	0.33	0	17,19,21	0.60	0
2	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1304	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1302	NAG	C4-C5-C6-O6
2	B	1302	NAG	C4-C5-C6-O6
2	B	1304	NAG	C4-C5-C6-O6
2	C	1301	NAG	O5-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	A	1301	NAG	C4-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6
2	A	1310	NAG	C4-C5-C6-O6
2	C	1303	NAG	O5-C5-C6-O6
2	A	1311	NAG	C4-C5-C6-O6
2	C	1307	NAG	C4-C5-C6-O6
2	A	1303	NAG	O5-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	B	1301	NAG	O5-C5-C6-O6
2	C	1304	NAG	O5-C5-C6-O6
2	A	1307	NAG	C4-C5-C6-O6
2	A	1305	NAG	O5-C5-C6-O6
2	A	1307	NAG	O5-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	C	1301	NAG	C4-C5-C6-O6
2	A	1311	NAG	O5-C5-C6-O6
2	B	1305	NAG	O5-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	A	1301	NAG	O5-C5-C6-O6
2	A	1308	NAG	O5-C5-C6-O6
2	A	1310	NAG	O5-C5-C6-O6
2	C	1307	NAG	O5-C5-C6-O6
2	B	1301	NAG	C4-C5-C6-O6
2	C	1303	NAG	C4-C5-C6-O6
2	A	1309	NAG	C4-C5-C6-O6
2	C	1304	NAG	C4-C5-C6-O6

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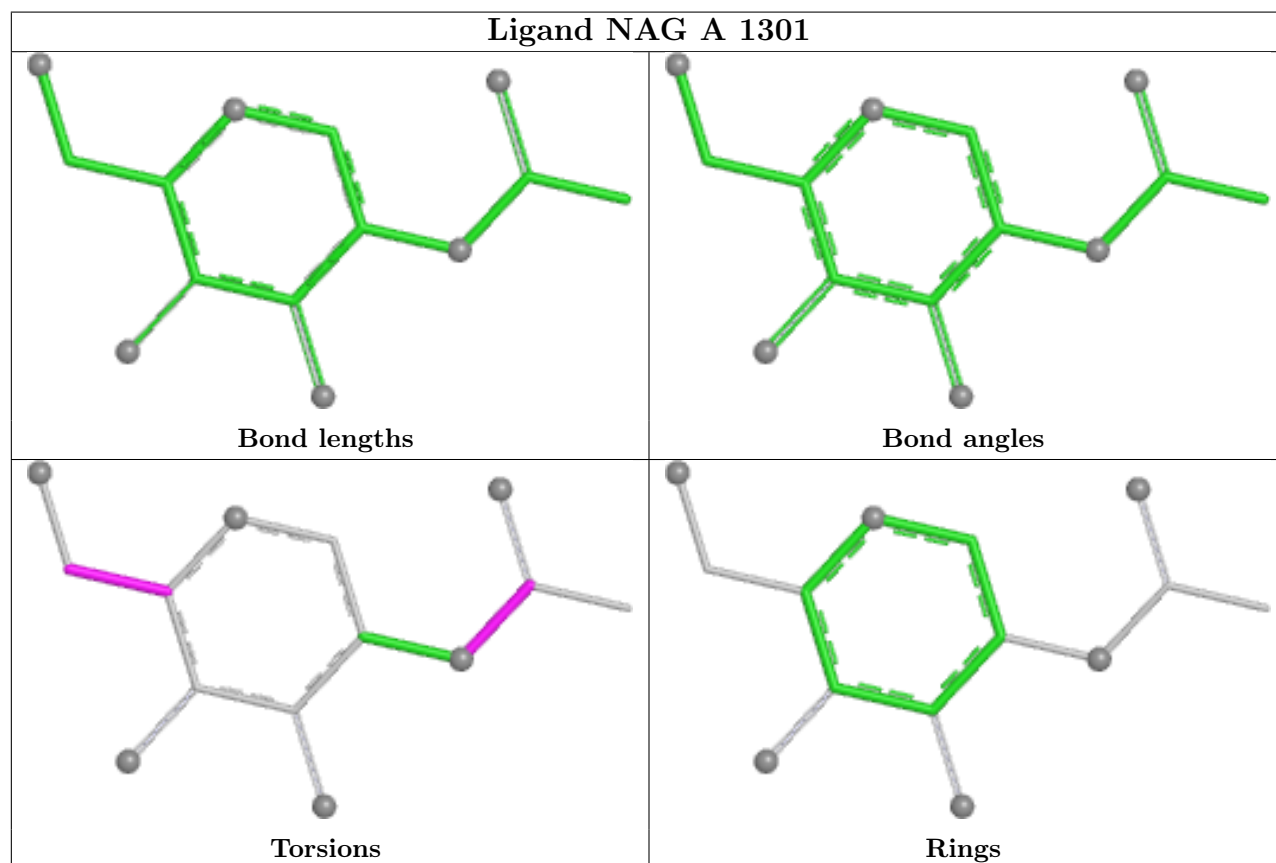
Mol	Chain	Res	Type	Atoms
2	A	1301	NAG	C8-C7-N2-C2
2	A	1301	NAG	O7-C7-N2-C2
2	A	1303	NAG	C8-C7-N2-C2
2	A	1303	NAG	O7-C7-N2-C2
2	A	1307	NAG	C8-C7-N2-C2
2	A	1307	NAG	O7-C7-N2-C2
2	B	1304	NAG	C8-C7-N2-C2
2	B	1304	NAG	O7-C7-N2-C2
2	B	1305	NAG	C8-C7-N2-C2
2	B	1305	NAG	O7-C7-N2-C2
2	B	1306	NAG	C8-C7-N2-C2
2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

There are no ring outliers.

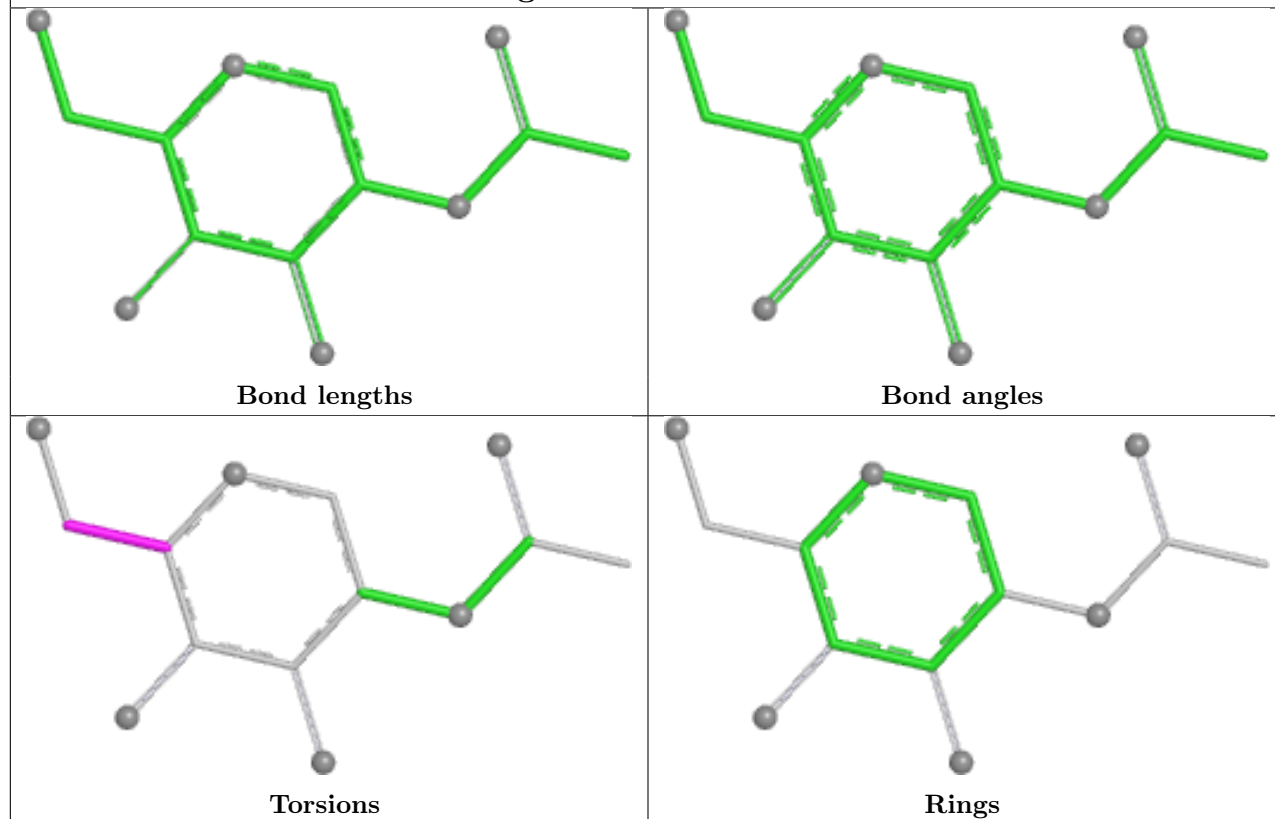
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0
2	B	1308	NAG	2	0
2	A	1307	NAG	1	0

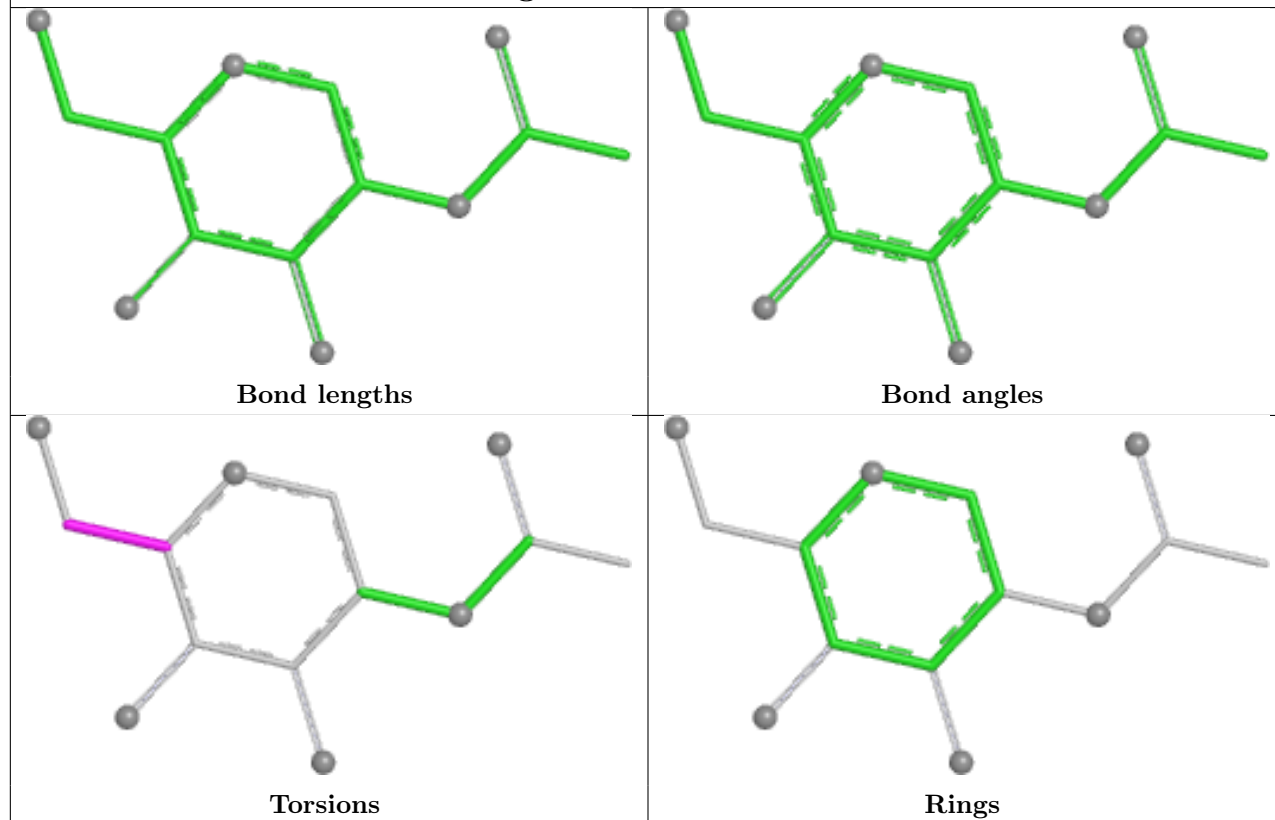
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



