Full wwPDB EM Validation Report ⓘ

Jun 19, 2023 – 10:40 PM JST

PDB ID	:	7YVI
EMDB ID	:	EMD-34128
Title	:	Omicron BA.4/5 SARS-CoV-2 S in complex with TH236 Fab
Authors	:	Guo, Y.; Zhang, G.; Liang, J.; Liu, F.; Rao, Z.
Deposited on	:	2022-08-19
Resolution	:	3.70 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:

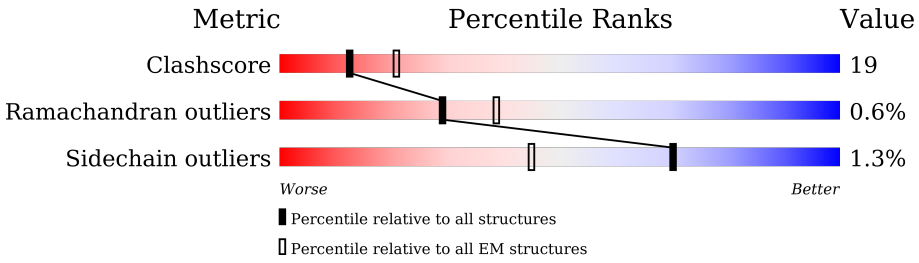
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1288	7% 55% 22% • 20%
1	B	1288	57% 21% • 20%
1	C	1288	• 55% 23% • 20%
2	H	111	33% 50% 47% ••
2	I	111	17% 43% 54% ••
2	N	111	• 46% 50% ••
3	J	125	70% 49% 51%
3	K	125	23% 45% 54% •

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Mol	Chain	Length	Quality of chain
3	O	125	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28961 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	C	1024	Total	C	N	O	S	0	0
			7705	4947	1283	1440	35		
1	B	1024	Total	C	N	O	S	0	0
			7705	4947	1283	1440	35		
1	A	1024	Total	C	N	O	S	0	0
			7705	4947	1283	1440	35		

There are 354 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called TH236 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	110	Total	C	N	O	S	0	0
			805	498	132	172	3		

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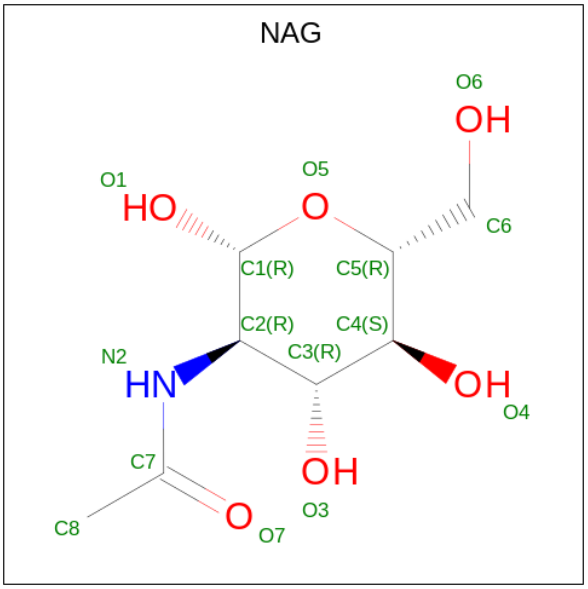
Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	110	Total	C	N	O	S	0	0
			805	498	132	172	3		
2	I	110	Total	C	N	O	S	0	0
			805	498	132	172	3		

- Molecule 3 is a protein called TH236 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	125	Total	C	N	O	S	0	0
			971	616	164	186	5		
3	O	125	Total	C	N	O	S	0	0
			971	616	164	186	5		
3	K	125	Total	C	N	O	S	0	0
			971	616	164	186	5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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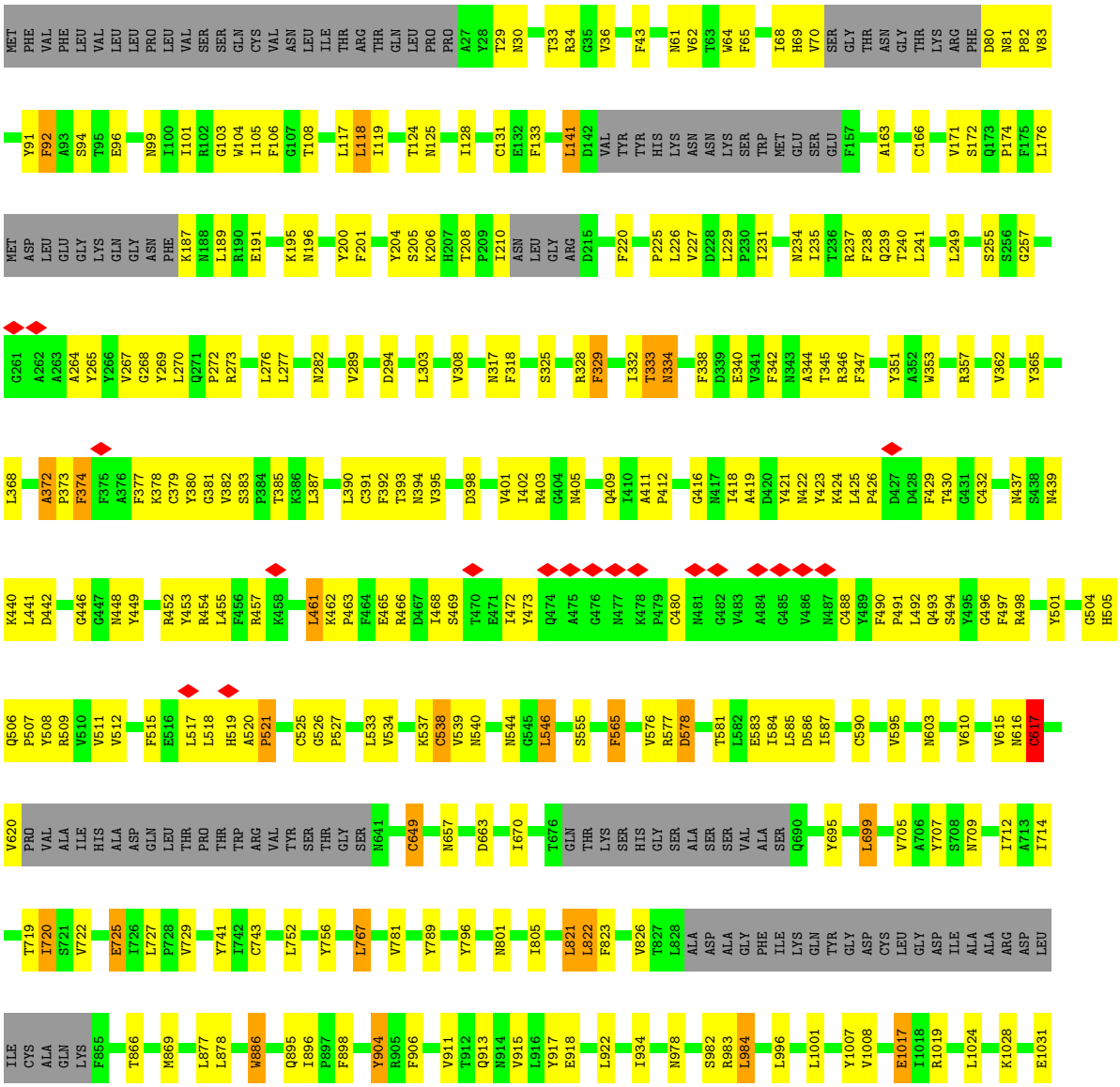
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total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

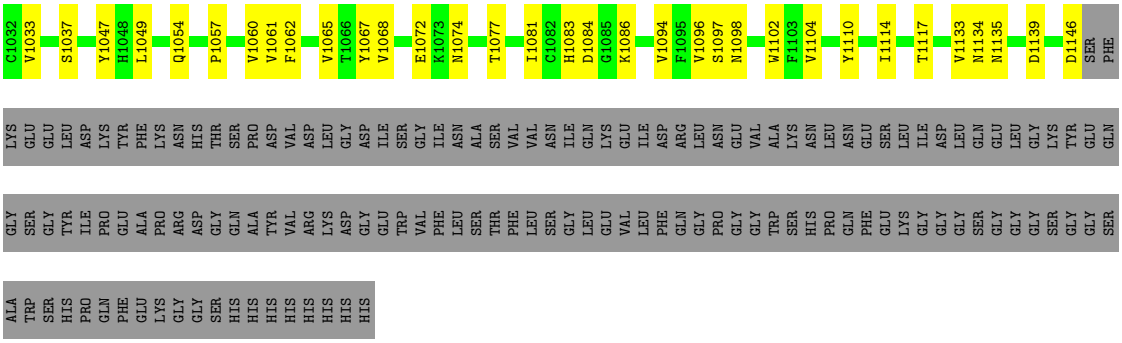
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

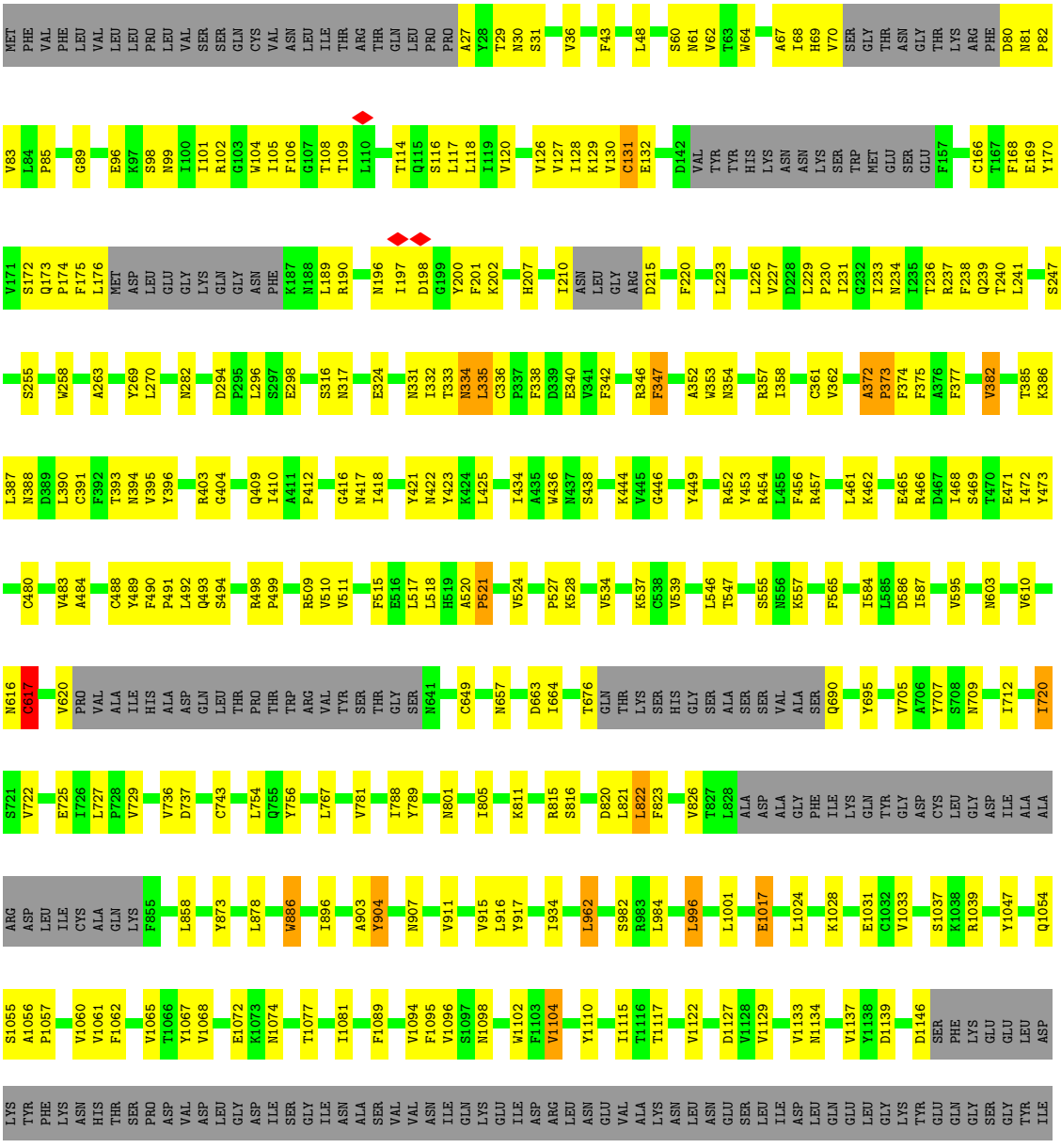
Chain C:

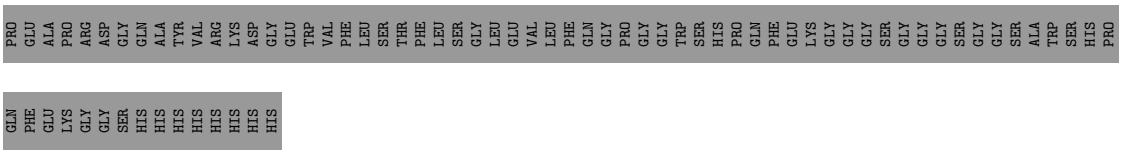




• Molecule 1: Spike glycoprotein

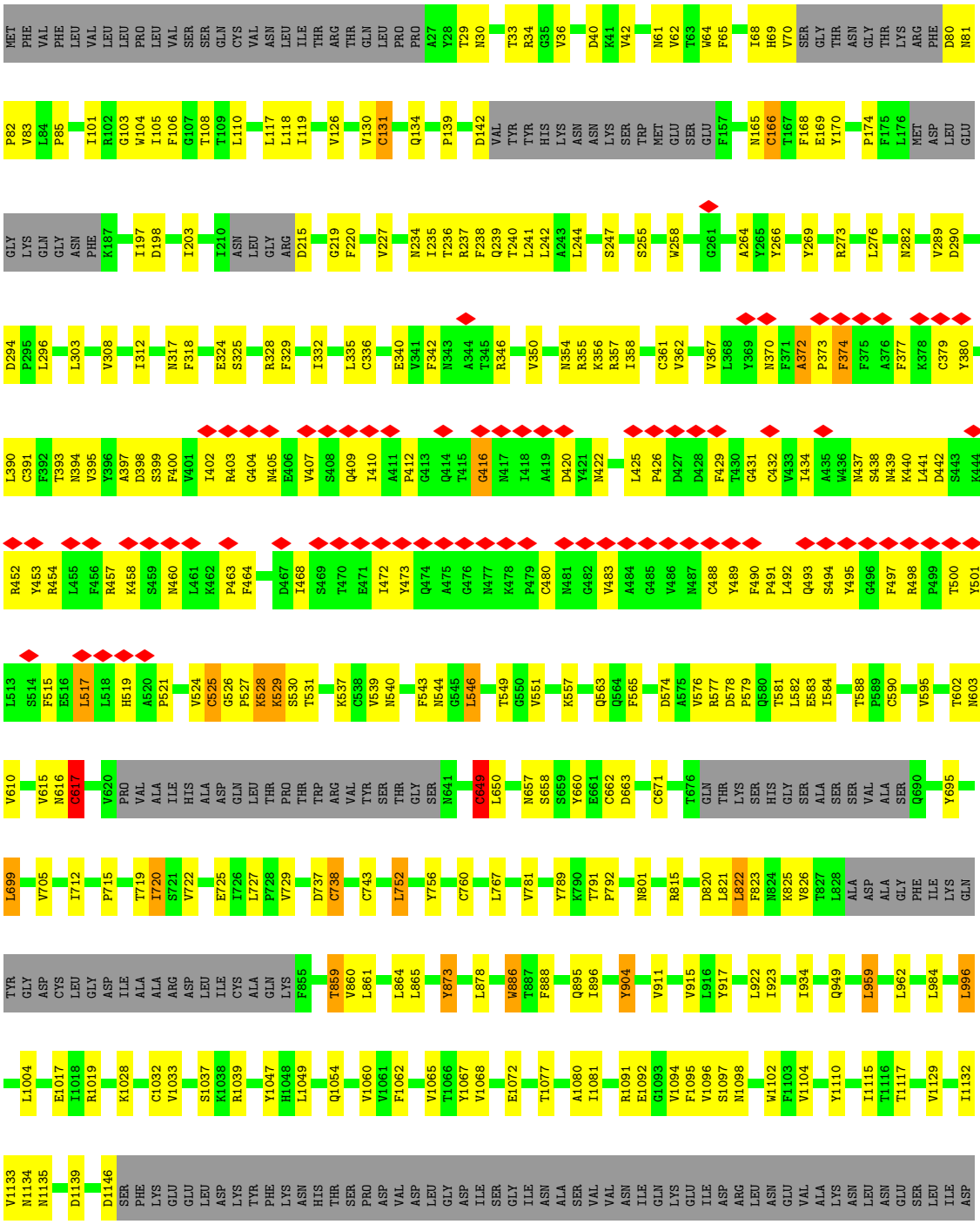
Chain B:

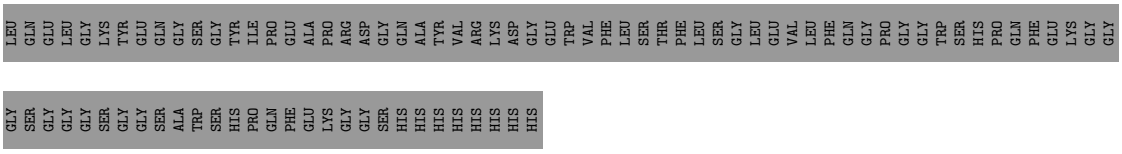




• Molecule 1: Spike glycoprotein

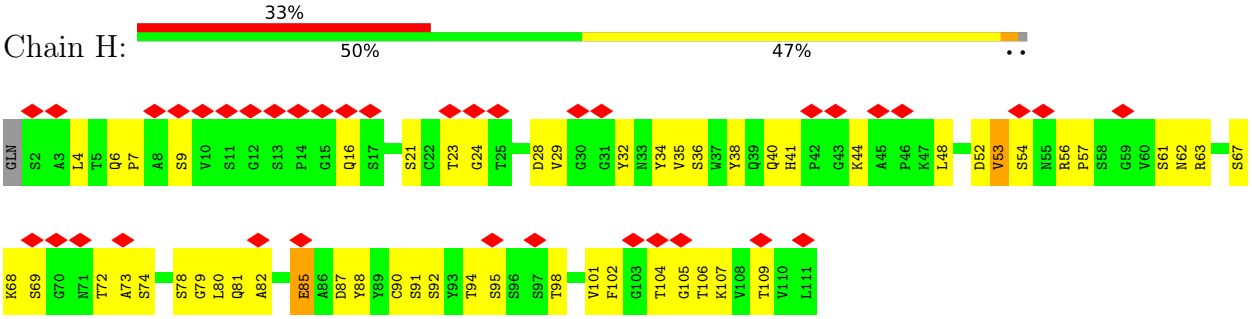
Chain A:





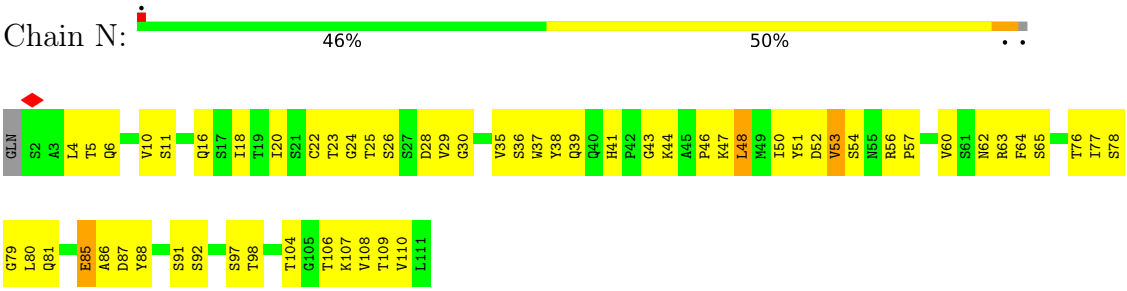
• Molecule 2: TH236 Fab light chain

Chain H:



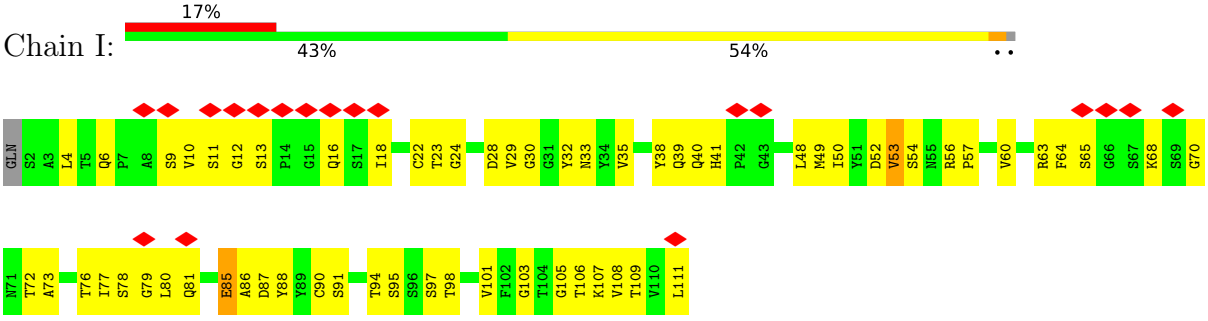
• Molecule 2: TH236 Fab light chain

Chain N:



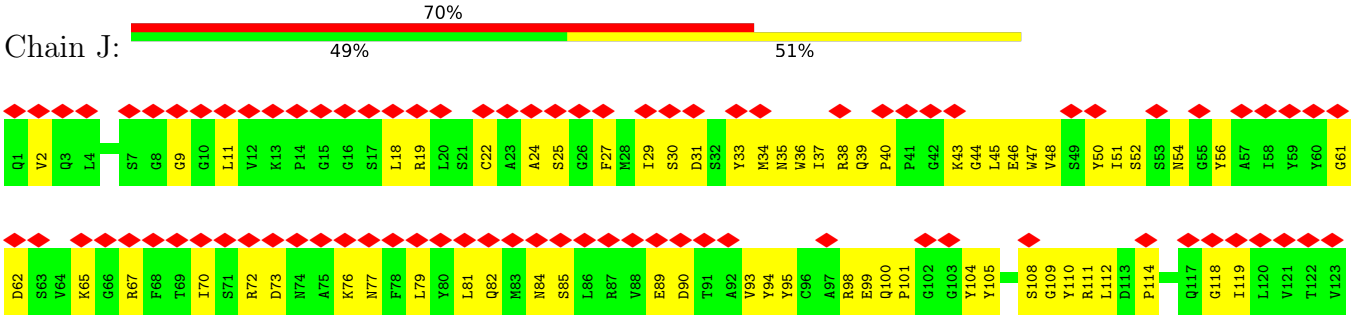
• Molecule 2: TH236 Fab light chain

Chain I:



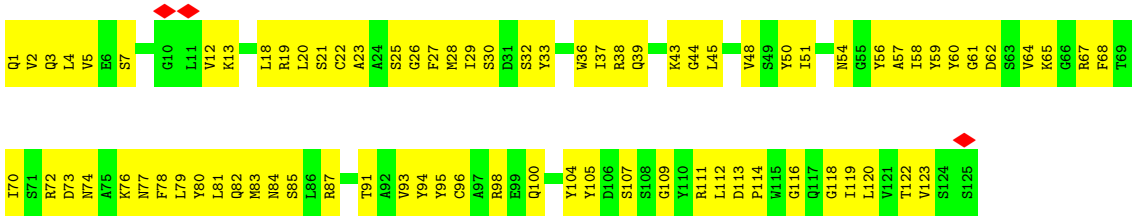
• Molecule 3: TH236 Fab heavy chain

Chain J:



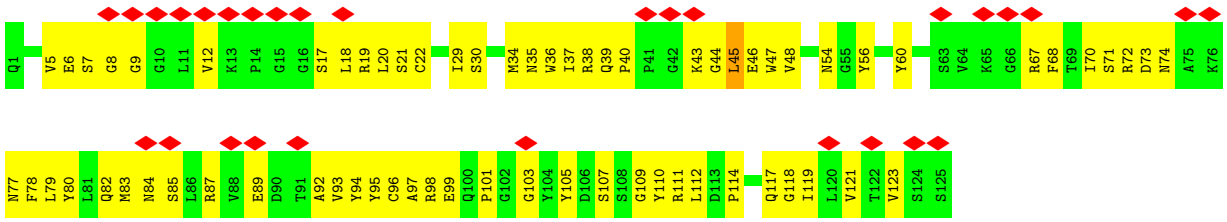
• Molecule 3: TH236 Fab heavy chain

Chain O:



• Molecule 3: TH236 Fab heavy chain

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210867	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 ($e^-/Å^2$)	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	2.280	Depositor
Minimum map value	-1.275	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.26	52/7890 (0.7%)	0.95	24/10782 (0.2%)
1	B	1.33	59/7890 (0.7%)	0.92	9/10782 (0.1%)
1	C	1.30	65/7890 (0.8%)	0.95	19/10782 (0.2%)
2	H	0.34	0/822	0.63	0/1119
2	I	0.39	0/822	0.58	0/1119
2	N	0.56	0/822	0.75	0/1119
3	J	0.37	0/995	0.68	0/1347
3	K	0.40	0/995	0.68	0/1347
3	O	0.59	0/995	0.75	0/1347
All	All	1.19	176/29121 (0.6%)	0.90	52/39744 (0.1%)

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	617	CYS	CB-SG	-9.78	1.65	1.82
1	C	617	CYS	CB-SG	-8.97	1.67	1.82
1	C	649	CYS	CB-SG	-8.54	1.67	1.82
1	B	391	CYS	CB-SG	-7.70	1.69	1.82
1	C	917	TYR	CD1-CE1	-7.51	1.28	1.39
1	C	1094	VAL	CB-CG2	-7.37	1.37	1.52
1	A	1032	CYS	CB-SG	-7.26	1.70	1.82
1	B	1033	VAL	CB-CG2	-7.18	1.37	1.52
1	A	1094	VAL	CB-CG2	-7.15	1.37	1.52
1	C	1094	VAL	CB-CG1	-7.10	1.38	1.52
1	B	1094	VAL	CB-CG1	-7.08	1.38	1.52
1	A	917	TYR	CD1-CE1	-6.99	1.28	1.39
1	A	911	VAL	CB-CG2	-6.99	1.38	1.52
1	B	1094	VAL	CB-CG2	-6.98	1.38	1.52
1	B	917	TYR	CD1-CE1	-6.84	1.29	1.39
1	C	911	VAL	CB-CG2	-6.78	1.38	1.52
1	C	565	PHE	CB-CG	-6.60	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	781	VAL	CB-CG2	-6.60	1.39	1.52
1	B	1096	VAL	CB-CG1	-6.54	1.39	1.52
1	B	743	CYS	CB-SG	-6.51	1.71	1.82
1	A	1094	VAL	CB-CG1	-6.46	1.39	1.52
1	A	695	TYR	CE1-CZ	-6.46	1.30	1.38
1	B	707	TYR	CE2-CZ	-6.40	1.30	1.38
1	B	1104	VAL	CB-CG2	-6.40	1.39	1.52
1	C	1065	VAL	CB-CG2	-6.39	1.39	1.52
1	A	1067	TYR	CE1-CZ	-6.39	1.30	1.38
1	A	590	CYS	CB-SG	-6.38	1.71	1.82
1	A	1033	VAL	CB-CG2	-6.35	1.39	1.52
1	C	1104	VAL	CB-CG2	-6.34	1.39	1.52
1	C	1060	VAL	CB-CG1	-6.32	1.39	1.52
1	B	915	VAL	CB-CG1	-6.29	1.39	1.52
1	A	1104	VAL	CB-CG2	-6.29	1.39	1.52
1	C	917	TYR	CE2-CZ	-6.28	1.30	1.38
1	C	1067	TYR	CE1-CZ	-6.24	1.30	1.38
1	B	1060	VAL	CB-CG1	-6.23	1.39	1.52
1	A	781	VAL	CB-CG2	-6.22	1.39	1.52
1	C	743	CYS	CB-SG	-6.21	1.71	1.82
1	A	1060	VAL	CB-CG1	-6.20	1.39	1.52
1	B	1129	VAL	CB-CG1	-6.18	1.39	1.52
1	A	904	TYR	CD2-CE2	-6.16	1.30	1.39
1	B	789	TYR	CD2-CE2	-6.14	1.30	1.39
1	B	1104	VAL	CB-CG1	-6.13	1.40	1.52
1	C	917	TYR	CE1-CZ	-6.13	1.30	1.38
1	C	707	TYR	CE2-CZ	-6.12	1.30	1.38
1	C	707	TYR	CE1-CZ	-6.10	1.30	1.38
1	C	917	TYR	CD2-CE2	-6.03	1.30	1.39
1	B	917	TYR	CD2-CE2	-6.03	1.30	1.39
1	B	722	VAL	CB-CG1	-6.02	1.40	1.52
1	C	610	VAL	CB-CG1	-6.01	1.40	1.52
1	A	760	CYS	CB-SG	-6.00	1.72	1.82
1	C	595	VAL	CB-CG2	-5.96	1.40	1.52
1	B	1062	PHE	CD1-CE1	-5.95	1.27	1.39
1	B	917	TYR	CE2-CZ	-5.93	1.30	1.38
1	A	1096	VAL	CB-CG1	-5.92	1.40	1.52
1	A	917	TYR	CE1-CZ	-5.92	1.30	1.38
1	A	1017	GLU	CG-CD	-5.92	1.43	1.51
1	C	1060	VAL	CB-CG2	-5.92	1.40	1.52
1	A	743	CYS	CB-SG	-5.89	1.72	1.81
1	C	915	VAL	CB-CG1	-5.88	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1047	TYR	CD2-CE2	-5.86	1.30	1.39
1	B	729	VAL	CB-CG1	-5.85	1.40	1.52
1	C	906	PHE	CE1-CZ	-5.85	1.26	1.37
1	A	1104	VAL	CB-CG1	-5.83	1.40	1.52
1	B	617	CYS	CB-SG	-5.83	1.72	1.81
1	B	1065	VAL	CB-CG2	-5.82	1.40	1.52
1	A	595	VAL	CB-CG2	-5.82	1.40	1.52
1	A	610	VAL	CB-CG1	-5.81	1.40	1.52
1	A	915	VAL	CB-CG1	-5.80	1.40	1.52
1	B	1102	TRP	CB-CG	-5.79	1.39	1.50
1	C	823	PHE	CB-CG	-5.78	1.41	1.51
1	B	1047	TYR	CE2-CZ	-5.77	1.31	1.38
1	C	1104	VAL	CB-CG1	-5.77	1.40	1.52
1	B	707	TYR	CD2-CE2	-5.76	1.30	1.39
1	B	1047	TYR	CD1-CE1	-5.74	1.30	1.39
1	A	695	TYR	CG-CD2	-5.71	1.31	1.39
1	B	1047	TYR	CE1-CZ	-5.71	1.31	1.38
1	B	1067	TYR	CE1-CZ	-5.70	1.31	1.38
1	B	1033	VAL	CB-CG1	-5.68	1.41	1.52
1	C	1062	PHE	CD1-CE1	-5.68	1.27	1.39
1	C	1068	VAL	CB-CG1	-5.67	1.41	1.52
1	C	898	PHE	CE1-CZ	-5.65	1.26	1.37
1	A	722	VAL	CB-CG1	-5.65	1.41	1.52
1	C	1110	TYR	CE1-CZ	-5.64	1.31	1.38
1	C	911	VAL	CB-CG1	-5.64	1.41	1.52
1	B	781	VAL	CB-CG2	-5.63	1.41	1.52
1	C	1072	GLU	CG-CD	-5.60	1.43	1.51
1	C	1096	VAL	CB-CG1	-5.60	1.41	1.52
1	C	904	TYR	CD2-CE2	-5.58	1.30	1.39
1	C	1133	VAL	CB-CG2	-5.58	1.41	1.52
1	A	1033	VAL	CB-CG1	-5.56	1.41	1.52
1	C	789	TYR	CD2-CE2	-5.55	1.31	1.39
1	B	789	TYR	CD1-CE1	-5.53	1.31	1.39
1	C	1072	GLU	CB-CG	-5.52	1.41	1.52
1	B	1133	VAL	CB-CG2	-5.51	1.41	1.52
1	C	1033	VAL	CB-CG2	-5.51	1.41	1.52
1	B	907	ASN	CB-CG	-5.49	1.38	1.51
1	A	1047	TYR	CD2-CE2	-5.48	1.31	1.39
1	C	1007	TYR	CE2-CZ	-5.45	1.31	1.38
1	A	911	VAL	CB-CG1	-5.45	1.41	1.52
1	A	705	VAL	CB-CG2	-5.43	1.41	1.52
1	B	1062	PHE	CD2-CE2	-5.43	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	695	TYR	CE1-CZ	-5.42	1.31	1.38
1	C	918	GLU	CB-CG	-5.42	1.41	1.52
1	A	904	TYR	CE2-CZ	-5.42	1.31	1.38
1	B	911	VAL	CB-CG2	-5.41	1.41	1.52
1	B	1110	TYR	CE1-CZ	-5.41	1.31	1.38
1	C	714	ILE	CB-CG2	-5.39	1.36	1.52
1	B	298	GLU	CB-CG	-5.39	1.42	1.52
1	C	1065	VAL	CB-CG1	-5.39	1.41	1.52
1	B	789	TYR	CE2-CZ	-5.38	1.31	1.38
1	C	1047	TYR	CD1-CE1	-5.37	1.31	1.39
1	A	917	TYR	CD2-CE2	-5.36	1.31	1.39
1	A	1047	TYR	CE2-CZ	-5.36	1.31	1.38
1	A	1065	VAL	CB-CG2	-5.36	1.41	1.52
1	A	729	VAL	CB-CG2	-5.36	1.41	1.52
1	B	610	VAL	CB-CG1	-5.34	1.41	1.52
1	A	1017	GLU	CB-CG	-5.33	1.42	1.52
1	B	1068	VAL	CB-CG1	-5.33	1.41	1.52
1	B	695	TYR	CE2-CZ	-5.28	1.31	1.38
1	B	823	PHE	CB-CG	-5.28	1.42	1.51
1	A	1068	VAL	CB-CG1	-5.28	1.41	1.52
1	C	906	PHE	CE2-CZ	-5.27	1.27	1.37
1	B	707	TYR	CE1-CZ	-5.27	1.31	1.38
1	A	738	CYS	CB-SG	-5.27	1.73	1.81
1	C	92	PHE	CB-CG	-5.26	1.42	1.51
1	A	873	TYR	CD2-CE2	-5.25	1.31	1.39
1	A	1129	VAL	CB-CG1	-5.25	1.41	1.52
1	C	1062	PHE	CD2-CE2	-5.25	1.28	1.39
1	C	1017	GLU	CG-CD	-5.25	1.44	1.51
1	C	1133	VAL	CB-CG1	-5.24	1.41	1.52
1	A	823	PHE	CB-CG	-5.24	1.42	1.51
1	B	1061	VAL	CB-CG1	-5.23	1.41	1.52
1	A	888	PHE	CD1-CE1	-5.23	1.28	1.39
1	C	1061	VAL	CB-CG2	-5.22	1.41	1.52
1	B	873	TYR	CD2-CE2	-5.22	1.31	1.39
1	A	1060	VAL	CB-CG2	-5.22	1.41	1.52
1	C	695	TYR	CE2-CZ	-5.21	1.31	1.38
1	B	1122	VAL	CB-CG1	-5.21	1.41	1.52
1	C	707	TYR	CD2-CE2	-5.21	1.31	1.39
1	A	1110	TYR	CE1-CZ	-5.21	1.31	1.38
1	A	1095	PHE	CB-CG	-5.20	1.42	1.51
1	A	1133	VAL	CB-CG1	-5.20	1.42	1.52
1	B	1017	GLU	CG-CD	-5.20	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	705	VAL	CB-CG2	-5.19	1.42	1.52
1	B	382	VAL	CB-CG2	-5.19	1.42	1.52
1	C	741	TYR	CE1-CZ	-5.17	1.31	1.38
1	A	917	TYR	CG-CD1	-5.15	1.32	1.39
1	C	906	PHE	CG-CD1	-5.15	1.31	1.38
1	C	906	PHE	CG-CD2	-5.14	1.31	1.38
1	A	917	TYR	CE2-CZ	-5.13	1.31	1.38
1	A	789	TYR	CD2-CE2	-5.13	1.31	1.39
1	B	1072	GLU	CB-CG	-5.12	1.42	1.52
1	B	1060	VAL	CB-CG2	-5.11	1.42	1.52
1	A	873	TYR	CE2-CZ	-5.11	1.31	1.38
1	B	695	TYR	CD1-CE1	-5.11	1.31	1.39
1	C	904	TYR	CE2-CZ	-5.10	1.31	1.38
1	B	595	VAL	CB-CG2	-5.10	1.42	1.52
1	B	904	TYR	CD2-CE2	-5.09	1.31	1.39
1	B	1089	PHE	CG-CD1	-5.09	1.31	1.38
1	C	1068	VAL	CB-CG2	-5.09	1.42	1.52
1	C	789	TYR	CD1-CE1	-5.08	1.31	1.39
1	B	705	VAL	CB-CG2	-5.08	1.42	1.52
1	B	917	TYR	CE1-CZ	-5.07	1.31	1.38
1	C	1047	TYR	CE2-CZ	-5.07	1.31	1.38
1	B	1065	VAL	CB-CG1	-5.07	1.42	1.52
1	A	1133	VAL	CB-CG2	-5.07	1.42	1.52
1	C	918	GLU	CG-CD	-5.06	1.44	1.51
1	C	1008	VAL	CB-CG2	-5.05	1.42	1.52
1	C	725	GLU	CB-CG	-5.04	1.42	1.52
1	C	729	VAL	CB-CG1	-5.04	1.42	1.52
1	A	729	VAL	CB-CG1	-5.03	1.42	1.52
1	C	1047	TYR	CD2-CE2	-5.01	1.31	1.39
1	C	781	VAL	CB-CG1	-5.01	1.42	1.52
1	B	649	CYS	CB-SG	-5.01	1.73	1.81
1	A	1062	PHE	CD1-CE1	-5.01	1.29	1.39
1	C	722	VAL	CB-CG1	-5.00	1.42	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	878	LEU	CB-CG-CD2	-11.33	91.74	111.00
1	C	878	LEU	CB-CG-CD2	-9.75	94.42	111.00
1	A	878	LEU	CB-CG-CD2	-8.67	96.26	111.00
1	A	649	CYS	CA-CB-SG	8.43	129.17	114.00
1	C	118	LEU	CB-CG-CD2	-8.38	96.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	546	LEU	CA-CB-CG	8.20	134.17	115.30
1	C	538	CYS	CA-CB-SG	8.02	128.43	114.00
1	C	767	LEU	CA-CB-CG	-7.80	97.36	115.30
1	A	720	ILE	CG1-CB-CG2	-7.57	94.74	111.40
1	C	720	ILE	CG1-CB-CG2	-7.55	94.78	111.40
1	A	590	CYS	CA-CB-SG	7.40	127.31	114.00
1	B	720	ILE	CG1-CB-CG2	-7.12	95.73	111.40
1	A	416	GLY	N-CA-C	-6.79	96.12	113.10
1	A	617	CYS	CA-CB-SG	-6.70	101.95	114.00
1	C	590	CYS	CA-CB-SG	6.64	125.95	114.00
1	C	565	PHE	CB-CA-C	-6.63	97.14	110.40
1	A	760	CYS	CA-CB-SG	-6.50	102.31	114.00
1	C	649	CYS	CA-CB-SG	6.47	125.65	114.00
1	A	727	LEU	CB-CG-CD1	-6.35	100.20	111.00
1	C	546	LEU	CB-CG-CD1	-6.29	100.31	111.00
1	C	877	LEU	CB-CG-CD2	-6.19	100.47	111.00
1	A	650	LEU	CA-CB-CG	6.17	129.49	115.30
1	C	277	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	B	727	LEU	CB-CG-CD1	-6.14	100.56	111.00
1	A	1115	ILE	CG1-CB-CG2	-5.97	98.26	111.40
1	A	699	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	A	996	LEU	CA-CB-CG	-5.92	101.69	115.30
1	C	878	LEU	CA-CB-CG	-5.88	101.79	115.30
1	A	756	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	B	996	LEU	CA-CB-CG	-5.82	101.92	115.30
1	A	767	LEU	CA-CB-CG	-5.79	101.98	115.30
1	C	461	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	508	TYR	CA-CB-CG	5.60	124.05	113.40
1	C	727	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	B	962	LEU	CB-CG-CD1	-5.57	101.52	111.00
1	C	699	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	A	1049	LEU	CB-CG-CD2	-5.49	101.68	111.00
1	A	962	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	B	767	LEU	CA-CB-CG	-5.32	103.07	115.30
1	B	822	LEU	CA-CB-CG	-5.29	103.14	115.30
1	C	984	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	878	LEU	CA-CB-CG	-5.26	103.20	115.30
1	B	48	LEU	CA-CB-CG	-5.25	103.23	115.30
1	A	756	TYR	CB-CG-CD2	5.24	124.15	121.00
1	A	752	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	B	878	LEU	CA-CB-CG	-5.14	103.47	115.30
1	A	959	LEU	CB-CG-CD2	-5.13	102.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	923	ILE	CG1-CB-CG2	-5.12	100.13	111.40
1	A	822	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	C	805	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	C	822	LEU	CA-CB-CG	-5.01	103.78	115.30
1	C	821	LEU	CB-CG-CD1	-5.00	102.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7705	0	7283	248	0
1	B	7705	0	7283	227	0
1	C	7705	0	7283	257	0
2	H	805	0	763	46	0
2	I	805	0	763	58	0
2	N	805	0	763	57	0
3	J	971	0	933	56	0
3	K	971	0	933	67	0
3	O	971	0	933	83	0
4	A	168	0	156	21	0
4	B	182	0	169	18	0
4	C	168	0	156	22	0
All	All	28961	0	27418	1064	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 19.