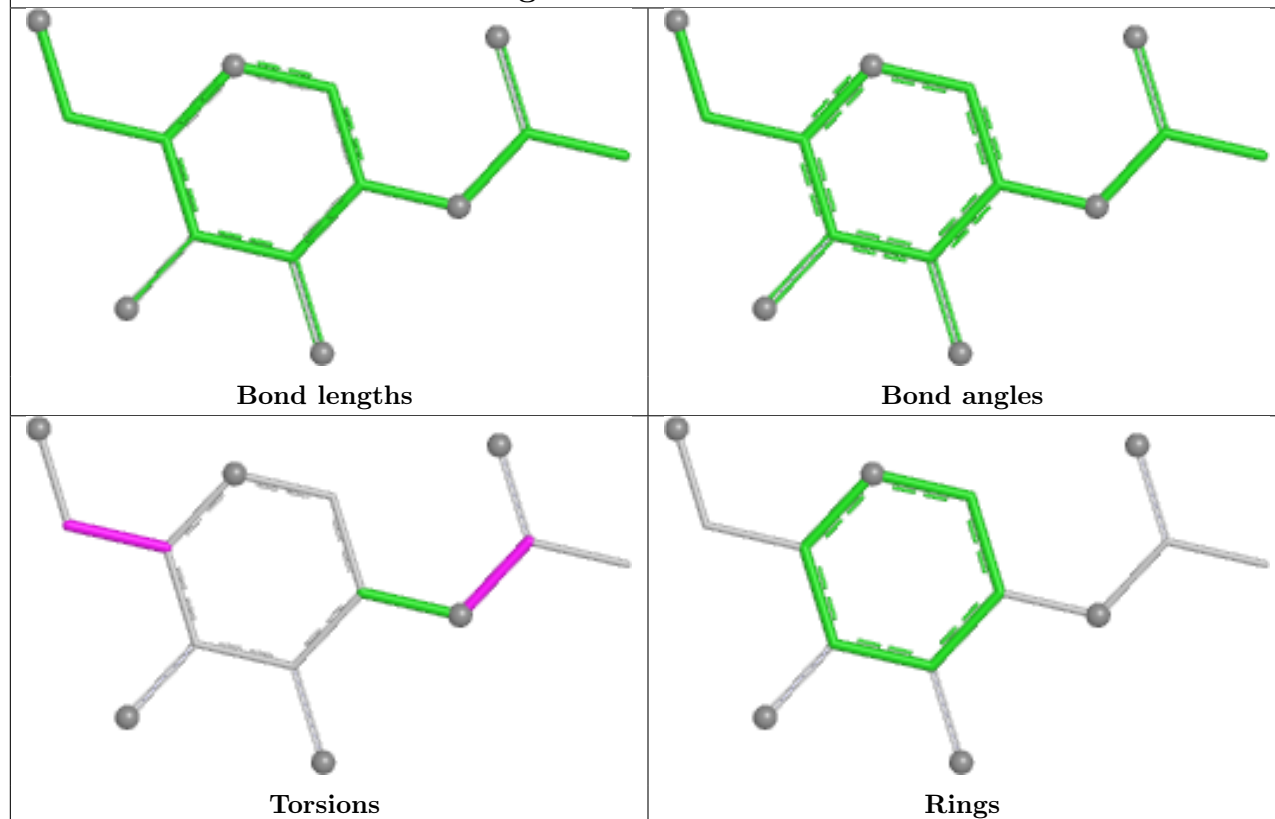
Ligand NAG A 1311



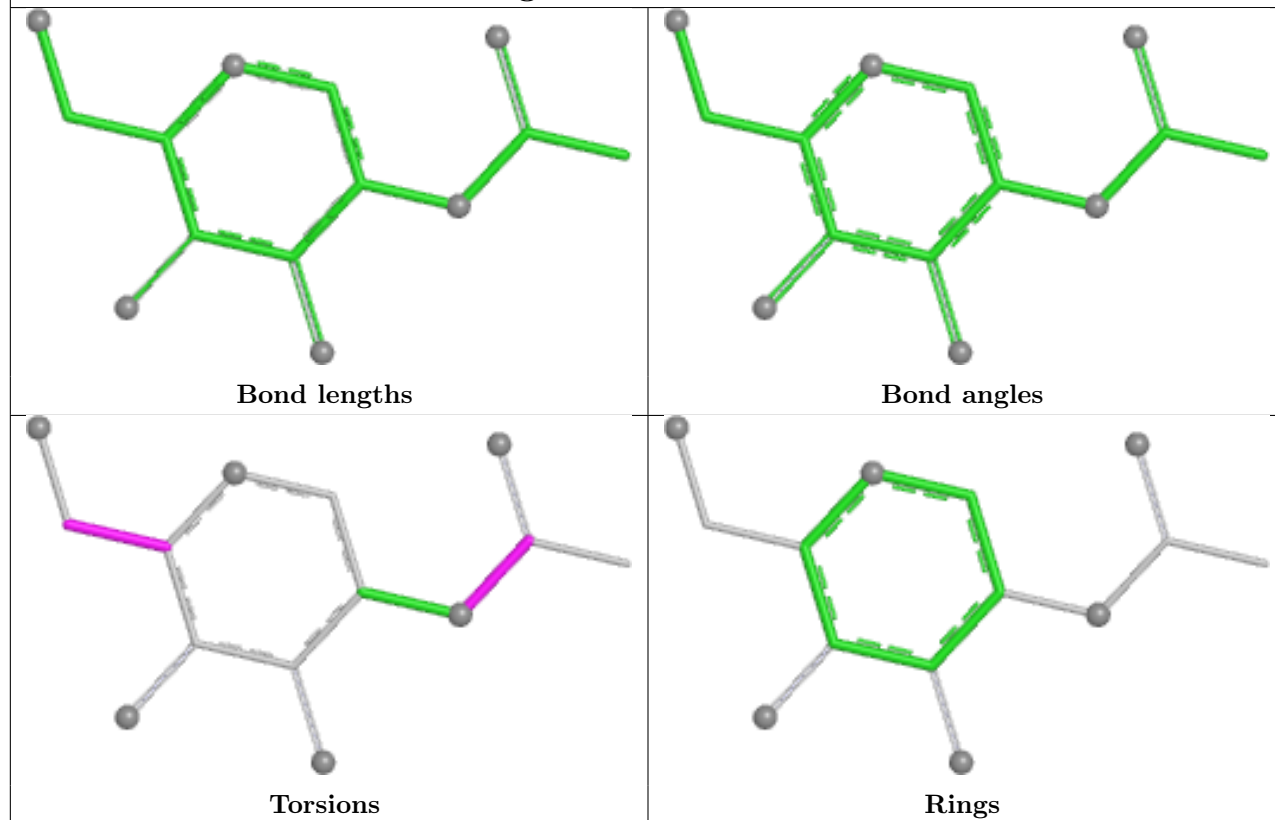
Ligand NAG A 1302



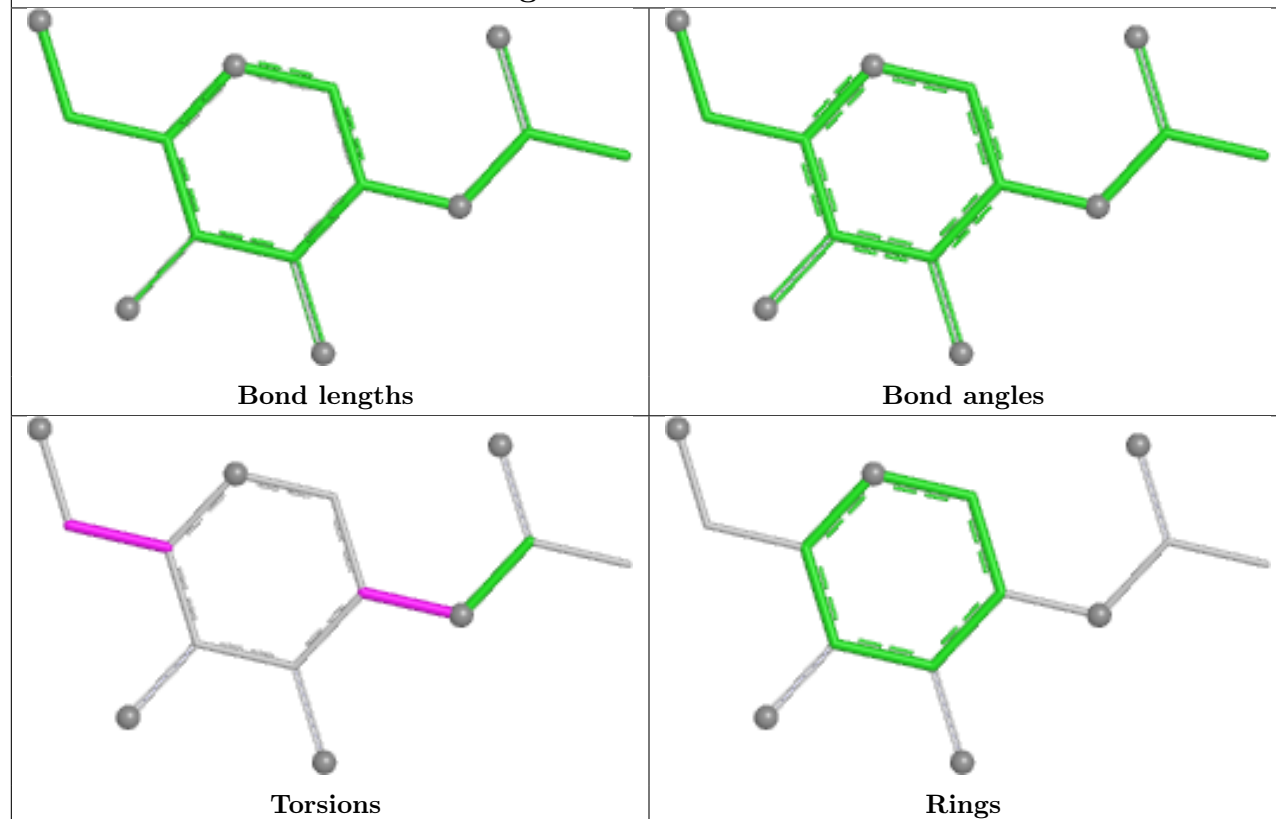
Ligand NAG B 1306



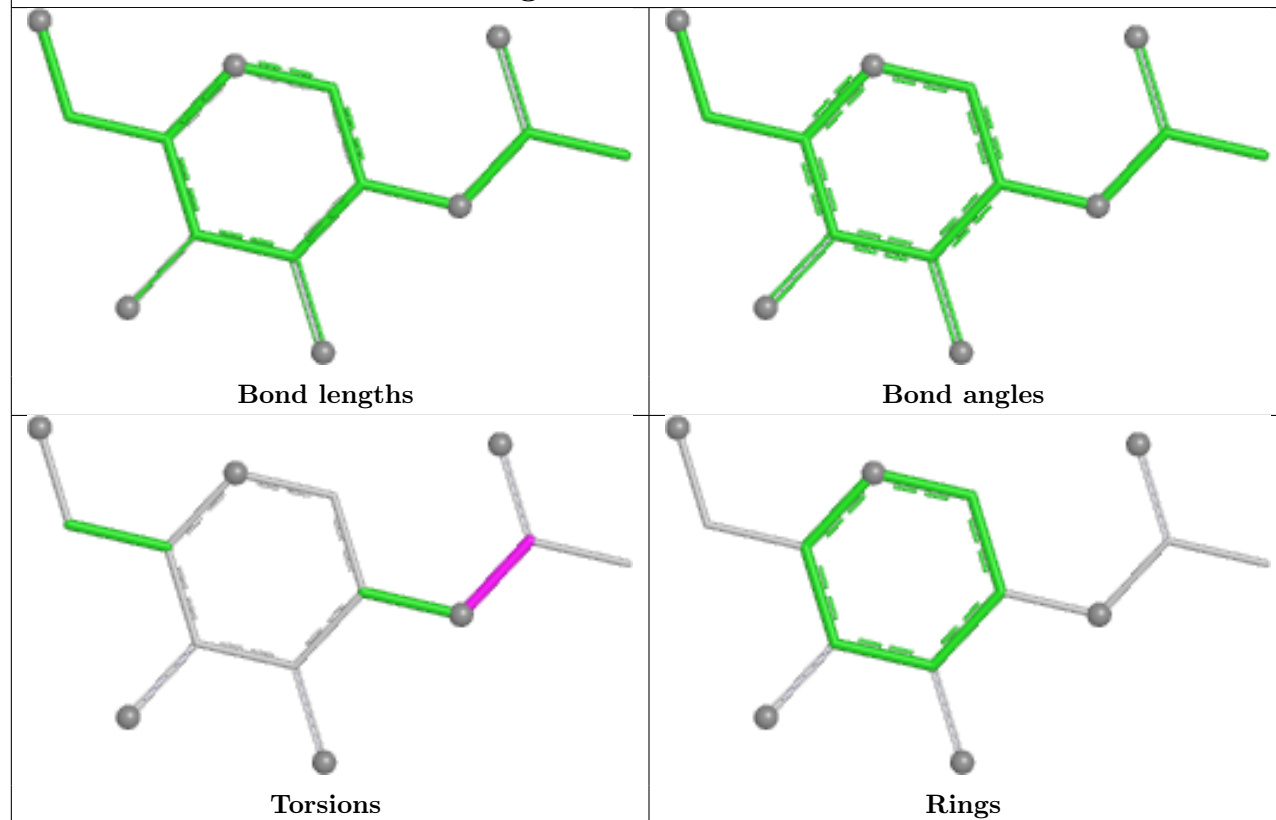
Ligand NAG C 1303

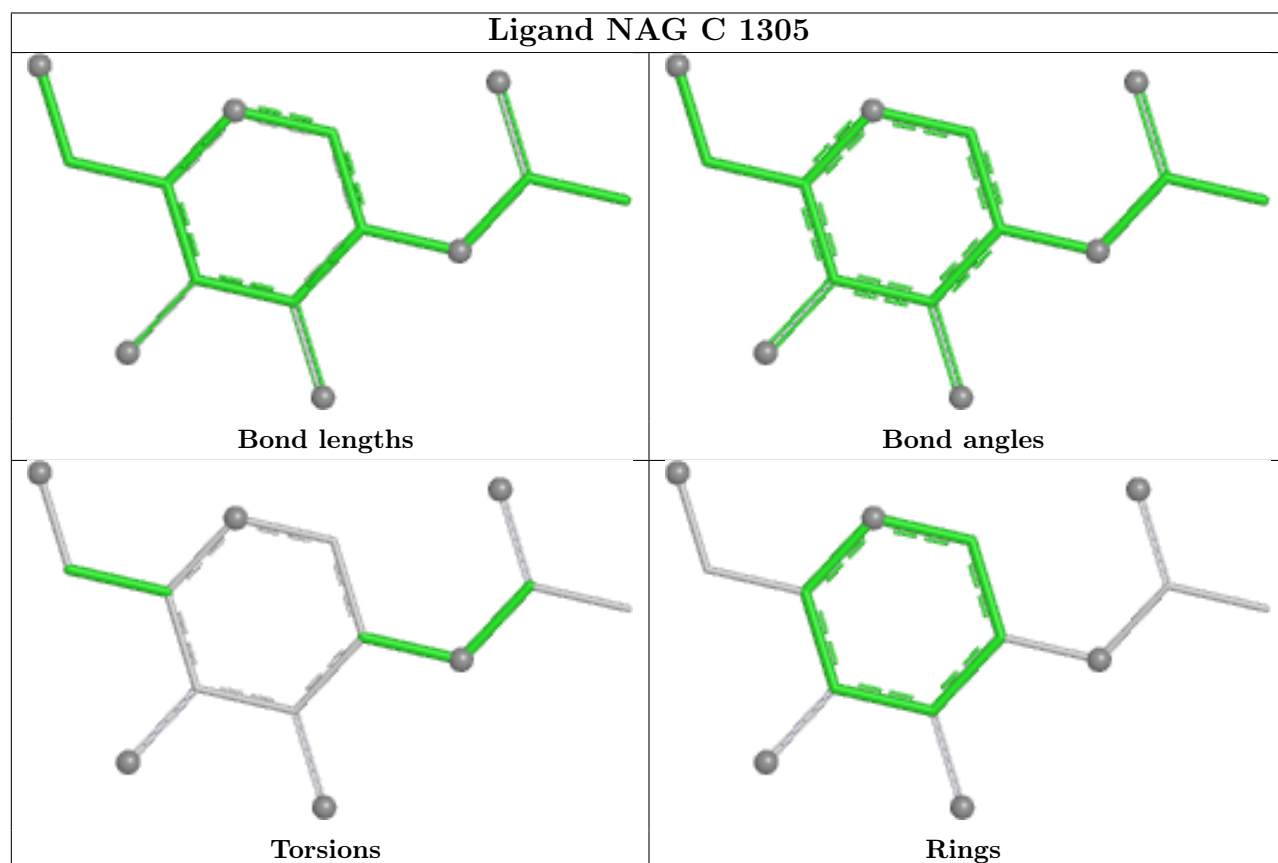
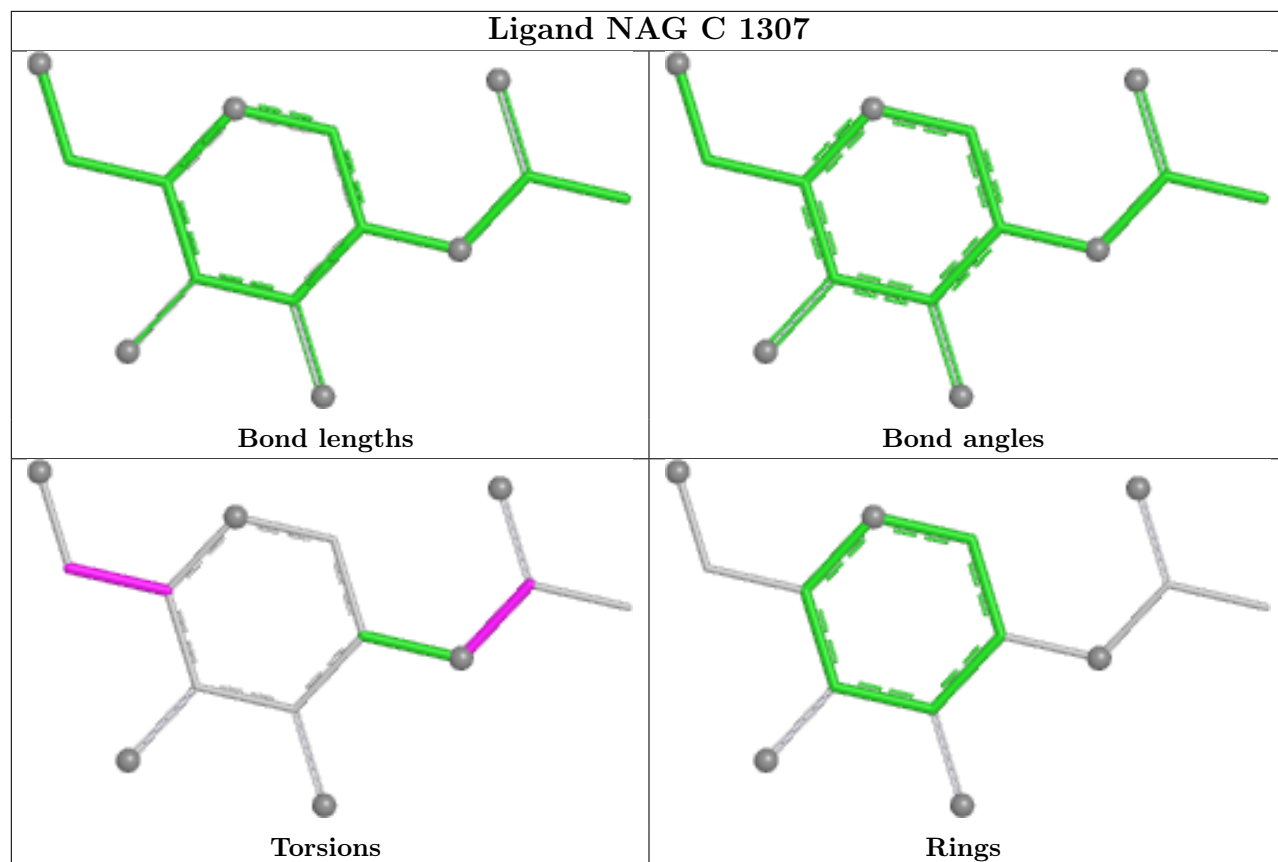