All (1064) 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)
3:O:82:GLN:HE22	3:O:84:ASN:HB3	1.24	1.00
1:A:362:VAL:HG23	1:A:526:GLY:HA3	1.50	0.93
1:B:737:ASP:OD2	1:A:317:ASN:ND2	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ARG:HG2	1:B:494:SER:HA	1.54	0.90
3:O:43:LYS:HD3	3:O:44:GLY:H	1.37	0.90
1:A:1134:ASN:ND2	4:A:1308:NAG:O7	2.05	0.90
2:N:63:ARG:NH2	2:N:79:GLY:O	2.05	0.89
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.06	0.89
1:A:422:ASN:O	1:A:454:ARG:NH1	2.06	0.88
3:O:70:ILE:HD11	3:O:79:LEU:HD21	1.55	0.88
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.38	0.85
1:A:1098:ASN:ND2	4:A:1309:NAG:O3	2.08	0.85
3:K:22:CYS:HB3	3:K:79:LEU:HB3	1.59	0.85
2:H:63:ARG:NH2	2:H:79:GLY:O	2.09	0.84
2:H:6:GLN:HB3	2:H:104:THR:HG22	1.60	0.84
1:B:358:ILE:HG13	1:B:395:VAL:HG23	1.60	0.84
1:B:118:LEU:HB3	1:B:129:LYS:HB2	1.60	0.84
2:N:38:TYR:HD1	2:N:48:LEU:HA	1.43	0.84
1:C:452:ARG:HG2	1:C:494:SER:HA	1.59	0.83
1:C:81:ASN:ND2	1:C:265:TYR:OH	2.11	0.82
1:C:353:TRP:O	1:C:466:ARG:NH2	2.11	0.82
2:H:41:HIS:H	2:H:44:LYS:HE3	1.42	0.82
2:I:38:TYR:HD1	2:I:48:LEU:HA	1.44	0.82
1:A:328:ARG:NH2	1:A:531:THR:O	2.13	0.82
3:O:98:ARG:HB3	3:O:114:PRO:HG2	1.62	0.82
3:O:54:ASN:HB3	3:O:56:TYR:HD2	1.46	0.81
2:N:6:GLN:HG2	2:N:106:THR:HG23	1.64	0.80
1:B:453:TYR:OH	1:B:493:GLN:NE2	2.15	0.80
3:J:37:ILE:HD11	3:J:112:LEU:HD13	1.62	0.80
2:I:6:GLN:HG2	2:I:106:THR:HG23	1.64	0.80
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.44	0.79
1:A:358:ILE:HG13	1:A:395:VAL:HG13	1.64	0.79
1:B:454:ARG:NH1	1:B:469:SER:O	2.17	0.78
3:O:82:GLN:NE2	3:O:84:ASN:HB3	1.99	0.77
1:C:342:PHE:HE1	1:C:511:VAL:HG21	1.49	0.77
1:B:200:TYR:HD2	1:B:230:PRO:HA	1.50	0.76
1:B:316:SER:OG	1:B:317:ASN:N	2.18	0.76
2:H:63:ARG:NH2	2:H:81:GLN:HG3	2.00	0.76
1:C:440:LYS:O	2:I:32:TYR:OH	2.03	0.76
1:B:200:TYR:CD2	1:B:230:PRO:HA	2.21	0.76
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.13	0.76
2:N:6:GLN:NE2	2:N:88:TYR:O	2.19	0.75
2:I:50:ILE:HG22	2:I:56:ARG:HG3	1.67	0.75
1:C:1019:ARG:NH1	1:B:1017:GLU:OE2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:NH2	1:A:530:SER:OG	2.19	0.75
3:K:5:VAL:HG22	3:K:117:GLN:HE22	1.50	0.75
1:C:234:ASN:ND2	4:C:1310:NAG:O7	2.19	0.75
1:B:417:ASN:O	1:B:422:ASN:ND2	2.20	0.75
3:O:7:SER:OG	3:O:21:SER:OG	2.03	0.75
3:O:22:CYS:HB3	3:O:79:LEU:HB3	1.69	0.75
1:C:195:LYS:HE3	1:C:204:TYR:CE1	2.22	0.74
1:B:483:VAL:HG22	1:B:484:ALA:H	1.52	0.74
1:C:353:TRP:CE2	1:C:466:ARG:HB3	2.22	0.74
1:A:563:GLN:O	1:A:577:ARG:NH1	2.20	0.74
3:K:36:TRP:HE1	3:K:79:LEU:HD22	1.53	0.74
3:O:19:ARG:HA	3:O:82:GLN:HA	1.69	0.74
1:B:1098:ASN:ND2	4:B:1310:NAG:O3	2.20	0.73
1:C:91:TYR:N	1:C:268:GLY:O	2.19	0.73
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.71	0.73
1:C:425:LEU:H	1:C:425:LEU:HD23	1.53	0.73
1:B:1098:ASN:ND2	4:B:1310:NAG:O7	2.22	0.73
1:A:165:ASN:HD21	4:A:1303:NAG:H4	1.54	0.72
2:H:94:THR:HG22	2:H:95:SER:H	1.54	0.72
1:B:709:ASN:HD21	4:B:1312:NAG:H4	1.54	0.72
1:C:461:LEU:HD13	1:C:465:GLU:HG3	1.70	0.72
2:H:38:TYR:HD1	2:H:48:LEU:HA	1.55	0.72
3:K:99:GLU:HG3	3:K:101:PRO:HD2	1.72	0.72
1:A:68:ILE:HG13	1:A:69:HIS:H	1.54	0.72
3:O:20:LEU:HD12	3:O:119:ILE:HD11	1.72	0.72
3:O:4:LEU:HB2	3:O:116:GLY:HA2	1.72	0.71
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.71	0.71
1:B:657:ASN:HD21	4:B:1305:NAG:H4	1.52	0.71
1:A:393:THR:OG1	1:A:394:ASN:OD1	2.07	0.71
2:N:53:VAL:HG23	2:N:54:SER:H	1.56	0.71
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.08	0.71
1:B:1031:GLU:OE2	1:A:1039:ARG:NH1	2.23	0.71
1:A:83:VAL:HG22	1:A:239:GLN:HE21	1.54	0.71
1:A:453:TYR:O	1:A:493:GLN:N	2.21	0.71
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.26	0.71
3:O:30:SER:O	3:O:72:ARG:NH1	2.23	0.70
2:I:13:SER:O	2:I:16:GLN:HG2	1.90	0.70
1:C:1098:ASN:ND2	4:C:1305:NAG:O3	2.24	0.70
1:B:129:LYS:NZ	1:B:169:GLU:HB3	2.06	0.70
3:O:30:SER:HB2	3:O:74:ASN:HD21	1.56	0.70
1:C:334:ASN:O	1:C:334:ASN:ND2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:37:ILE:HG22	3:K:95:TYR:HB2	1.73	0.70
1:A:409:GLN:N	1:A:409:GLN:OE1	2.24	0.70
2:N:6:GLN:H	2:N:104:THR:HG23	1.56	0.70
1:C:353:TRP:CZ2	1:C:466:ARG:HB3	2.27	0.69
1:C:546:LEU:HD11	1:C:565:PHE:CE1	2.27	0.69
3:O:54:ASN:HB3	3:O:56:TYR:CD2	2.26	0.69
1:A:30:ASN:HA	1:A:61:ASN:HA	1.73	0.69
1:B:886:TRP:CH2	1:B:904:TYR:HD2	2.10	0.69
1:A:617:CYS:N	1:A:649:CYS:SG	2.65	0.69
3:K:30:SER:O	3:K:72:ARG:NH1	2.25	0.69
1:B:377:PHE:HD1	1:B:434:ILE:HG12	1.58	0.69
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.25	0.69
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.28	0.69
1:C:663:ASP:OD1	1:C:663:ASP:N	2.24	0.69
1:B:231:ILE:HD12	1:B:233:ILE:HG12	1.75	0.69
2:I:63:ARG:NH2	2:I:79:GLY:O	2.26	0.69
1:C:490:PHE:CD1	1:C:491:PRO:HD2	2.28	0.69
2:N:80:LEU:HD12	2:N:110:VAL:HG12	1.74	0.69
4:C:1309:NAG:HO6	4:B:1312:NAG:HO6	1.41	0.69
3:J:19:ARG:HE	3:J:82:GLN:HB3	1.58	0.68
3:K:19:ARG:NH1	3:K:82:GLN:OE1	2.26	0.68
1:A:403:ARG:NE	1:A:405:ASN:OD1	2.26	0.68
1:B:229:LEU:HG	1:B:231:ILE:HG23	1.75	0.68
1:B:200:TYR:OH	1:A:394:ASN:ND2	2.27	0.68
1:B:1074:ASN:HD21	4:B:1308:NAG:C1	2.06	0.68
1:A:501:TYR:HB2	1:A:506:GLN:NE2	2.09	0.68
1:C:36:VAL:HG21	1:C:220:PHE:CZ	2.29	0.68
3:O:98:ARG:HH21	3:O:100:GLN:HA	1.59	0.68
1:A:236:THR:HG23	1:A:237:ARG:HG3	1.76	0.67
3:K:54:ASN:HB3	3:K:56:TYR:HD2	1.60	0.67
3:K:43:LYS:HG2	3:K:44:GLY:H	1.59	0.67
1:B:725:GLU:OE1	1:B:1028:LYS:NZ	2.24	0.67
1:A:390:LEU:HD23	1:A:390:LEU:H	1.59	0.67
1:A:1098:ASN:ND2	4:A:1309:NAG:O7	2.27	0.67
1:B:473:TYR:O	1:B:488:CYS:HA	1.94	0.67
2:H:9:SER:HB2	2:H:107:LYS:HE3	1.77	0.67
2:H:23:THR:HG22	2:H:24:GLY:H	1.59	0.67
2:N:36:SER:OG	2:N:91:SER:OG	2.12	0.67
3:O:48:VAL:O	3:O:61:GLY:N	2.26	0.67
2:I:94:THR:HG22	2:I:95:SER:H	1.58	0.67
3:J:109:GLY:O	3:J:111:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ALA:O	1:C:509:ARG:NH1	2.28	0.67
3:O:43:LYS:HD3	3:O:44:GLY:N	2.09	0.67
1:A:616:ASN:ND2	4:A:1310:NAG:O7	2.28	0.66
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.42	0.66
2:H:6:GLN:HG2	2:H:106:THR:HG23	1.76	0.66
1:C:62:VAL:HB	1:C:267:VAL:O	1.95	0.66
2:H:6:GLN:NE2	2:H:88:TYR:O	2.22	0.66
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.75	0.66
2:N:29:VAL:HG23	2:N:35:VAL:HG11	1.78	0.66
1:A:526:GLY:H	1:A:527:PRO:HD3	1.59	0.66
2:N:36:SER:HA	2:N:51:TYR:HA	1.78	0.66
2:N:37:TRP:N	2:N:50:ILE:O	2.27	0.66
3:K:99:GLU:OE2	3:K:110:TYR:HB3	1.96	0.66
1:C:362:VAL:HG23	1:C:526:GLY:HA3	1.78	0.66
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.61	0.66
1:B:886:TRP:HH2	1:B:904:TYR:HD2	1.40	0.66
3:O:36:TRP:CH2	3:O:96:CYS:HB2	2.31	0.66
1:C:437:ASN:HB2	1:C:508:TYR:CZ	2.32	0.65
3:K:39:GLN:HB2	3:K:45:LEU:HD13	1.78	0.65
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.31	0.65
1:A:712:ILE:HG13	1:A:1077:THR:HG21	1.78	0.65
1:B:896:ILE:HG13	1:A:712:ILE:HD11	1.79	0.65
1:B:68:ILE:HG13	1:B:69:HIS:H	1.60	0.65
3:K:36:TRP:CH2	3:K:96:CYS:HB2	2.32	0.65
1:C:101:ILE:HD11	1:C:240:THR:OG1	1.97	0.65
1:C:546:LEU:HD21	1:C:565:PHE:CZ	2.32	0.65
4:C:1309:NAG:O6	4:B:1312:NAG:O6	2.10	0.65
1:B:446:GLY:O	1:B:498:ARG:NH1	2.29	0.65
3:O:109:GLY:O	3:O:111:ARG:NH1	2.29	0.65
1:C:496:GLY:O	1:C:501:TYR:OH	2.06	0.65
1:C:174:PRO:HB2	1:C:176:LEU:HD13	1.78	0.65
1:B:373:PRO:O	1:A:405:ASN:ND2	2.27	0.65
3:O:91:THR:HG22	3:O:123:VAL:H	1.61	0.65
1:C:81:ASN:OD1	1:C:82:PRO:HD2	1.96	0.64
3:K:29:ILE:HD11	3:K:34:MET:SD	2.37	0.64
1:B:395:VAL:HG12	1:B:515:PHE:HB3	1.78	0.64
1:C:378:LYS:NZ	1:C:379:CYS:H	1.96	0.64
1:C:518:LEU:HD11	1:C:520:ALA:HB2	1.79	0.64
2:N:107:LYS:HZ2	2:N:108:VAL:N	1.95	0.64
2:N:41:HIS:HB2	2:N:44:LYS:HE2	1.78	0.64
1:A:85:PRO:O	1:A:269:TYR:OH	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:HG2	1:C:505:HIS:HA	1.78	0.64
3:J:99:GLU:CD	3:J:110:TYR:HB3	2.19	0.63
3:O:93:VAL:HA	3:O:120:LEU:HA	1.81	0.63
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.33	0.63
1:B:282:ASN:HD21	4:B:1304:NAG:H5	1.63	0.63
1:A:583:GLU:OE2	1:A:584:ILE:N	2.31	0.63
1:C:30:ASN:HA	1:C:61:ASN:HA	1.79	0.63
1:C:346:ARG:NE	3:K:101:PRO:O	2.32	0.62
1:B:172:SER:OG	1:B:173:GLN:N	2.32	0.62
1:B:712:ILE:HG13	1:B:1077:THR:HG21	1.81	0.62
1:A:282:ASN:ND2	4:A:1304:NAG:O7	2.32	0.62
2:I:10:VAL:HG12	2:I:108:VAL:HA	1.81	0.62
1:B:200:TYR:CZ	1:A:394:ASN:ND2	2.67	0.62
2:I:40:GLN:O	2:I:87:ASP:N	2.27	0.62
4:C:1305:NAG:C7	4:C:1305:NAG:HO3	2.13	0.62
1:B:96:GLU:OE1	1:B:98:SER:N	2.31	0.62
2:N:88:TYR:HB2	2:N:106:THR:OG1	1.99	0.62
1:A:537:LYS:O	1:A:539:VAL:HG23	1.99	0.62
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.65	0.62
2:H:40:GLN:HG2	2:H:87:ASP:HB2	1.81	0.62
1:A:403:ARG:CZ	1:A:405:ASN:HD21	2.13	0.62
1:A:394:ASN:OD1	1:A:394:ASN:N	2.32	0.62
1:A:457:ARG:HE	1:A:458:LYS:H	1.48	0.61
1:B:118:LEU:N	1:B:129:LYS:O	2.22	0.61
3:K:67:ARG:HE	3:K:85:SER:HG	1.48	0.61
1:C:709:ASN:HD21	4:C:1307:NAG:H2	1.65	0.61
4:C:1305:NAG:O3	4:C:1305:NAG:O7	2.17	0.61
1:A:526:GLY:O	1:A:528:LYS:N	2.34	0.61
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.82	0.61
3:O:51:ILE:HA	3:O:58:ILE:HD13	1.82	0.61
1:C:195:LYS:HE3	1:C:204:TYR:HE1	1.66	0.61
1:A:70:VAL:HG21	1:A:255:SER:HA	1.82	0.61
1:B:663:ASP:OD1	1:B:663:ASP:N	2.29	0.61
1:A:108:THR:HA	1:A:236:THR:HG22	1.82	0.61
1:A:130:VAL:CG1	1:A:168:PHE:HB3	2.31	0.61
2:I:23:THR:HA	2:I:72:THR:HA	1.82	0.61
1:C:372:ALA:O	1:C:374:PHE:N	2.34	0.60
1:B:518:LEU:HD11	1:B:520:ALA:HB2	1.82	0.60
1:C:68:ILE:HG23	1:C:69:HIS:H	1.66	0.60
1:C:83:VAL:HB	1:C:239:GLN:HE21	1.67	0.60
1:C:978:ASN:HB3	1:B:547:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ARG:HH21	1:A:490:PHE:HE2	1.49	0.60
3:K:98:ARG:HB3	3:K:114:PRO:HG2	1.83	0.60
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.83	0.60
2:H:16:GLN:O	2:H:80:LEU:HD23	2.01	0.60
1:B:354:ASN:ND2	3:O:105:TYR:OH	2.34	0.60
1:B:70:VAL:HG21	1:B:255:SER:HA	1.83	0.60
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.33	0.60
3:K:70:ILE:HG13	3:K:79:LEU:HD21	1.83	0.60
1:C:393:THR:OG1	1:C:394:ASN:OD1	2.17	0.60
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.66	0.60
2:H:4:LEU:HG	2:H:101:VAL:HG12	1.83	0.60
1:B:196:ASN:ND2	1:B:201:PHE:HB2	2.16	0.60
2:I:68:LYS:NZ	2:I:70:GLY:O	2.34	0.60
1:C:379:CYS:HA	1:C:432:CYS:HA	1.84	0.60
1:B:108:THR:HB	1:B:234:ASN:O	2.01	0.60
1:B:324:GLU:HB3	1:B:539:VAL:HG12	1.84	0.60
2:N:6:GLN:O	2:N:104:THR:OG1	2.17	0.60
3:O:30:SER:HB2	3:O:74:ASN:ND2	2.17	0.60
1:C:91:TYR:OH	1:C:191:GLU:OE2	2.19	0.60
3:K:79:LEU:HD23	3:K:80:TYR:N	2.17	0.59
1:A:497:PHE:CD1	1:A:507:PRO:HD3	2.37	0.59
1:B:462:LYS:N	1:B:465:GLU:OE1	2.35	0.59
1:A:361:CYS:O	1:A:524:VAL:HG23	2.03	0.59
3:O:20:LEU:N	3:O:81:LEU:O	2.26	0.59
3:O:20:LEU:CD2	3:O:83:MET:HG3	2.32	0.59
1:C:1017:GLU:OE2	1:A:1019:ARG:NH1	2.35	0.59
1:A:442:ASP:O	1:A:448:ASN:ND2	2.35	0.59
2:N:39:GLN:NE2	2:N:88:TYR:OH	2.35	0.59
3:J:70:ILE:HG13	3:J:81:LEU:HD13	1.83	0.59
1:C:709:ASN:ND2	4:C:1307:NAG:H2	2.18	0.59
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.38	0.59
1:A:657:ASN:HD21	4:A:1305:NAG:H2	1.66	0.59
1:C:83:VAL:CB	1:C:239:GLN:HE21	2.15	0.59
1:C:454:ARG:HA	1:C:491:PRO:O	2.02	0.59
1:B:393:THR:HG23	1:B:520:ALA:HB3	1.84	0.59
3:K:67:ARG:NE	3:K:85:SER:OG	2.31	0.59
1:C:424:LYS:H	1:C:461:LEU:HD11	1.68	0.59
1:C:555:SER:OG	1:C:584:ILE:HB	2.03	0.59
1:B:294:ASP:N	1:B:294:ASP:OD1	2.36	0.59
1:A:103:GLY:HA3	1:A:241:LEU:HD12	1.85	0.59
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:SER:HG	3:J:104:TYR:HH	1.51	0.58
1:A:663:ASP:N	1:A:663:ASP:OD1	2.28	0.58
1:C:796:TYR:CE2	4:C:1309:NAG:H2	2.37	0.58
2:H:29:VAL:HG13	2:H:35:VAL:HG21	1.84	0.58
1:C:338:PHE:C	1:C:340:GLU:H	2.06	0.58
1:B:116:SER:HB2	1:B:132:GLU:HA	1.84	0.58
1:B:198:ASP:OD1	1:B:202:LYS:NZ	2.32	0.58
1:B:390:LEU:HD12	1:B:390:LEU:H	1.68	0.58
1:B:372:ALA:HB1	1:B:436:TRP:CG	2.38	0.58
1:C:712:ILE:HD11	1:A:896:ILE:HG13	1.85	0.58
1:B:490:PHE:CD1	1:B:491:PRO:HD2	2.39	0.58
1:C:201:PHE:HD2	1:C:229:LEU:HB2	1.69	0.58
1:A:412:PRO:HB3	1:A:426:PRO:O	2.04	0.58
2:I:22:CYS:N	2:I:73:ALA:O	2.28	0.58
3:J:38:ARG:O	3:J:46:GLU:N	2.37	0.58
2:I:6:GLN:NE2	2:I:88:TYR:O	2.36	0.58
1:B:129:LYS:HZ3	1:B:169:GLU:HB3	1.68	0.58
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.22	0.58
1:B:347:PHE:CD2	1:B:509:ARG:HD3	2.39	0.57
1:B:586:ASP:OD1	1:B:587:ILE:N	2.37	0.57
1:B:982:SER:O	1:A:386:LYS:HD2	2.03	0.57
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.85	0.57
2:I:88:TYR:HB2	2:I:106:THR:OG1	2.04	0.57
3:K:73:ASP:O	3:K:77:ASN:N	2.37	0.57
1:A:404:GLY:HA2	1:A:508:TYR:CD1	2.38	0.57
3:J:73:ASP:HB3	3:J:76:LYS:HG2	1.86	0.57
3:O:18:LEU:N	3:O:83:MET:O	2.37	0.57
3:K:7:SER:OG	3:K:21:SER:OG	2.18	0.57
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.70	0.57
1:B:352:ALA:HB2	1:B:468:ILE:HD12	1.85	0.57
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.69	0.57
4:A:1309:NAG:HO3	4:A:1309:NAG:C7	2.18	0.57
1:C:70:VAL:H	1:C:80:ASP:HA	1.70	0.57
1:B:189:LEU:HB2	1:B:210:ILE:HD11	1.86	0.57
4:B:1310:NAG:C7	4:B:1310:NAG:HO3	2.17	0.57
1:C:982:SER:O	1:B:386:LYS:HD3	2.05	0.57
1:A:801:ASN:ND2	4:A:1312:NAG:O7	2.37	0.57
3:K:39:GLN:HG3	3:K:44:GLY:O	2.05	0.57
1:C:395:VAL:HG22	1:C:515:PHE:HB3	1.87	0.57
1:B:421:TYR:HA	1:B:461:LEU:HD22	1.86	0.57
3:O:60:TYR:HB2	3:O:65:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:67:ARG:HD3	3:K:68:PHE:CE1	2.40	0.57
3:J:54:ASN:CG	3:J:56:TYR:H	2.08	0.56
2:N:46:PRO:HG2	3:O:45:LEU:HD11	1.86	0.56
3:O:19:ARG:HD3	3:O:80:TYR:HD2	1.69	0.56
3:O:95:TYR:CE1	3:O:118:GLY:HA3	2.39	0.56
2:I:63:ARG:HH22	2:I:81:GLN:HB2	1.70	0.56
1:C:801:ASN:ND2	4:C:1308:NAG:N2	2.52	0.56
1:B:805:ILE:O	1:B:816:SER:OG	2.16	0.56
1:C:896:ILE:HG13	1:B:712:ILE:HD11	1.85	0.56
2:H:102:PHE:CZ	3:J:45:LEU:HD12	2.40	0.56
3:J:98:ARG:HB3	3:J:114:PRO:HG2	1.85	0.56
2:I:4:LEU:HG	2:I:101:VAL:HG23	1.87	0.56
3:K:36:TRP:HE1	3:K:79:LEU:CD2	2.18	0.56
1:C:390:LEU:HB2	1:C:392:PHE:CZ	2.41	0.56
2:H:35:VAL:HG22	2:H:92:SER:HB2	1.87	0.56
1:C:886:TRP:CH2	1:C:904:TYR:HD2	2.24	0.56
1:A:379:CYS:HA	1:A:432:CYS:HA	1.88	0.56
1:A:398:ASP:O	1:A:511:VAL:HA	2.03	0.56
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.40	0.56
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.41	0.56
1:C:616:ASN:OD1	1:C:617:CYS:N	2.38	0.56
1:B:472:ILE:HD11	1:B:490:PHE:HD1	1.71	0.56
1:A:420:ASP:O	1:A:460:ASN:ND2	2.39	0.56
2:N:43:GLY:C	2:N:44:LYS:HD3	2.26	0.56
1:B:99:ASN:OD1	1:B:102:ARG:HG2	2.06	0.56
1:B:826:VAL:CG2	1:B:1057:PRO:HG2	2.35	0.56
3:O:3:GLN:OE1	3:O:25:SER:OG	2.13	0.56
1:C:342:PHE:CE1	1:C:511:VAL:HG21	2.37	0.56
1:C:418:ILE:HA	1:C:422:ASN:ND2	2.15	0.56
1:C:421:TYR:HA	1:C:457:ARG:HD2	1.86	0.56
2:H:35:VAL:HB	2:H:68:LYS:HE2	1.88	0.56
2:N:56:ARG:HH21	2:N:62:ASN:HA	1.71	0.56
1:C:546:LEU:HD21	1:C:565:PHE:HZ	1.68	0.56
3:O:98:ARG:NH2	3:O:100:GLN:HA	2.20	0.56
1:C:128:ILE:HD13	1:C:229:LEU:HD21	1.88	0.55
1:A:501:TYR:HB2	1:A:506:GLN:HE21	1.70	0.55
2:N:28:ASP:OD1	2:N:29:VAL:N	2.34	0.55
2:N:53:VAL:HG23	2:N:54:SER:N	2.21	0.55
1:C:395:VAL:HA	1:C:515:PHE:HB3	1.88	0.55
1:B:101:ILE:HD11	1:B:240:THR:OG1	2.04	0.55
1:C:106:PHE:HB3	1:C:235:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.41	0.55
1:A:404:GLY:HA2	1:A:508:TYR:CE1	2.41	0.55
1:C:282:ASN:ND2	4:C:1312:NAG:O5	2.33	0.55
1:B:43:PHE:HB3	1:A:565:PHE:O	2.07	0.55
1:B:128:ILE:O	1:B:129:LYS:HE2	2.06	0.55
1:B:546:LEU:HD13	1:B:565:PHE:CE1	2.41	0.55
4:A:1309:NAG:O3	4:A:1309:NAG:O7	2.23	0.55
3:K:38:ARG:O	3:K:46:GLU:N	2.40	0.55
1:C:712:ILE:HG13	1:C:1077:THR:HG21	1.88	0.55
1:A:402:ILE:O	1:A:508:TYR:N	2.40	0.55
1:A:440:LYS:O	1:A:441:LEU:HD23	2.07	0.55
2:N:38:TYR:CD1	2:N:48:LEU:HA	2.34	0.55
2:N:51:TYR:CD2	2:N:52:ASP:HB2	2.42	0.55
1:A:34:ARG:NH2	1:A:219:GLY:O	2.39	0.55
3:O:73:ASP:O	3:O:77:ASN:N	2.40	0.55
1:C:353:TRP:HE1	1:C:423:TYR:HB2	1.72	0.55
1:B:31:SER:N	1:B:60:SER:O	2.26	0.55
3:O:113:ASP:HB3	3:O:114:PRO:HD3	1.88	0.55
1:C:81:ASN:HD22	1:C:240:THR:HG22	1.72	0.54
1:B:197:ILE:HG13	1:B:198:ASP:H	1.73	0.54
1:A:403:ARG:HB2	1:A:495:TYR:CE1	2.41	0.54
2:N:65:SER:OG	2:N:76:THR:HB	2.08	0.54
1:B:176:LEU:HD13	1:B:190:ARG:HH12	1.71	0.54
1:A:215:ASP:N	1:A:215:ASP:OD1	2.41	0.54
1:A:657:ASN:HD21	4:A:1305:NAG:C2	2.20	0.54
1:B:131:CYS:HB3	1:B:166:CYS:N	2.22	0.54
1:C:617:CYS:HA	1:C:620:VAL:HB	1.89	0.54
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.89	0.54
1:B:403:ARG:HG2	1:B:404:GLY:H	1.73	0.54
1:B:444:LYS:O	1:B:499:PRO:HD3	2.08	0.54
1:A:517:LEU:C	1:A:519:HIS:H	2.10	0.54
1:C:34:ARG:NE	1:C:191:GLU:OE2	2.31	0.54
1:B:197:ILE:HG13	1:B:198:ASP:N	2.22	0.54
1:A:64:TRP:HE1	1:A:264:ALA:CB	2.17	0.54
1:C:68:ILE:HG12	1:C:69:HIS:CD2	2.43	0.54
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.43	0.54
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.90	0.54
3:O:107:SER:O	3:O:107:SER:OG	2.24	0.54
4:B:1313:NAG:O7	4:B:1313:NAG:O3	2.25	0.54
1:A:434:ILE:O	1:A:510:VAL:HG23	2.06	0.54
1:B:377:PHE:CD1	1:B:434:ILE:HG12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:41:HIS:HB2	2:N:44:LYS:CE	2.37	0.54
3:K:18:LEU:O	3:K:83:MET:N	2.41	0.54
1:C:117:LEU:HD21	1:C:119:ILE:HG13	1.89	0.53
1:C:141:LEU:O	1:C:249:LEU:HD13	2.08	0.53
1:C:345:THR:HG23	3:K:107:SER:HA	1.90	0.53
1:C:372:ALA:C	1:C:374:PHE:H	2.11	0.53
1:A:342:PHE:CE2	1:A:511:VAL:HG11	2.43	0.53
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.42	0.53
1:B:546:LEU:HD13	1:B:565:PHE:HE1	1.72	0.53
4:B:1310:NAG:O3	4:B:1310:NAG:O7	2.26	0.53
2:N:107:LYS:NZ	2:N:108:VAL:O	2.41	0.53
1:C:983:ARG:HH21	1:B:517:LEU:HD12	1.73	0.53
1:B:70:VAL:HG13	1:B:80:ASP:O	2.08	0.53
1:B:616:ASN:OD1	1:B:617:CYS:N	2.41	0.53
1:A:70:VAL:HA	1:A:80:ASP:O	2.08	0.53
2:N:52:ASP:O	2:N:54:SER:N	2.42	0.53
3:J:22:CYS:SG	3:J:79:LEU:HD12	2.48	0.53
3:O:43:LYS:CD	3:O:44:GLY:H	2.17	0.53
1:B:801:ASN:HD21	4:B:1313:NAG:C2	2.21	0.53
2:N:35:VAL:HG12	2:N:92:SER:HB2	1.90	0.53
3:O:22:CYS:HB2	3:O:36:TRP:CZ2	2.43	0.53
1:C:1102:TRP:HB2	1:C:1135:ASN:HD22	1.73	0.53
2:N:16:GLN:O	2:N:80:LEU:HD23	2.09	0.53
2:N:25:THR:OG1	2:N:26:SER:N	2.41	0.53
1:C:105:ILE:HG23	1:C:241:LEU:HD21	1.91	0.53
1:A:431:GLY:HA2	1:A:515:PHE:CZ	2.43	0.53
3:K:5:VAL:HG22	3:K:117:GLN:NE2	2.23	0.53
1:B:89:GLY:HA3	1:B:270:LEU:HD12	1.91	0.53
1:A:142:ASP:O	1:A:244:LEU:N	2.34	0.53
1:A:437:ASN:HD21	1:A:506:GLN:HB2	1.73	0.53
3:O:36:TRP:CZ3	3:O:96:CYS:HB2	2.44	0.53
3:K:36:TRP:HB2	3:K:48:VAL:HB	1.91	0.53
1:C:537:LYS:O	1:C:539:VAL:HG13	2.09	0.52
1:B:231:ILE:HG13	1:B:231:ILE:O	2.09	0.52
1:A:498:ARG:HD2	1:A:500:THR:H	1.73	0.52
1:C:294:ASP:OD1	1:C:294:ASP:N	2.40	0.52
1:B:338:PHE:HE1	1:B:358:ILE:HD12	1.75	0.52
1:A:81:ASN:OD1	1:A:82:PRO:HD2	2.08	0.52
2:N:63:ARG:HB3	2:N:78:SER:O	2.08	0.52
3:O:37:ILE:O	3:O:95:TYR:N	2.39	0.52
3:O:85:SER:HB3	3:O:87:ARG:HH11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD13	1:B:336:CYS:H	1.74	0.52
1:B:456:PHE:HE2	1:B:489:TYR:HB2	1.73	0.52
2:N:18:ILE:HB	2:N:77:ILE:HG23	1.91	0.52
3:O:3:GLN:OE1	3:O:3:GLN:N	2.42	0.52
2:I:33:ASN:OD1	2:I:68:LYS:HD3	2.10	0.52
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.91	0.52
1:C:1117:THR:O	1:C:1117:THR:HG22	2.09	0.52
1:B:1134:ASN:HD21	4:B:1309:NAG:C2	2.22	0.52
1:C:131:CYS:HA	1:C:166:CYS:HA	1.90	0.52
1:A:131:CYS:HB3	1:A:166:CYS:CA	2.38	0.52
1:A:409:GLN:HG3	1:A:416:GLY:HA3	1.91	0.52
2:I:10:VAL:O	2:I:109:THR:OG1	2.20	0.52
1:C:362:VAL:HG23	1:C:526:GLY:CA	2.40	0.52
1:A:356:LYS:HB2	3:J:105:TYR:OH	2.10	0.52
2:I:11:SER:HA	2:I:109:THR:O	2.07	0.52
1:A:294:ASP:OD1	1:A:294:ASP:N	2.42	0.52
1:A:332:ILE:O	1:A:362:VAL:HB	2.10	0.52
1:C:205:SER:O	1:C:206:LYS:HG2	2.10	0.52
1:A:801:ASN:HD21	4:A:1312:NAG:C2	2.23	0.52
1:C:96:GLU:HG2	1:C:101:ILE:HG22	1.92	0.52
1:B:118:LEU:O	1:B:129:LYS:N	2.32	0.52
1:A:234:ASN:ND2	4:A:1302:NAG:O7	2.43	0.52
3:J:62:ASP:O	3:J:65:LYS:HG2	2.08	0.52
1:C:303:LEU:HD12	1:C:308:VAL:HG12	1.92	0.52
1:B:1037:SER:O	1:B:1037:SER:OG	2.28	0.52
1:A:1037:SER:O	1:A:1037:SER:OG	2.27	0.52
3:O:28:MET:HG3	3:O:30:SER:H	1.75	0.52
1:B:106:PHE:CE1	1:B:238:PHE:HB2	2.45	0.51
1:B:372:ALA:HB3	1:B:374:PHE:CE1	2.45	0.51
1:A:169:GLU:HG2	1:A:170:TYR:N	2.25	0.51
1:C:124:THR:HG23	1:C:125:ASN:OD1	2.10	0.51
2:H:52:ASP:O	2:H:54:SER:N	2.44	0.51
3:K:78:PHE:HB2	3:K:80:TYR:HE1	1.74	0.51
1:B:480:CYS:HB3	1:B:483:VAL:HG12	1.92	0.51
3:J:2:VAL:HG23	3:J:25:SER:O	2.10	0.51
1:C:334:ASN:O	1:C:362:VAL:HG12	2.10	0.51
1:B:736:VAL:HG23	1:B:858:LEU:HD23	1.93	0.51
1:A:473:TYR:HB2	1:A:489:TYR:O	2.11	0.51
2:N:39:GLN:O	2:N:47:LYS:N	2.33	0.51
3:O:79:LEU:HD23	3:O:80:TYR:N	2.25	0.51
2:I:88:TYR:HB2	2:I:106:THR:HG1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ALA:C	1:C:374:PHE:N	2.63	0.51
1:C:439:ASN:OD1	1:C:507:PRO:HD2	2.10	0.51
2:H:85:GLU:OE1	2:H:109:THR:HA	2.11	0.51
3:O:36:TRP:HB2	3:O:48:VAL:HB	1.92	0.51
3:K:39:GLN:O	3:K:93:VAL:HG12	2.10	0.51
1:B:196:ASN:HD22	1:B:201:PHE:HB2	1.75	0.51
3:J:43:LYS:CG	3:J:44:GLY:H	2.23	0.51
1:C:378:LYS:HZ3	1:C:379:CYS:H	1.58	0.51
1:C:393:THR:OG1	1:C:394:ASN:N	2.43	0.51
1:C:402:ILE:HG22	1:C:403:ARG:H	1.76	0.51
1:A:240:THR:HG22	1:A:241:LEU:N	2.25	0.51
1:A:578:ASP:O	1:A:582:LEU:HA	2.11	0.51
1:C:174:PRO:HB2	1:C:176:LEU:CD1	2.41	0.51
1:C:333:THR:HG23	1:C:334:ASN:H	1.76	0.51
1:B:335:LEU:O	1:B:361:CYS:HB2	2.10	0.51
1:C:96:GLU:OE1	1:C:99:ASN:N	2.44	0.50
1:C:128:ILE:HG21	1:C:229:LEU:HD21	1.94	0.50
1:C:204:TYR:N	1:C:204:TYR:CD1	2.79	0.50
1:B:555:SER:OG	1:B:584:ILE:HB	2.11	0.50
1:A:422:ASN:HA	1:A:454:ARG:HE	1.77	0.50
1:A:480:CYS:HB3	1:A:483:VAL:HG22	1.93	0.50
3:J:29:ILE:HG22	3:J:77:ASN:OD1	2.11	0.50
1:B:109:THR:HA	1:B:237:ARG:HD2	1.92	0.50
1:A:318:PHE:CZ	1:A:615:VAL:HG11	2.46	0.50
1:A:425:LEU:HG	1:A:464:PHE:HE1	1.76	0.50
1:C:1146:ASP:OD2	1:B:1146:ASP:N	2.43	0.50
3:O:20:LEU:HD21	3:O:83:MET:HE3	1.93	0.50
1:C:422:ASN:OD1	1:C:453:TYR:HB2	2.11	0.50
1:B:480:CYS:HB3	1:B:483:VAL:CG1	2.41	0.50
3:O:28:MET:HE2	3:O:30:SER:H	1.76	0.50
1:C:454:ARG:NH2	1:C:469:SER:O	2.45	0.50
4:C:1308:NAG:HO3	4:C:1308:NAG:C7	2.22	0.50
2:H:34:TYR:CE1	3:J:109:GLY:HA3	2.46	0.50
3:O:87:ARG:O	3:O:123:VAL:HG11	2.11	0.50
1:C:117:LEU:HD23	1:C:118:LEU:N	2.26	0.50
1:C:393:THR:HG21	1:C:518:LEU:HG	1.93	0.50
1:B:342:PHE:CE1	1:B:511:VAL:HG11	2.47	0.50
1:B:472:ILE:CD1	1:B:490:PHE:HA	2.42	0.50
3:J:37:ILE:HB	3:J:95:TYR:HB2	1.93	0.50
2:I:32:TYR:OH	2:I:95:SER:HB3	2.11	0.50
3:K:19:ARG:HA	3:K:82:GLN:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.77	0.50
1:A:438:SER:OG	1:A:509:ARG:HG3	2.12	0.50
1:A:752:LEU:HD23	1:A:752:LEU:O	2.11	0.50
3:O:20:LEU:N	3:O:20:LEU:HD22	2.27	0.50
1:B:1134:ASN:HD21	4:B:1309:NAG:C7	2.25	0.50
2:H:69:SER:O	2:H:72:THR:HG22	2.12	0.50
3:O:20:LEU:HD23	3:O:83:MET:HG3	1.93	0.50
1:C:353:TRP:NE1	1:C:423:TYR:HB2	2.26	0.49
1:C:446:GLY:O	1:C:449:TYR:OH	2.18	0.49
1:C:1074:ASN:HD21	4:C:1303:NAG:C1	2.25	0.49
1:A:308:VAL:HG22	1:A:602:THR:CG2	2.42	0.49
2:H:82:ALA:O	2:H:85:GLU:HG2	2.12	0.49
2:N:86:ALA:H	2:N:107:LYS:NZ	2.09	0.49
3:O:5:VAL:HG23	3:O:23:ALA:HB3	1.94	0.49
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.45	0.49
4:C:1308:NAG:O7	4:C:1308:NAG:O3	2.24	0.49
1:B:215:ASP:OD1	1:B:215:ASP:N	2.45	0.49
2:I:40:GLN:N	2:I:87:ASP:O	2.39	0.49
3:K:97:ALA:HB3	3:K:112:LEU:HD13	1.94	0.49
1:C:269:TYR:CD1	1:C:269:TYR:N	2.79	0.49
1:C:398:ASP:HB2	1:C:512:VAL:CG1	2.42	0.49
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.94	0.49
1:B:446:GLY:O	1:B:449:TYR:OH	2.19	0.49
3:O:36:TRP:CD1	3:O:81:LEU:HD22	2.47	0.49
1:C:385:THR:HG21	1:B:473:TYR:CE2	2.47	0.49
1:B:130:VAL:O	1:B:166:CYS:HA	2.12	0.49
1:A:83:VAL:CG2	1:A:239:GLN:HE21	2.23	0.49
3:O:64:VAL:HB	3:O:68:PHE:CD1	2.48	0.49
1:A:405:ASN:ND2	1:A:504:GLY:O	2.45	0.49
1:A:1117:THR:HG22	1:A:1117:THR:O	2.12	0.49
3:O:36:TRP:O	3:O:37:ILE:HD13	2.13	0.49
1:B:886:TRP:HH2	1:B:904:TYR:CD2	2.24	0.49
1:A:29:THR:O	1:A:62:VAL:N	2.33	0.49
1:A:454:ARG:HA	1:A:491:PRO:O	2.12	0.49
3:J:35:ASN:HB3	3:J:50:TYR:HD1	1.77	0.49
2:N:38:TYR:O	2:N:88:TYR:HA	2.13	0.49
3:K:22:CYS:HB2	3:K:36:TRP:CZ2	2.48	0.49
1:C:401:VAL:O	1:C:402:ILE:HD13	2.13	0.49
1:C:437:ASN:HB2	1:C:508:TYR:CE2	2.48	0.49
1:B:394:ASN:OD1	1:B:394:ASN:N	2.44	0.49
1:A:110:LEU:O	1:A:134:GLN:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:85:GLU:OE1	2:I:109:THR:HA	2.13	0.49