Ligand NAG C 1304

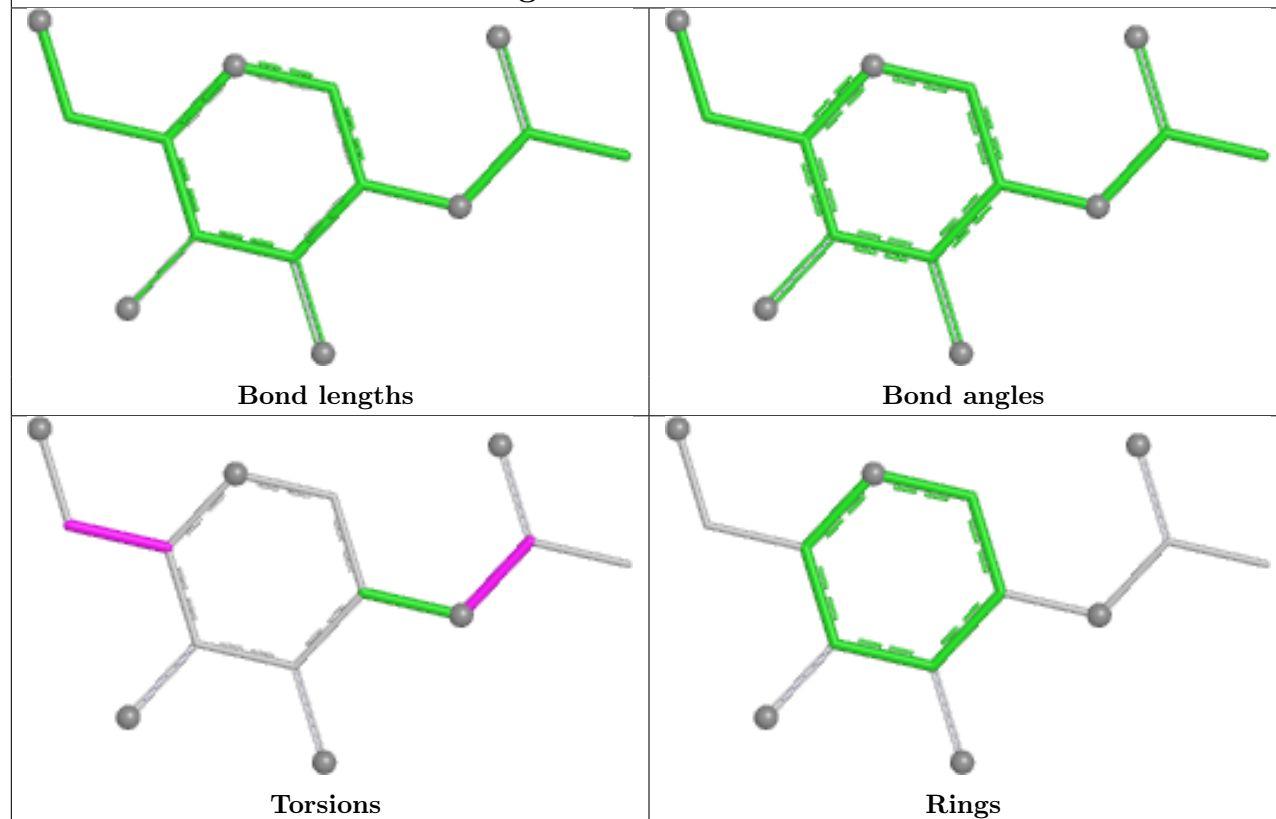


Ligand NAG B 1308

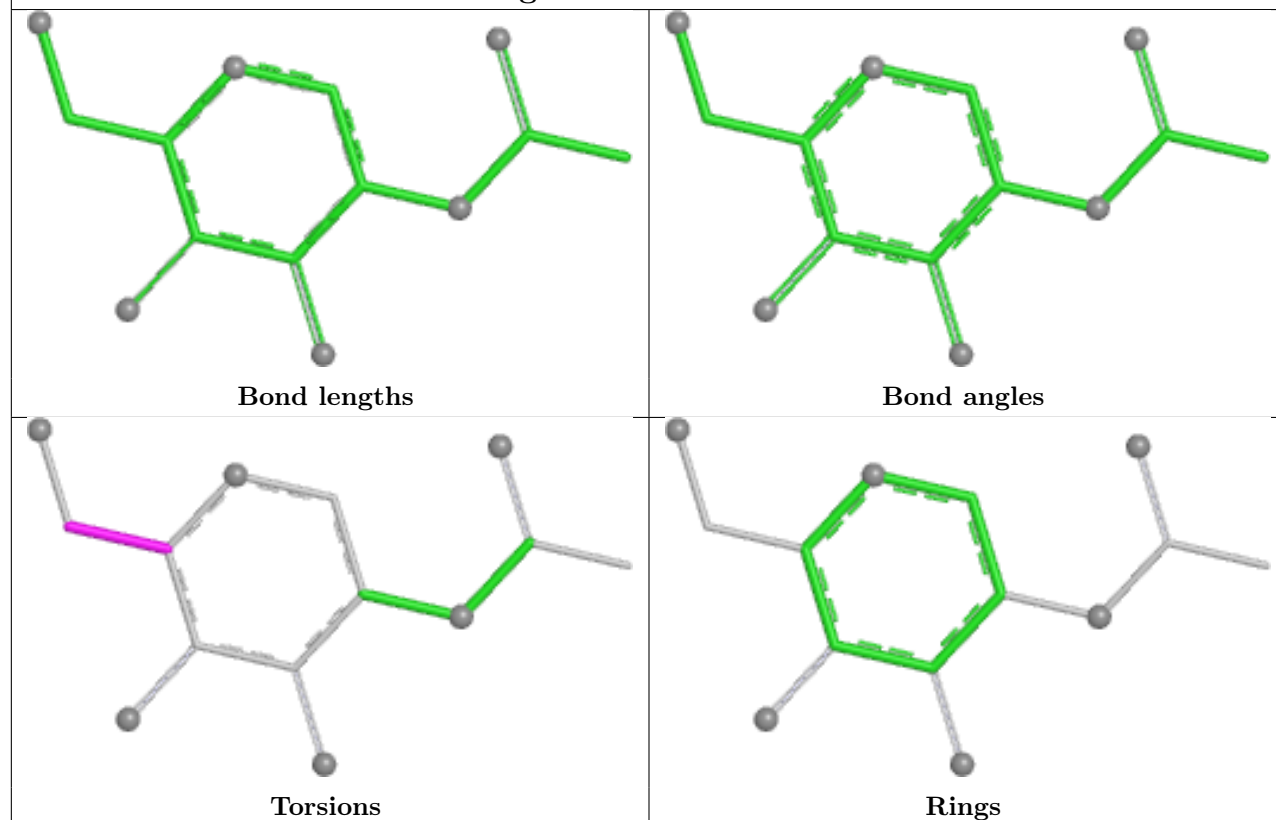




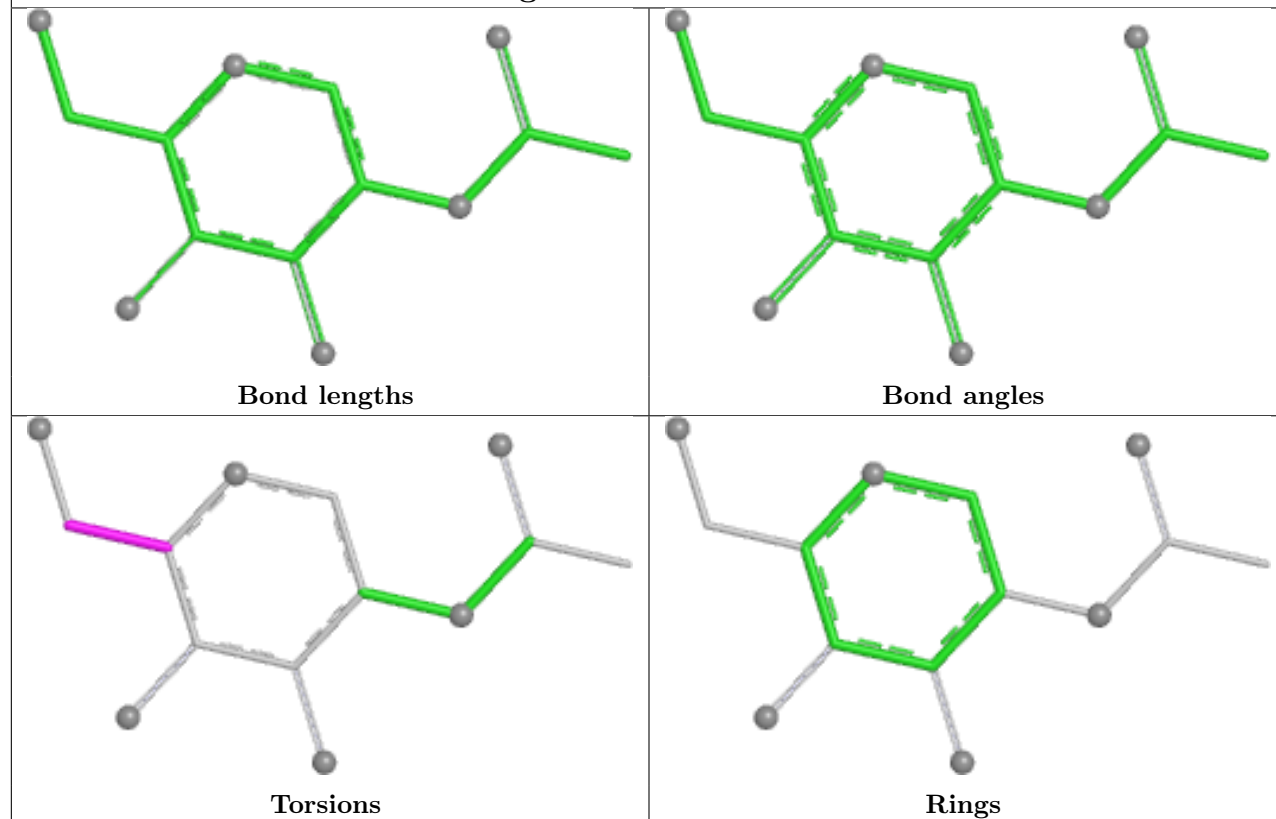
Ligand NAG A 1303



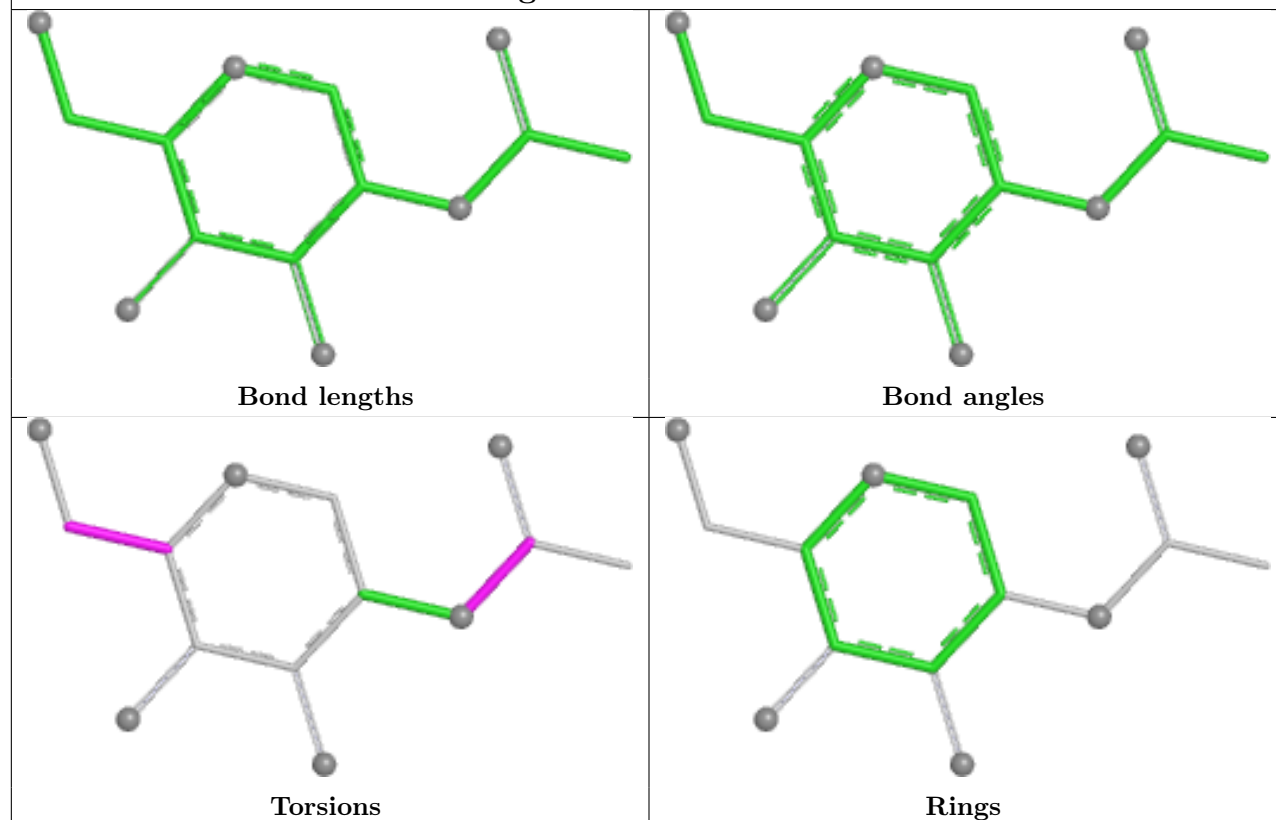
Ligand NAG C 1301

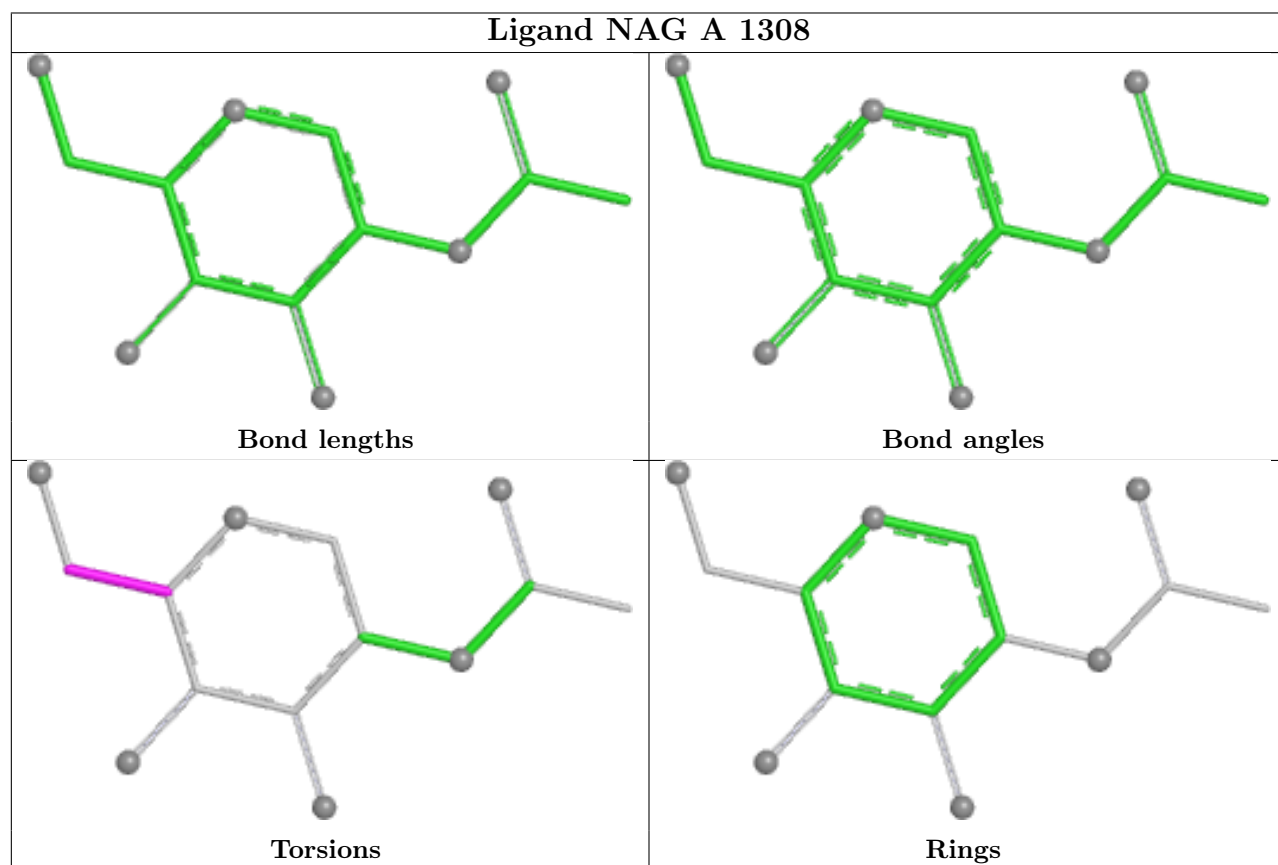