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.77	0.49
1:C:1098:ASN:ND2	4:C:1305:NAG:O7	2.45	0.49
2:H:32:TYR:HH	2:H:95:SER:HG	1.60	0.49
3:O:67:ARG:HB3	3:O:84:ASN:OD1	2.13	0.49
1:C:461:LEU:HD12	1:C:462:LYS:O	2.13	0.48
1:C:204:TYR:CE2	1:C:225:PRO:HB3	2.48	0.48
1:C:1134:ASN:ND2	4:C:1304:NAG:N2	2.61	0.48
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.48	0.48
3:J:43:LYS:HG3	3:J:44:GLY:H	1.78	0.48
1:A:1054:GLN:HA	1:A:1054:GLN:NE2	2.28	0.48
3:J:18:LEU:HD23	3:J:19:ARG:N	2.29	0.48
2:N:97:SER:O	2:N:98:THR:OG1	2.28	0.48
1:C:402:ILE:HG22	1:C:403:ARG:N	2.28	0.48
1:C:616:ASN:OD1	1:C:616:ASN:C	2.51	0.48
1:B:200:TYR:CE2	1:A:394:ASN:ND2	2.82	0.48
1:B:353:TRP:NE1	1:B:423:TYR:CD1	2.81	0.48
2:I:35:VAL:HG12	2:I:53:VAL:HG22	1.96	0.48
1:A:403:ARG:HD2	1:A:505:HIS:HD2	1.79	0.48
1:A:410:ILE:HG23	1:A:410:ILE:O	2.13	0.48
2:N:107:LYS:HE3	2:N:109:THR:HG23	1.96	0.48
1:A:247:SER:HB3	1:A:258:TRP:CG	2.49	0.48
2:H:63:ARG:O	2:H:78:SER:N	2.44	0.48
2:N:57:PRO:HD2	2:N:60:VAL:HG21	1.95	0.48
3:O:76:LYS:HE3	3:O:78:PHE:CE2	2.48	0.48
1:A:165:ASN:ND2	4:A:1303:NAG:H4	2.25	0.48
2:I:39:GLN:OE1	2:I:49:MET:HB2	2.14	0.48
1:C:69:HIS:HB3	1:C:257:GLY:HA3	1.96	0.48
1:B:81:ASN:OD1	1:B:82:PRO:HD2	2.14	0.48
1:B:196:ASN:HA	1:B:200:TYR:O	2.14	0.48
3:K:38:ARG:N	3:K:46:GLU:O	2.39	0.48
1:C:196:ASN:HA	1:C:200:TYR:O	2.14	0.48
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.68	0.48
1:B:30:ASN:HA	1:B:61:ASN:HA	1.94	0.48
1:B:83:VAL:HG22	1:B:239:GLN:HE21	1.78	0.47
1:A:354:ASN:O	1:A:398:ASP:HA	2.15	0.47
3:J:77:ASN:O	3:J:77:ASN:ND2	2.46	0.47
2:I:97:SER:O	2:I:98:THR:HB	2.13	0.47
1:A:247:SER:HB3	1:A:258:TRP:CD1	2.49	0.47
1:A:454:ARG:N	1:A:492:LEU:HD13	2.28	0.47
2:N:63:ARG:NH1	2:N:77:ILE:HD11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:41:HIS:CD2	2:I:86:ALA:HB2	2.49	0.47
3:K:94:TYR:O	3:K:118:GLY:HA2	2.14	0.47
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.95	0.47
1:B:409:GLN:OE1	1:B:416:GLY:HA3	2.14	0.47
2:H:94:THR:HG22	2:H:95:SER:N	2.28	0.47
1:C:83:VAL:HB	1:C:239:GLN:NE2	2.29	0.47
1:C:124:THR:O	1:C:174:PRO:HD3	2.14	0.47
1:C:398:ASP:O	1:C:511:VAL:HA	2.14	0.47
1:C:419:ALA:HA	1:C:423:TYR:O	2.14	0.47
1:C:472:ILE:HG21	1:C:480:CYS:O	2.14	0.47
1:A:581:THR:O	1:A:581:THR:HG22	2.14	0.47
2:H:36:SER:N	2:H:91:SER:O	2.41	0.47
2:N:63:ARG:O	2:N:77:ILE:HA	2.14	0.47
3:O:57:ALA:HB1	3:O:59:TYR:HE1	1.80	0.47
1:A:81:ASN:HB2	1:A:242:LEU:HD11	1.96	0.47
1:A:725:GLU:OE1	1:A:1028:LYS:NZ	2.46	0.47
1:A:859:THR:OG1	1:A:860:VAL:N	2.47	0.47
3:J:29:ILE:HD11	3:J:34:MET:HG3	1.96	0.47
2:N:10:VAL:HG12	2:N:11:SER:H	1.79	0.47
1:C:103:GLY:HA3	1:C:241:LEU:HD12	1.95	0.47
1:C:983:ARG:NH2	1:B:517:LEU:HD12	2.29	0.47
1:A:325:SER:OG	1:A:540:ASN:HB2	2.15	0.47
2:H:35:VAL:HA	2:H:91:SER:O	2.14	0.47
2:N:48:LEU:HD12	2:N:48:LEU:O	2.14	0.47
3:O:20:LEU:HB2	3:O:81:LEU:HB3	1.97	0.47
2:I:29:VAL:HG22	2:I:68:LYS:NZ	2.30	0.47
3:K:71:SER:OG	3:K:72:ARG:N	2.48	0.47
1:B:231:ILE:HA	1:A:357:ARG:NH2	2.30	0.47
1:A:437:ASN:HD21	1:A:506:GLN:CB	2.28	0.47
3:O:29:ILE:HD11	3:O:79:LEU:HB2	1.97	0.47
2:I:65:SER:N	2:I:76:THR:O	2.46	0.47
1:C:380:TYR:CZ	1:C:412:PRO:HD3	2.49	0.47
1:C:448:ASN:N	1:C:497:PHE:O	2.47	0.47
1:C:1031:GLU:OE2	1:B:1039:ARG:NH1	2.37	0.47
1:C:409:GLN:OE1	1:C:416:GLY:HA3	2.15	0.47
1:C:720:ILE:HD13	1:C:720:ILE:HG21	1.40	0.47
1:B:346:ARG:NH2	3:O:33:TYR:CZ	2.83	0.47
1:B:412:PRO:HA	1:B:425:LEU:HD11	1.97	0.47
1:A:68:ILE:HG13	1:A:69:HIS:N	2.27	0.47
1:A:473:TYR:O	1:A:488:CYS:HA	2.15	0.47
3:J:98:ARG:CZ	3:J:114:PRO:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:ILE:HG21	2:N:106:THR:HG21	1.97	0.47
2:I:49:MET:O	2:I:60:VAL:HG21	2.15	0.47
1:C:83:VAL:CG1	1:C:239:GLN:HE21	2.27	0.46
1:C:455:LEU:HD12	1:C:493:GLN:CG	2.45	0.46
1:B:200:TYR:N	1:B:200:TYR:CD1	2.83	0.46
2:H:63:ARG:HB3	2:H:78:SER:O	2.15	0.46
3:K:60:TYR:CE1	3:K:70:ILE:HG22	2.50	0.46
3:K:92:ALA:O	3:K:121:VAL:HG12	2.15	0.46
1:A:117:LEU:HD23	1:A:118:LEU:N	2.29	0.46
3:J:30:SER:HA	3:J:72:ARG:CZ	2.45	0.46
1:C:699:LEU:HA	1:C:699:LEU:HD23	1.71	0.46
1:B:438:SER:O	1:B:438:SER:OG	2.33	0.46
1:A:367:VAL:O	1:A:370:ASN:ND2	2.48	0.46
1:A:581:THR:O	1:A:582:LEU:HG	2.15	0.46
1:C:81:ASN:HD22	1:C:240:THR:CG2	2.29	0.46
1:C:267:VAL:HG12	1:C:269:TYR:HE1	1.80	0.46
1:C:402:ILE:O	1:C:508:TYR:N	2.45	0.46
1:C:455:LEU:HD12	1:C:493:GLN:HG2	1.97	0.46
1:B:67:ALA:N	1:B:263:ALA:O	2.37	0.46
1:B:120:VAL:HG23	1:B:127:VAL:HB	1.97	0.46
2:I:10:VAL:HG11	2:I:18:ILE:HD13	1.97	0.46
2:I:18:ILE:HD11	2:I:80:LEU:HD11	1.96	0.46
1:C:69:HIS:ND1	1:C:255:SER:O	2.49	0.46
1:C:108:THR:HB	1:C:234:ASN:O	2.16	0.46
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.70	0.46
1:B:373:PRO:HB3	1:A:505:HIS:HB2	1.96	0.46
2:H:67:SER:N	2:H:74:SER:O	2.47	0.46
2:I:22:CYS:O	2:I:73:ALA:N	2.41	0.46
1:C:351:TYR:HE1	1:C:468:ILE:HG23	1.81	0.46
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.80	0.46
1:A:117:LEU:HD21	1:A:119:ILE:HG13	1.97	0.46
2:N:80:LEU:HD12	2:N:110:VAL:CG1	2.44	0.46
2:I:29:VAL:HG13	2:I:30:GLY:N	2.31	0.46
1:B:815:ARG:NH2	1:B:820:ASP:OD1	2.48	0.46
1:A:340:GLU:OE2	3:J:105:TYR:HB3	2.16	0.46
3:J:24:ALA:HB1	3:J:27:PHE:CE1	2.50	0.46
3:J:52:SER:HB2	3:J:54:ASN:OD1	2.16	0.46
3:J:82:GLN:HG3	3:J:84:ASN:HD22	1.80	0.46
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.98	0.46
1:A:452:ARG:HA	1:A:494:SER:HA	1.97	0.46
3:O:18:LEU:O	3:O:83:MET:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:O	1:C:268:GLY:N	2.48	0.46
1:C:452:ARG:HH12	3:K:56:TYR:CB	2.29	0.46
1:C:1081:ILE:HD12	1:C:1081:ILE:HG23	1.61	0.46
1:A:473:TYR:HB3	1:A:489:TYR:N	2.30	0.46
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.50	0.46
2:I:90:CYS:O	2:I:103:GLY:N	2.49	0.46
1:C:424:LYS:N	1:C:461:LEU:HD11	2.31	0.46
1:B:456:PHE:HB3	1:B:473:TYR:CD1	2.51	0.46
2:I:64:PHE:CE1	2:I:77:ILE:HD13	2.50	0.46
3:K:72:ARG:NE	3:K:74:ASN:HD21	2.14	0.46
1:C:377:PHE:O	1:B:489:TYR:OH	2.35	0.45
1:C:886:TRP:HH2	1:C:904:TYR:HD2	1.63	0.45
1:B:1117:THR:HG22	1:B:1117:THR:O	2.15	0.45
1:A:801:ASN:ND2	4:A:1312:NAG:C7	2.80	0.45
2:N:85:GLU:N	2:N:85:GLU:OE1	2.49	0.45
3:O:39:GLN:O	3:O:93:VAL:HG12	2.16	0.45
3:O:94:TYR:O	3:O:118:GLY:HA2	2.16	0.45
1:C:329:PHE:CE1	1:C:544:ASN:HA	2.52	0.45
1:C:382:VAL:HG22	1:C:383:SER:N	2.31	0.45
1:C:461:LEU:HB2	1:C:465:GLU:OE2	2.16	0.45
1:C:670:ILE:HD12	1:C:670:ILE:HG23	1.69	0.45
1:B:83:VAL:HG13	1:B:239:GLN:HG2	1.99	0.45
1:B:96:GLU:OE1	1:B:99:ASN:N	2.49	0.45
1:B:754:LEU:HD13	1:B:754:LEU:HA	1.73	0.45
1:A:380:TYR:HD2	1:A:429:PHE:HD2	1.63	0.45
2:H:32:TYR:OH	2:H:95:SER:OG	2.28	0.45
3:O:70:ILE:HD12	3:O:80:TYR:O	2.17	0.45
2:I:6:GLN:HB3	2:I:105:GLY:H	1.81	0.45
3:K:17:SER:HG	3:K:84:ASN:HA	1.81	0.45
1:C:657:ASN:HD21	4:C:1301:NAG:C7	2.28	0.45
1:C:1037:SER:O	1:C:1037:SER:OG	2.34	0.45
1:A:372:ALA:O	1:A:374:PHE:N	2.49	0.45
1:C:340:GLU:OE1	3:K:105:TYR:HB3	2.17	0.45
1:C:405:ASN:CG	1:C:504:GLY:HA3	2.37	0.45
1:C:497:PHE:CE2	1:C:507:PRO:HB3	2.51	0.45
1:C:520:ALA:O	1:C:521:PRO:C	2.55	0.45
1:C:821:LEU:HD12	1:C:821:LEU:HA	1.57	0.45
1:B:334:ASN:ND2	1:B:361:CYS:HA	2.32	0.45
1:B:524:VAL:O	1:B:524:VAL:HG13	2.16	0.45
1:B:903:ALA:HB2	1:B:916:LEU:HD23	1.99	0.45
1:A:103:GLY:CA	1:A:241:LEU:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ASN:OD1	1:A:579:PRO:HB3	2.16	0.45
1:A:551:VAL:HG12	1:A:588:THR:O	2.15	0.45
1:A:616:ASN:ND2	4:A:1310:NAG:C7	2.80	0.45
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.78	0.45
3:J:39:GLN:HB3	3:J:93:VAL:HG13	1.98	0.45
3:O:1:GLN:OE1	3:O:2:VAL:HG23	2.17	0.45
2:I:28:ASP:OD1	2:I:29:VAL:N	2.42	0.45
4:C:1307:NAG:O3	4:A:1301:NAG:H5	2.16	0.45
1:B:347:PHE:HD1	1:B:347:PHE:HA	1.63	0.45
1:B:357:ARG:HG3	1:B:396:TYR:HE1	1.81	0.45
1:B:801:ASN:OD1	4:B:1313:NAG:H82	2.17	0.45
3:J:36:TRP:HB2	3:J:48:VAL:HB	1.99	0.45
3:K:40:PRO:HA	3:K:92:ALA:HA	1.99	0.45
1:C:473:TYR:O	1:C:488:CYS:HA	2.16	0.45
1:B:372:ALA:O	1:B:374:PHE:N	2.49	0.45
1:B:471:GLU:H	1:B:491:PRO:HG3	1.81	0.45
2:H:7:PRO:HD3	2:H:21:SER:O	2.16	0.45
2:I:88:TYR:O	2:I:105:GLY:HA2	2.17	0.45
1:B:127:VAL:HG13	1:B:129:LYS:HE3	1.99	0.45
1:B:822:LEU:HD23	1:B:822:LEU:HA	1.71	0.45
1:A:106:PHE:CE1	1:A:238:PHE:HB2	2.52	0.45
1:A:468:ILE:HG22	1:A:468:ILE:O	2.17	0.45
1:A:546:LEU:HD21	1:A:565:PHE:CZ	2.52	0.45
3:J:89:GLU:O	3:J:89:GLU:HG3	2.17	0.45
3:J:98:ARG:HB3	3:J:114:PRO:CG	2.46	0.45
3:O:12:VAL:HG12	3:O:13:LYS:N	2.31	0.45
1:B:821:LEU:HD12	1:B:821:LEU:HA	1.72	0.45
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.49	0.45
1:A:203:ILE:HB	1:A:227:VAL:HG12	1.97	0.45
3:O:20:LEU:HD21	3:O:83:MET:HG3	1.97	0.45
3:O:50:TYR:N	3:O:59:TYR:O	2.50	0.45
1:C:33:THR:HG23	1:C:33:THR:O	2.17	0.45
1:B:114:THR:O	1:B:116:SER:N	2.48	0.45
1:B:117:LEU:HA	1:B:130:VAL:HA	1.99	0.45
1:B:353:TRP:O	1:B:466:ARG:NH2	2.50	0.45
1:A:447:GLY:HA2	1:A:497:PHE:O	2.17	0.45
3:K:98:ARG:O	3:K:114:PRO:HD2	2.17	0.45
1:C:276:LEU:HB3	1:C:289:VAL:CG2	2.47	0.45
1:C:382:VAL:HG21	1:C:387:LEU:HD13	1.99	0.45
1:C:699:LEU:HD22	1:A:873:TYR:OH	2.17	0.45
1:C:866:THR:HG22	1:C:869:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:THR:HA	1:B:362:VAL:HG21	1.99	0.45
1:B:434:ILE:O	1:B:510:VAL:HG23	2.17	0.45
1:B:805:ILE:HD13	1:B:805:ILE:HG21	1.65	0.45
2:H:28:ASP:OD2	2:H:92:SER:HB3	2.17	0.45
3:J:35:ASN:ND2	3:J:112:LEU:HD21	2.31	0.45
2:N:63:ARG:NH2	2:N:81:GLN:HG3	2.32	0.45
2:I:38:TYR:CD1	2:I:48:LEU:HA	2.36	0.45
1:B:190:ARG:HH21	1:B:207:HIS:CD2	2.35	0.44
1:A:403:ARG:CZ	1:A:405:ASN:ND2	2.80	0.44
1:A:895:GLN:O	1:A:895:GLN:HG2	2.16	0.44
3:K:67:ARG:HD3	3:K:68:PHE:HE1	1.81	0.44
1:C:171:VAL:O	1:C:172:SER:OG	2.34	0.44
1:C:913:GLN:H	1:C:913:GLN:HG2	1.41	0.44
1:B:616:ASN:OD1	1:B:616:ASN:C	2.55	0.44
1:A:826:VAL:HG23	1:A:949:GLN:OE1	2.17	0.44
3:K:20:LEU:HD11	3:K:119:ILE:HD11	1.98	0.44
3:K:38:ARG:HB3	3:K:48:VAL:HG22	1.98	0.44
1:C:996:LEU:HA	1:C:996:LEU:HD23	1.54	0.44
1:B:418:ILE:HA	1:B:422:ASN:ND2	2.33	0.44
1:B:537:LYS:O	1:B:539:VAL:HG13	2.16	0.44
1:A:165:ASN:HD21	4:A:1303:NAG:C4	2.27	0.44
1:A:825:LYS:HE3	1:A:825:LYS:HB3	1.87	0.44
1:A:865:LEU:HD23	1:A:865:LEU:HA	1.75	0.44
1:A:934:ILE:HD12	1:A:934:ILE:HG23	1.72	0.44
2:H:35:VAL:HB	2:H:68:LYS:CE	2.48	0.44
3:K:70:ILE:CG1	3:K:79:LEU:HD21	2.48	0.44
1:C:106:PHE:HB3	1:C:235:ILE:CD1	2.48	0.44
1:C:452:ARG:HH21	1:C:492:LEU:HD12	1.82	0.44
1:C:1049:LEU:HA	1:C:1049:LEU:HD23	1.68	0.44
1:B:421:TYR:CB	1:B:457:ARG:HD2	2.46	0.44
1:B:1024:LEU:HA	1:B:1024:LEU:HD12	1.75	0.44
1:A:403:ARG:HB2	1:A:495:TYR:OH	2.18	0.44
1:A:699:LEU:HA	1:A:699:LEU:HD23	1.69	0.44
2:H:68:LYS:HA	2:H:73:ALA:HA	1.98	0.44
3:O:84:ASN:OD1	3:O:84:ASN:N	2.49	0.44
3:K:37:ILE:HD12	3:K:47:TRP:HA	1.98	0.44
1:C:616:ASN:HD21	4:C:1306:NAG:H83	1.81	0.44
2:N:64:PHE:CE2	2:N:77:ILE:HD13	2.52	0.44
1:C:83:VAL:HG12	1:C:239:GLN:HE21	1.82	0.44
1:C:92:PHE:HE1	1:C:94:SER:OG	2.01	0.44
1:C:752:LEU:HA	1:C:752:LEU:HD12	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1306:NAG:O7	4:C:1306:NAG:H3	2.17	0.44
1:B:353:TRP:NE1	1:B:423:TYR:HD1	2.15	0.44
1:A:329:PHE:HB2	1:A:529:LYS:O	2.18	0.44
3:J:47:TRP:HE1	3:J:62:ASP:H	1.65	0.44
2:I:49:MET:SD	2:I:50:ILE:HG23	2.57	0.44
3:K:8:GLY:O	3:K:18:LEU:HD11	2.17	0.44
3:K:89:GLU:OE2	3:K:89:GLU:N	2.51	0.44
1:C:338:PHE:C	1:C:340:GLU:N	2.69	0.44
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.52	0.44
1:B:1139:ASP:OD1	1:B:1139:ASP:N	2.43	0.44
1:A:720:ILE:HG21	1:A:720:ILE:HD13	1.40	0.44
2:N:50:ILE:HG22	2:N:51:TYR:N	2.32	0.44
3:K:9:GLY:HA2	3:K:18:LEU:HD21	1.98	0.44
1:C:385:THR:HG21	1:B:473:TYR:HE2	1.82	0.44
1:C:442:ASP:O	1:C:448:ASN:ND2	2.51	0.44
1:A:662:CYS:HB2	1:A:671:CYS:HB3	1.82	0.44
2:H:98:THR:HG23	3:J:47:TRP:CZ3	2.53	0.44
2:I:28:ASP:HA	2:I:94:THR:HG23	2.00	0.44
1:C:411:ALA:C	1:C:425:LEU:HD11	2.39	0.44
1:C:1084:ASP:HB2	1:C:1086:LYS:HE3	1.99	0.44
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.52	0.44
1:B:603:ASN:OD1	1:B:603:ASN:O	2.36	0.44
1:B:1055:SER:OG	1:B:1056:ALA:N	2.51	0.44
1:A:616:ASN:C	1:A:616:ASN:OD1	2.56	0.44
2:H:24:GLY:HA3	2:H:29:VAL:CG2	2.48	0.44
3:O:38:ARG:HH22	3:O:64:VAL:HG11	1.83	0.44
3:K:12:VAL:CG2	3:K:123:VAL:HG12	2.48	0.44
3:K:72:ARG:HG3	3:K:74:ASN:HD21	1.81	0.44
1:B:236:THR:OG1	4:B:1302:NAG:H82	2.18	0.43
1:B:492:LEU:HD23	1:B:492:LEU:HA	1.79	0.43
1:B:1146:ASP:OD2	1:A:1146:ASP:N	2.52	0.43
2:H:53:VAL:CG2	2:H:68:LYS:HD3	2.48	0.43
1:C:34:ARG:NH1	1:C:191:GLU:OE1	2.43	0.43
2:H:63:ARG:HH22	2:H:81:GLN:HG3	1.78	0.43
3:J:35:ASN:HD21	3:J:112:LEU:HD21	1.83	0.43
2:I:85:GLU:OE2	2:I:109:THR:HA	2.17	0.43
1:C:351:TYR:CE1	1:C:468:ILE:HG23	2.53	0.43
1:C:934:ILE:HD12	1:C:934:ILE:HG23	1.67	0.43
1:C:1054:GLN:HA	1:C:1054:GLN:NE2	2.34	0.43
1:B:1081:ILE:HG23	1:B:1081:ILE:HD12	1.64	0.43
1:A:139:PRO:HB3	1:A:241:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HG2	1:A:170:TYR:H	1.82	0.43
1:A:397:ALA:HA	1:A:512:VAL:O	2.18	0.43
3:J:38:ARG:NH2	3:J:40:PRO:HG3	2.34	0.43
2:I:24:GLY:HA3	2:I:29:VAL:CG1	2.49	0.43
1:C:517:LEU:C	1:C:519:HIS:H	2.22	0.43
1:B:36:VAL:HG21	1:B:220:PHE:HZ	1.80	0.43
1:B:223:LEU:HD12	1:B:223:LEU:N	2.33	0.43
1:B:934:ILE:HA	1:B:934:ILE:HD13	1.74	0.43
1:A:335:LEU:HD12	1:A:335:LEU:H	1.83	0.43
1:A:616:ASN:OD1	1:A:617:CYS:N	2.50	0.43
1:C:346:ARG:HH11	3:K:101:PRO:HG2	1.83	0.43
1:C:555:SER:OG	1:C:584:ILE:O	2.26	0.43
1:B:375:PHE:CZ	1:A:503:VAL:HB	2.53	0.43
1:B:788:ILE:HD13	1:B:788:ILE:HA	1.76	0.43
1:A:40:ASP:O	1:A:42:VAL:HG13	2.17	0.43
1:A:197:ILE:HG23	1:A:198:ASP:N	2.34	0.43
1:A:324:GLU:O	1:A:539:VAL:HG13	2.18	0.43
1:A:603:ASN:OD1	1:A:603:ASN:O	2.36	0.43
1:C:1024:LEU:HD12	1:C:1024:LEU:HA	1.73	0.43
1:B:226:LEU:HA	1:B:226:LEU:HD12	1.71	0.43
1:B:335:LEU:HD22	1:B:335:LEU:HA	1.70	0.43
1:A:101:ILE:HD11	1:A:240:THR:CG2	2.48	0.43
1:A:118:LEU:HD12	1:A:119:ILE:H	1.84	0.43
3:O:18:LEU:HD12	3:O:19:ARG:H	1.83	0.43
2:I:63:ARG:O	2:I:78:SER:N	2.47	0.43
1:C:984:LEU:HA	1:C:984:LEU:HD23	1.81	0.43
1:B:425:LEU:C	1:B:425:LEU:HD12	2.39	0.43
1:B:449:TYR:OH	1:B:498:ARG:NH1	2.52	0.43
1:A:36:VAL:HG11	1:A:220:PHE:CE2	2.53	0.43
1:A:457:ARG:NE	1:A:458:LYS:H	2.14	0.43
1:A:822:LEU:HA	1:A:822:LEU:HD23	1.82	0.43
3:J:38:ARG:HH22	3:J:40:PRO:HG3	1.82	0.43
3:O:120:LEU:HD21	3:O:122:THR:HG23	2.00	0.43
2:I:12:GLY:O	2:I:111:LEU:N	2.47	0.43
3:K:54:ASN:HB3	3:K:56:TYR:CD2	2.48	0.43
1:C:353:TRP:CZ3	1:C:466:ARG:HD3	2.54	0.43
1:C:378:LYS:HD2	1:C:378:LYS:HA	1.59	0.43
1:C:395:VAL:HG22	1:C:515:PHE:CB	2.48	0.43
1:C:398:ASP:HB2	1:C:512:VAL:HG12	2.00	0.43
1:C:425:LEU:H	1:C:425:LEU:CD2	2.28	0.43
1:C:441:LEU:HD13	2:I:32:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1001:LEU:HA	1:C:1001:LEU:HD12	1.74	0.43
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.60	0.43
1:B:801:ASN:HD21	4:B:1313:NAG:C7	2.32	0.43
1:B:1095:PHE:CE1	1:B:1104:VAL:HG22	2.54	0.43
3:J:38:ARG:HB2	3:J:48:VAL:HG22	2.00	0.43
2:I:29:VAL:HG22	2:I:68:LYS:HZ1	1.84	0.43
1:C:43:PHE:CE2	1:B:557:LYS:HD3	2.53	0.43
1:C:346:ARG:HD2	3:K:103:GLY:O	2.18	0.43
1:B:85:PRO:O	1:B:269:TYR:OH	2.19	0.43
1:B:128:ILE:HD13	1:B:170:TYR:CD1	2.54	0.43
1:B:1137:VAL:HG23	1:B:1137:VAL:O	2.18	0.43
1:A:130:VAL:O	1:A:130:VAL:HG13	2.18	0.43
1:A:658:SER:OG	1:A:660:TYR:OH	2.28	0.43
1:A:1081:ILE:HD13	1:A:1081:ILE:HA	1.80	0.43
2:N:23:THR:OG1	2:N:24:GLY:N	2.51	0.43
2:I:10:VAL:HG22	2:I:11:SER:H	1.83	0.43
3:K:109:GLY:O	3:K:111:ARG:NH1	2.52	0.43
1:B:223:LEU:HD12	1:B:223:LEU:H	1.84	0.43
1:A:276:LEU:HB3	1:A:289:VAL:HG23	2.01	0.43
1:A:374:PHE:HE1	1:A:434:ILE:HG21	1.84	0.43
1:A:540:ASN:ND2	1:A:549:THR:OG1	2.51	0.43
1:A:657:ASN:HD21	4:A:1305:NAG:C1	2.32	0.43
3:J:108:SER:HB3	3:J:111:ARG:HH22	1.83	0.43
1:C:439:ASN:HB3	1:C:440:LYS:NZ	2.34	0.42
1:B:126:VAL:HG11	1:B:175:PHE:CE1	2.54	0.42
1:B:130:VAL:CG1	1:B:168:PHE:HB3	2.49	0.42
1:B:338:PHE:C	1:B:340:GLU:H	2.22	0.42
3:J:35:ASN:HB3	3:J:50:TYR:CD1	2.54	0.42
3:O:18:LEU:O	3:O:82:GLN:HG2	2.18	0.42
1:C:64:TRP:CD1	1:C:65:PHE:N	2.87	0.42
1:A:33:THR:HG23	1:A:33:THR:O	2.19	0.42
1:A:234:ASN:HD21	4:A:1302:NAG:C1	2.32	0.42
1:A:402:ILE:HD12	1:A:495:TYR:OH	2.19	0.42
1:A:407:VAL:O	1:A:410:ILE:HG22	2.19	0.42
1:A:896:ILE:HG21	1:A:896:ILE:HD13	1.70	0.42
3:J:33:TYR:CD2	3:J:52:SER:HA	2.55	0.42
2:N:39:GLN:HE21	2:N:86:ALA:HB3	1.84	0.42
3:O:36:TRP:HE1	3:O:79:LEU:CD2	2.32	0.42
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	2.02	0.42
1:A:355:ARG:HA	1:A:397:ALA:O	2.18	0.42
1:A:426:PRO:HG3	1:A:463:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:ILE:HD13	1:A:934:ILE:HA	1.82	0.42
2:N:4:LEU:HD13	2:N:22:CYS:SG	2.59	0.42
1:C:822:LEU:HD23	1:C:822:LEU:HA	1.73	0.42
1:B:382:VAL:HG21	1:B:387:LEU:HD13	2.00	0.42
1:A:403:ARG:HB2	1:A:495:TYR:HE1	1.83	0.42
1:A:526:GLY:N	1:A:527:PRO:CD	2.83	0.42
1:A:719:THR:HG23	1:A:719:THR:O	2.19	0.42
2:N:87:ASP:HA	2:N:106:THR:O	2.18	0.42
1:C:325:SER:HA	1:C:540:ASN:O	2.19	0.42
1:C:405:ASN:N	1:C:504:GLY:O	2.52	0.42
1:C:576:VAL:O	1:C:585:LEU:N	2.44	0.42
1:C:616:ASN:HD21	4:C:1306:NAG:C7	2.33	0.42
1:A:64:TRP:CD1	1:A:65:PHE:N	2.88	0.42
1:A:105:ILE:HD13	1:A:105:ILE:HG21	1.76	0.42
3:J:100:GLN:NE2	3:J:111:ARG:HH21	2.18	0.42
1:C:133:PHE:HA	1:C:163:ALA:O	2.20	0.42
1:A:821:LEU:HD12	1:A:821:LEU:HA	1.65	0.42
3:O:112:LEU:HD12	3:O:112:LEU:H	1.85	0.42
2:I:40:GLN:C	2:I:86:ALA:HB1	2.39	0.42
1:C:1114:ILE:HD13	1:C:1114:ILE:HA	1.83	0.42
1:C:1139:ASP:OD1	1:C:1139:ASP:N	2.44	0.42
1:B:334:ASN:HD21	1:B:361:CYS:HA	1.84	0.42
1:A:282:ASN:ND2	4:A:1304:NAG:C7	2.82	0.42
1:A:454:ARG:HA	1:A:492:LEU:HA	2.01	0.42
1:A:1081:ILE:HD12	1:A:1081:ILE:HG23	1.57	0.42
3:O:62:ASP:OD1	3:O:62:ASP:N	2.51	0.42
1:C:229:LEU:HB3	1:C:231:ILE:HG12	2.02	0.42
1:C:328:ARG:NE	1:C:578:ASP:OD2	2.50	0.42
1:B:534:VAL:HG21	1:B:539:VAL:HG11	2.00	0.42
1:A:350:VAL:HG23	1:A:400:PHE:CD2	2.55	0.42
1:A:1139:ASP:N	1:A:1139:ASP:OD1	2.40	0.42
2:H:61:SER:C	2:H:63:ARG:H	2.23	0.42
3:J:9:GLY:HA2	3:J:18:LEU:HD11	2.01	0.42
3:O:113:ASP:HB3	3:O:114:PRO:CD	2.49	0.42
1:C:83:VAL:HG21	1:C:237:ARG:NH1	2.35	0.42
1:A:517:LEU:C	1:A:519:HIS:N	2.73	0.42
2:H:29:VAL:HG13	2:H:35:VAL:CG2	2.50	0.42
3:J:34:MET:HB2	3:J:51:ILE:HG22	2.01	0.42
1:C:501:TYR:O	1:C:506:GLN:NE2	2.53	0.42
1:C:577:ARG:HA	1:C:583:GLU:O	2.20	0.42
1:B:520:ALA:O	1:B:521:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:THR:HA	1:B:690:GLN:N	2.35	0.42
1:A:1004:LEU:HA	1:A:1004:LEU:HD12	1.82	0.42
1:C:29:THR:O	1:C:61:ASN:HA	2.20	0.41
1:C:461:LEU:CD1	1:C:465:GLU:HG3	2.46	0.41
1:C:895:GLN:O	1:C:895:GLN:HG2	2.20	0.41
1:B:105:ILE:HD11	1:B:239:GLN:HB2	2.01	0.41
1:B:1054:GLN:HA	1:B:1054:GLN:NE2	2.35	0.41
1:A:815:ARG:NH2	1:A:820:ASP:OD1	2.53	0.41
2:H:62:ASN:OD1	2:H:62:ASN:N	2.53	0.41
2:I:9:SER:OG	2:I:107:LYS:HB2	2.20	0.41
1:C:934:ILE:HD13	1:C:934:ILE:HA	1.76	0.41
1:C:1083:HIS:O	1:C:1086:LYS:HG2	2.20	0.41
1:A:959:LEU:HA	1:A:959:LEU:HD23	1.78	0.41
3:O:2:VAL:HG22	3:O:26:GLY:HA3	2.01	0.41
3:O:39:GLN:HG3	3:O:44:GLY:O	2.19	0.41
2:I:35:VAL:CG1	2:I:53:VAL:HG22	2.50	0.41
1:C:826:VAL:CG1	1:C:1057:PRO:HG2	2.51	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:CE3	2.55	0.41
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.56	0.41
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.02	0.41
3:J:99:GLU:HG3	3:J:101:PRO:HD2	2.01	0.41
2:N:5:THR:HB	2:N:23:THR:HG22	2.01	0.41
1:C:380:TYR:HD2	1:C:429:PHE:HE2	1.69	0.41
1:B:82:PRO:C	1:B:239:GLN:NE2	2.74	0.41
1:B:388:ASN:O	1:B:527:PRO:HD2	2.20	0.41
3:J:37:ILE:O	3:J:95:TYR:N	2.45	0.41
3:O:3:GLN:HB2	3:O:25:SER:OG	2.21	0.41
1:C:317:ASN:ND2	1:A:737:ASP:OD2	2.54	0.41
1:C:498:ARG:NH2	1:C:501:TYR:OH	2.54	0.41
1:C:586:ASP:OD1	1:C:587:ILE:N	2.53	0.41
1:C:896:ILE:HD13	1:C:896:ILE:HG21	1.69	0.41
1:B:346:ARG:O	1:B:346:ARG:HG3	2.20	0.41
1:B:385:THR:OG1	1:A:420:ASP:OD2	2.30	0.41
1:B:586:ASP:OD1	1:B:586:ASP:C	2.59	0.41
1:A:543:PHE:CE2	1:A:576:VAL:HG11	2.56	0.41
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.56	0.41
3:J:118:GLY:O	3:J:119:ILE:HD13	2.21	0.41
3:O:27:PHE:HE2	3:O:32:SER:OG	2.03	0.41
2:I:40:GLN:HB3	2:I:87:ASP:HB2	2.01	0.41
1:B:962:LEU:HD12	1:B:962:LEU:HA	1.60	0.41
1:A:308:VAL:H	1:A:602:THR:CG2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:O	1:A:312:ILE:HG23	2.20	0.41
2:H:48:LEU:HD22	2:H:57:PRO:HG3	2.02	0.41
3:J:47:TRP:CD1	3:J:61:GLY:HA2	2.56	0.41
1:C:603:ASN:O	1:C:603:ASN:OD1	2.39	0.41
1:C:719:THR:HG23	1:C:719:THR:O	2.21	0.41
3:O:67:ARG:HH21	3:O:87:ARG:CZ	2.34	0.41
2:I:29:VAL:HG13	2:I:30:GLY:H	1.86	0.41
3:K:35:ASN:HB2	3:K:47:TRP:HE1	1.84	0.41
3:K:94:TYR:HE1	3:K:121:VAL:HG11	1.85	0.41
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.02	0.41
1:B:483:VAL:HG22	1:B:484:ALA:N	2.28	0.41
1:B:801:ASN:ND2	4:B:1313:NAG:N2	2.59	0.41
1:A:362:VAL:CG2	1:A:526:GLY:HA3	2.37	0.41
3:J:2:VAL:HG21	3:J:98:ARG:NH1	2.35	0.41
1:C:187:LYS:HA	1:C:210:ILE:HG22	2.03	0.41
1:C:353:TRP:CE3	1:C:466:ARG:HD3	2.56	0.41
4:C:1307:NAG:HO3	4:C:1307:NAG:C7	2.32	0.41
1:B:117:LEU:HD23	1:B:118:LEU:N	2.36	0.41
1:A:70:VAL:HG22	1:A:80:ASP:HA	2.02	0.41
1:A:452:ARG:HG2	1:A:494:SER:CB	2.51	0.41
1:A:472:ILE:HD13	1:A:472:ILE:HA	1.94	0.41
2:H:6:GLN:OE1	2:H:105:GLY:N	2.47	0.41
3:O:3:GLN:C	3:O:4:LEU:HD22	2.41	0.41
2:I:50:ILE:HA	2:I:57:PRO:HD3	2.03	0.41
3:K:72:ARG:NH1	3:K:74:ASN:OD1	2.49	0.41
1:B:620:VAL:O	1:B:620:VAL:HG22	2.21	0.41
2:H:56:ARG:HA	2:H:57:PRO:HD3	1.94	0.41
2:I:52:ASP:O	2:I:54:SER:N	2.53	0.41
3:K:6:GLU:OE2	3:K:96:CYS:HB3	2.20	0.41
1:C:353:TRP:CD1	1:C:423:TYR:HB2	2.56	0.40
1:C:357:ARG:NH1	1:C:394:ASN:HB3	2.35	0.40
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.84	0.40
1:B:438:SER:OG	1:B:509:ARG:HG3	2.21	0.40
1:B:664:ILE:HD13	1:B:664:ILE:HG21	1.75	0.40
3:J:29:ILE:HG13	3:J:29:ILE:O	2.22	0.40
3:J:67:ARG:NH1	3:J:90:ASP:OD2	2.53	0.40
2:N:39:GLN:HA	2:N:87:ASP:O	2.21	0.40
3:K:72:ARG:HG3	3:K:74:ASN:ND2	2.36	0.40
1:C:272:PRO:C	1:C:273:ARG:HG2	2.42	0.40
1:C:365:TYR:HA	1:C:368:LEU:HD13	2.03	0.40
1:B:29:THR:O	1:B:62:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:LEU:HD12	1:B:1001:LEU:HA	1.64	0.40
1:A:266:TYR:CD1	1:A:266:TYR:N	2.88	0.40
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.85	0.40
1:A:324:GLU:HG2	1:A:539:VAL:HG13	2.03	0.40
1:A:864:LEU:HA	1:A:864:LEU:HD12	1.79	0.40
1:A:1080:ALA:O	1:A:1132:ILE:HG13	2.21	0.40
2:N:44:LYS:HD3	2:N:44:LYS:N	2.36	0.40
1:B:472:ILE:HD13	1:B:490:PHE:HA	2.02	0.40
1:A:791:THR:HG22	1:A:792:PRO:HD2	2.02	0.40
1:A:922:LEU:HD12	1:A:922:LEU:HA	1.68	0.40
3:J:94:TYR:O	3:J:118:GLY:HA2	2.21	0.40
2:N:39:GLN:N	2:N:47:LYS:O	2.30	0.40
1:B:168:PHE:HB2	1:A:357:ARG:NH1	2.36	0.40
1:B:720:ILE:HG21	1:B:720:ILE:HD13	1.41	0.40
1:A:1091:ARG:O	1:A:1092:GLU:HG3	2.22	0.40
2:H:53:VAL:HG22	2:H:68:LYS:HD3	2.03	0.40
2:I:32:TYR:CZ	2:I:95:SER:HB3	2.56	0.40
3:K:37:ILE:CG2	3:K:95:TYR:HB2	2.48	0.40
1:C:189:LEU:HB2	1:C:208:THR:HG23	2.02	0.40
1:C:270:LEU:N	1:C:270:LEU:HD12	2.37	0.40
1:C:395:VAL:HG13	1:C:515:PHE:HD2	1.87	0.40
1:C:402:ILE:HD12	1:C:402:ILE:HG23	1.84	0.40
1:C:452:ARG:NH1	3:K:56:TYR:HB3	2.36	0.40
1:C:533:LEU:HG	1:C:534:VAL:N	2.37	0.40
1:C:581:THR:HG23	1:C:583:GLU:H	1.86	0.40
1:C:922:LEU:HD12	1:C:922:LEU:HA	1.77	0.40
1:B:247:SER:HB3	1:B:258:TRP:CD1	2.56	0.40
1:B:410:ILE:HD12	1:B:423:TYR:CE2	2.56	0.40
1:A:106:PHE:HB3	1:A:235:ILE:HD11	2.03	0.40
1:A:118:LEU:HD12	1:A:119:ILE:N	2.36	0.40
1:A:391:CYS:HA	1:A:525:CYS:HB3	2.03	0.40
2:H:36:SER:O	2:H:90:CYS:HA	2.21	0.40
3:J:67:ARG:NH2	3:J:85:SER:O	2.55	0.40
2:N:29:VAL:HG13	2:N:30:GLY:N	2.36	0.40
2:I:38:TYR:HE2	2:I:91:SER:HB3	1.86	0.40
3:K:98:ARG:HB3	3:K:114:PRO:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1008/1288 (78%)	955 (95%)	47 (5%)	6 (1%)	25	62
1	B	1008/1288 (78%)	961 (95%)	41 (4%)	6 (1%)	25	62
1	C	1008/1288 (78%)	958 (95%)	45 (4%)	5 (0%)	29	66
2	H	108/111 (97%)	94 (87%)	12 (11%)	2 (2%)	8	40
2	I	108/111 (97%)	95 (88%)	11 (10%)	2 (2%)	8	40
2	N	108/111 (97%)	92 (85%)	14 (13%)	2 (2%)	8	40
3	J	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
3	K	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
3	O	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
All	All	3717/4572 (81%)	3496 (94%)	198 (5%)	23 (1%)	29	62

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	527	PRO
2	H	53	VAL
2	N	53	VAL
1	B	528	LYS
1	A	525	CYS
1	A	528	LYS
2	I	53	VAL
1	C	373	PRO
2	H	85	GLU
2	N	85	GLU
2	I	85	GLU
1	C	332	ILE
1	C	372	ALA
1	B	331	ASN
1	B	372	ALA
1	B	373	PRO

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Mol	Chain	Res	Type
1	A	373	PRO
1	A	529	LYS
1	B	521	PRO
1	A	372	ALA
1	A	521	PRO
1	C	521	PRO
1	B	332	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	807/1113 (72%)	795 (98%)	12 (2%)	65	81
1	B	807/1113 (72%)	798 (99%)	9 (1%)	73	85
1	C	807/1113 (72%)	795 (98%)	12 (2%)	65	81
2	H	92/93 (99%)	92 (100%)	0	100	100
2	I	92/93 (99%)	92 (100%)	0	100	100
2	N	92/93 (99%)	91 (99%)	1 (1%)	73	85
3	J	103/103 (100%)	101 (98%)	2 (2%)	57	76
3	K	103/103 (100%)	101 (98%)	2 (2%)	57	76
3	O	103/103 (100%)	102 (99%)	1 (1%)	76	86
All	All	3006/3927 (76%)	2967 (99%)	39 (1%)	70	83

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	141	LEU
1	C	227	VAL
1	C	329	PHE
1	C	333	THR
1	C	334	ASN
1	C	374	PHE
1	C	538	CYS

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Mol	Chain	Res	Type
1	C	578	ASP
1	C	617	CYS
1	C	649	CYS
1	C	756	TYR
1	C	886	TRP
1	B	131	CYS
1	B	227	VAL
1	B	334	ASN
1	B	335	LEU
1	B	347	PHE
1	B	617	CYS
1	B	756	TYR
1	B	886	TRP
1	B	1127	ASP
1	A	131	CYS
1	A	166	CYS
1	A	336	CYS
1	A	346	ARG
1	A	374	PHE
1	A	517	LEU
1	A	617	CYS
1	A	649	CYS
1	A	738	CYS
1	A	859	THR
1	A	861	LEU
1	A	886	TRP
3	J	11	LEU
3	J	31	ASP
2	N	48	LEU
3	O	104	TYR
3	K	45	LEU
3	K	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	C	188	ASN
1	C	234	ASN
1	C	239	GLN
1	C	354	ASN
1	C	405	ASN

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Mol	Chain	Res	Type
1	C	422	ASN
1	C	448	ASN
1	C	505	HIS
1	C	641	ASN
1	C	657	ASN
1	C	751	ASN
1	C	801	ASN
1	C	1074	ASN
1	C	1098	ASN
1	C	1134	ASN
1	B	30	ASN
1	B	188	ASN
1	B	334	ASN
1	B	354	ASN
1	B	414	GLN
1	B	422	ASN
1	B	439	ASN
1	B	493	GLN
1	B	505	HIS
1	B	657	ASN
1	B	709	ASN
1	B	755	GLN
1	B	801	ASN
1	B	1074	ASN
1	B	1098	ASN
1	B	1134	ASN
1	A	165	ASN
1	A	234	ASN
1	A	317	ASN
1	A	370	ASN
1	A	437	ASN
1	A	505	HIS
1	A	540	ASN
1	A	657	ASN
1	A	801	ASN
1	A	1074	ASN
1	A	1098	ASN
2	H	33	ASN
2	H	39	GLN
3	J	84	ASN
2	N	39	GLN
3	O	74	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
4	NAG	B	1311	-	14,14,15	0.37	0	17,19,21	0.61	0
4	NAG	C	1303	-	14,14,15	0.55	0	17,19,21	0.50	0
4	NAG	B	1304	-	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	C	1312	-	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	B	1302	-	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	A	1301	-	14,14,15	0.49	0	17,19,21	0.61	0
4	NAG	B	1310	-	14,14,15	0.44	0	17,19,21	0.62	0
4	NAG	A	1305	-	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	A	1302	-	14,14,15	0.24	0	17,19,21	0.53	0
4	NAG	A	1309	-	14,14,15	0.41	0	17,19,21	0.68	0
4	NAG	C	1306	-	14,14,15	0.28	0	17,19,21	0.55	0
4	NAG	B	1305	-	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	A	1312	-	14,14,15	0.43	0	17,19,21	0.51	0
4	NAG	C	1304	-	14,14,15	0.59	0	17,19,21	0.51	0
4	NAG	B	1303	-	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	B	1309	-	14,14,15	0.69	1 (7%)	17,19,21	0.57	0
4	NAG	C	1310	-	14,14,15	0.33	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1310	-	14,14,15	0.30	0	17,19,21	0.71	0
4	NAG	A	1306	-	14,14,15	0.35	0	17,19,21	0.53	0
4	NAG	A	1303	-	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	C	1301	-	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	A	1311	-	14,14,15	0.51	0	17,19,21	0.76	0
4	NAG	A	1307	-	14,14,15	0.32	0	17,19,21	0.42	0
4	NAG	C	1308	-	14,14,15	0.47	0	17,19,21	0.46	0
4	NAG	B	1312	-	14,14,15	0.28	0	17,19,21	0.73	0
4	NAG	C	1309	-	14,14,15	0.53	0	17,19,21	0.69	0
4	NAG	C	1307	-	14,14,15	0.35	0	17,19,21	0.77	0
4	NAG	C	1311	-	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	B	1308	-	14,14,15	0.43	0	17,19,21	0.56	0
4	NAG	A	1308	-	14,14,15	0.55	0	17,19,21	0.54	0
4	NAG	C	1305	-	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	B	1307	-	14,14,15	0.35	0	17,19,21	0.62	0
4	NAG	B	1306	-	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	B	1313	-	14,14,15	0.39	0	17,19,21	0.47	0
4	NAG	A	1304	-	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1302	-	14,14,15	0.41	0	17,19,21	0.59	0
4	NAG	B	1301	-	14,14,15	0.57	0	17,19,21	0.64	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
4	NAG	B	1311	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1309	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1306	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	-	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1306	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1311	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1312	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1311	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1308	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1313	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1304	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	-	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1309	NAG	O5-C1	-2.23	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1306	NAG	C3-C2-N2-C7
4	B	1305	NAG	C4-C5-C6-O6

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

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

There are no ring outliers.

27 monomers are involved in 58 short contacts:

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

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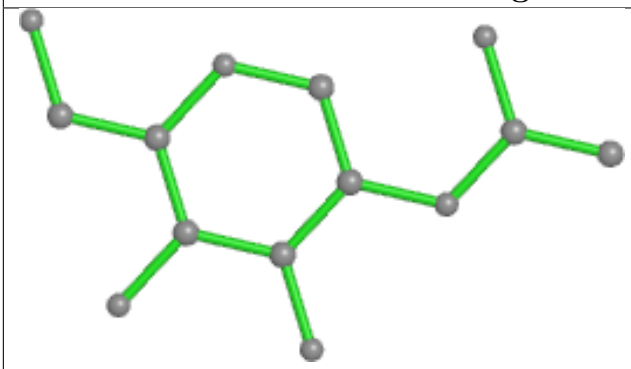
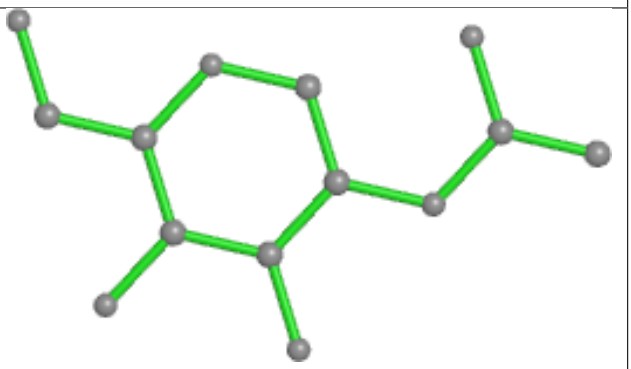
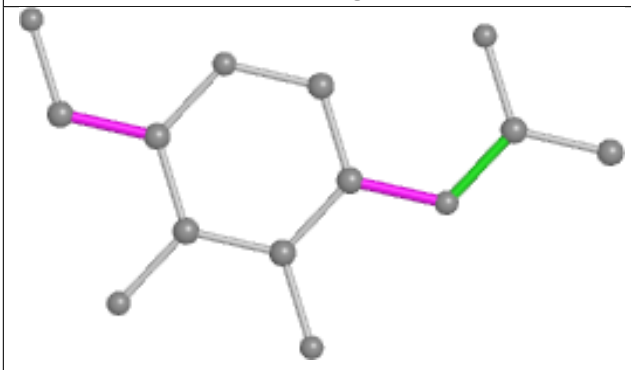
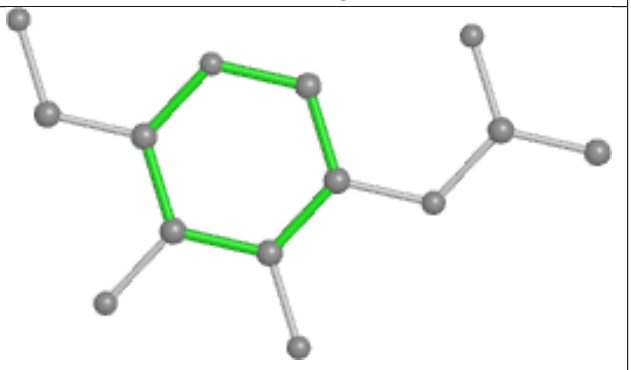
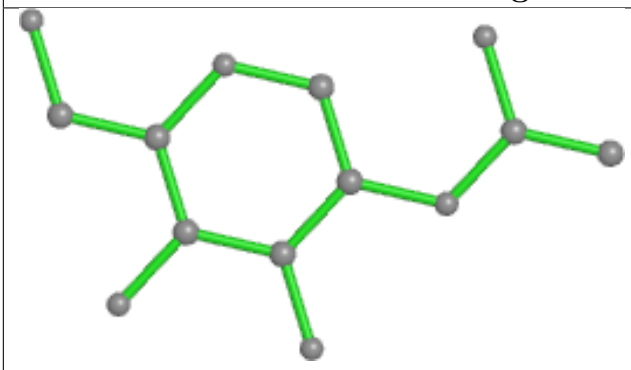
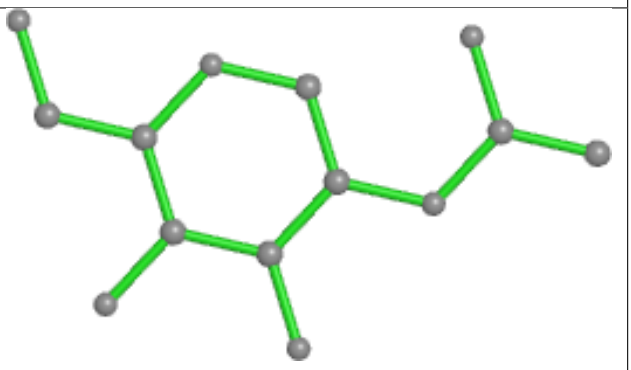
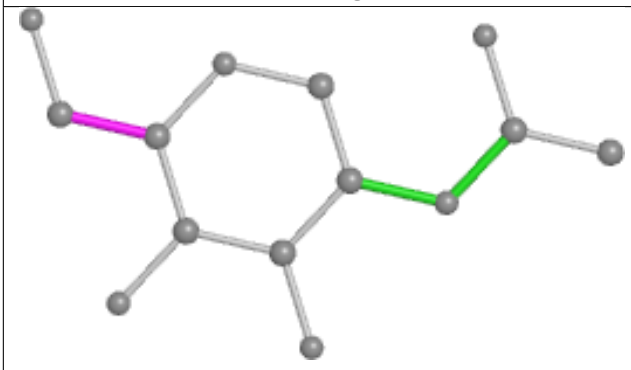
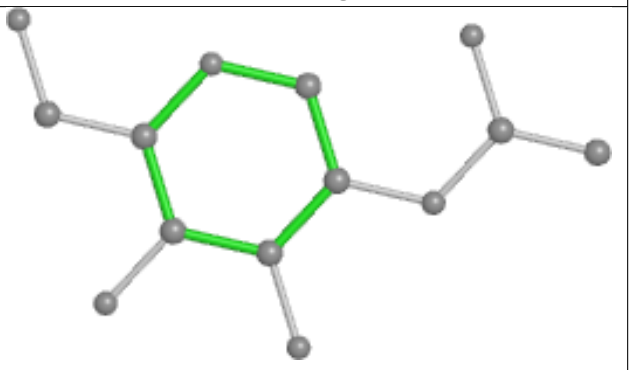
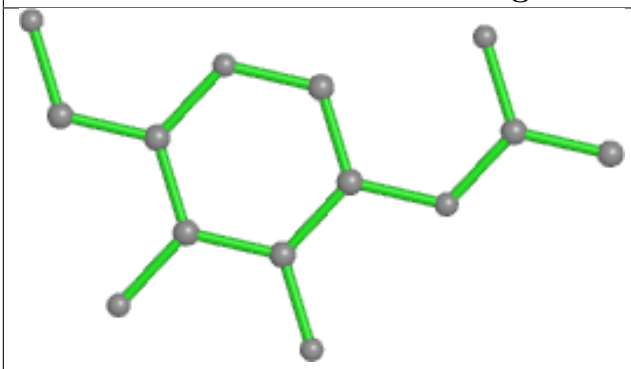
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1305	NAG	1	0
4	A	1312	NAG	3	0
4	C	1304	NAG	1	0
4	B	1309	NAG	2	0
4	C	1310	NAG	1	0
4	A	1310	NAG	2	0
4	A	1303	NAG	3	0
4	C	1301	NAG	1	0
4	C	1308	NAG	3	0
4	B	1312	NAG	3	0
4	C	1309	NAG	3	0
4	C	1307	NAG	4	0
4	B	1308	NAG	1	0
4	A	1308	NAG	1	0
4	C	1305	NAG	4	0
4	B	1313	NAG	5	0
4	A	1304	NAG	2	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

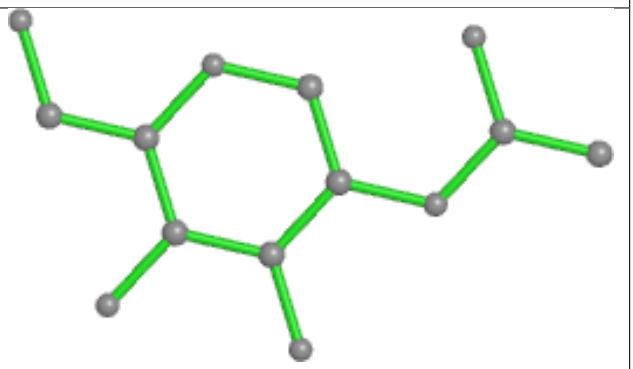
Ligand NAG B 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