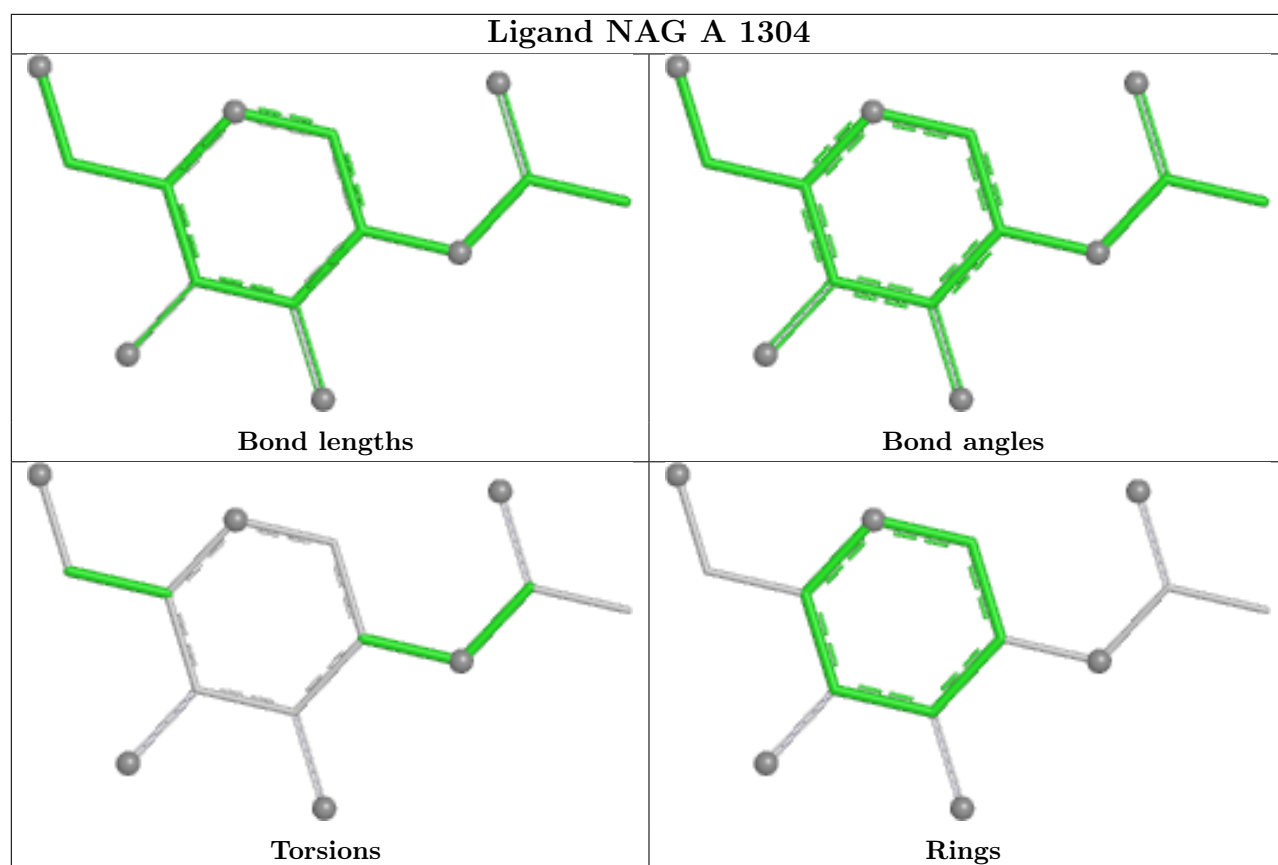


Ligand NAG C 1302

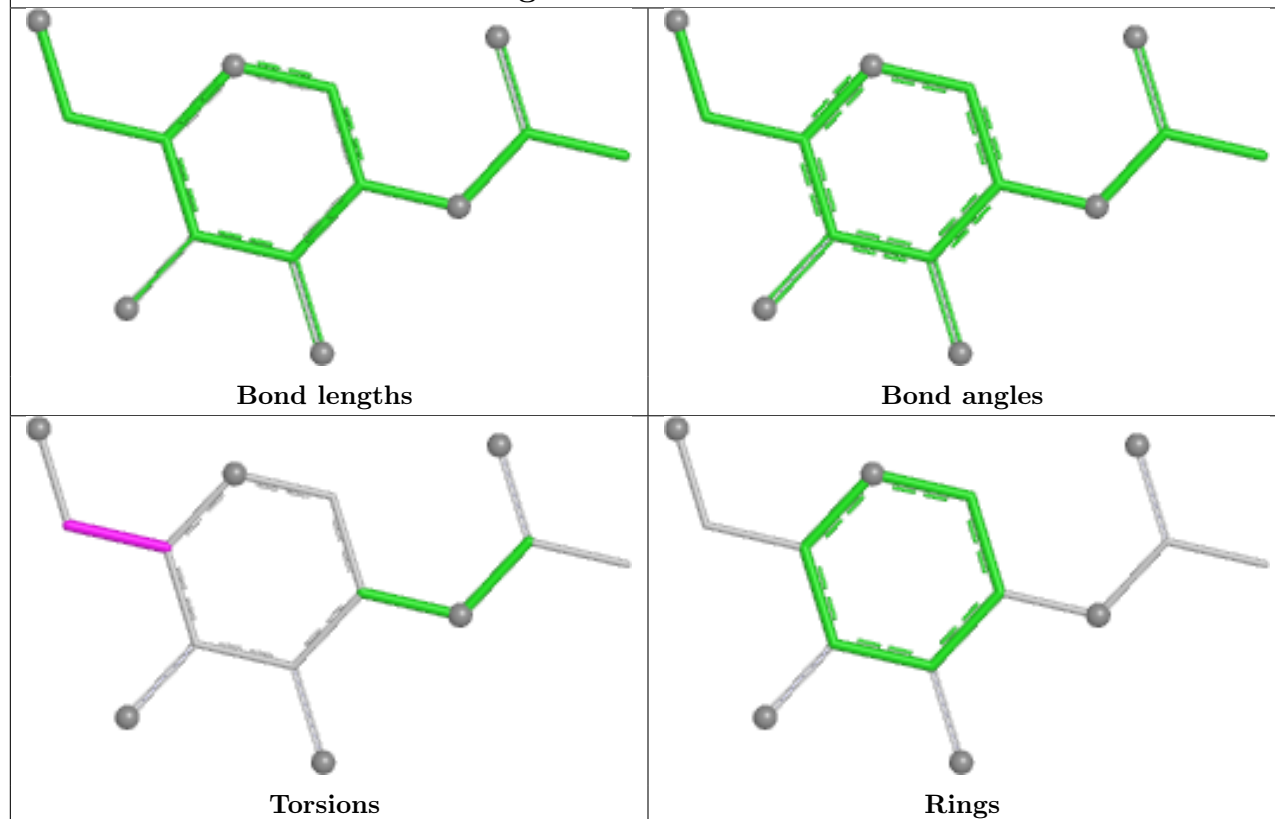


Ligand NAG A 1307

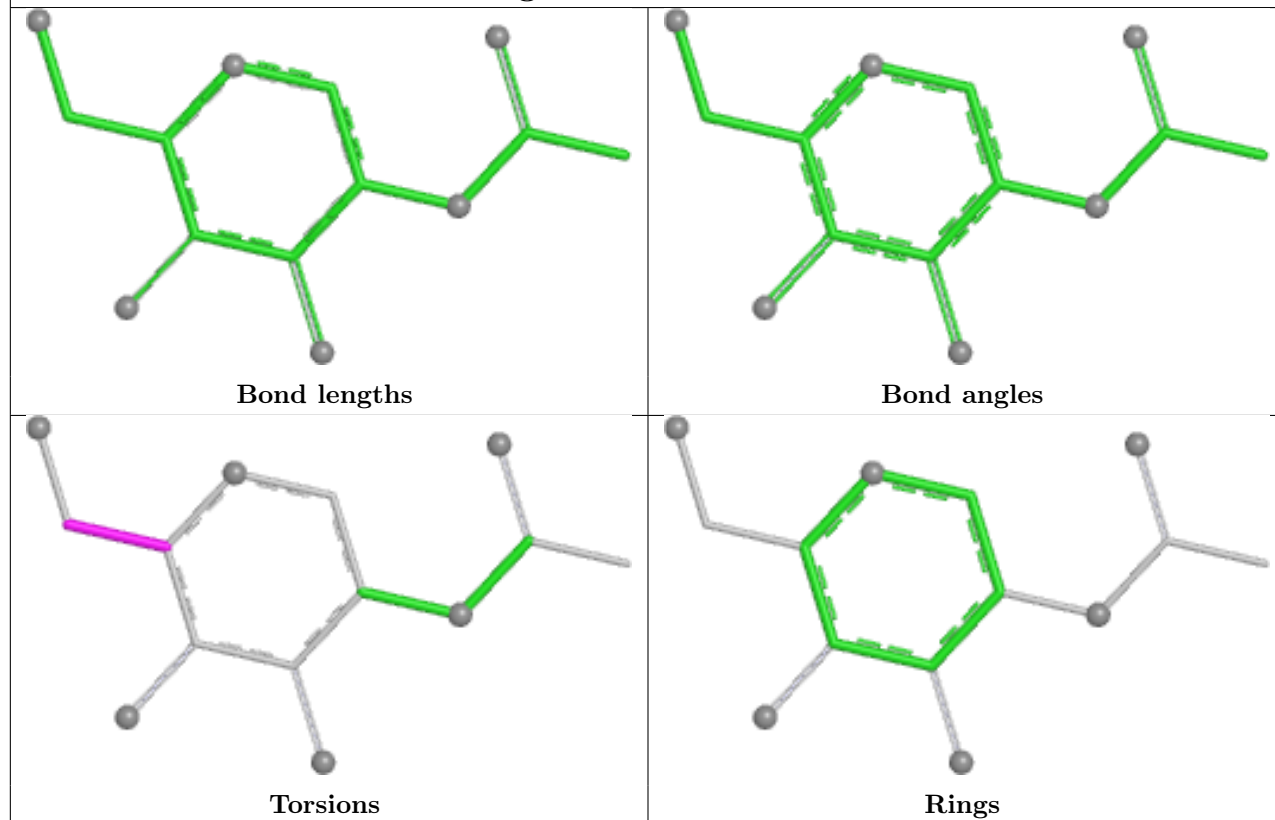


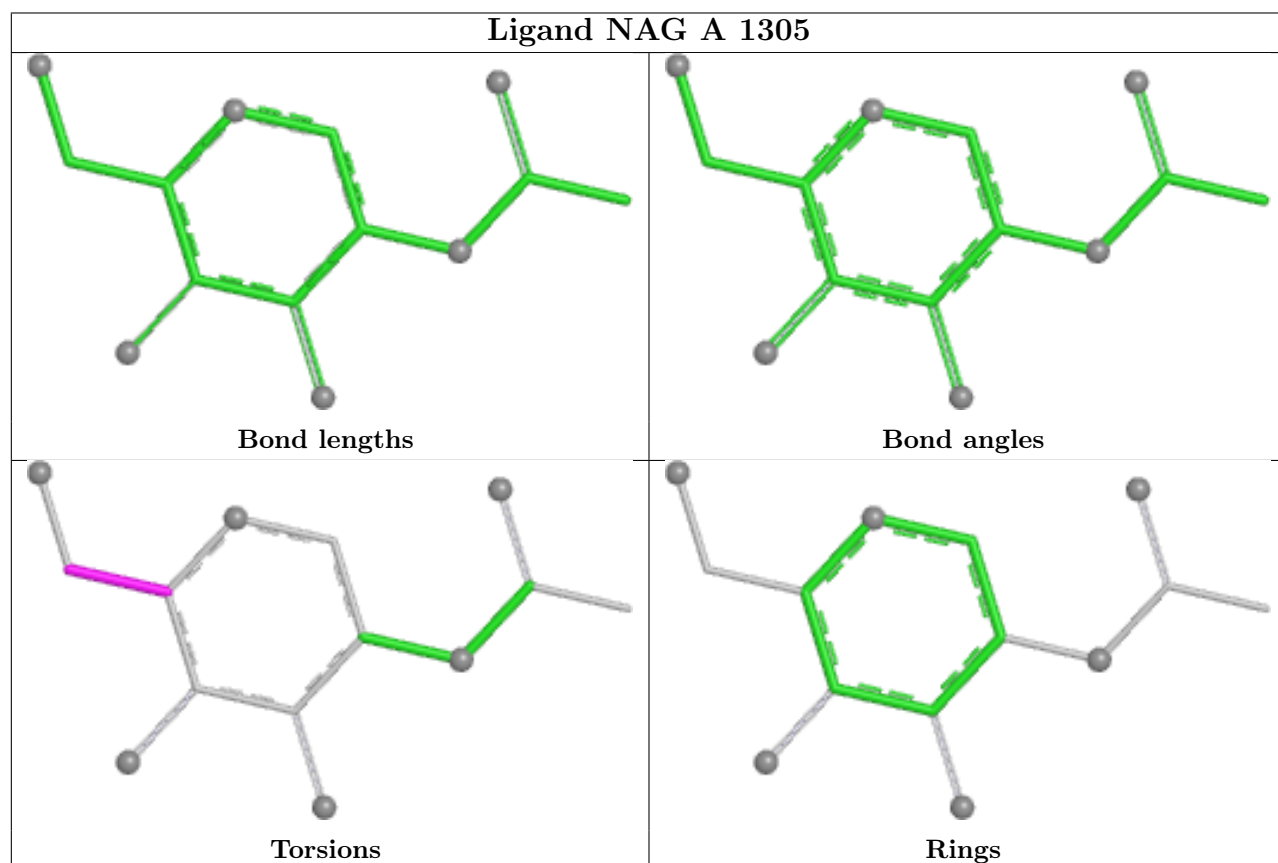
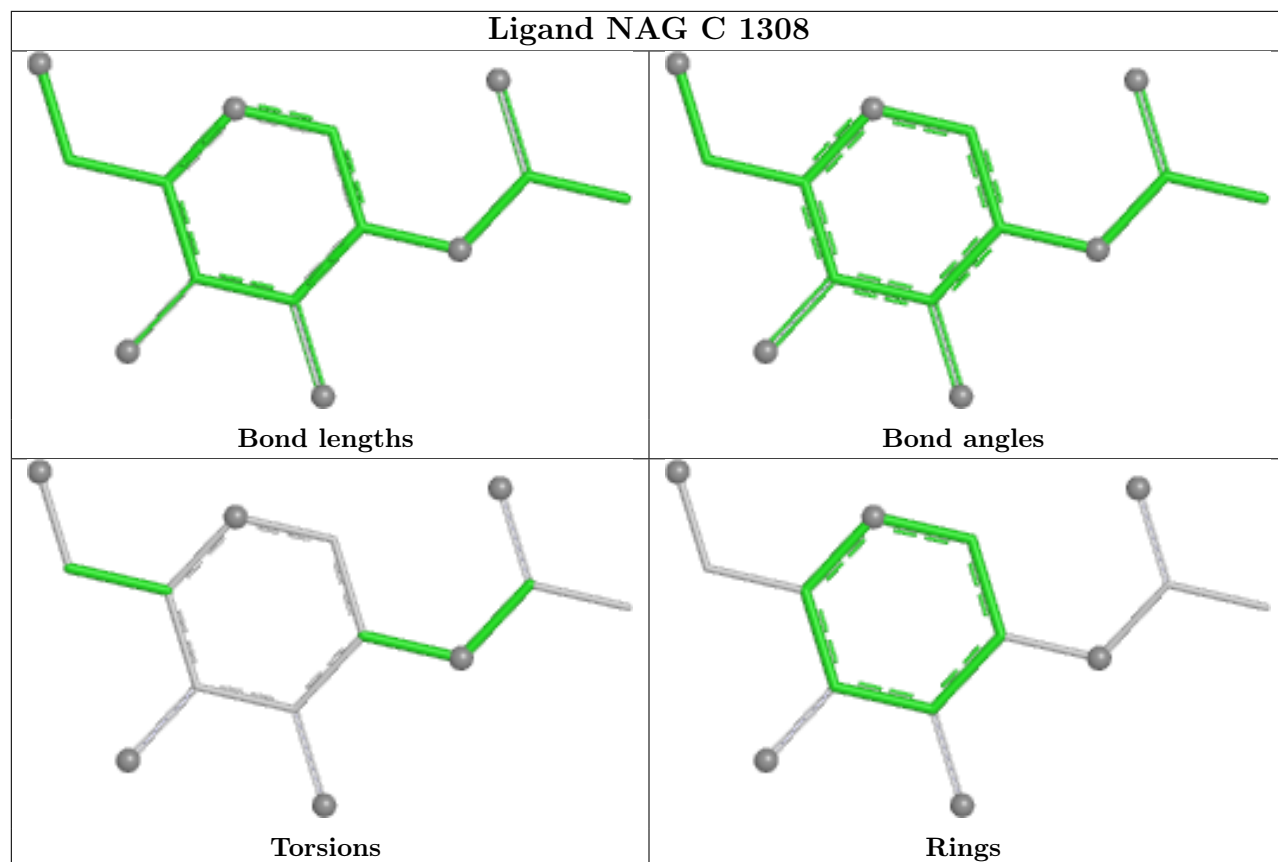


Ligand NAG B 1302

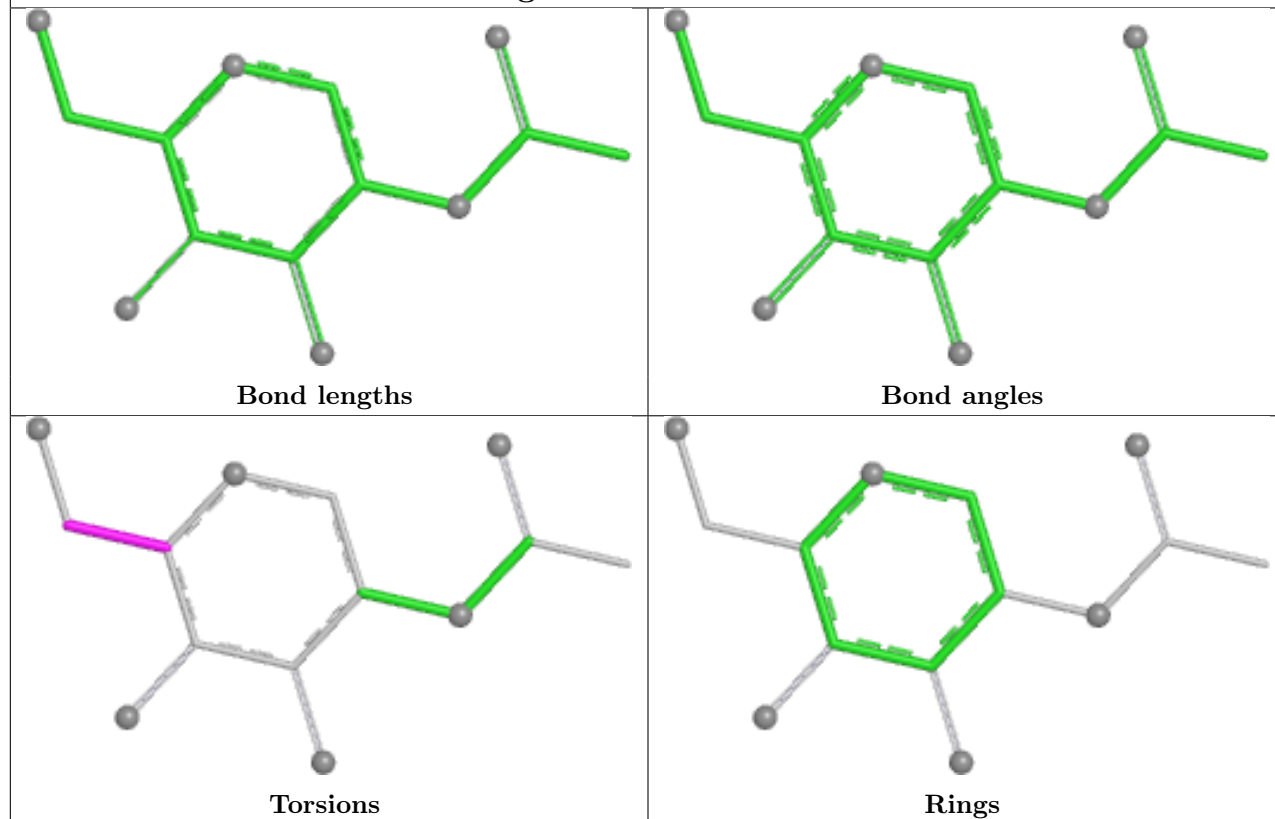


Ligand NAG C 1306

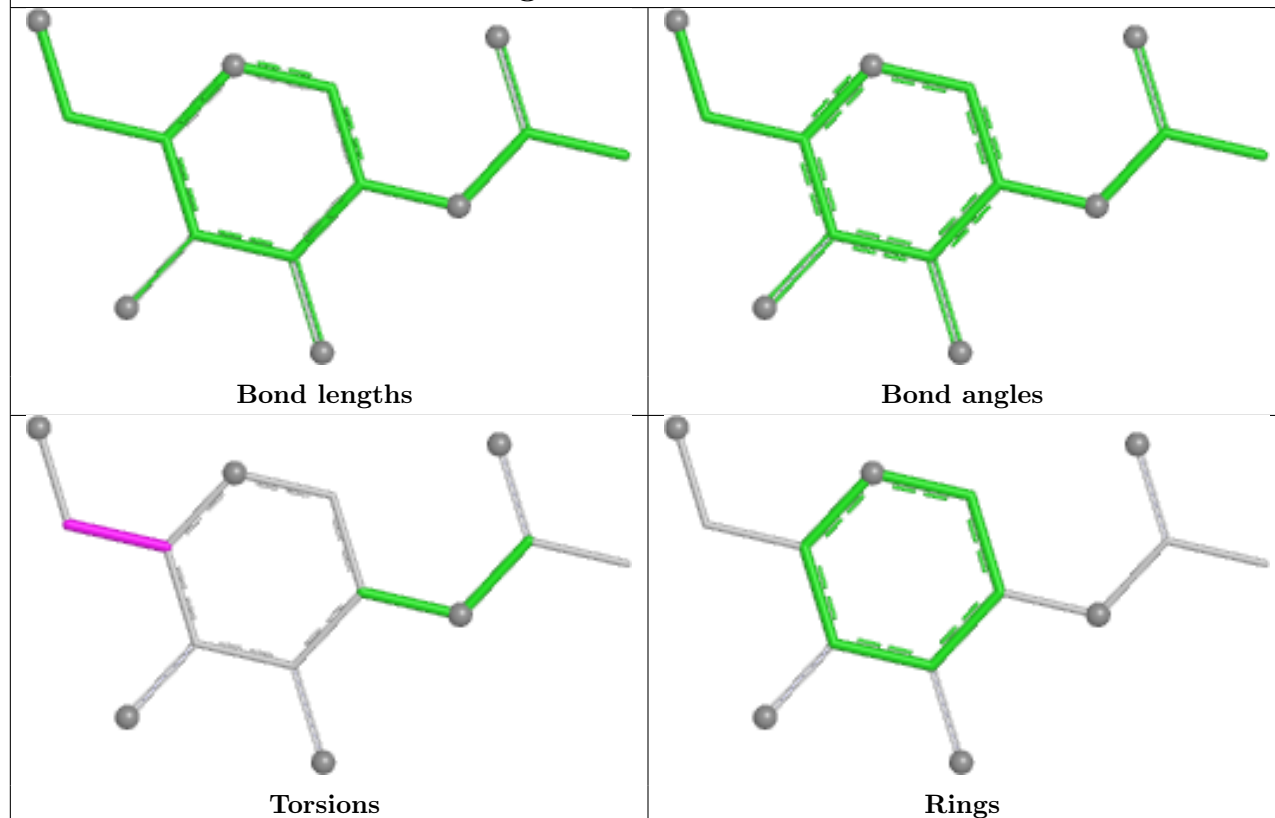




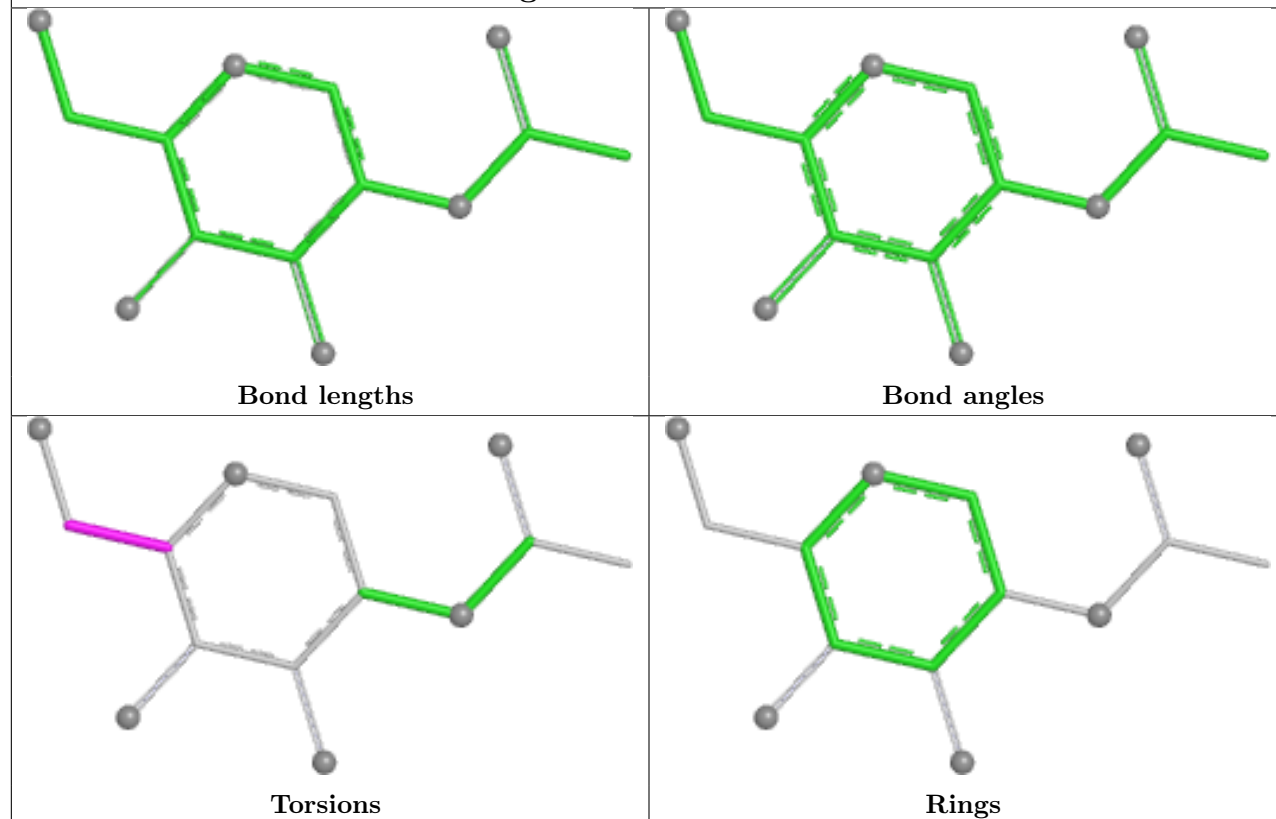
Ligand NAG A 1310



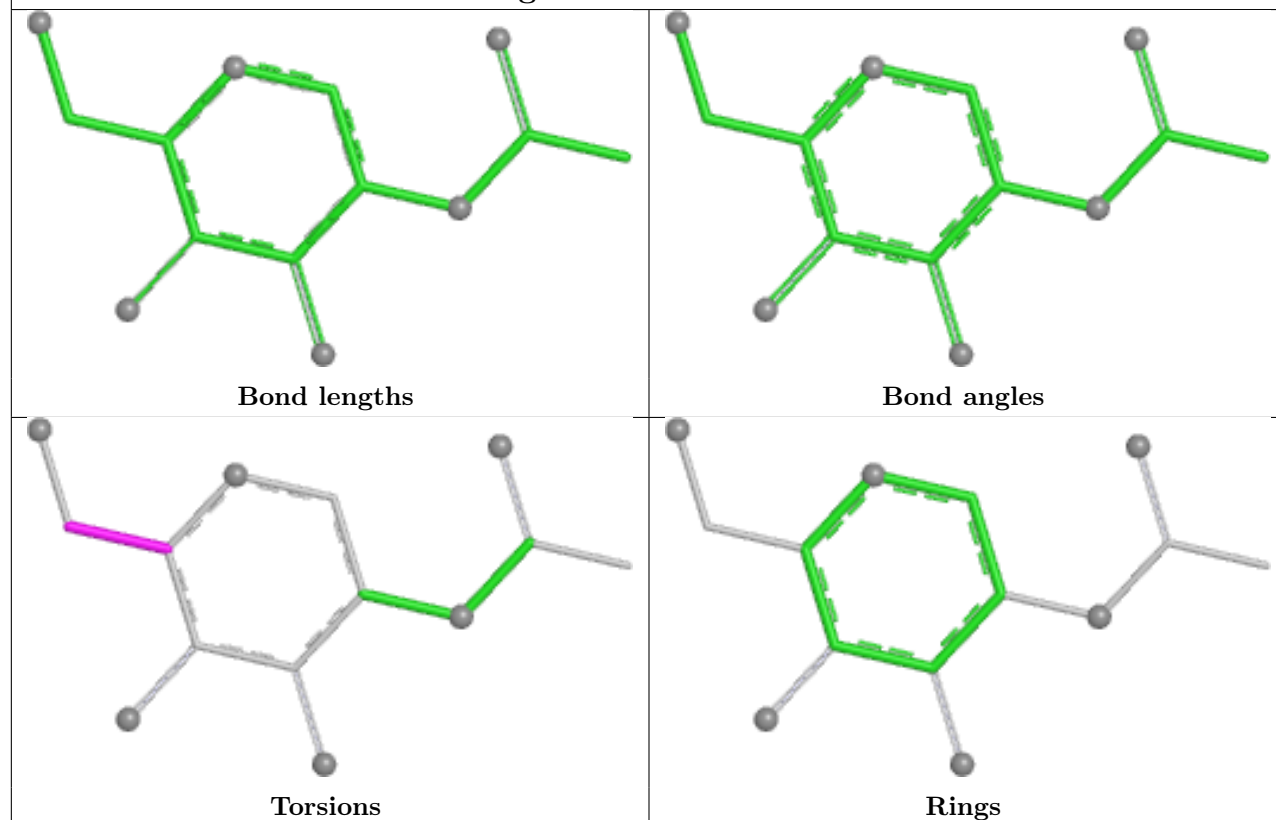
Ligand NAG B 1303



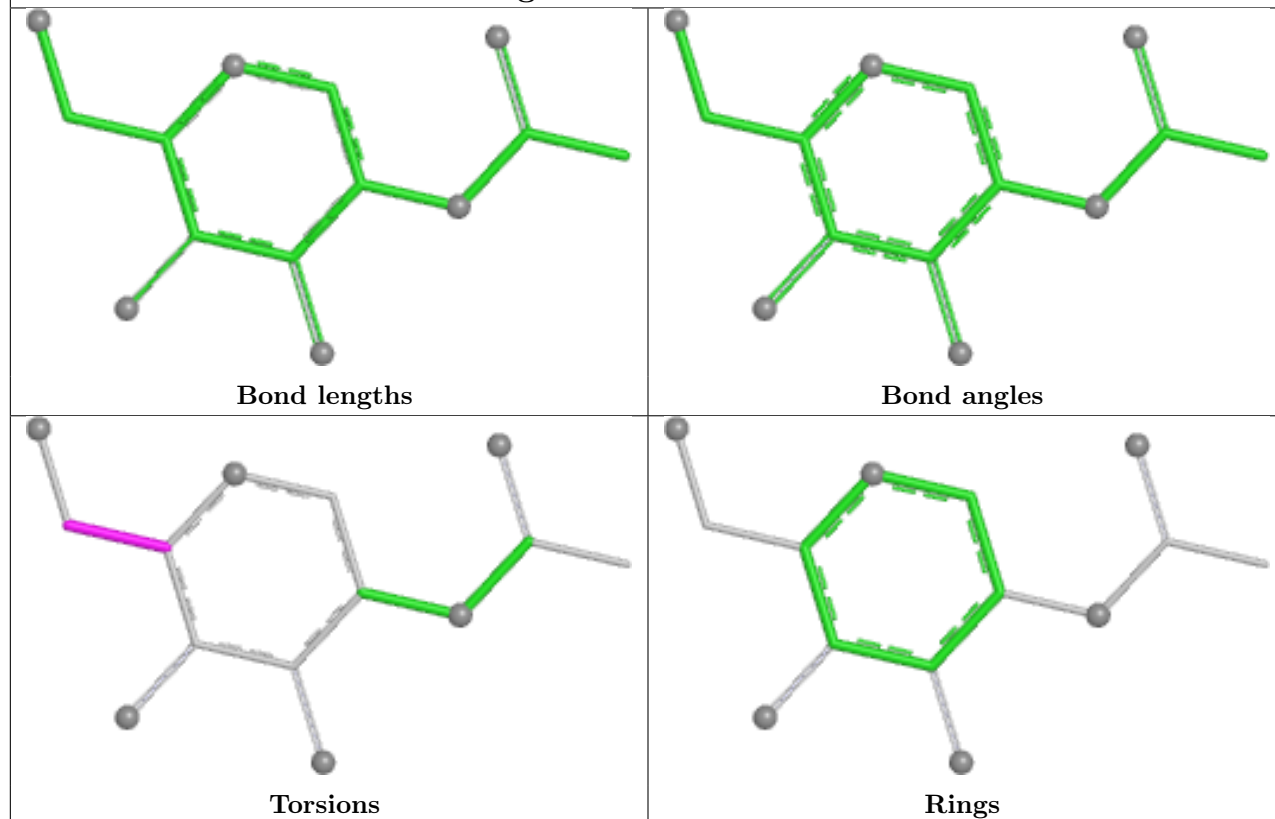
Ligand NAG B 1307



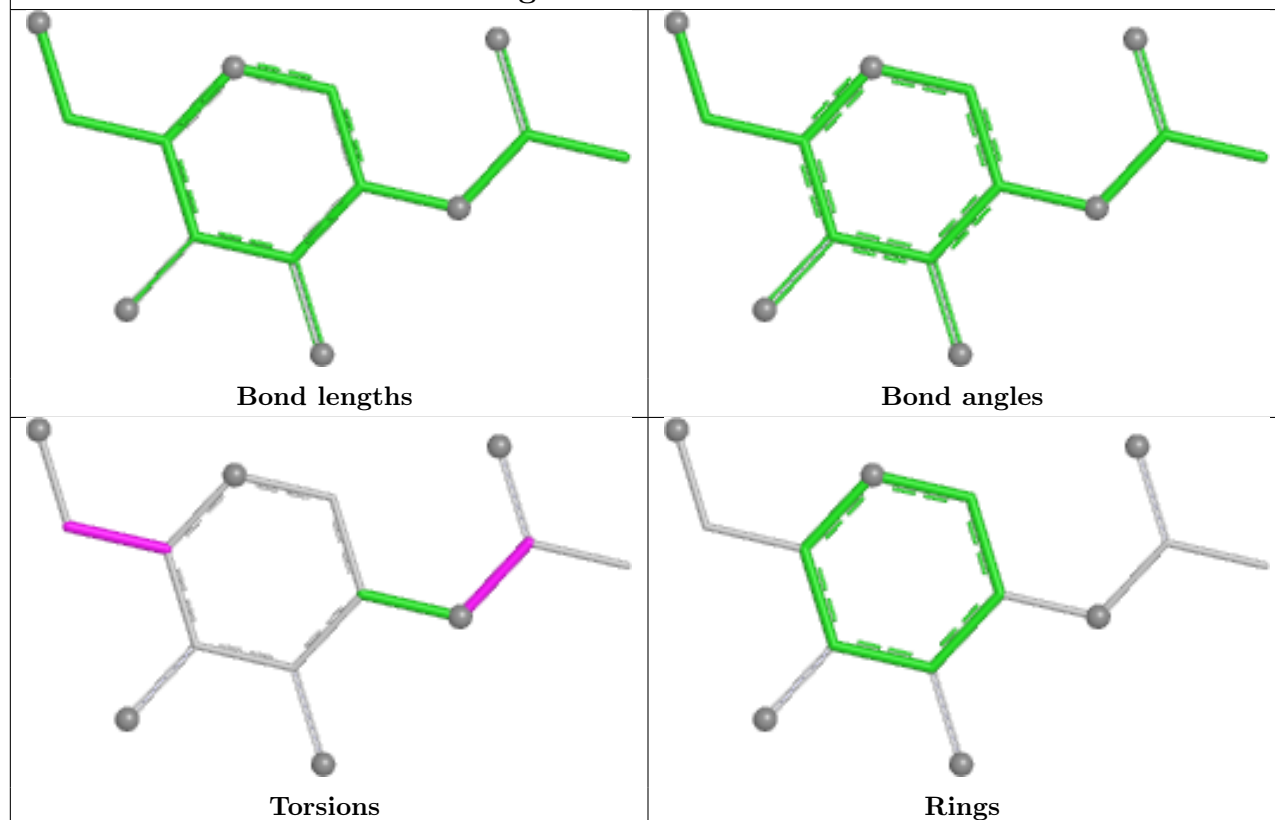
Ligand NAG A 1309

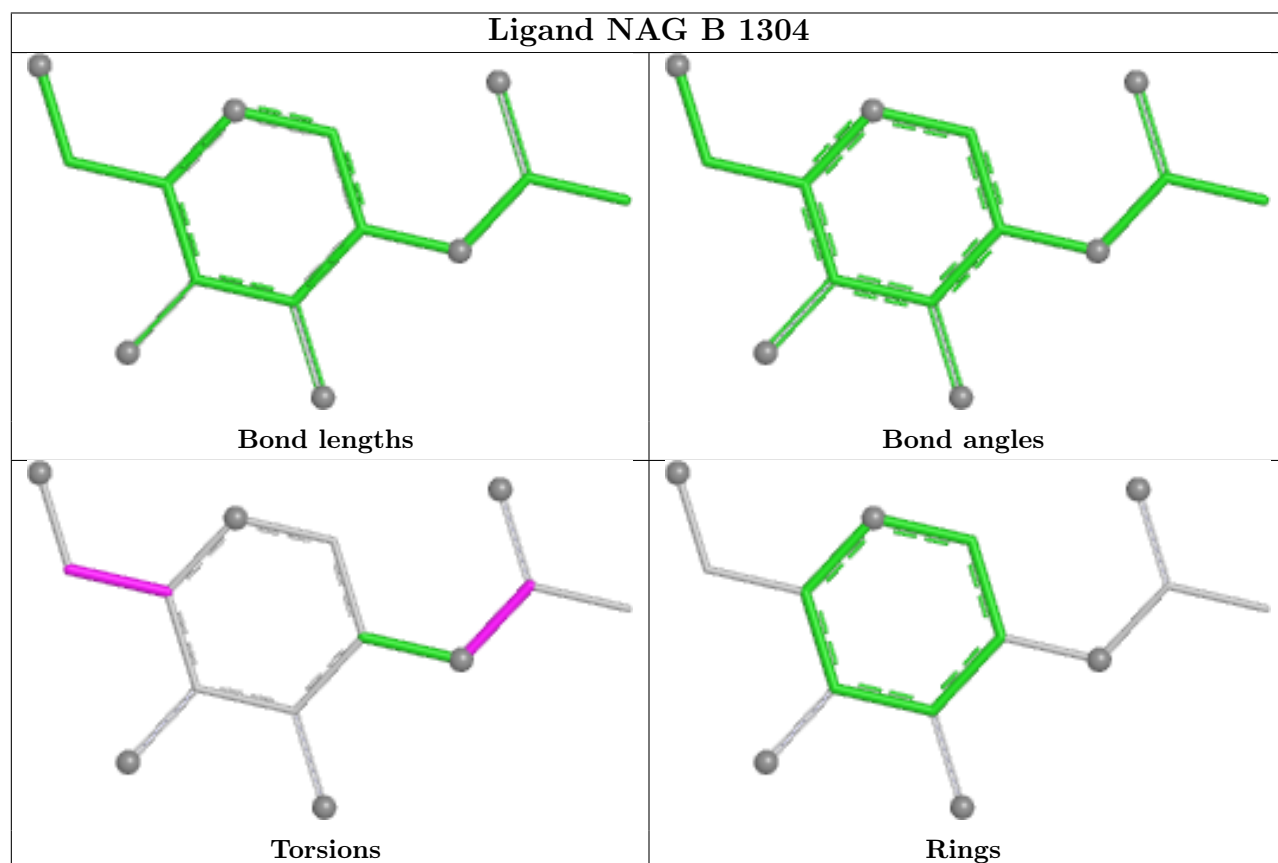
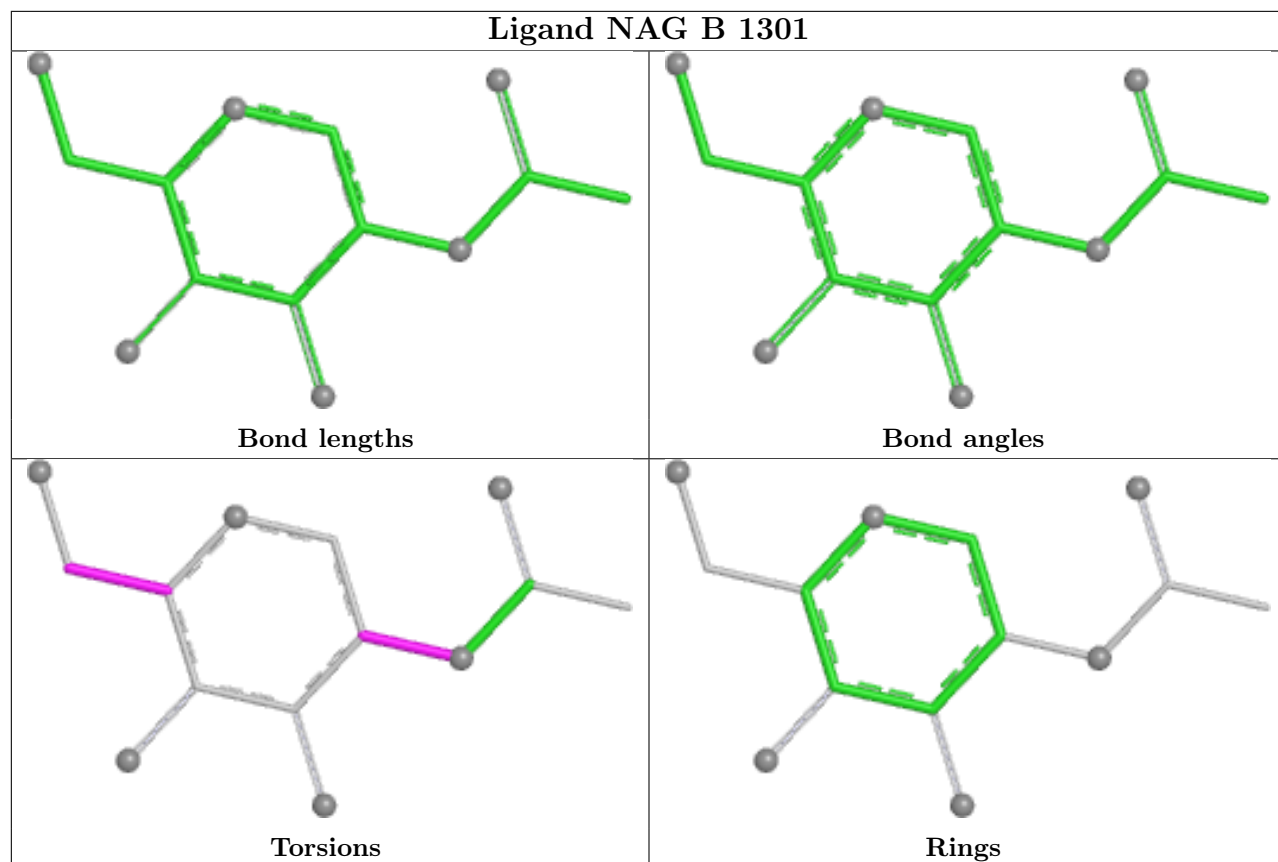


Ligand NAG A 1306



Ligand NAG B 1305





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.