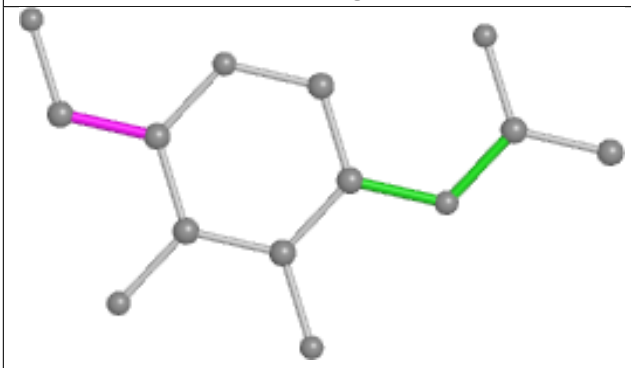
Ligand NAG B 1304



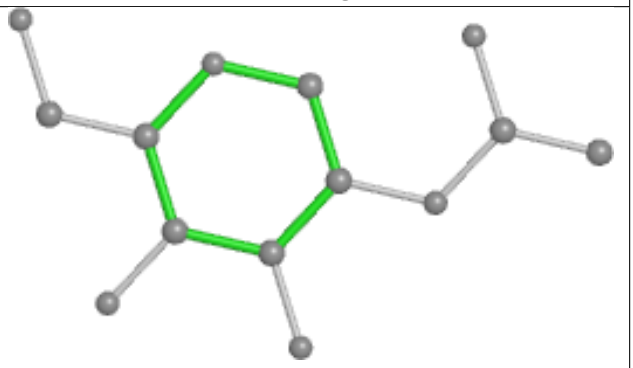
Bond lengths



Bond angles

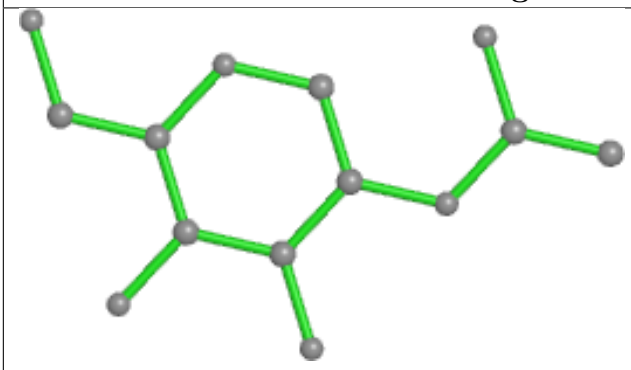


Torsions

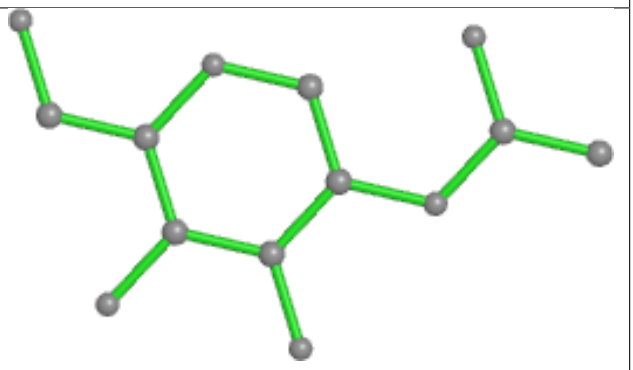


Rings

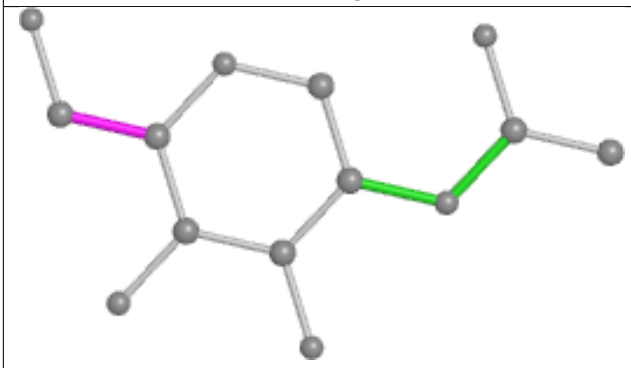
Ligand NAG C 1312



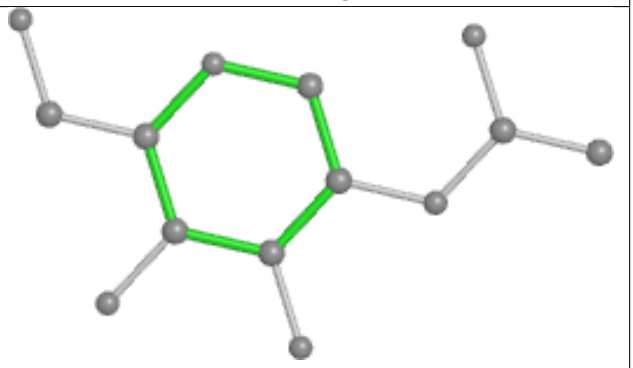
Bond lengths



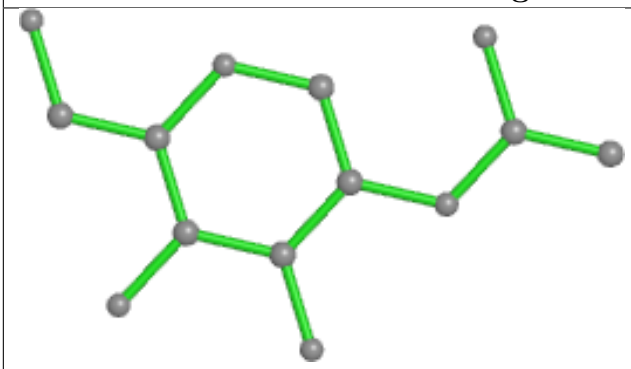
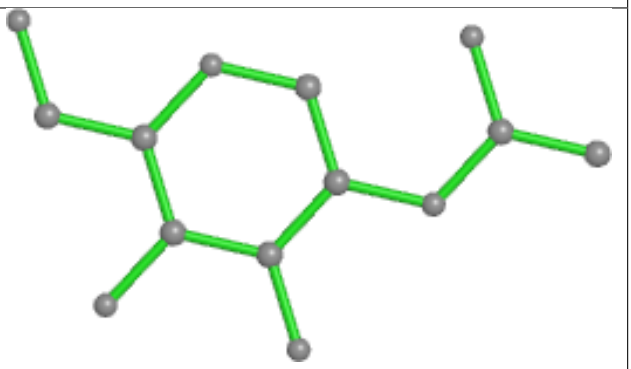
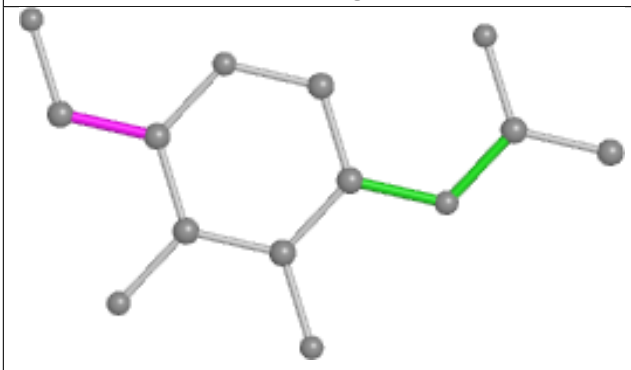
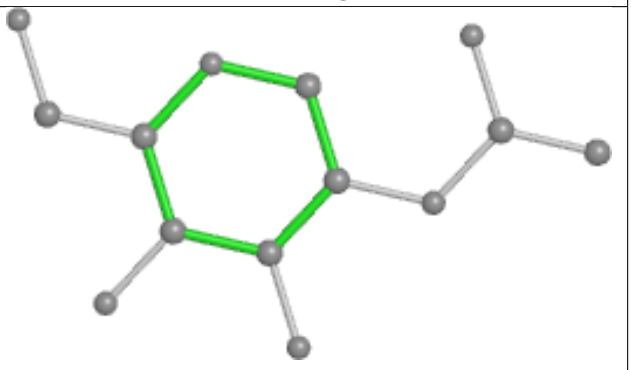
Bond angles

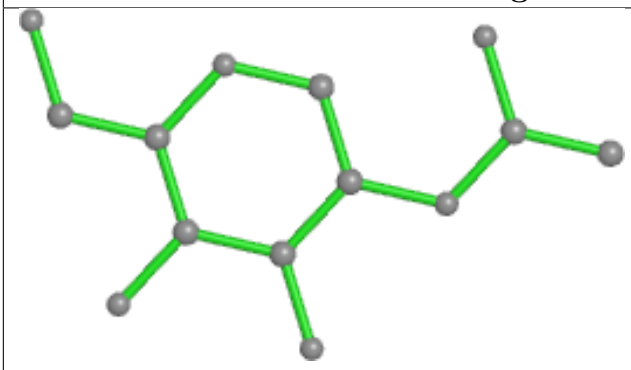
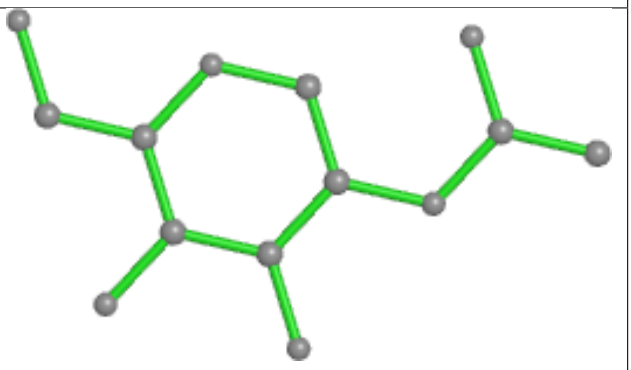
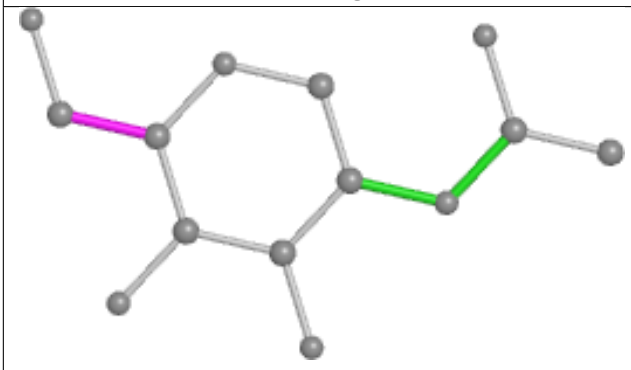
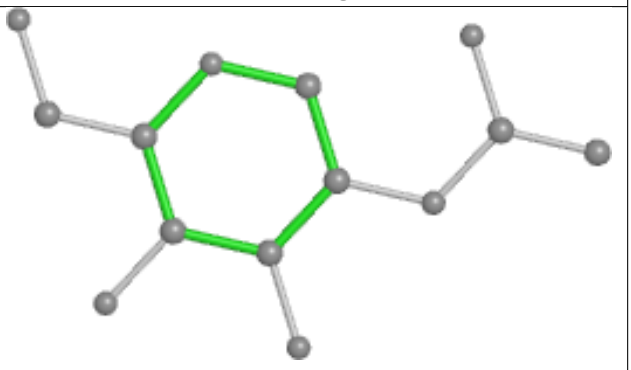


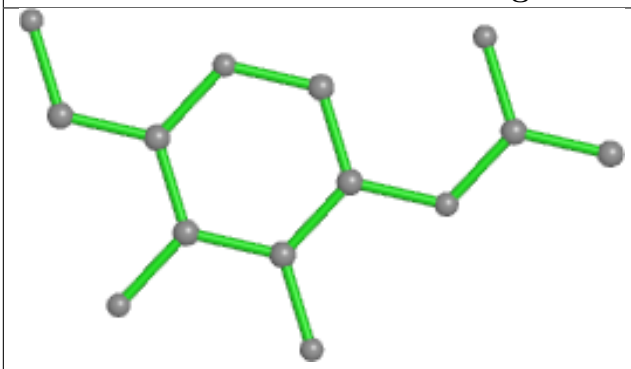
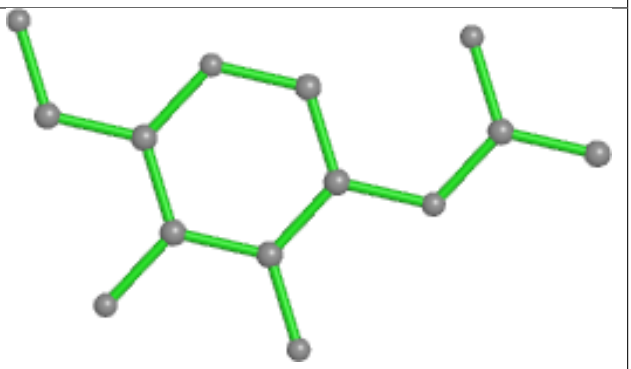
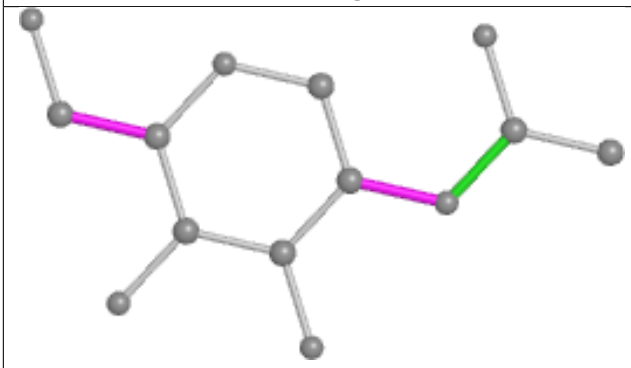
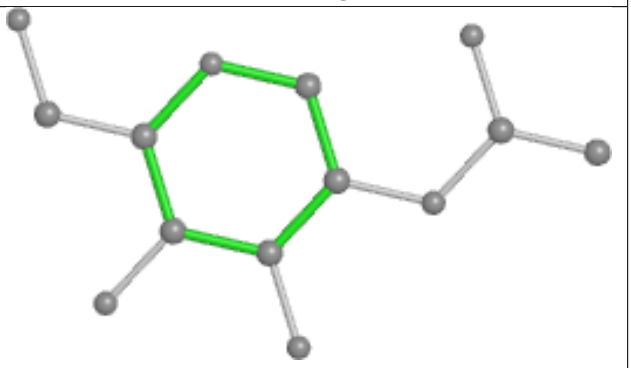
Torsions

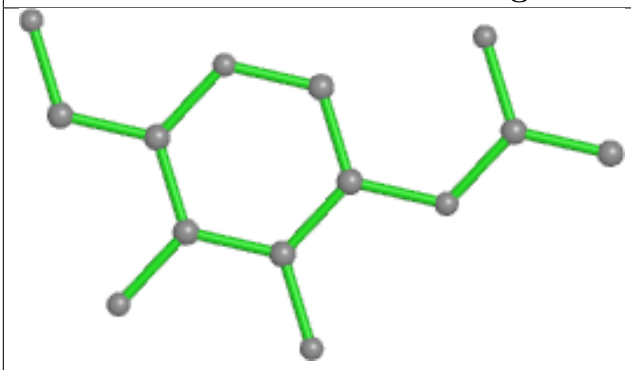
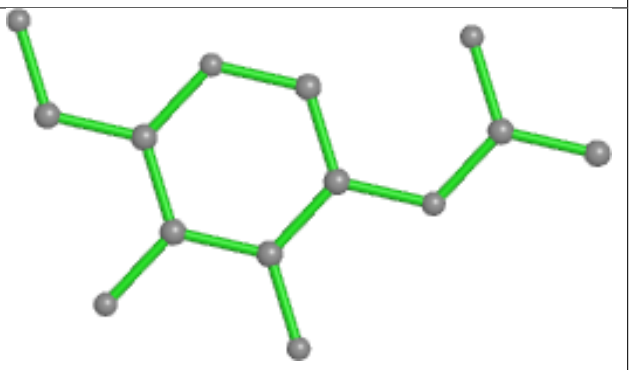
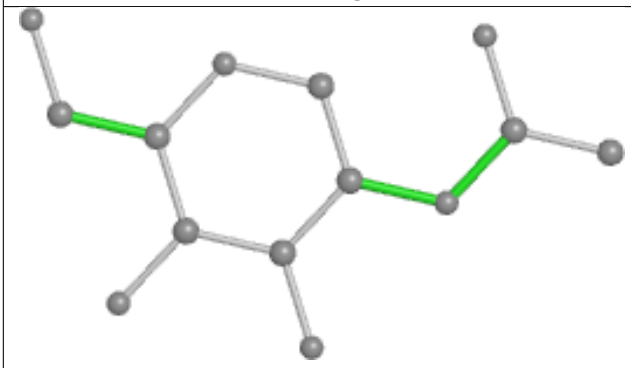
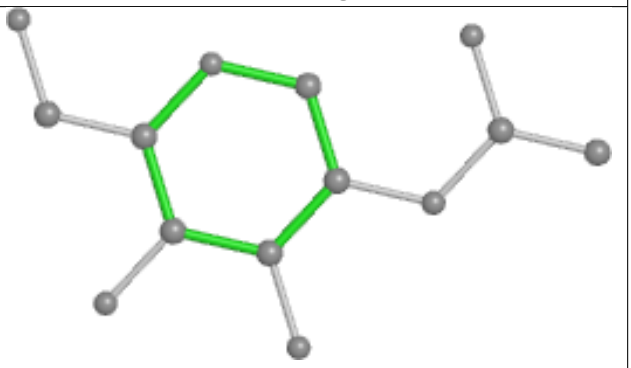


Rings

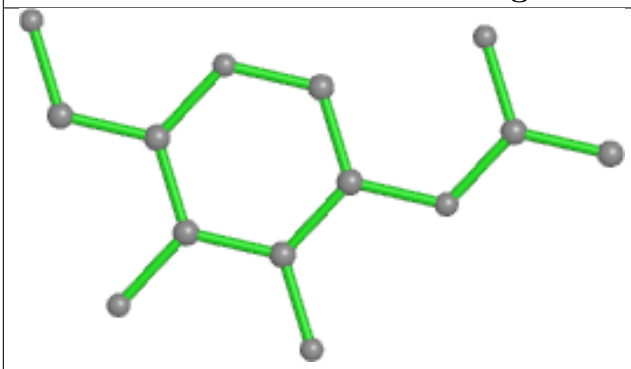
Ligand NAG B 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

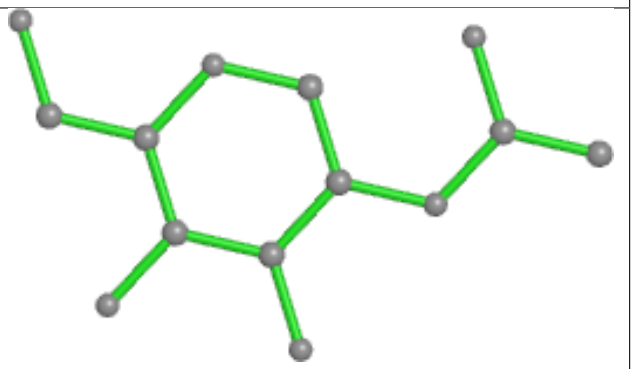
Ligand NAG B 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

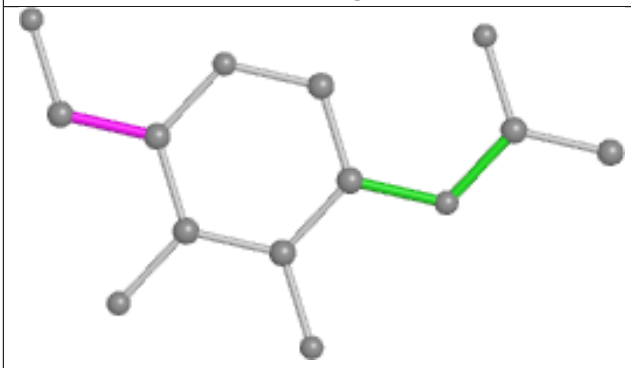
Ligand NAG A 1302



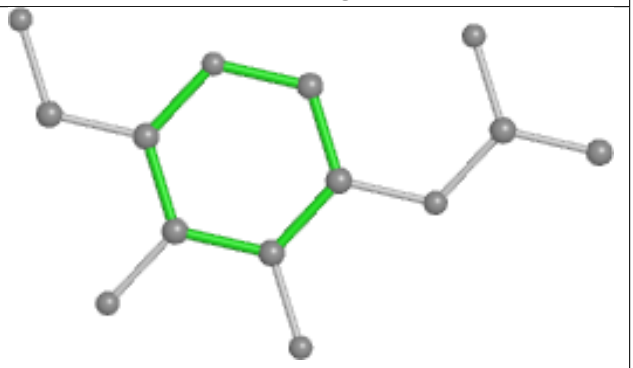
Bond lengths



Bond angles

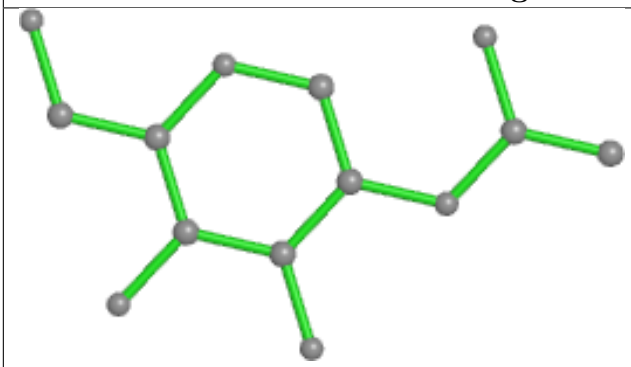


Torsions



Rings

Ligand NAG A 1309



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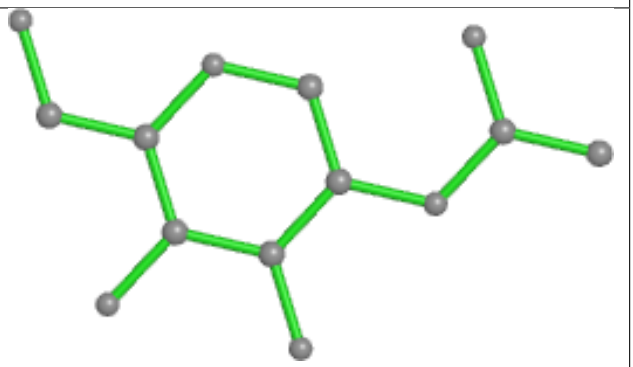
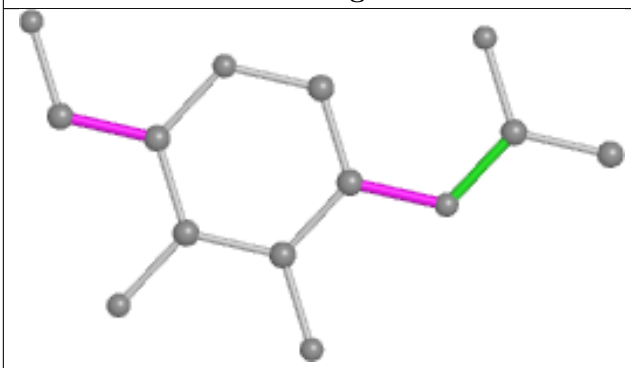


Bond angles



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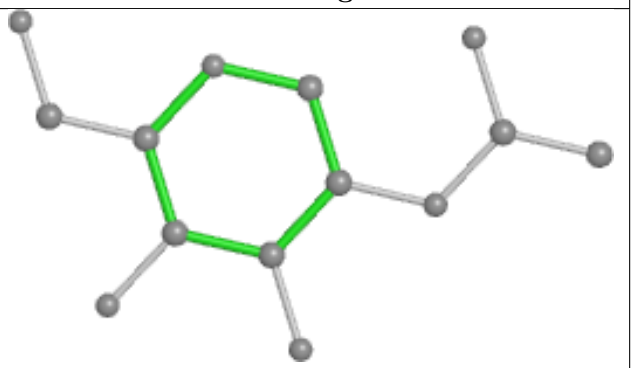
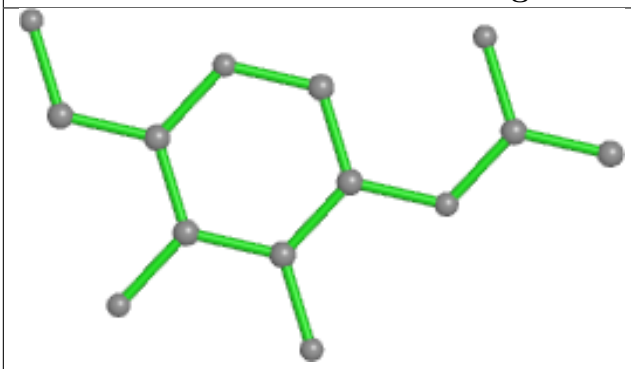


Rings

Ligand NAG C 1306



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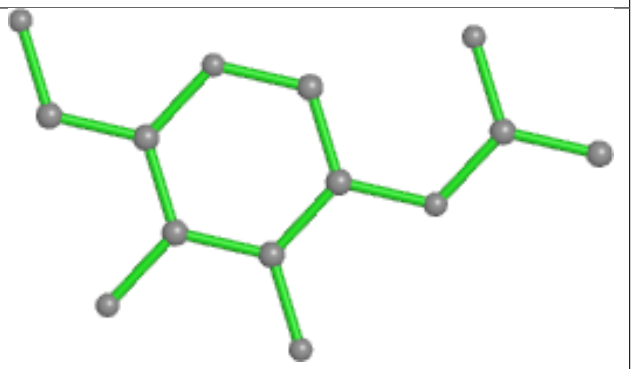
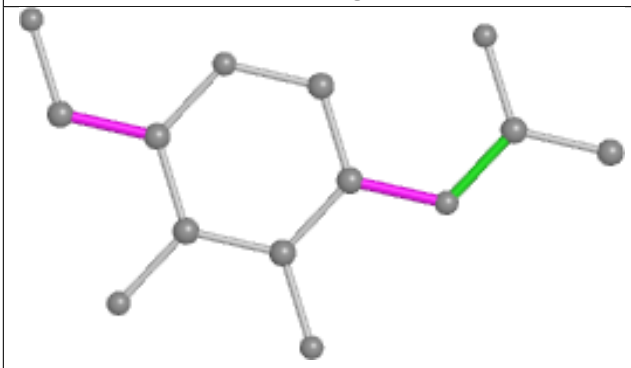


Bond angles



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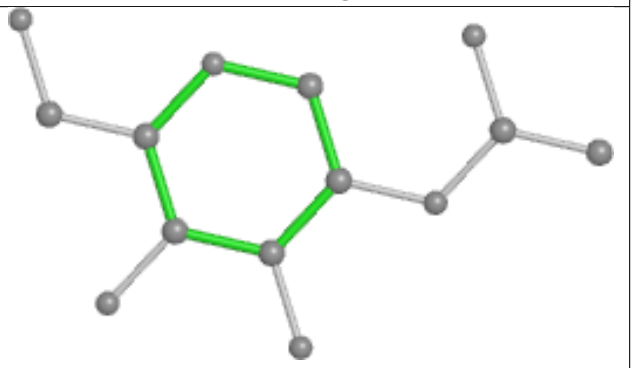
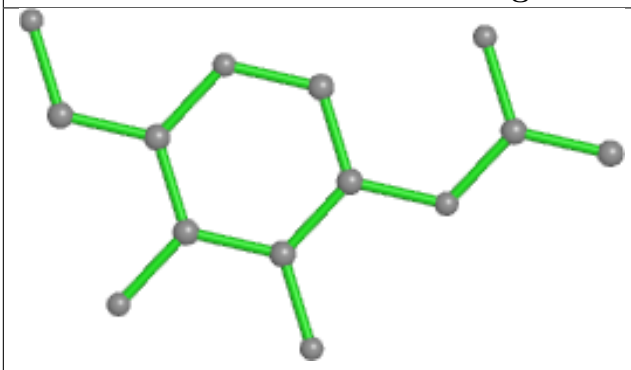


Rings

Ligand NAG B 1305



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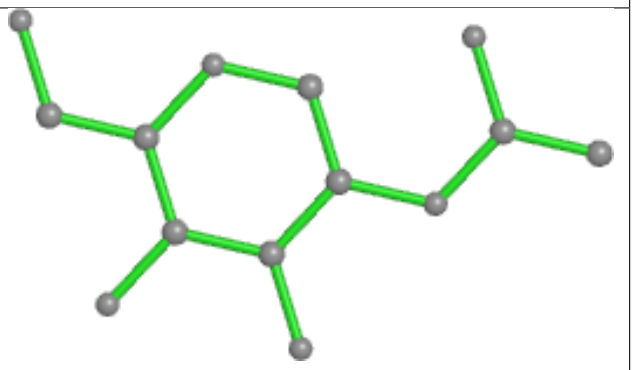
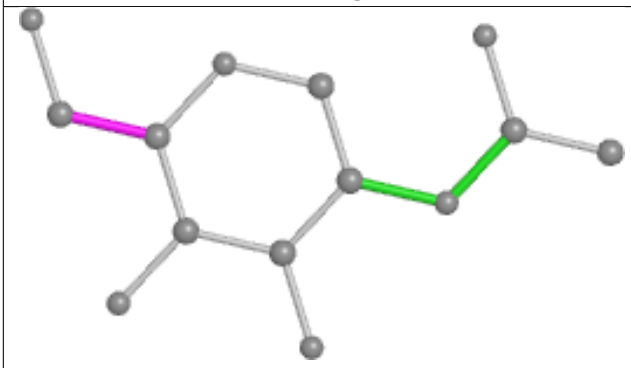
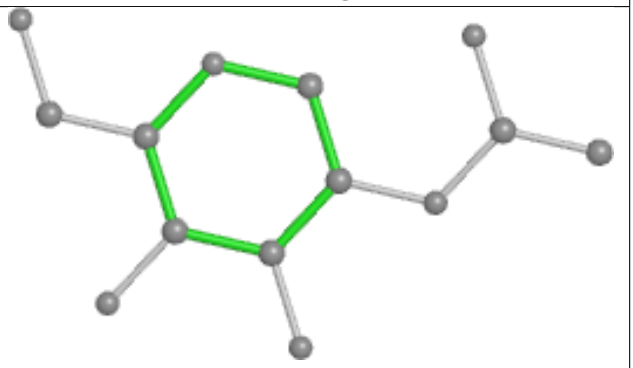