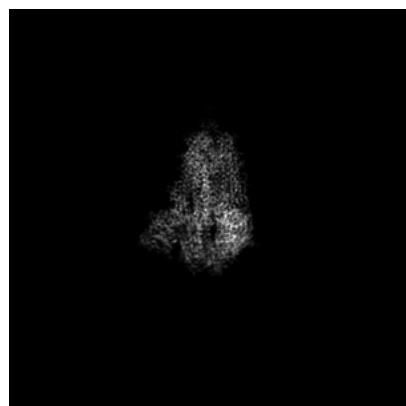
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38488. These allow visual inspection of the internal detail of the map and identification of artifacts.

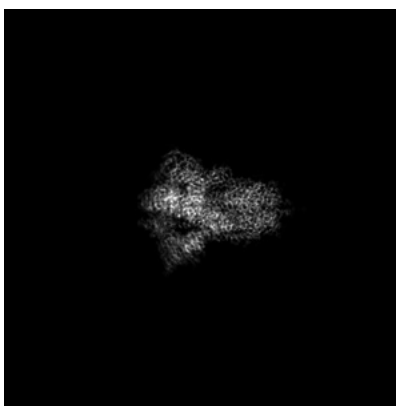
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

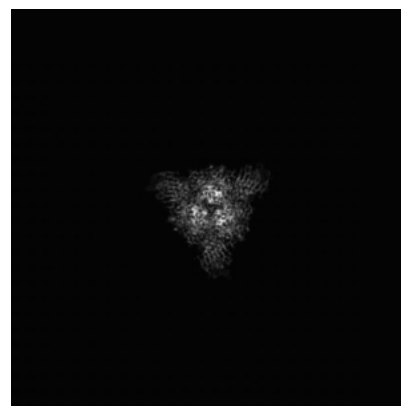
6.1.1 Primary map



X

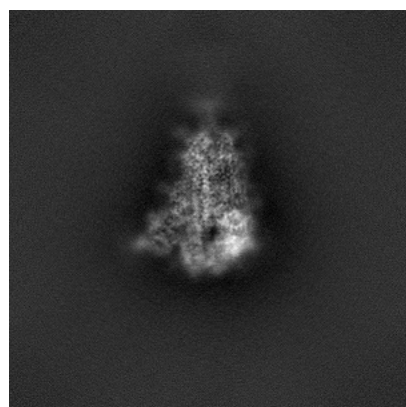


Y

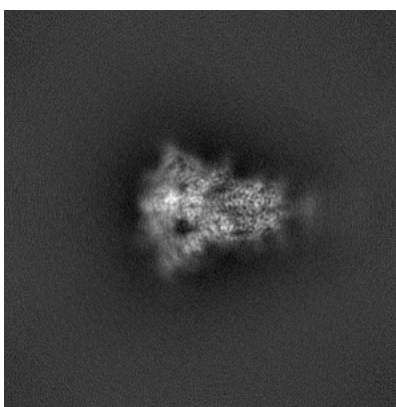


Z

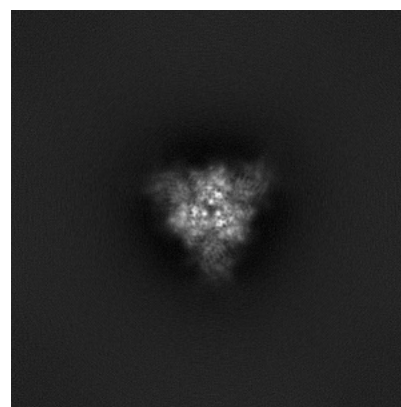
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