Bond angles

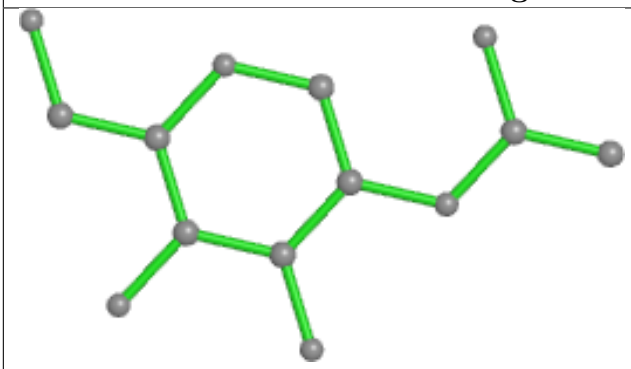


Torsions

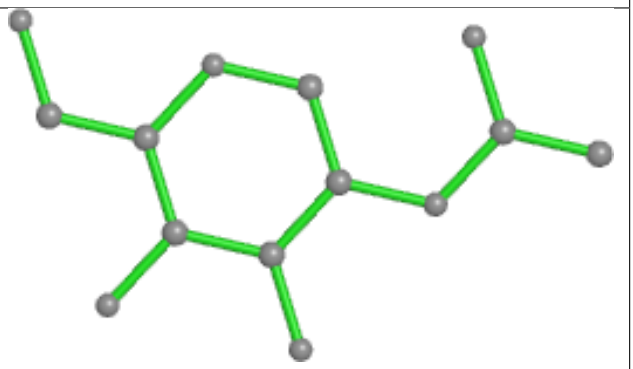


Rings

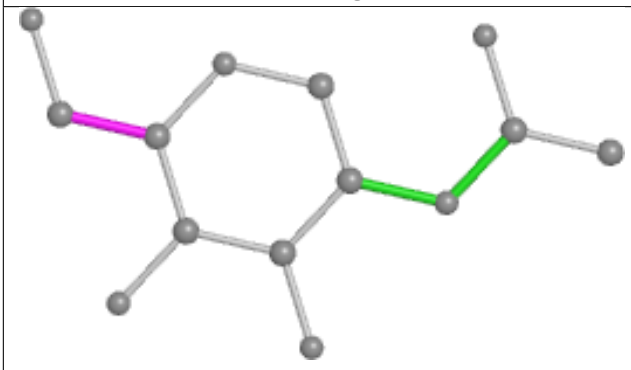
Ligand NAG A 1312



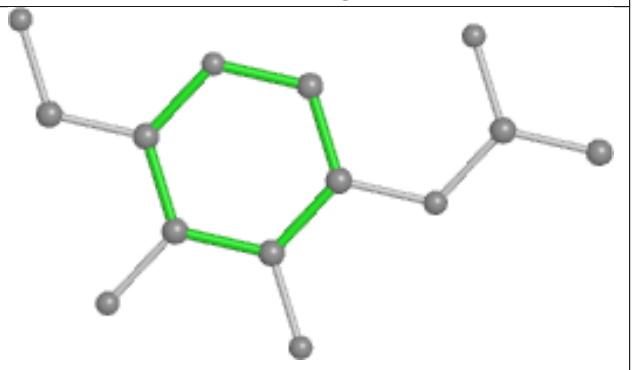
Bond lengths



Bond angles

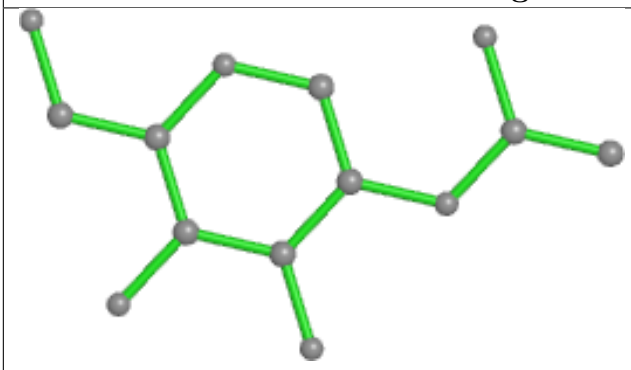


Torsions

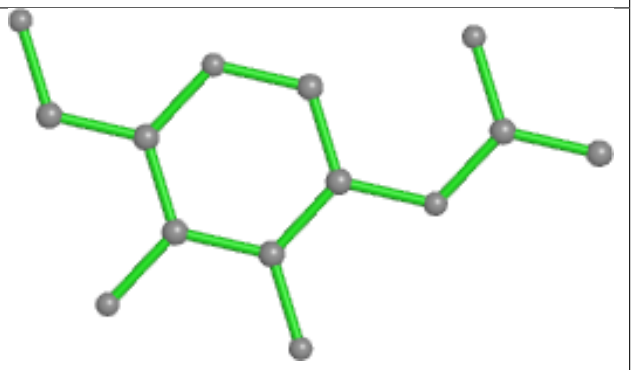


Rings

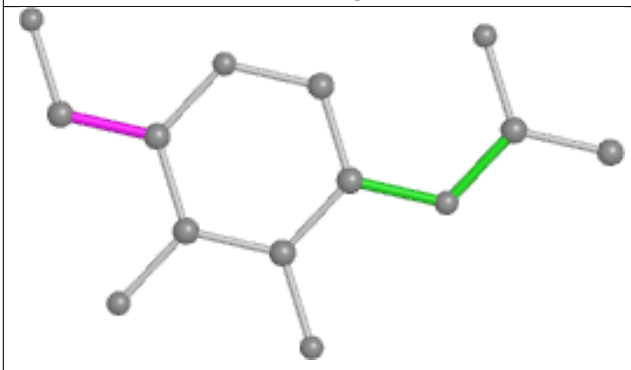
Ligand NAG C 1304



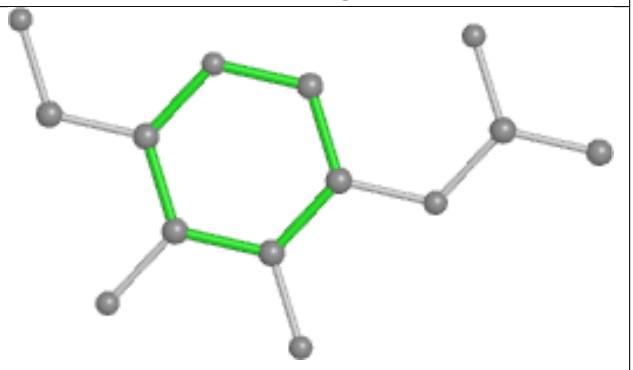
Bond lengths



Bond angles

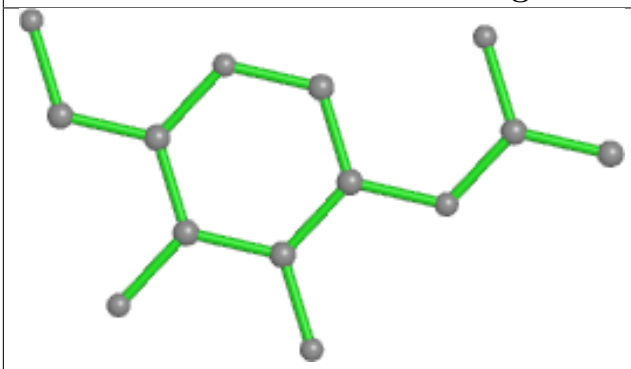


Torsions

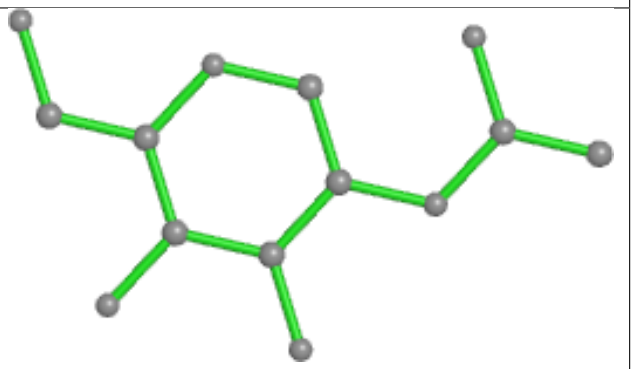


Rings

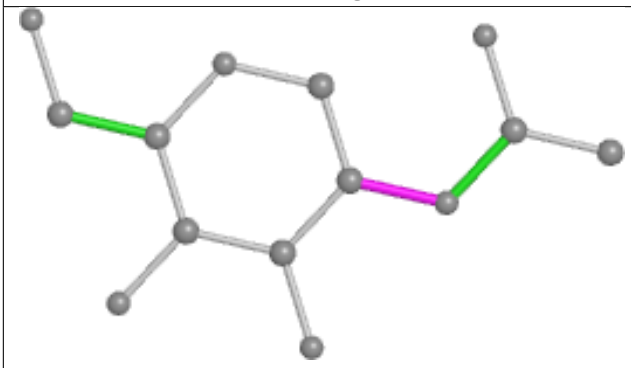
Ligand NAG B 1303



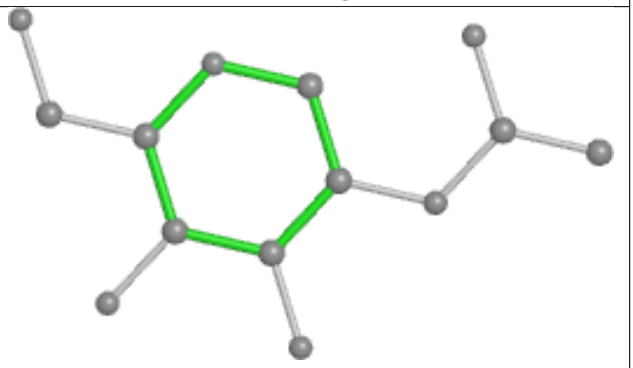
Bond lengths



Bond angles

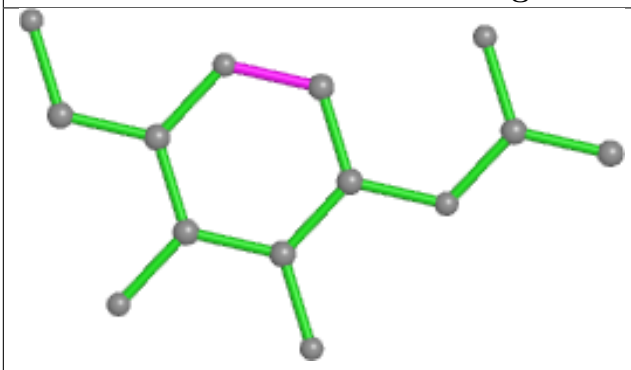


Torsions

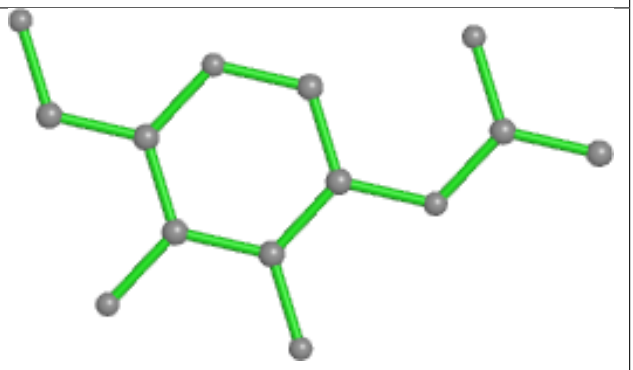


Rings

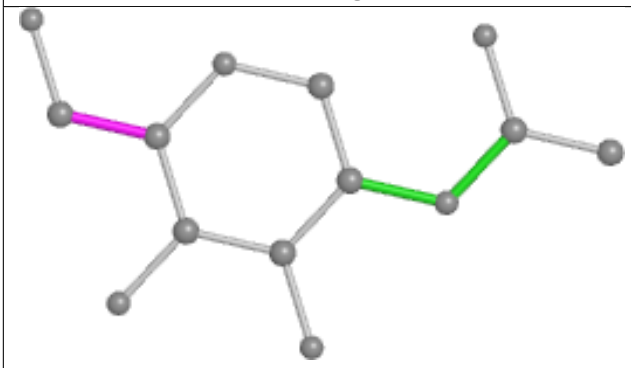
Ligand NAG B 1309



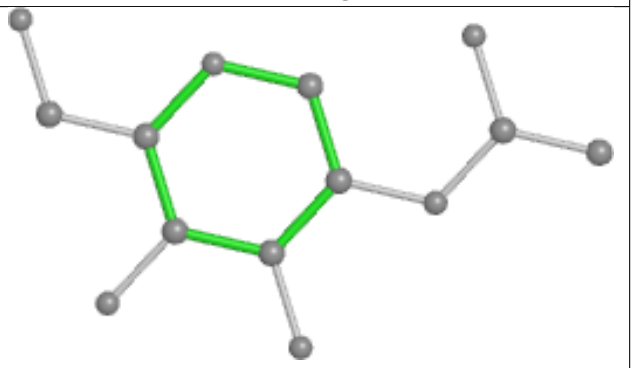
Bond lengths



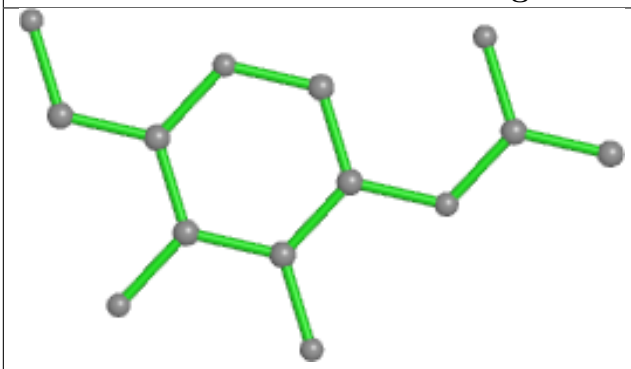
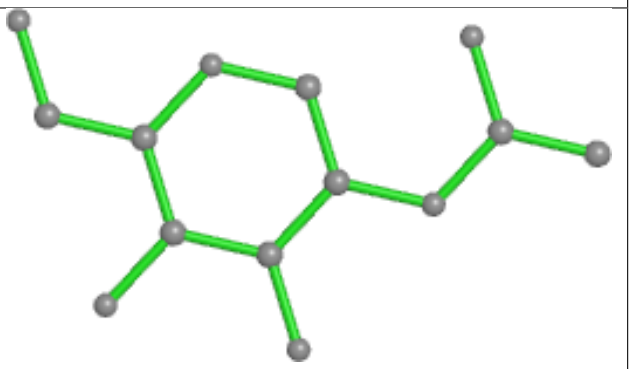
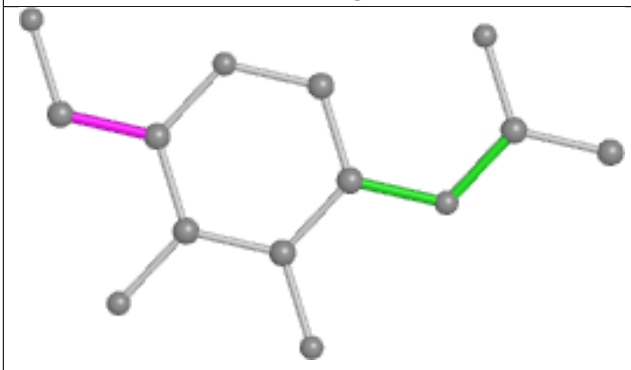
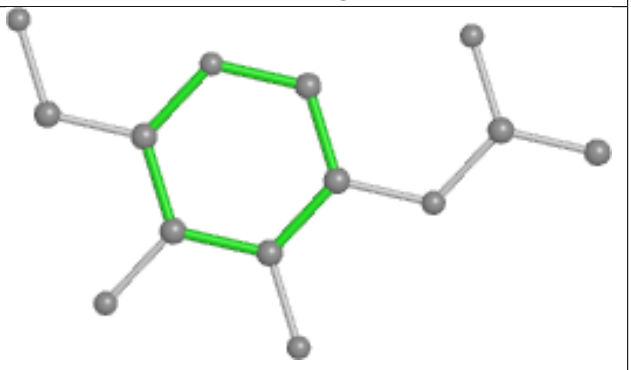
Bond angles

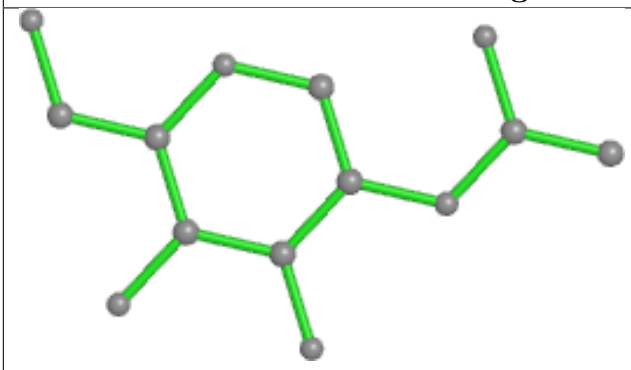
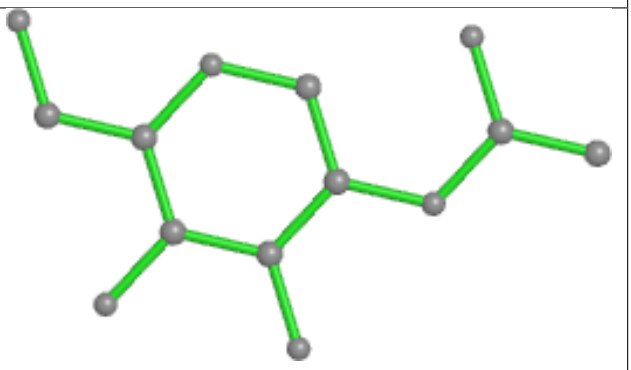
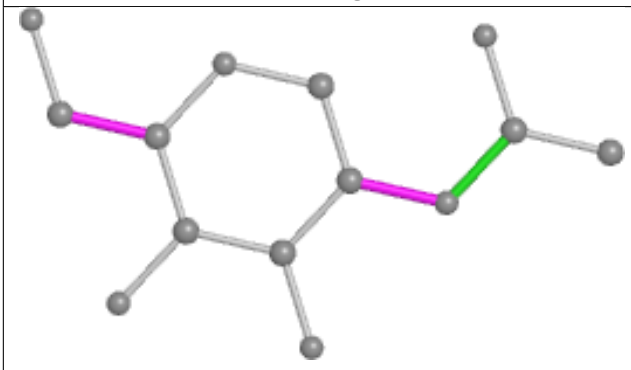
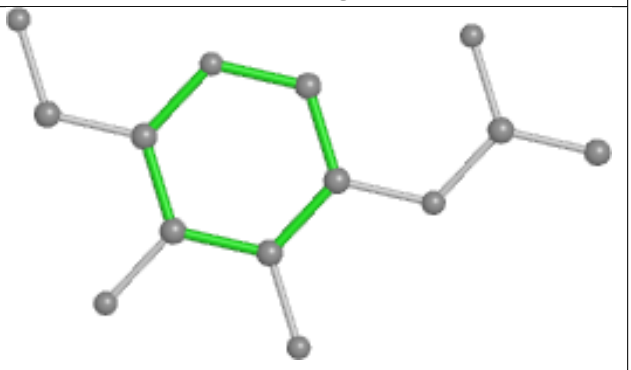


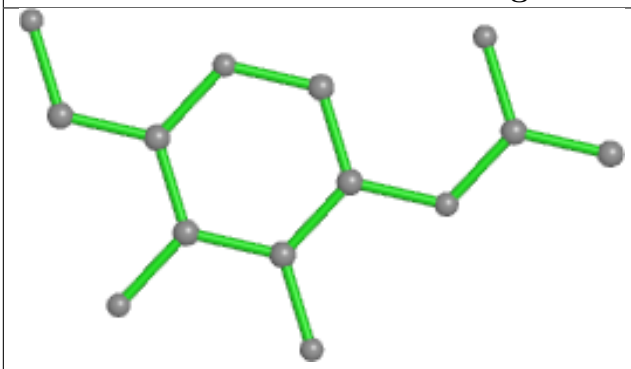
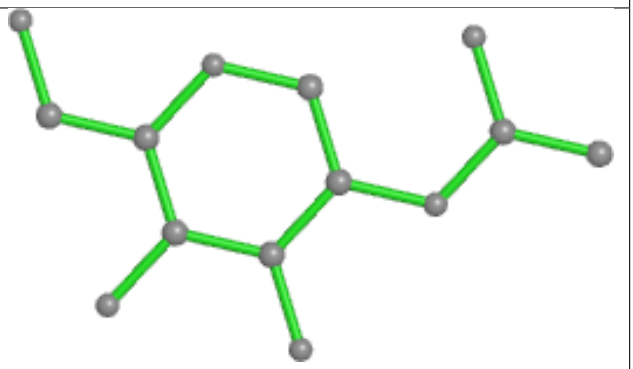
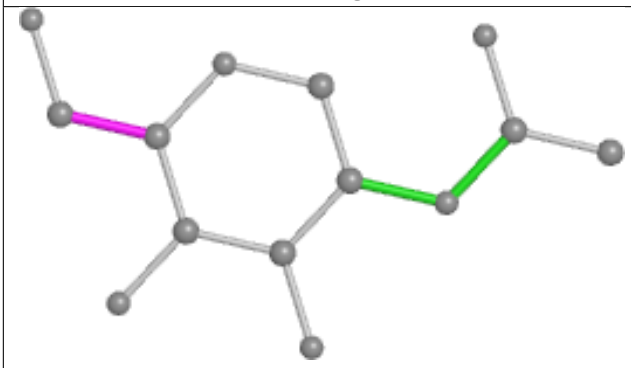
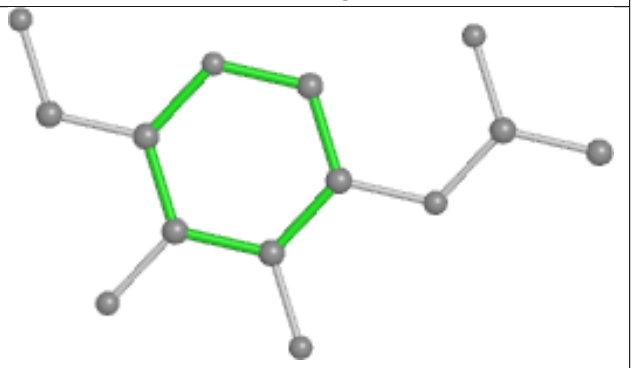
Torsions



Rings

Ligand NAG C 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1306	
	
Bond lengths	Bond angles
	
Torsions	Rings

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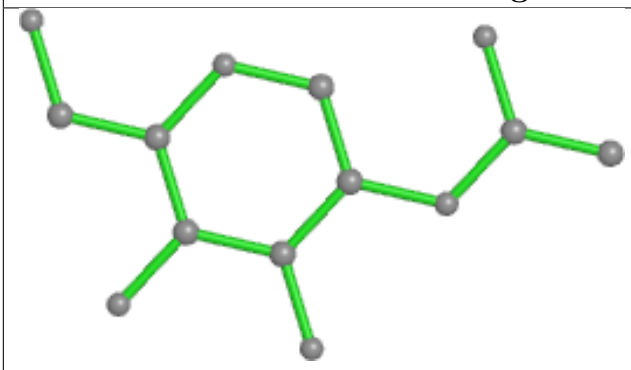
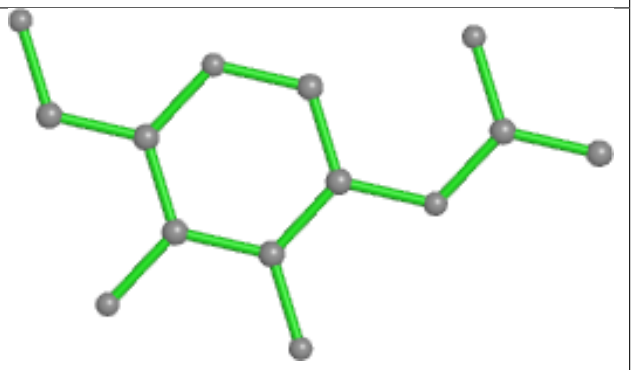
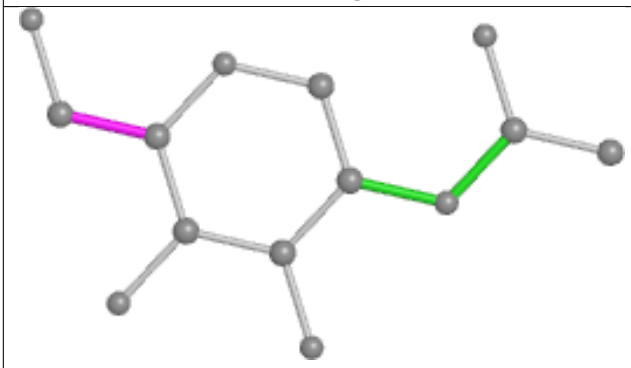
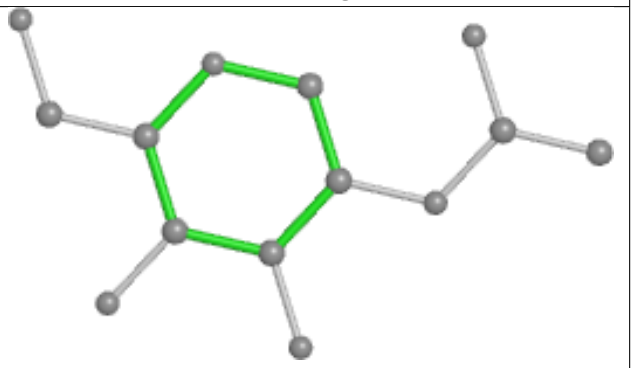
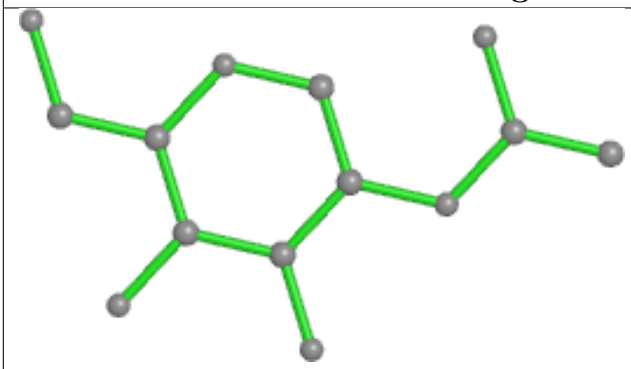
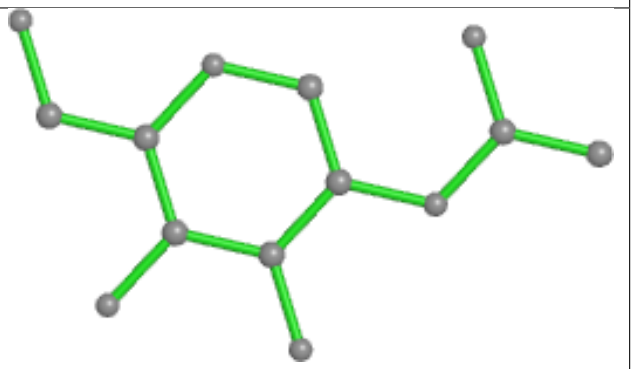
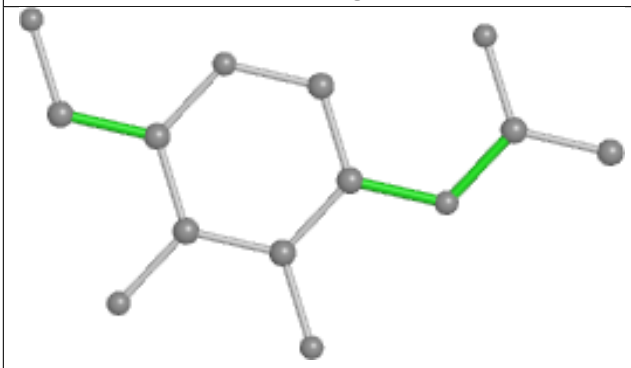
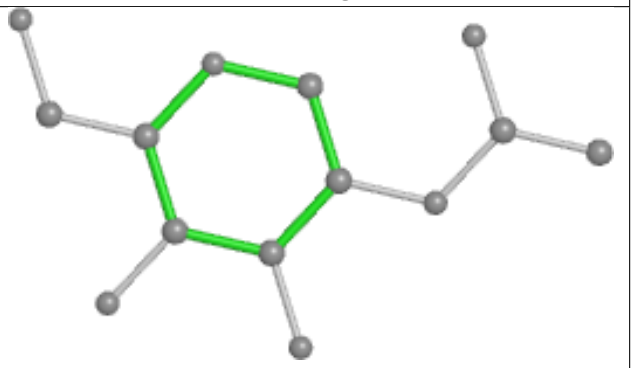
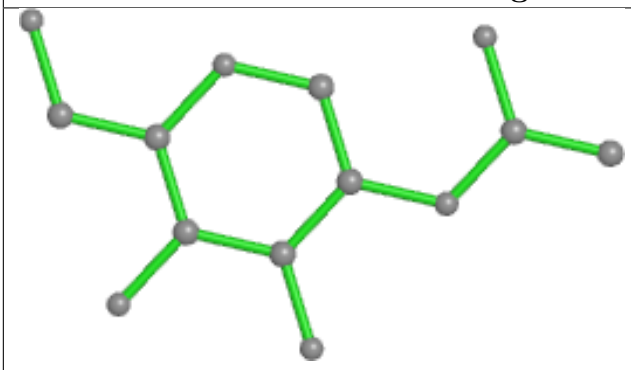
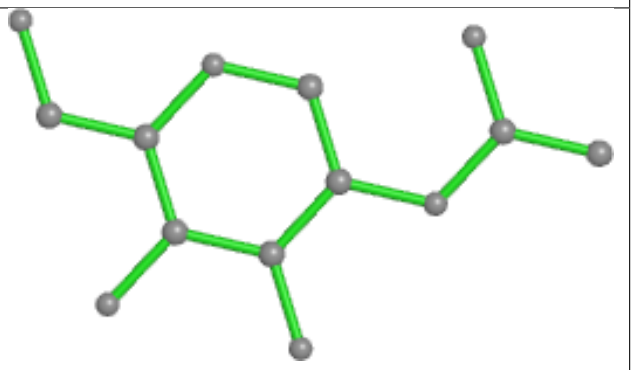
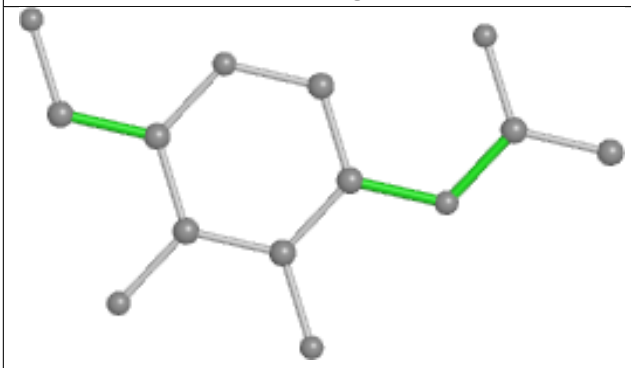
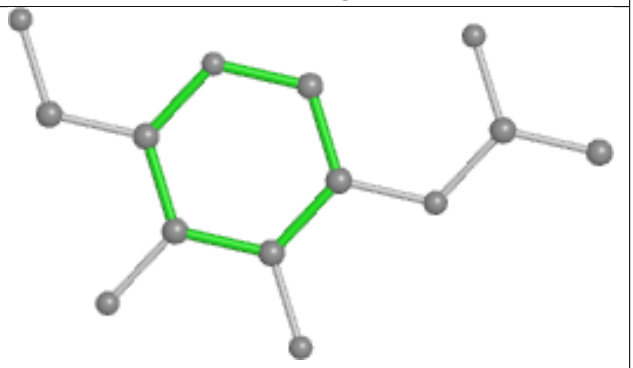
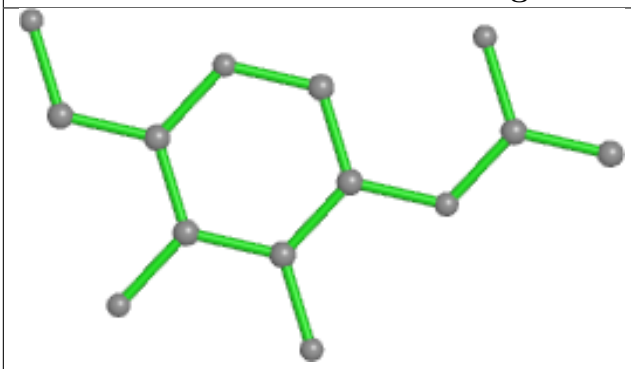
	
Bond lengths	Bond angles
	
Torsions	Rings

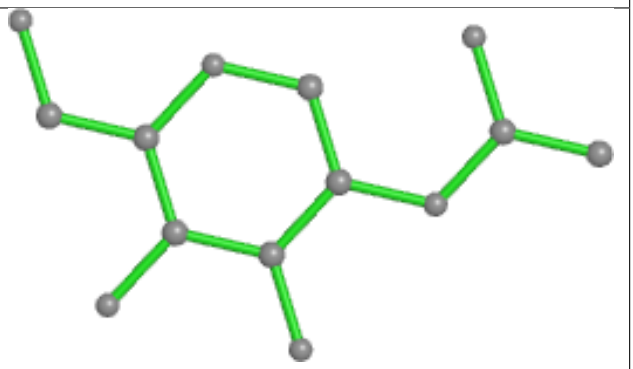
Ligand NAG C 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

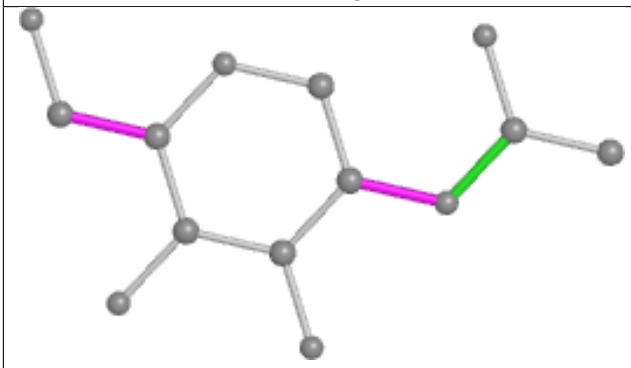
Ligand NAG A 1307



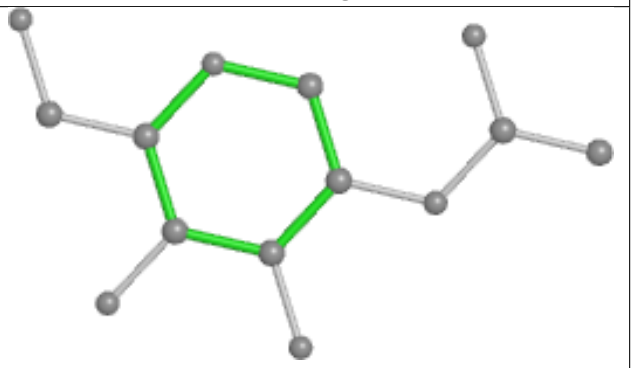
Bond lengths



Bond angles

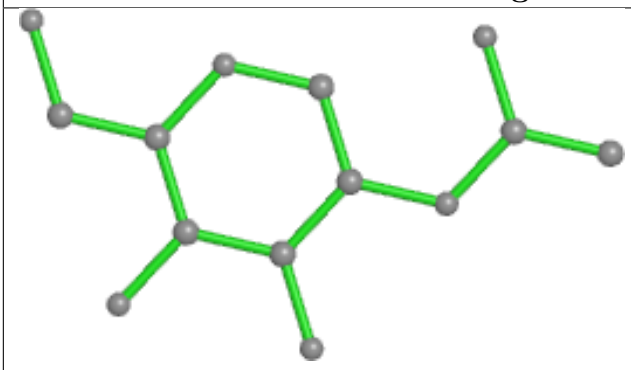


Torsions



Rings

Ligand NAG C 1308



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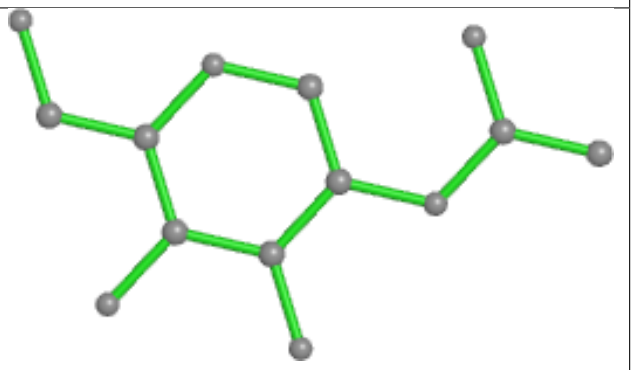
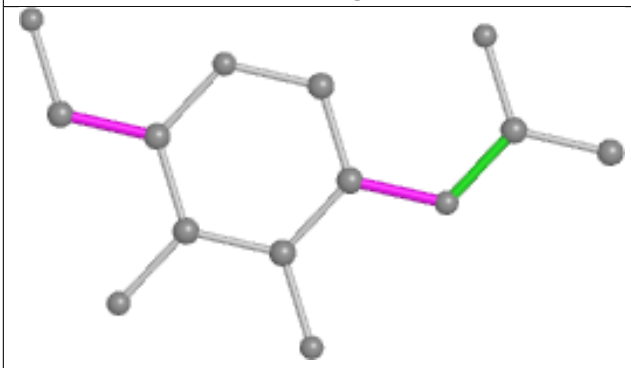


Bond angles



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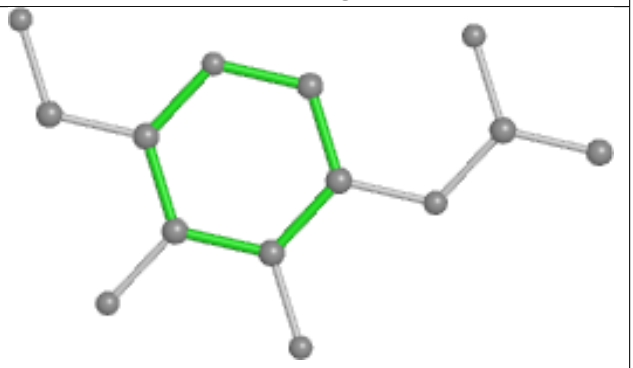
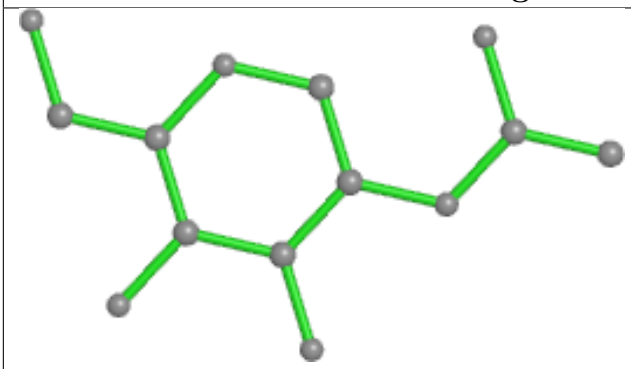


Rings

Ligand NAG B 1312



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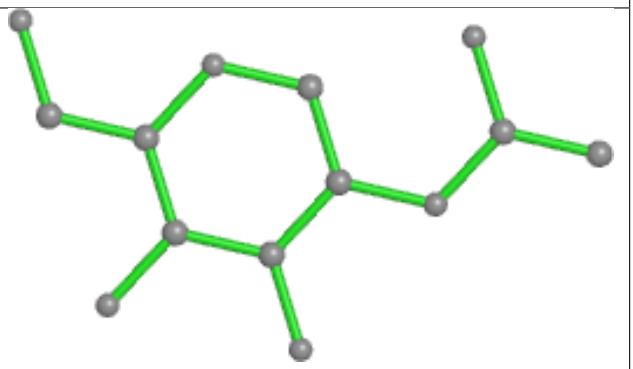
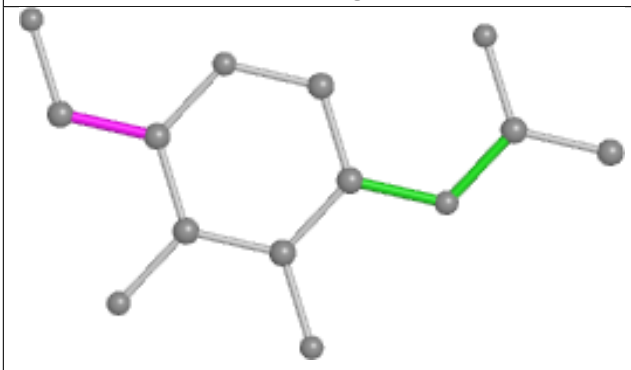


Bond angles



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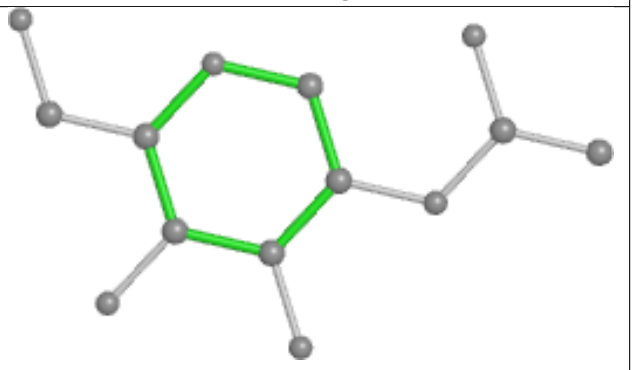
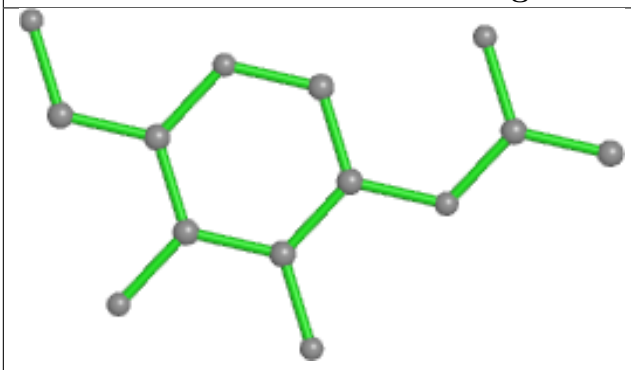


Rings

Ligand NAG C 1309



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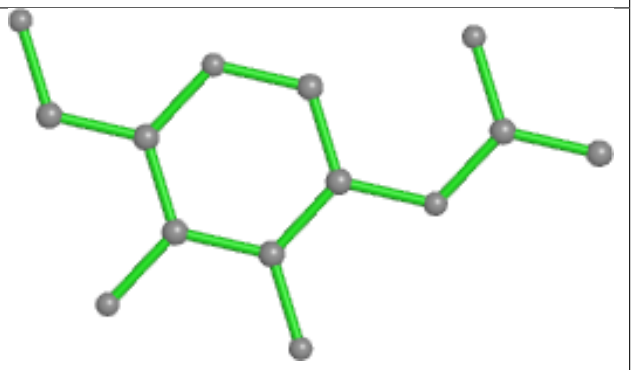
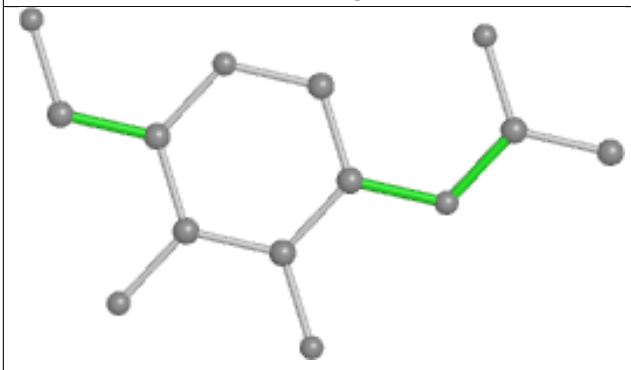


Bond angles



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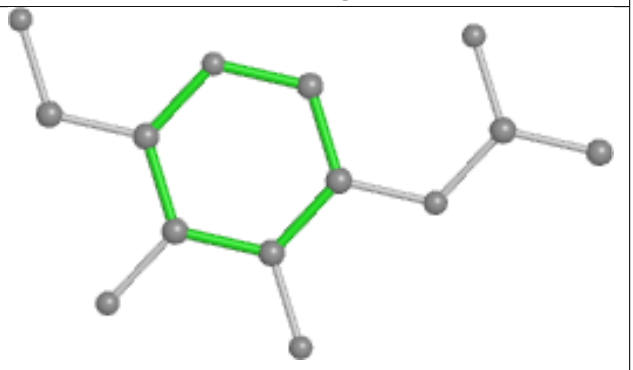
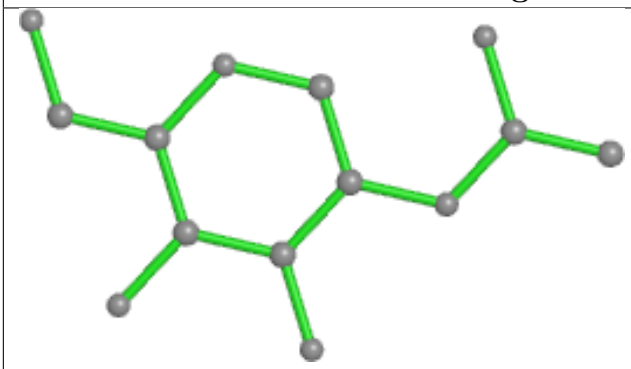


Rings

Ligand NAG C 1307



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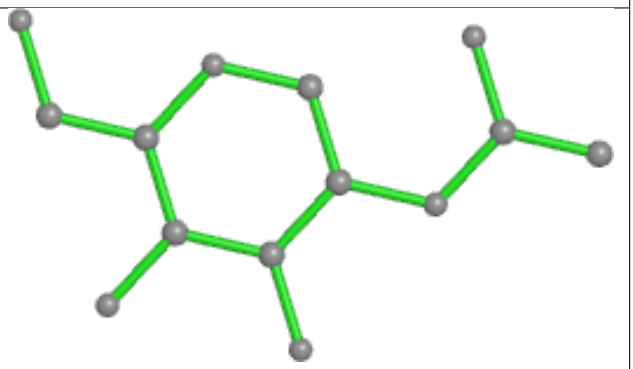
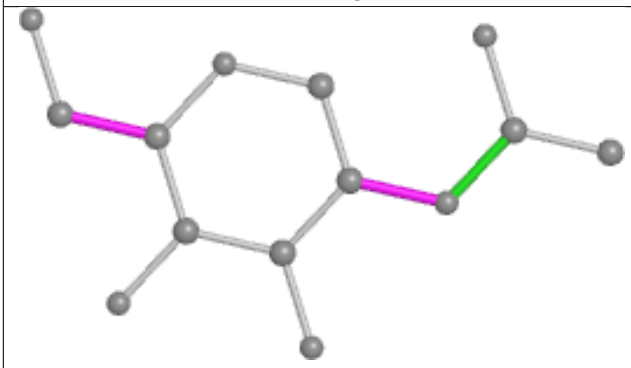
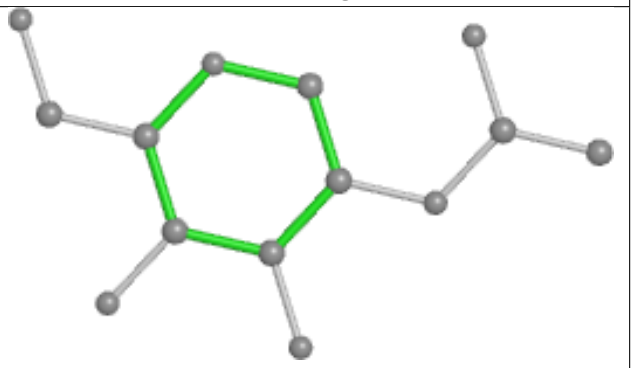