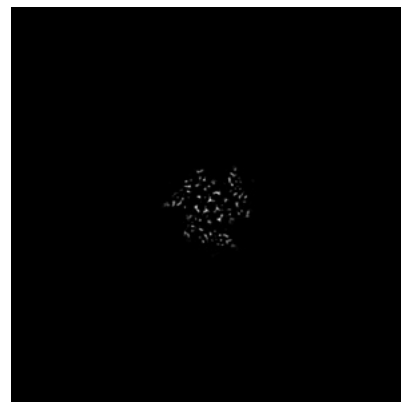
6.2.1 Primary map



X Index: 256

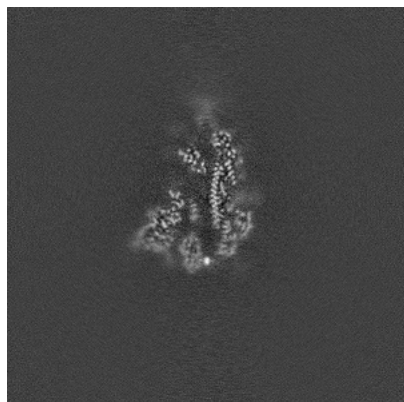


Y Index: 256

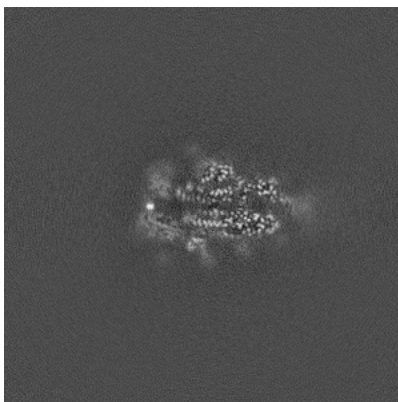


Z Index: 256

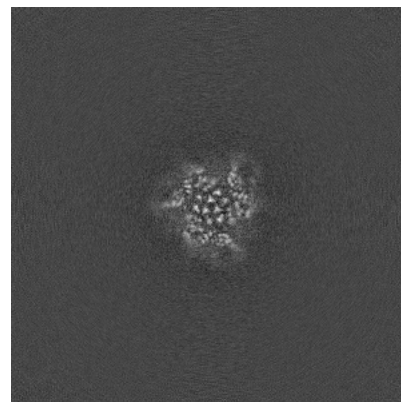
6.2.2 Raw map



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](#)

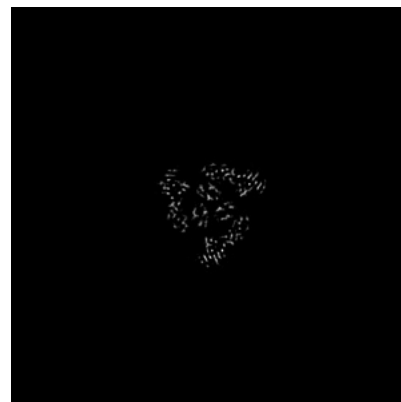
6.3.1 Primary map



X Index: 267

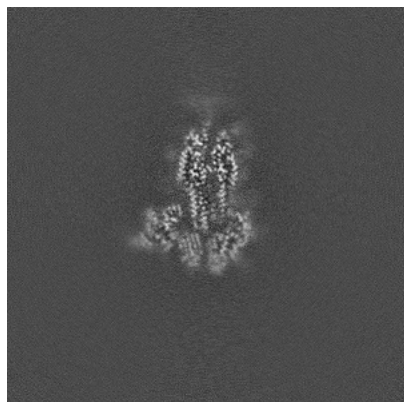


Y Index: 251

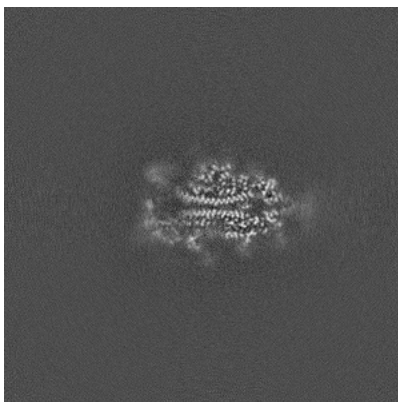


Z Index: 236

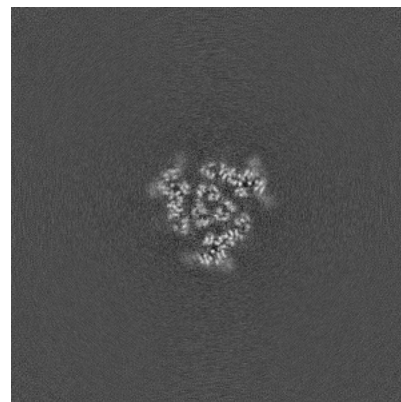
6.3.2 Raw map



X Index: 268



Y Index: 251

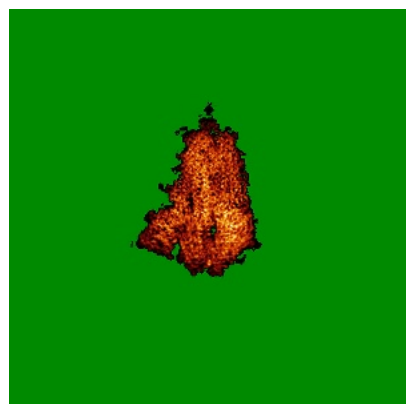


Z Index: 238

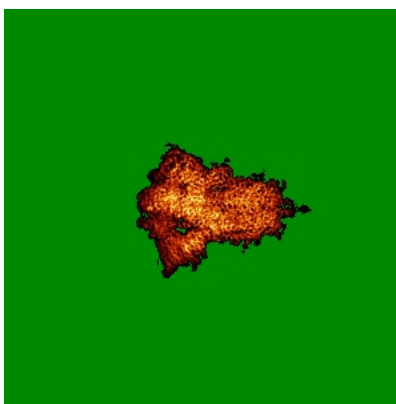
The images above show the largest variance slices of the map in three orthogonal directions.

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

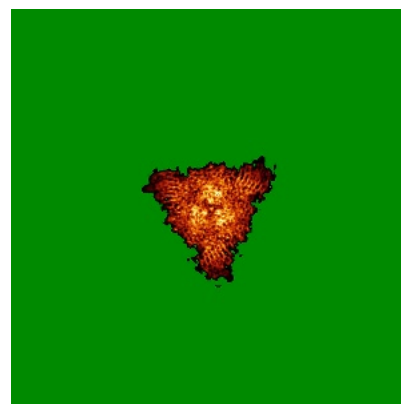
6.4.1 Primary map



X

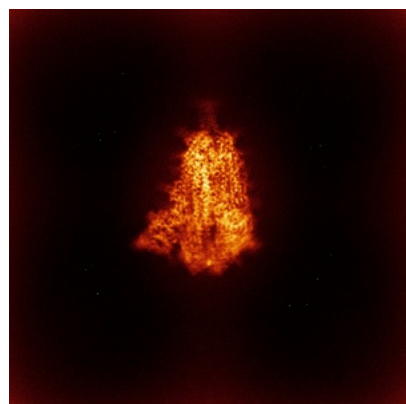


Y

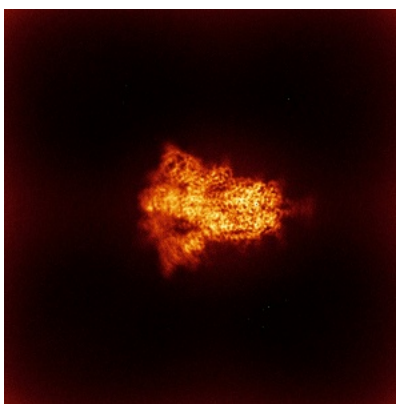


Z

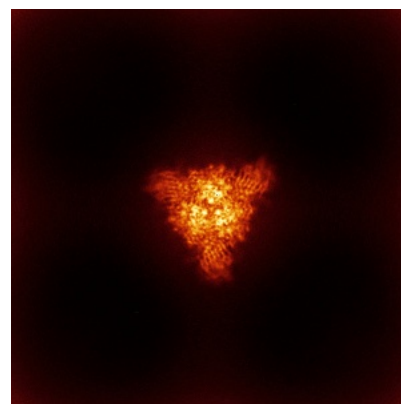
6.4.2 Raw map



X



Y

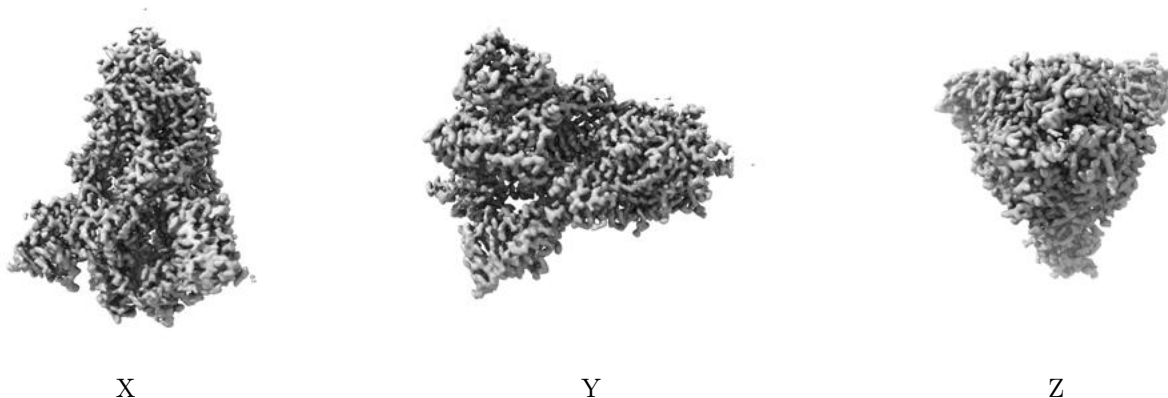


Z

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 0.1. 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.

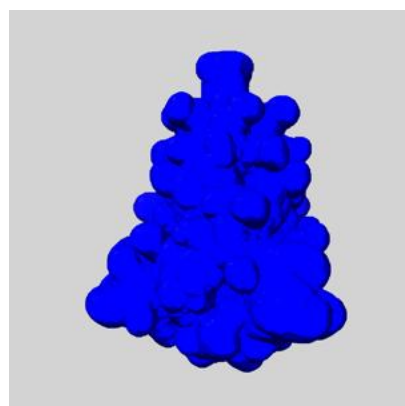
6.6 Mask visualisation [i](#)

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

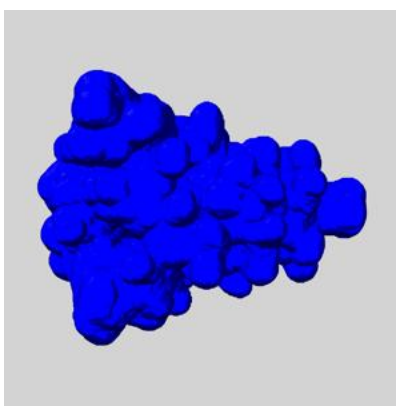
A mask typically either:

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

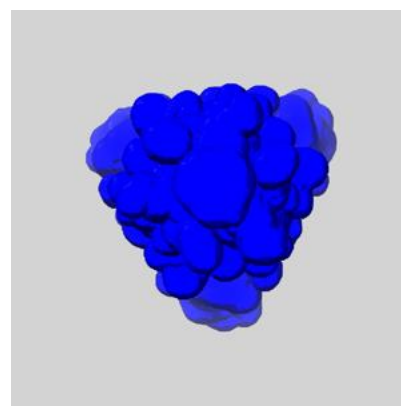
6.6.1 emd_38488_msk_1.map [i](#)



X



Y

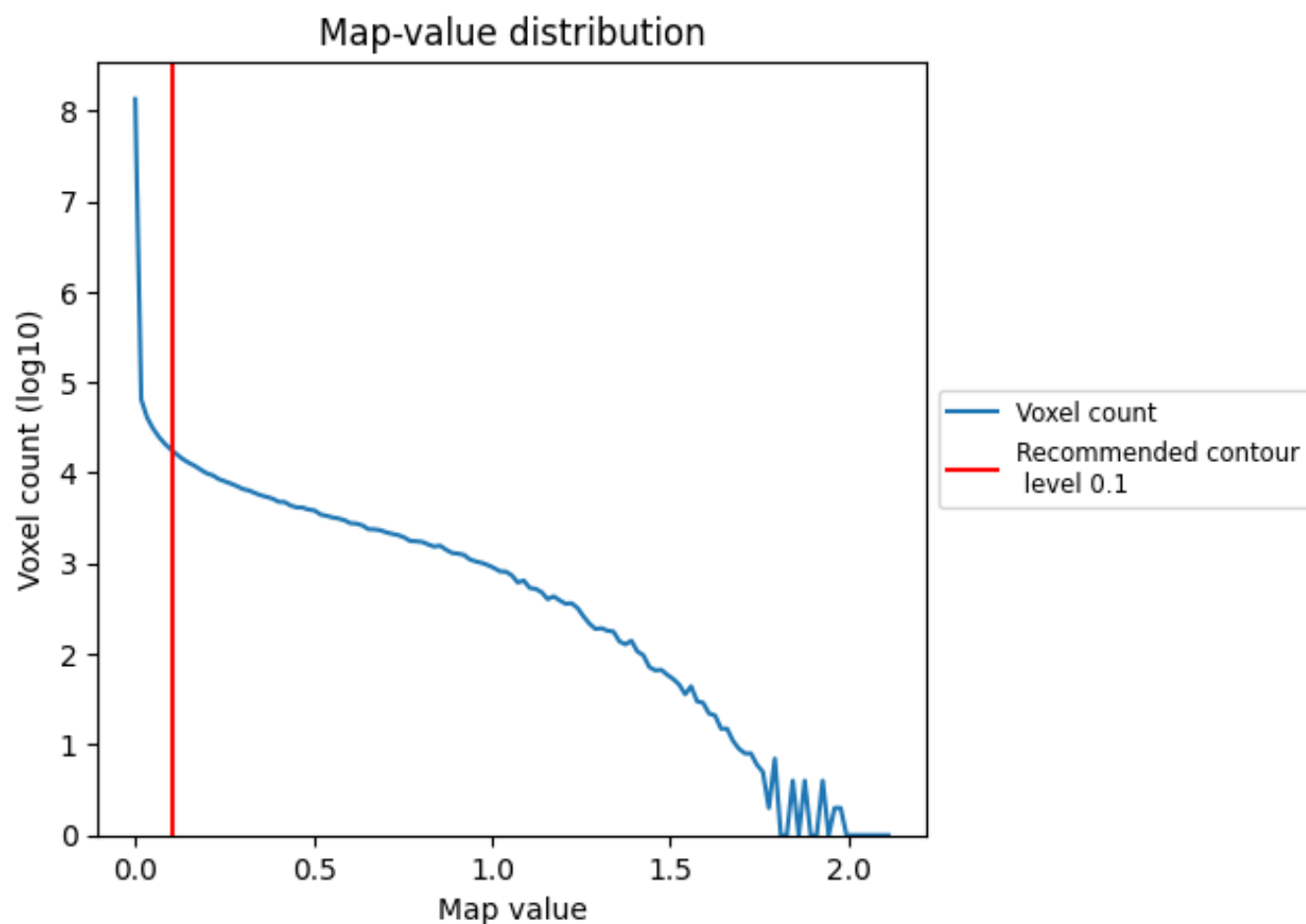


Z

7 Map analysis [i](#)

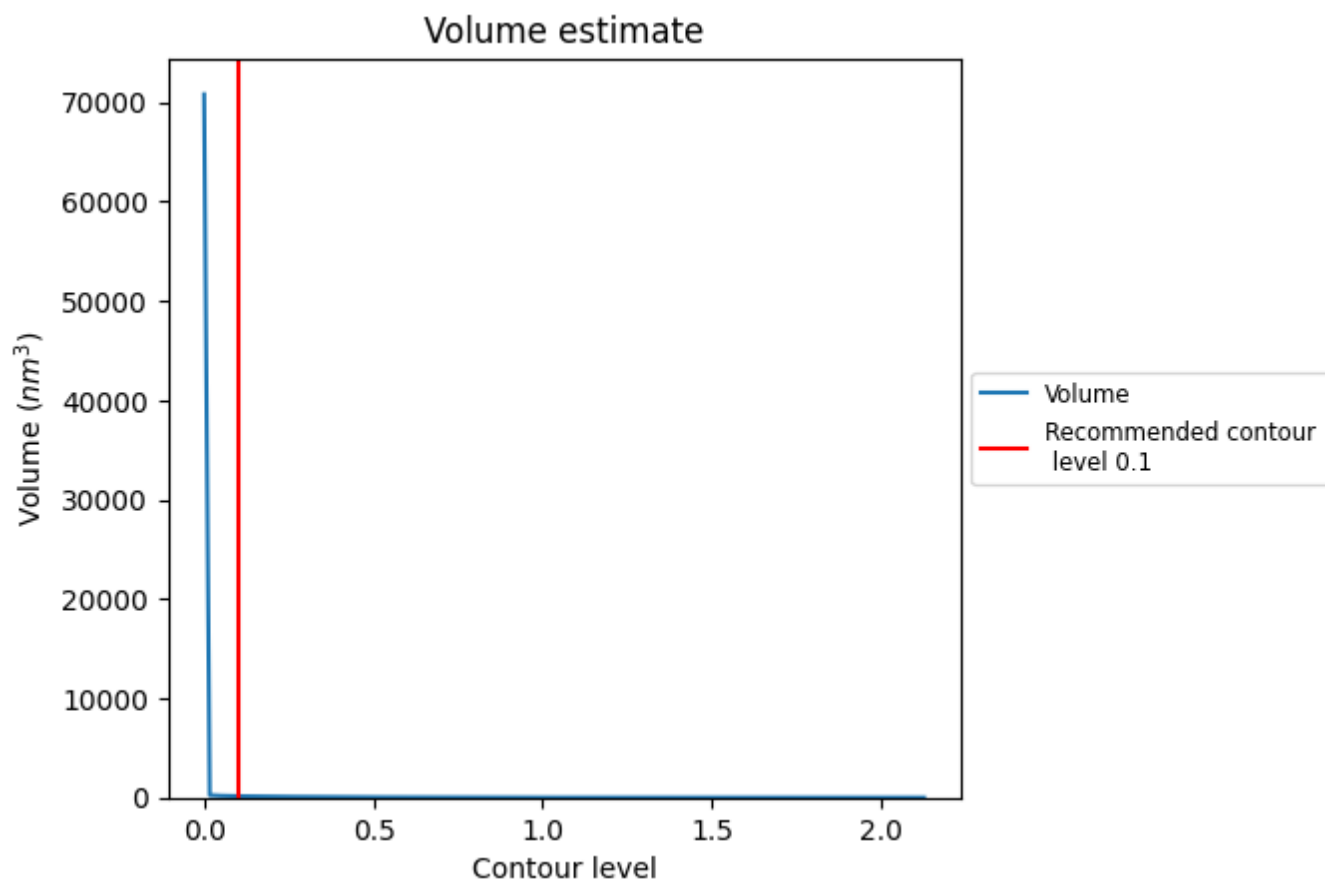
This section contains the results of statistical analysis of the map.