Bond angles

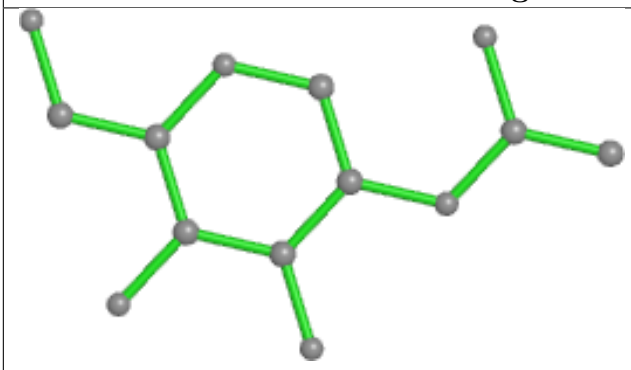


Torsions



Rings

Ligand NAG C 1311



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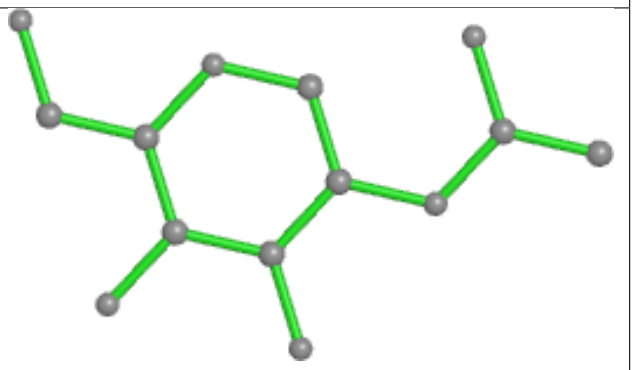
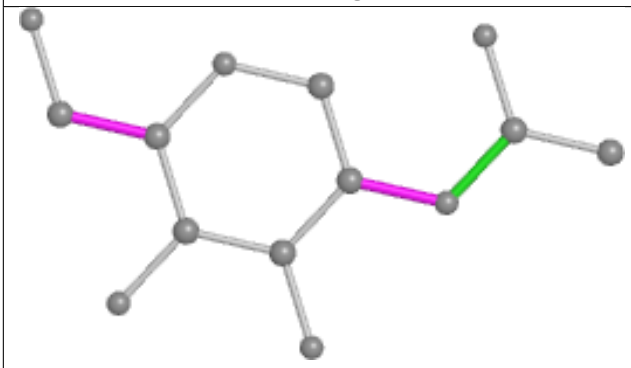


Bond angles



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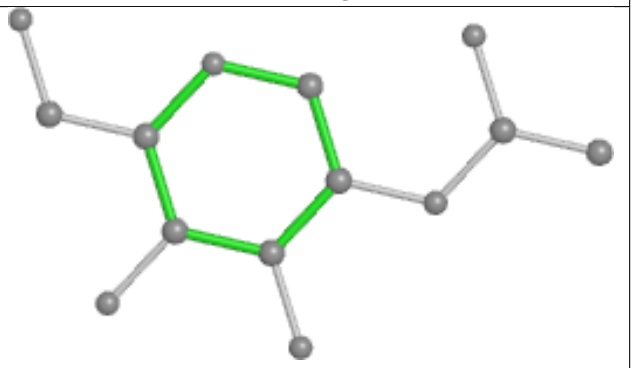
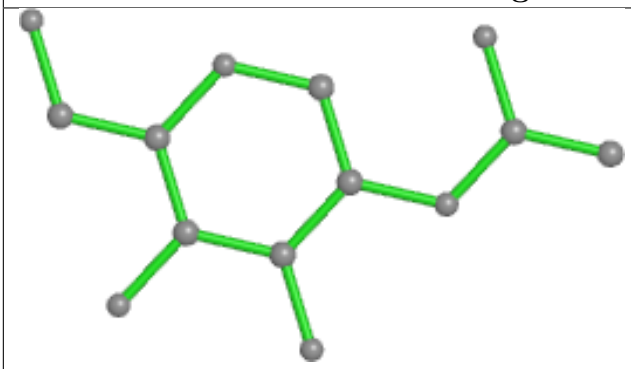


Rings

Ligand NAG B 1308



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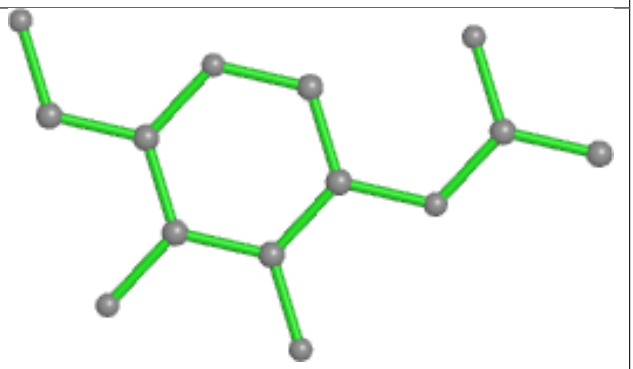
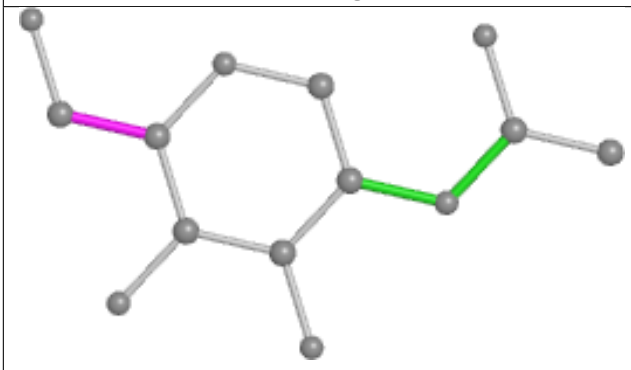


Bond angles



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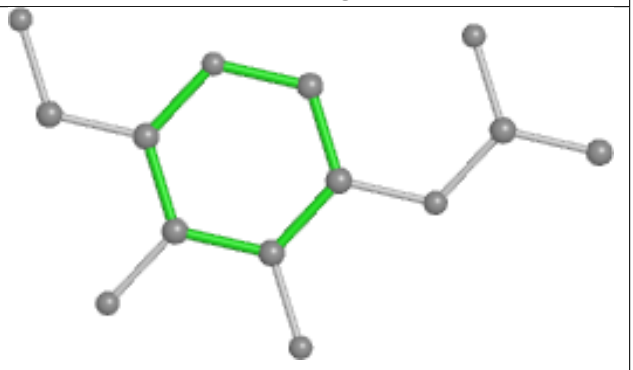
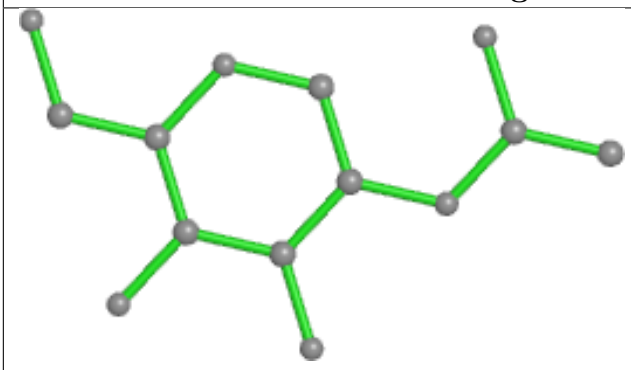


Rings

Ligand NAG A 1308



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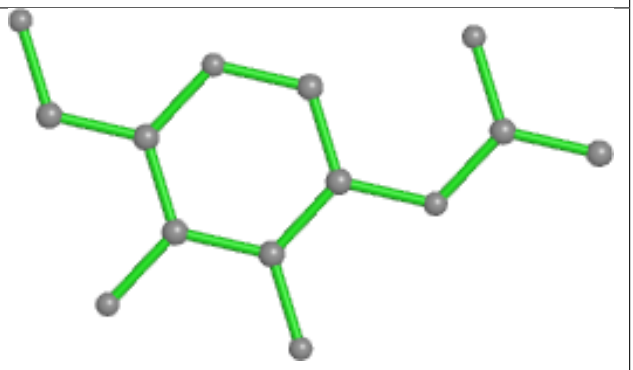
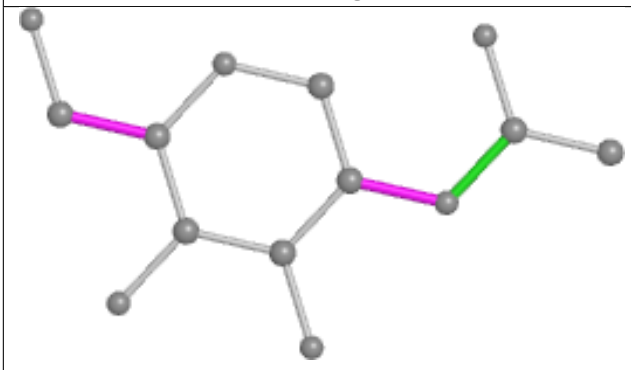


Bond angles



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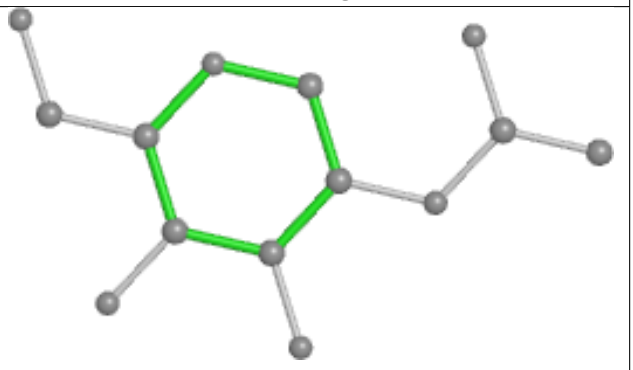
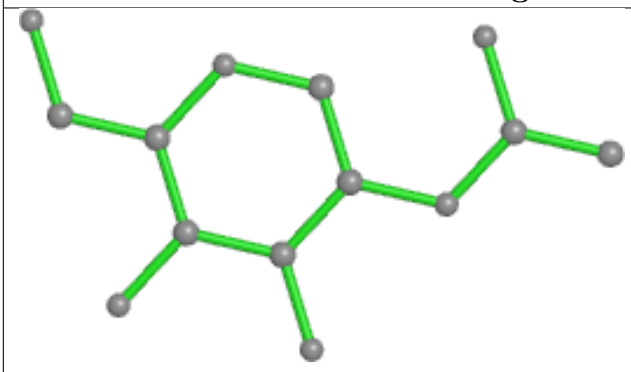
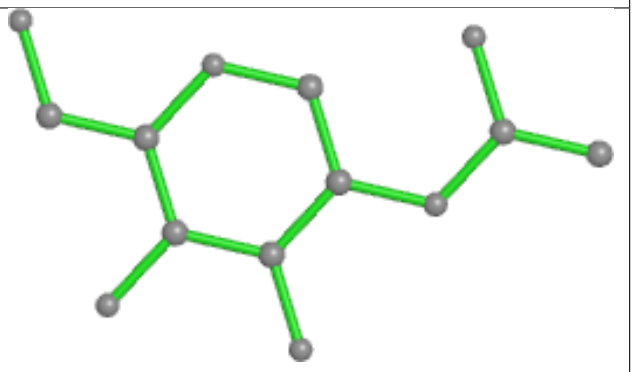


Rings

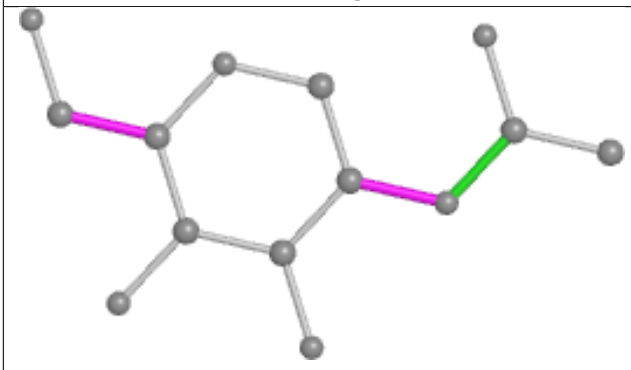
Ligand NAG C 1305



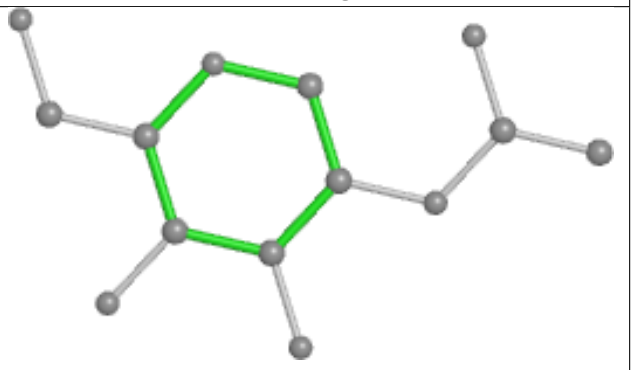
Bond lengths



Bond angles

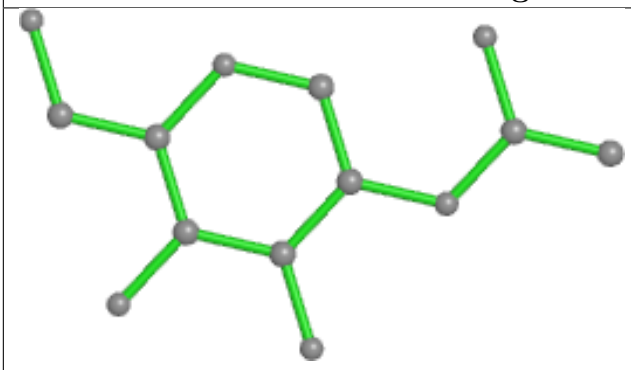


Torsions

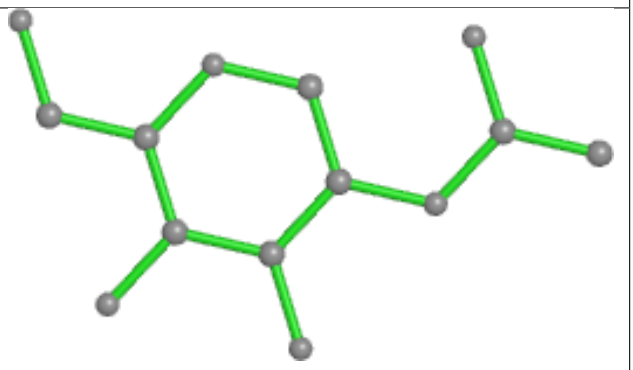


Rings

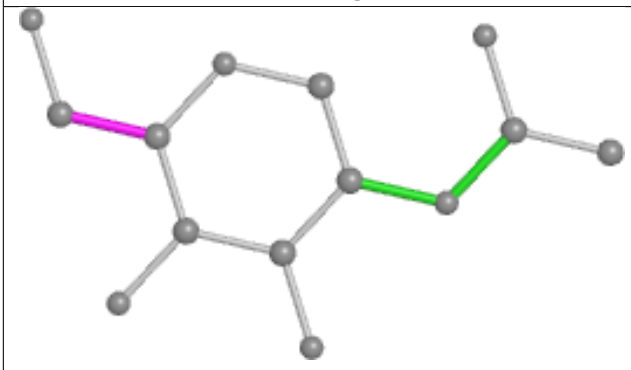
Ligand NAG B 1307



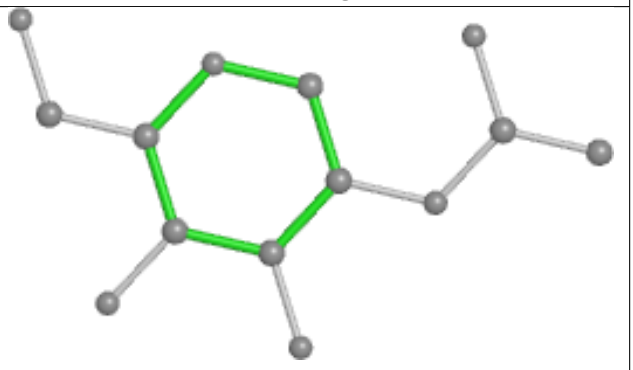
Bond lengths



Bond angles

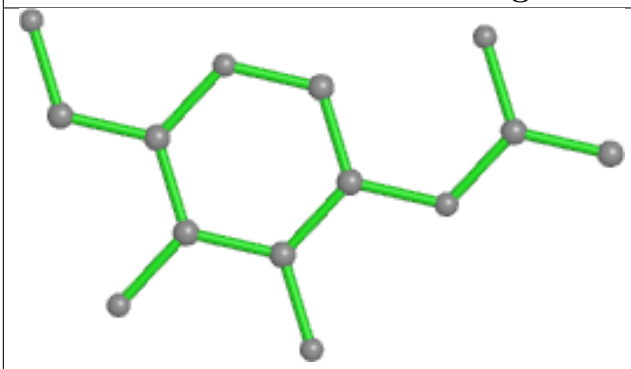


Torsions

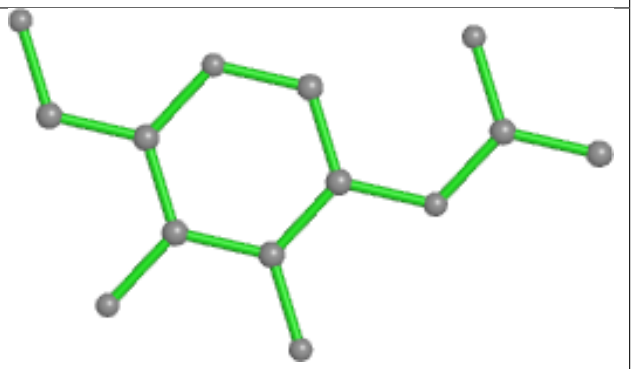


Rings

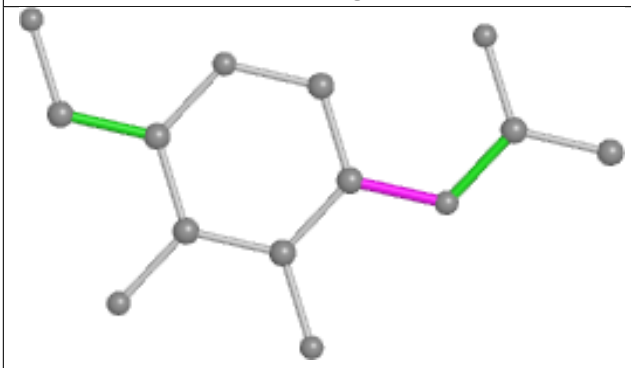
Ligand NAG B 1306



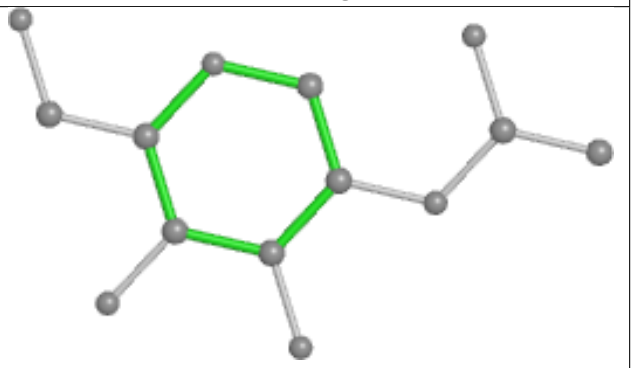
Bond lengths



Bond angles

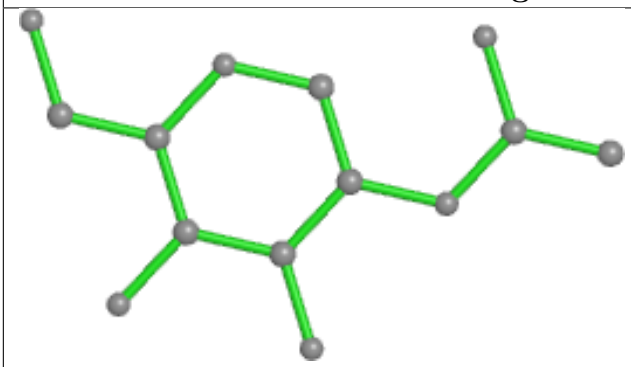


Torsions

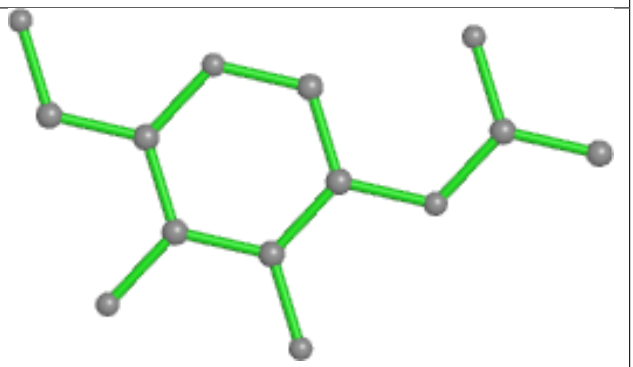


Rings

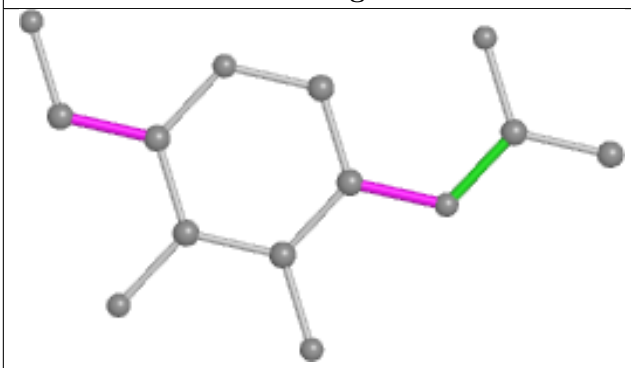
Ligand NAG B 1313



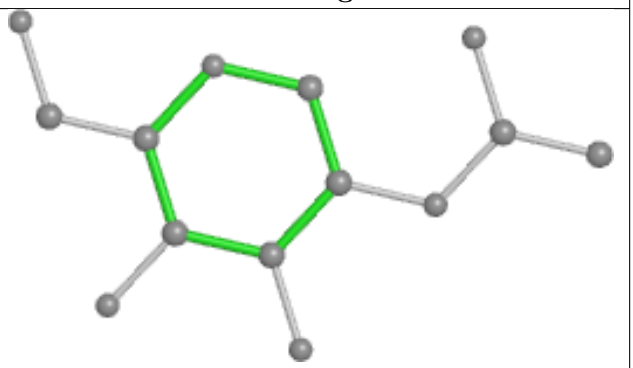
Bond lengths



Bond angles

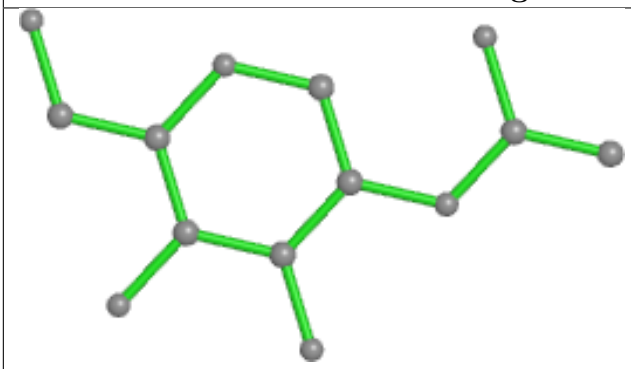


Torsions

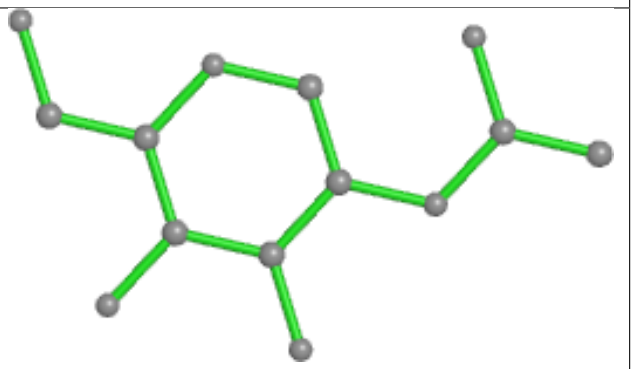


Rings

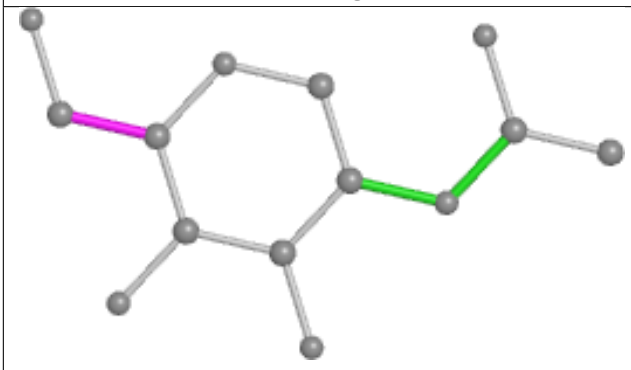
Ligand NAG A 1304



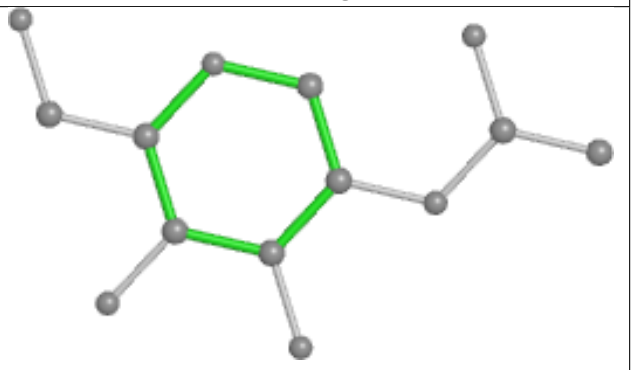
Bond lengths



Bond angles

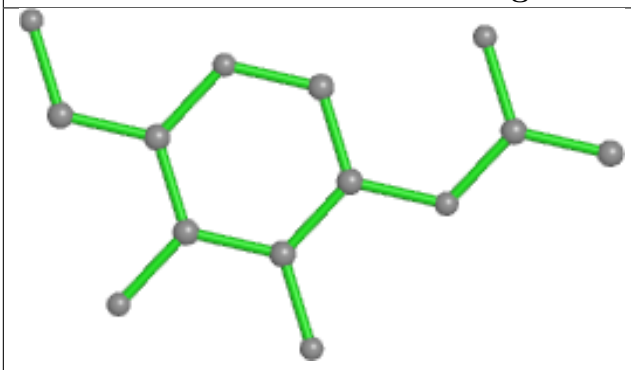


Torsions

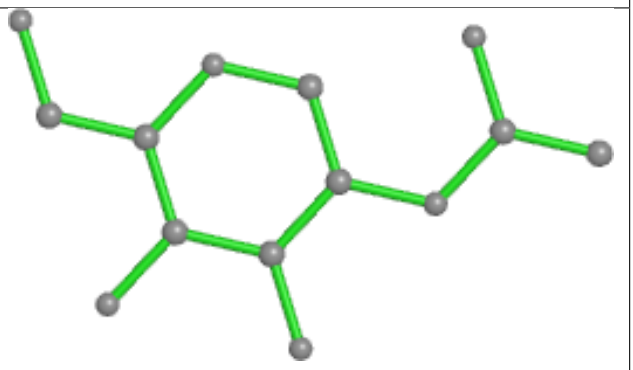


Rings

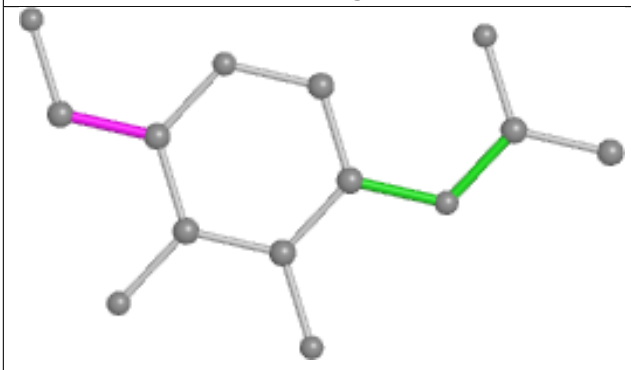
Ligand NAG C 1302



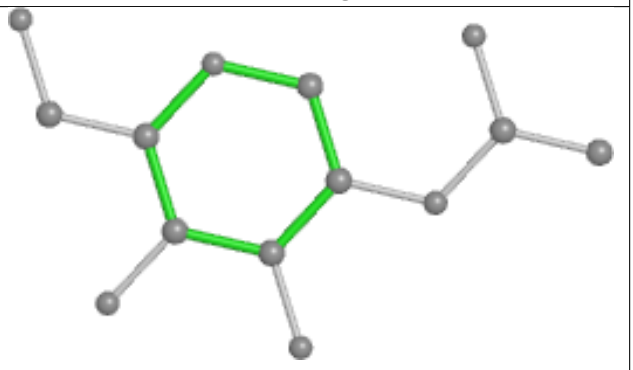
Bond lengths



Bond angles

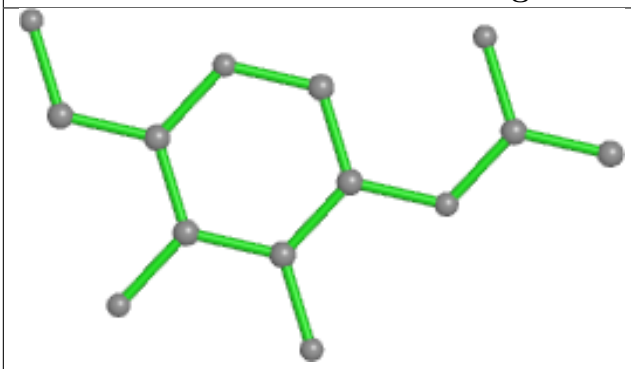


Torsions

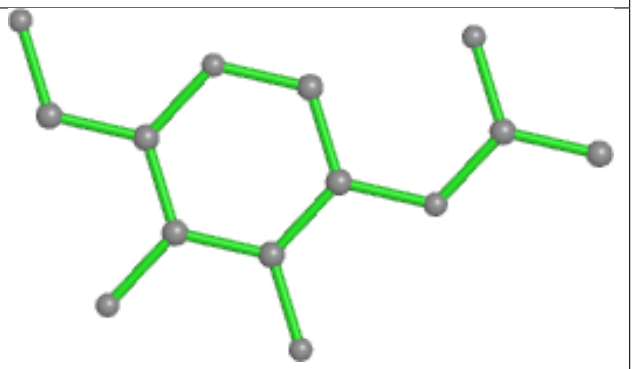


Rings

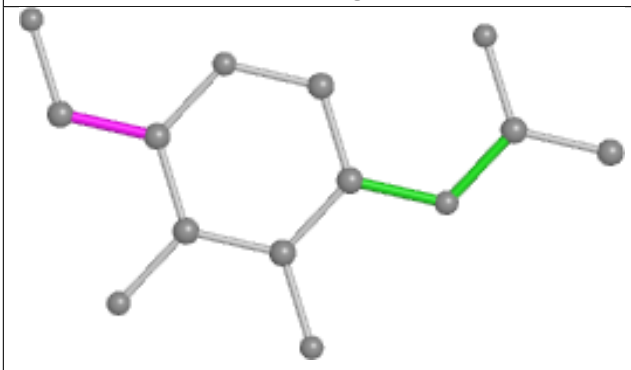
Ligand NAG B 1301



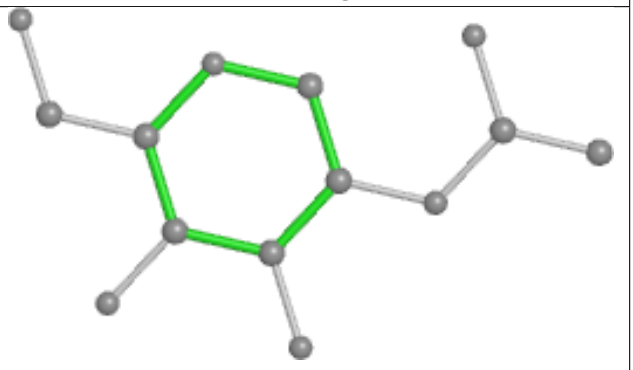
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

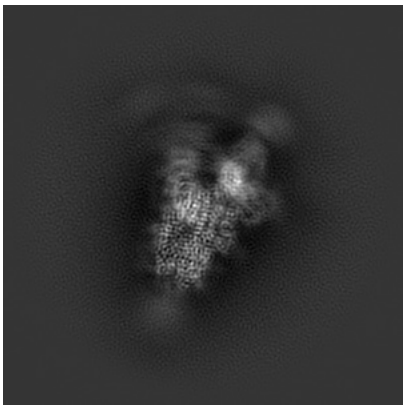
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34128. These allow visual inspection of the internal detail of the map and identification of artifacts.

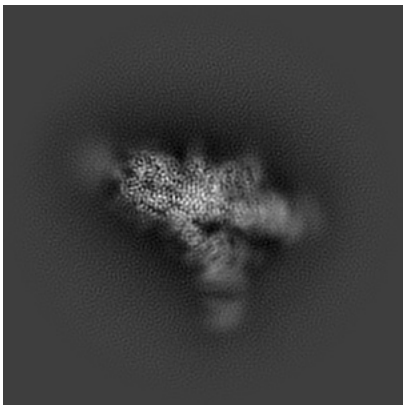
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

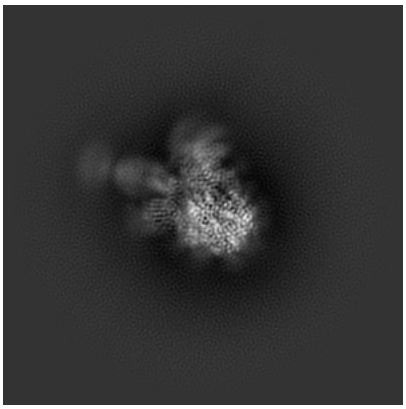
6.1.1 Primary map



X

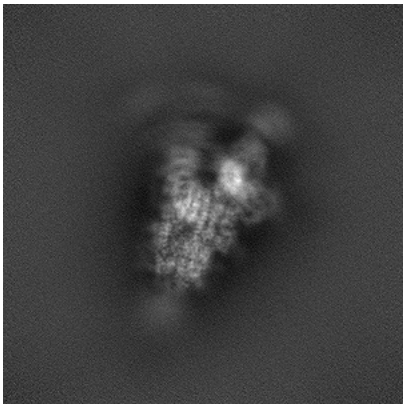


Y

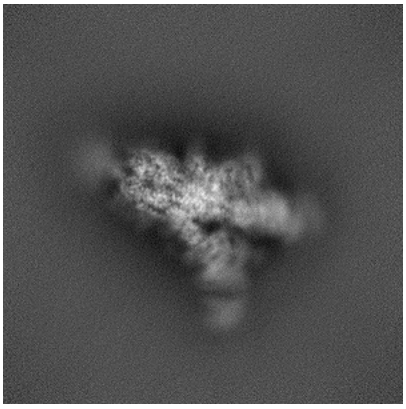


Z

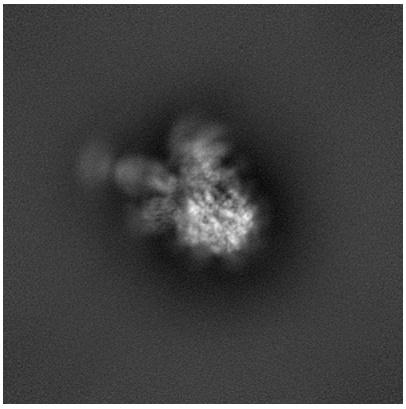
6.1.2 Raw map



X



Y

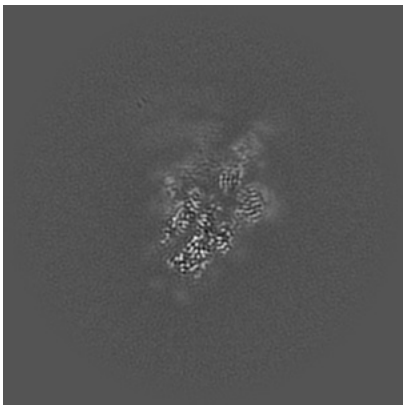


Z

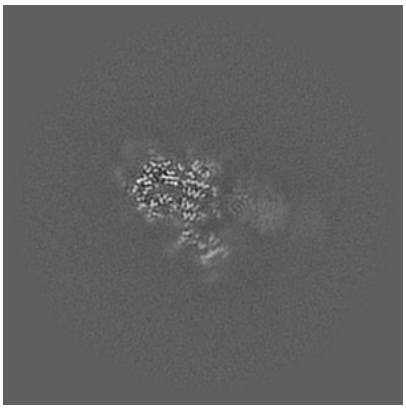
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

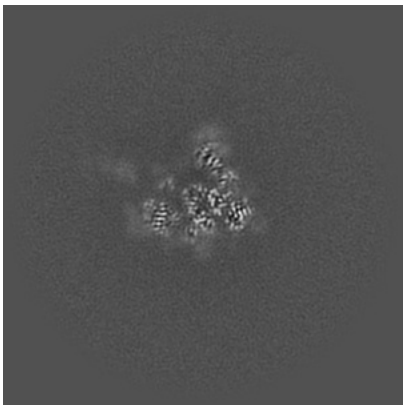
6.2.1 Primary map



X Index: 256

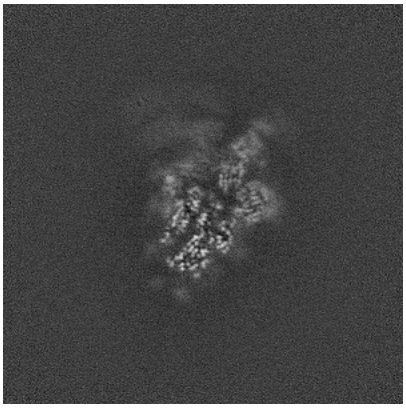


Y Index: 256

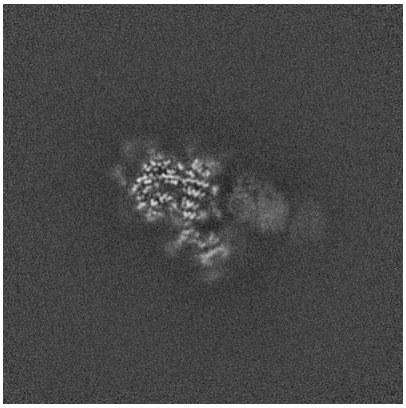


Z Index: 256

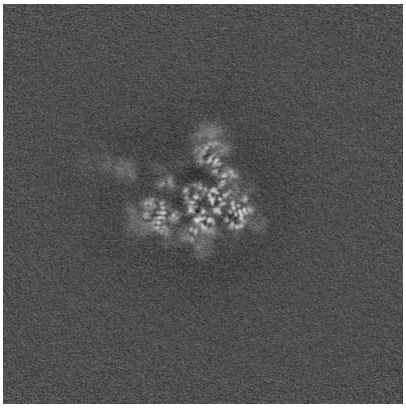
6.2.2 Raw map



X Index: 256



Y Index: 256

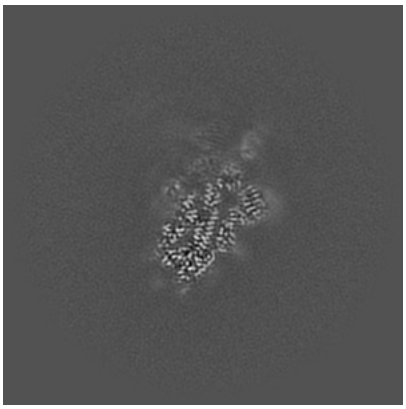


Z Index: 256

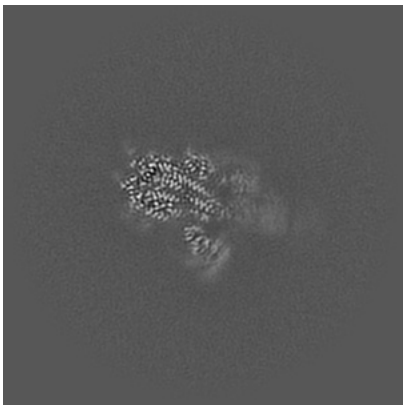
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

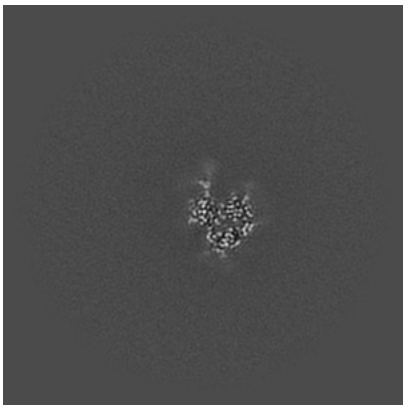
6.3.1 Primary map



X Index: 263

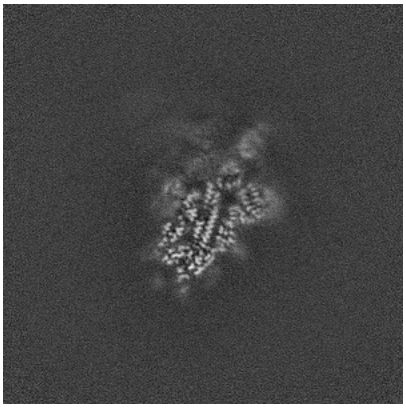


Y Index: 246

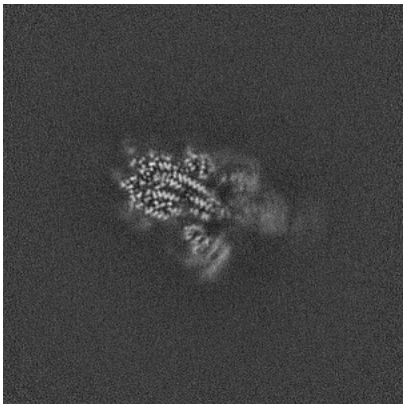


Z Index: 196

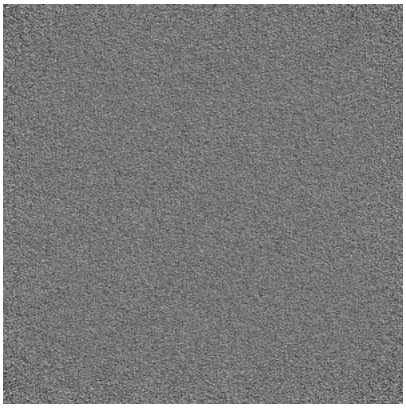
6.3.2 Raw map



X Index: 262



Y Index: 246

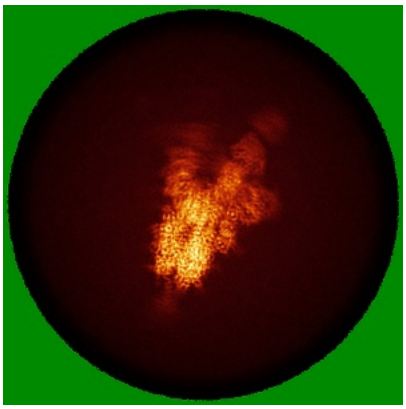


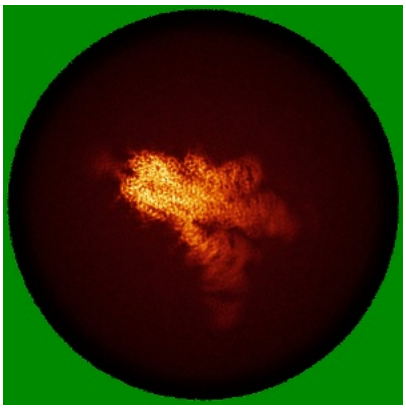
Z Index: 0

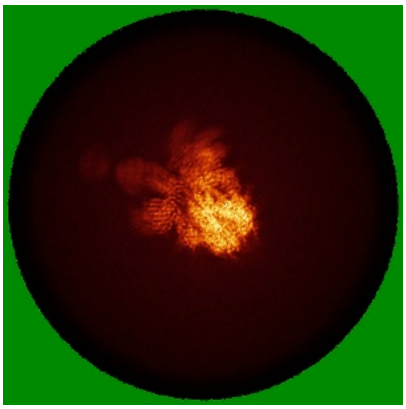
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

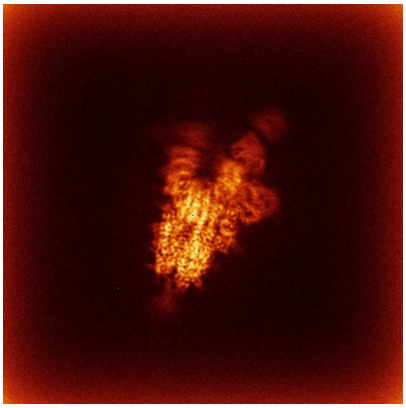
6.4.1 Primary map

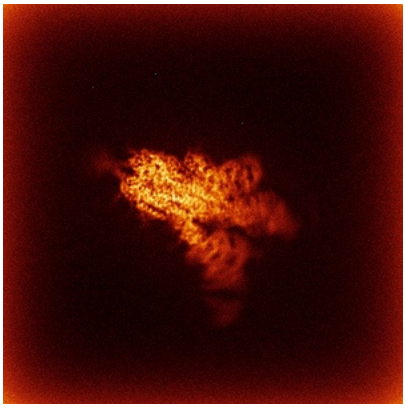

X

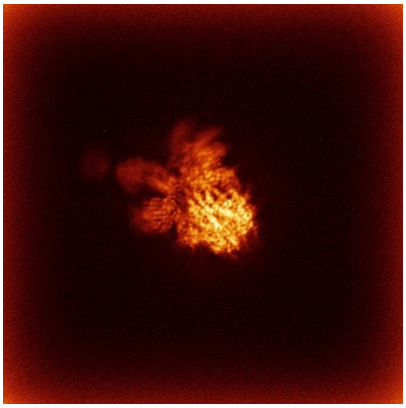

Y


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

X Y Z

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

X Y Z

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.

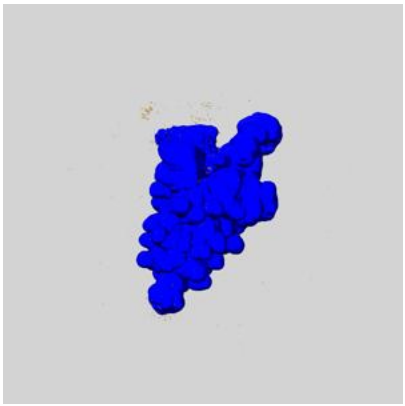
6.6 Mask visualisation (i)

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

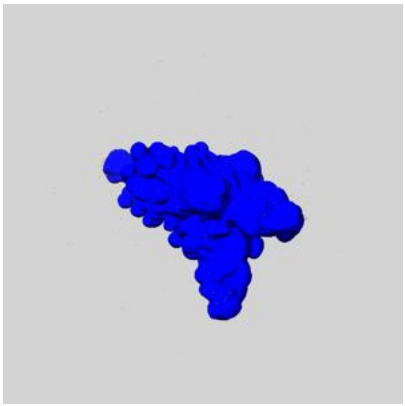
A mask typically either:

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

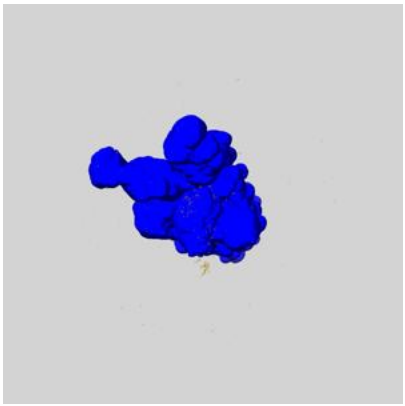
6.6.1 emd_34128_msk_1.map (i)



X



Y

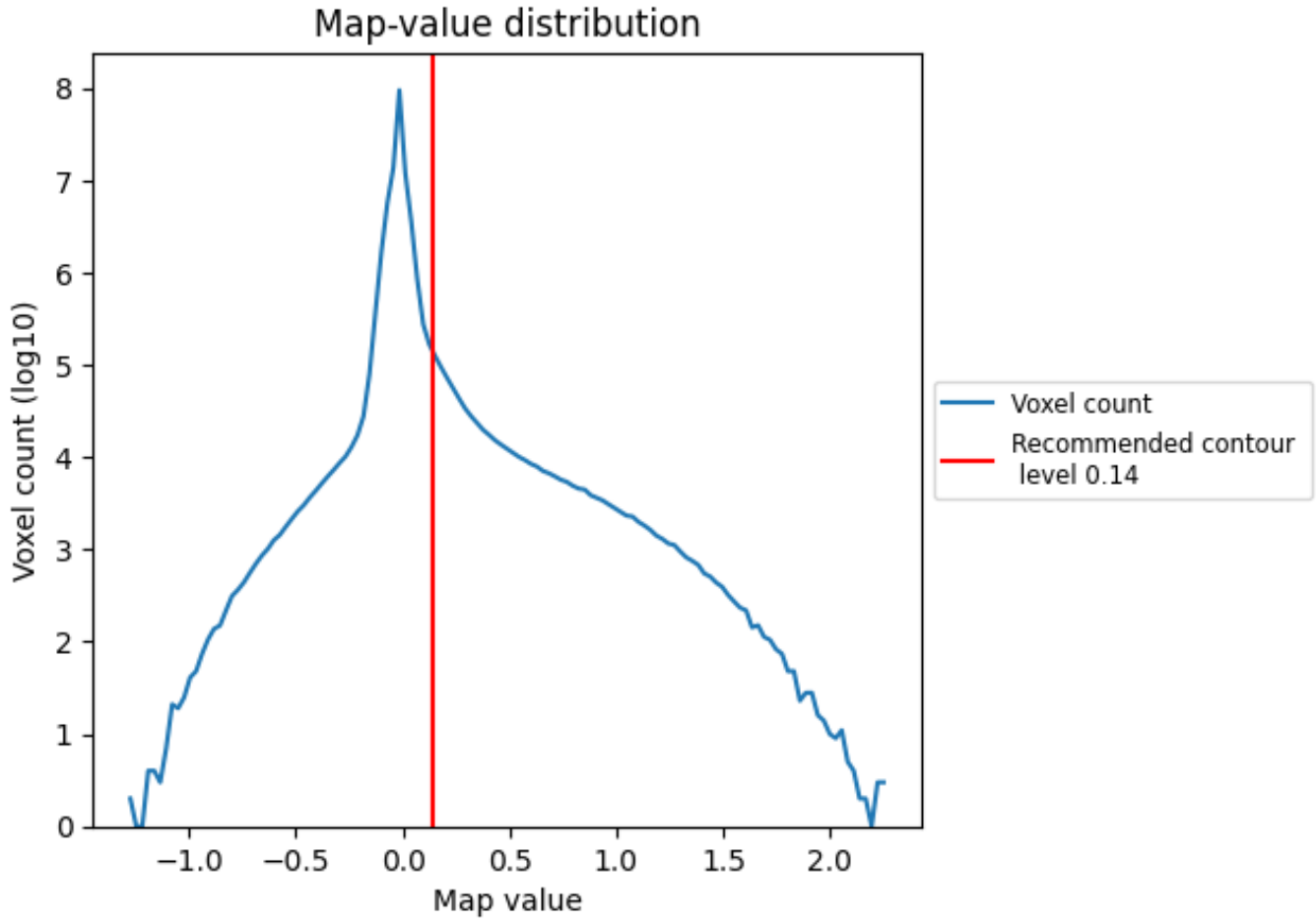


Z

7 Map analysis

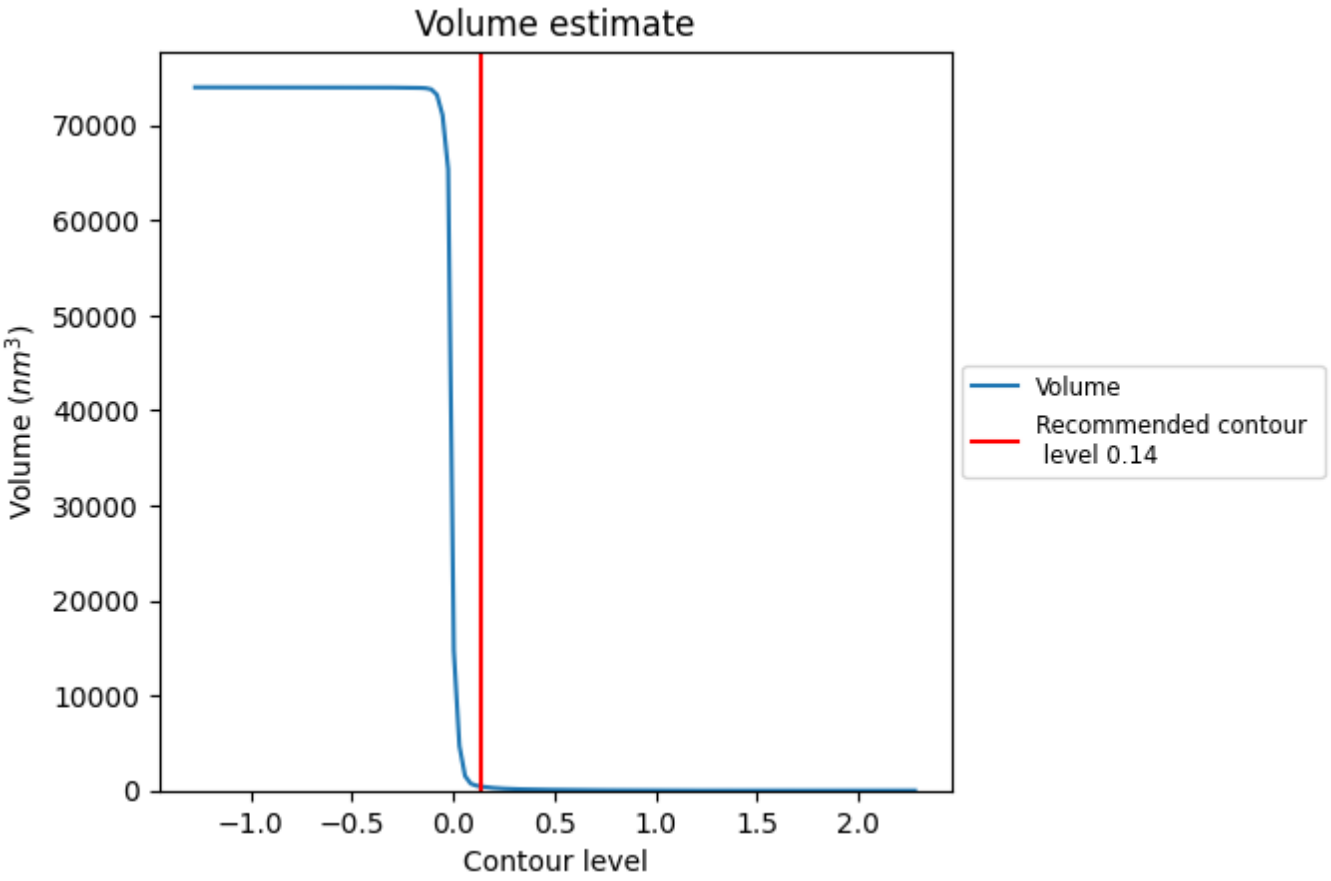
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

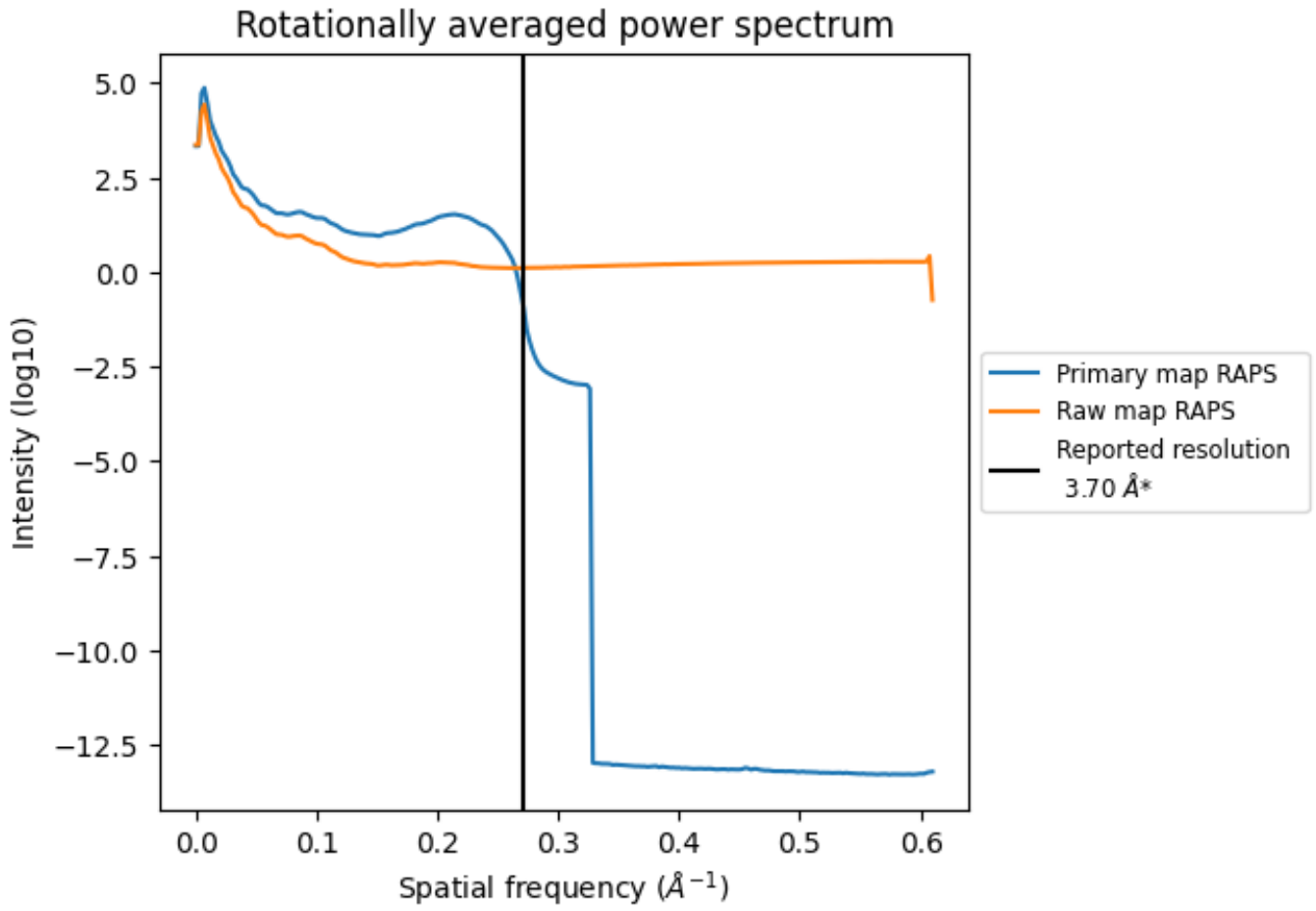
7.2 Volume estimate



The volume at the recommended contour level is 418 nm^3; this corresponds to an approximate mass of 377 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)

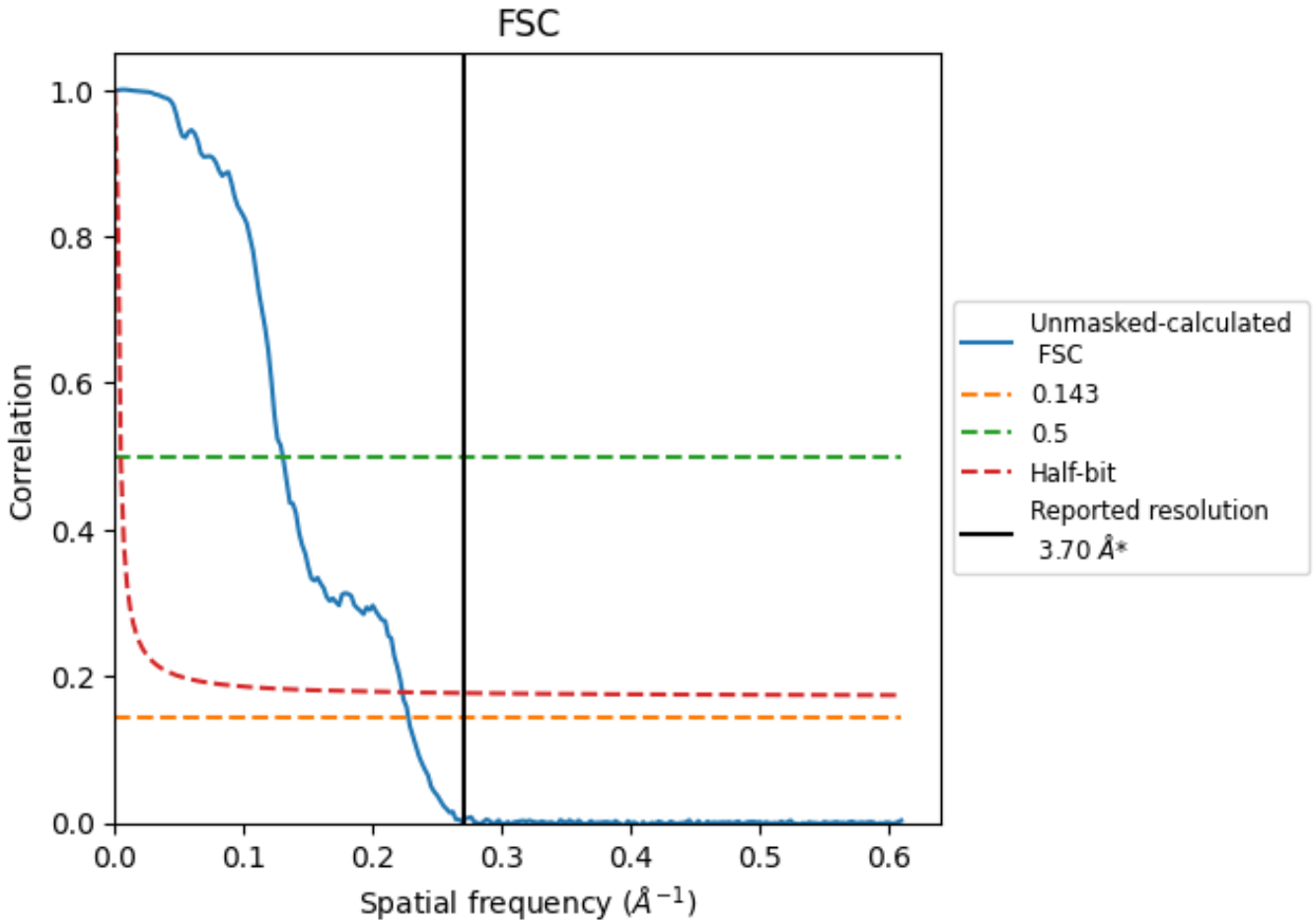


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

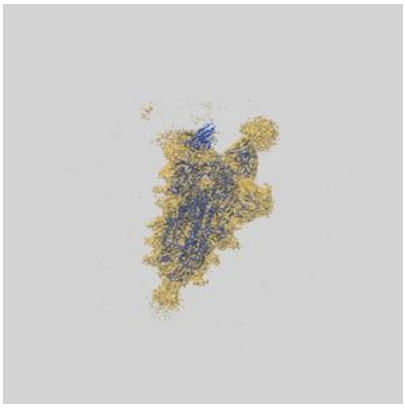
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.39	7.68	4.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.7 by more than 10 %

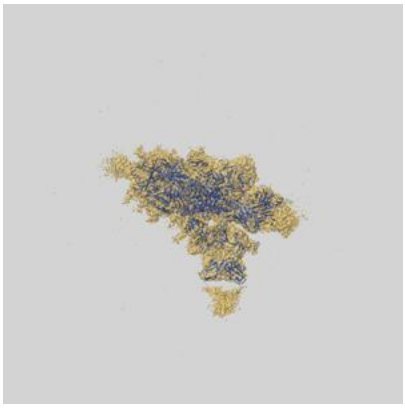
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34128 and PDB model 7YVI. Per-residue inclusion information can be found in section 3 on page 16.

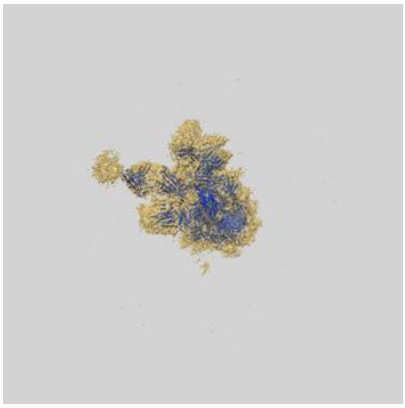
9.1 Map-model overlay



X



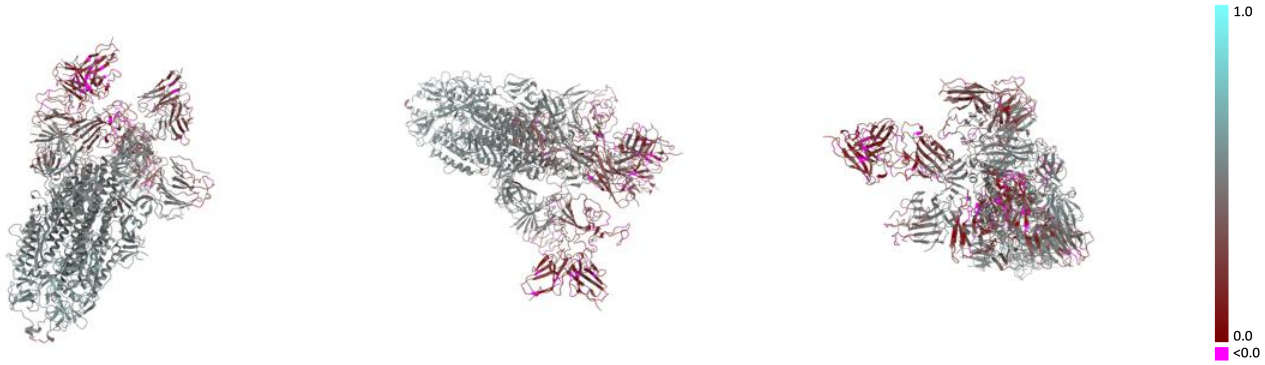
Y



Z

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.

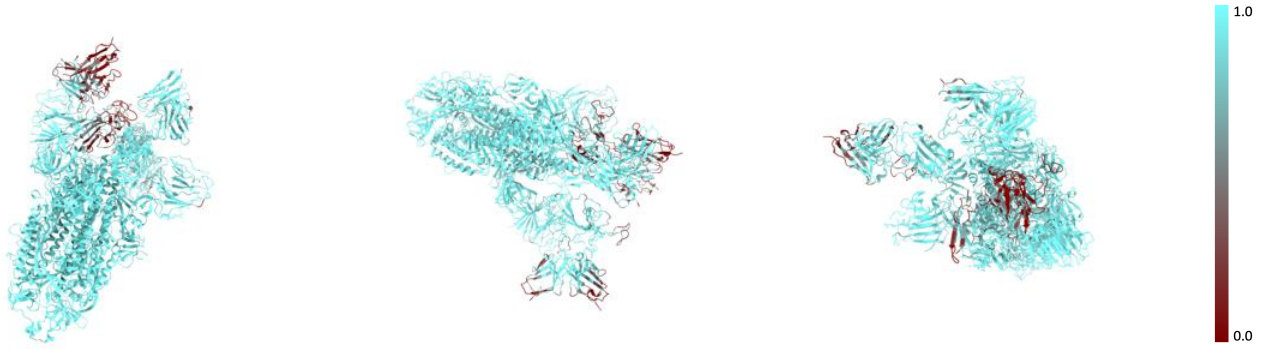
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

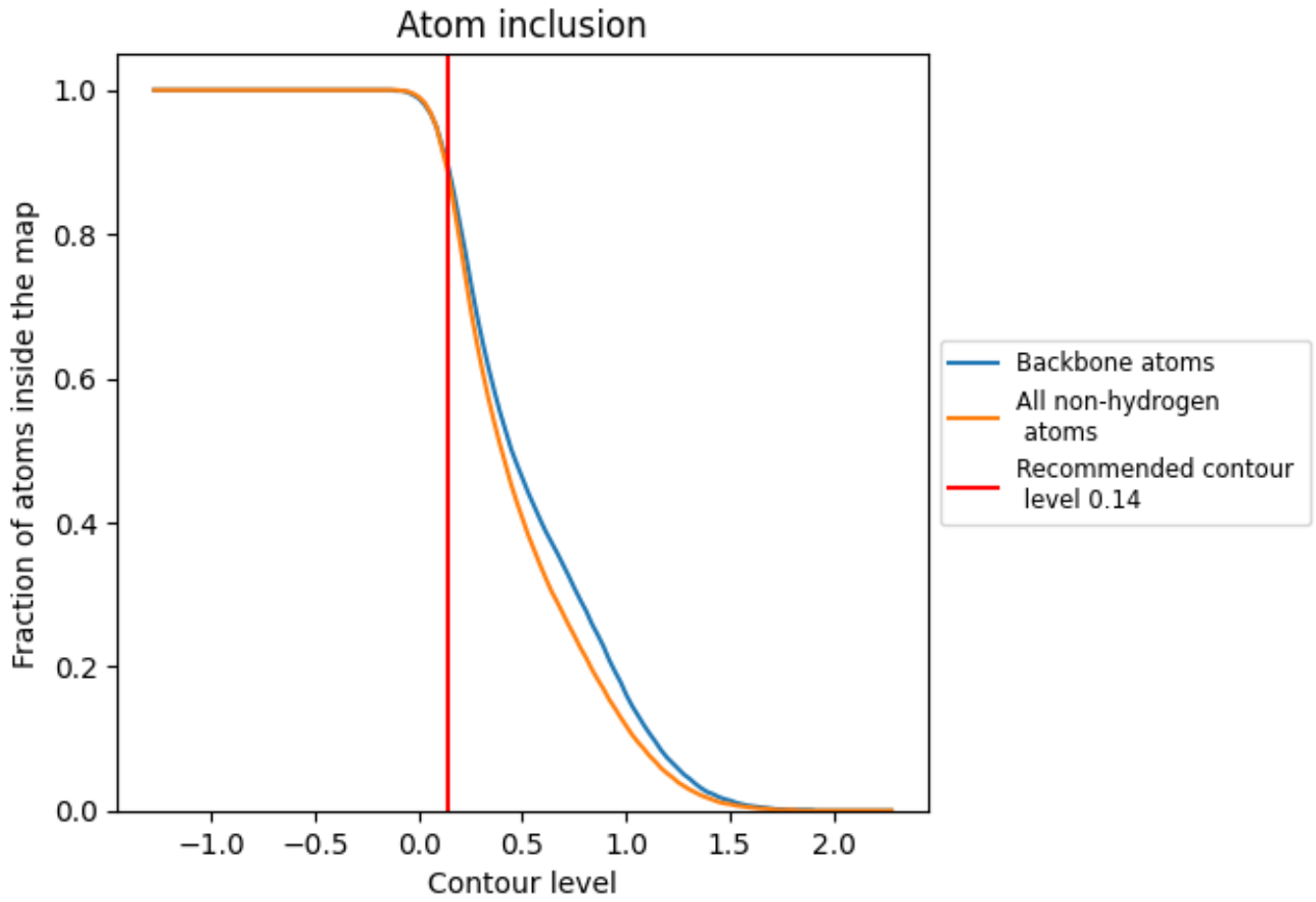
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% 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	0.8880	0.4140
A	0.8790	0.4440
B	0.9660	0.4750
C	0.9510	0.4430
H	0.6040	0.1830
I	0.7690	0.1850
J	0.2830	0.1660
K	0.6830	0.1970
N	0.9460	0.3190
O	0.8920	0.3450