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.

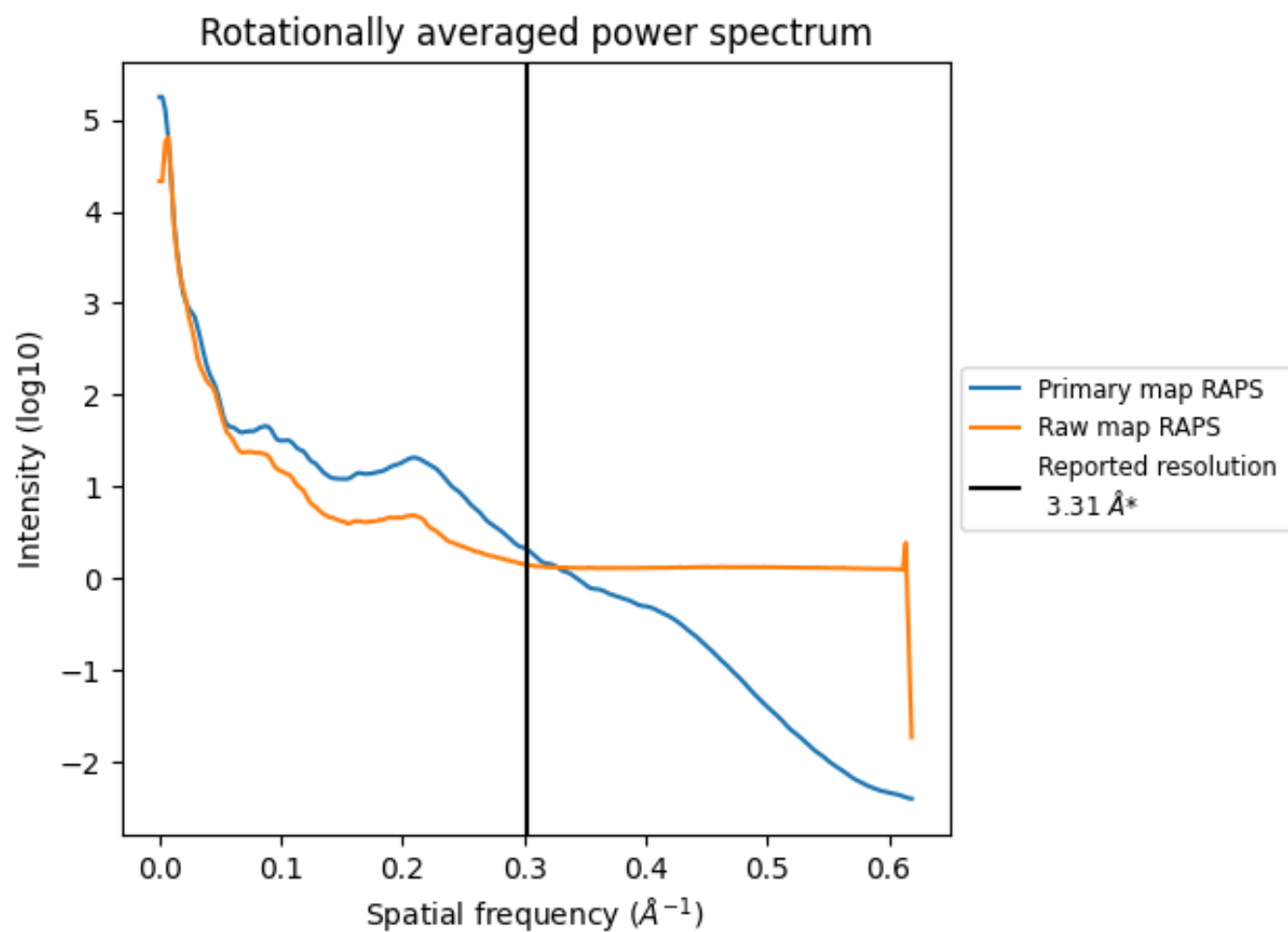
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 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 [i](#)

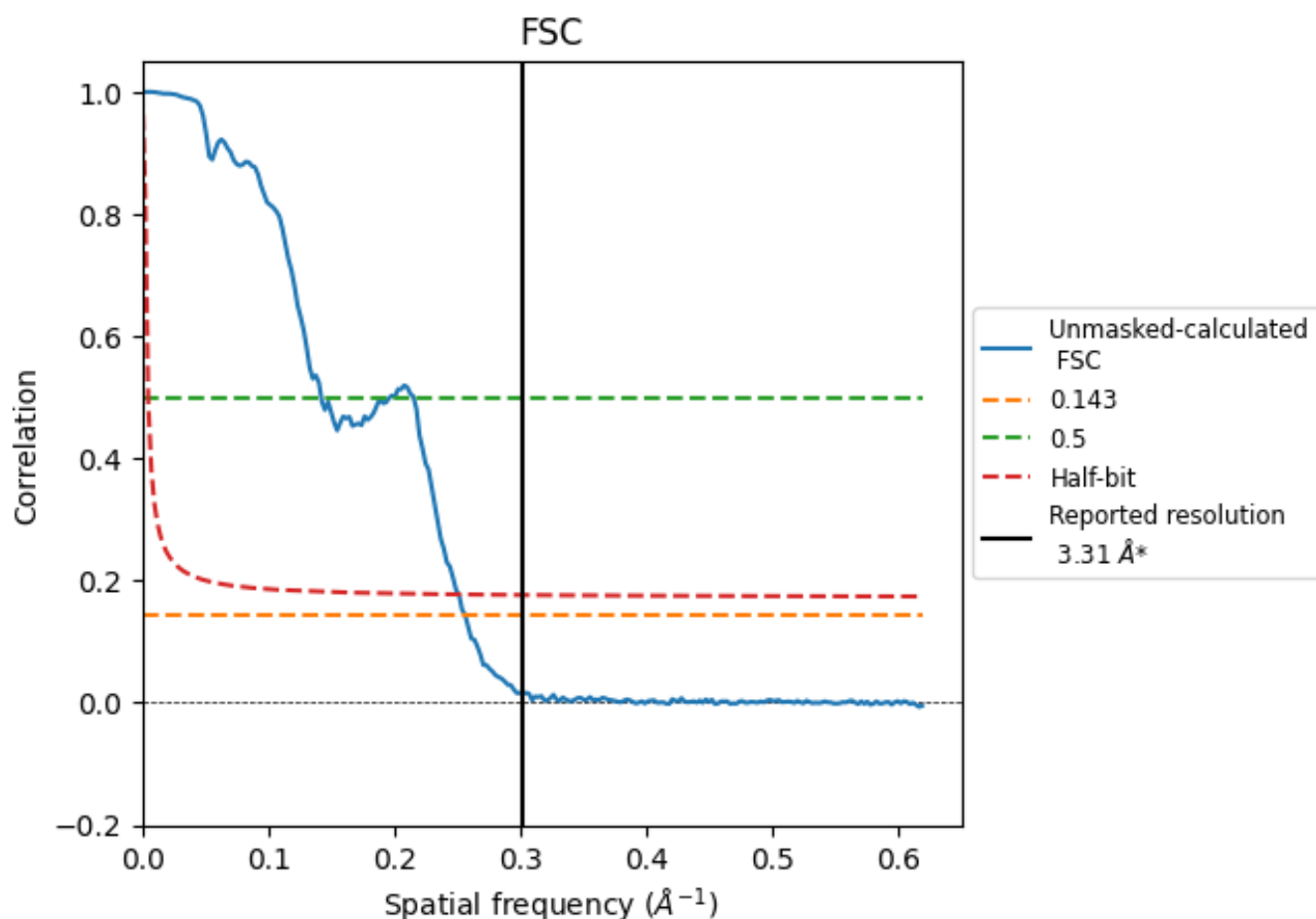


*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

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 $0.302 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.90	7.04	3.98

*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 3.90 differs from the reported value 3.31 by more than 10 %

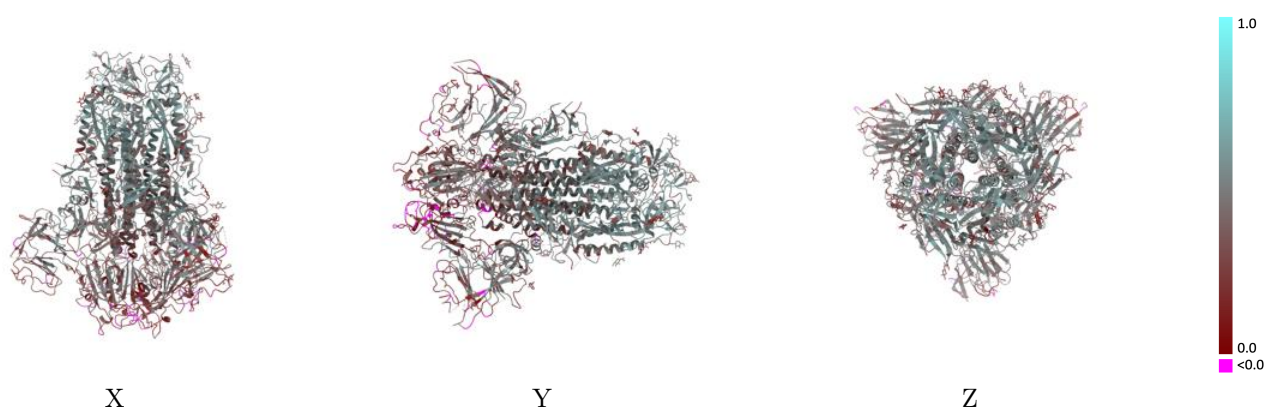
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38488 and PDB model 8XMT. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

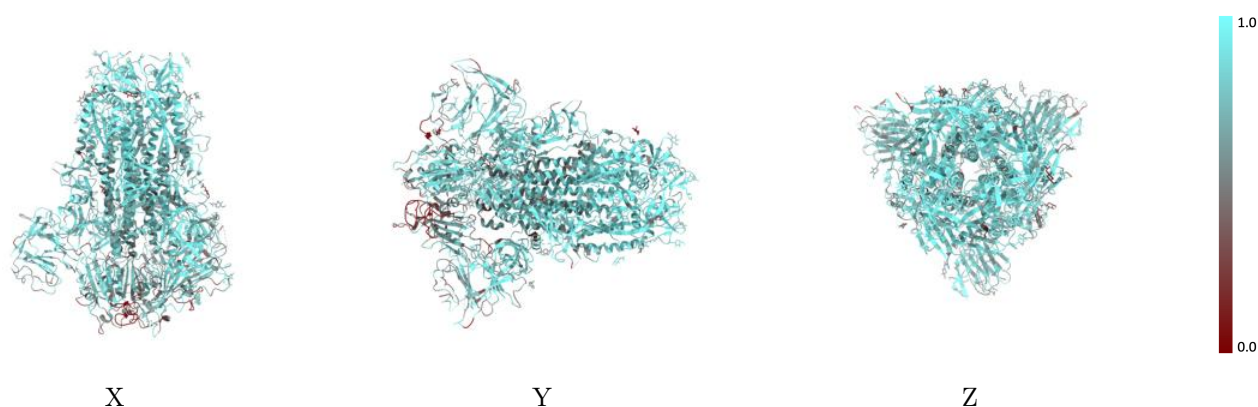
This section was not generated.

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



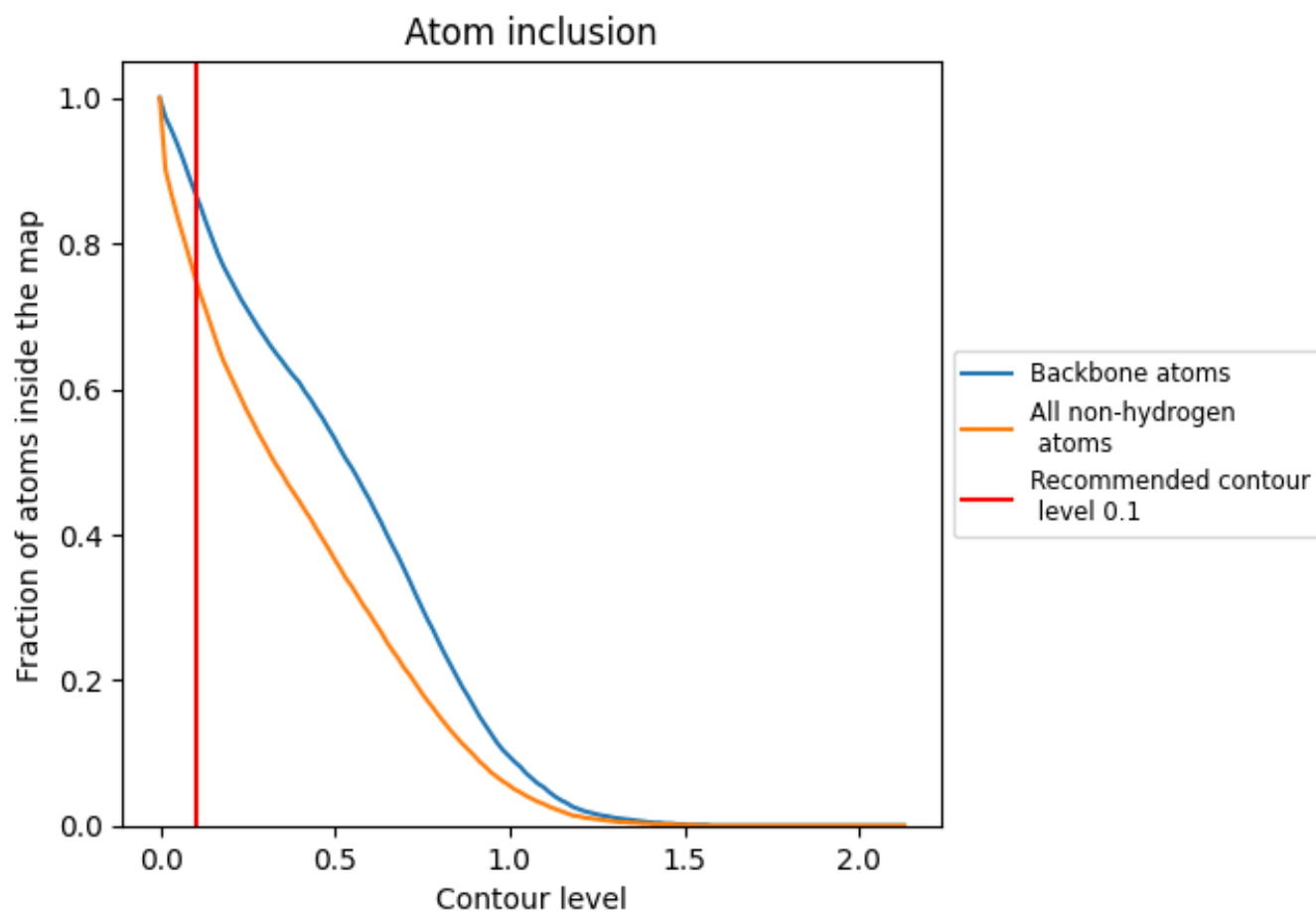
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.3990
A	0.7670	0.4090
B	0.7330	0.3910
C	0.7560	0.3980

