Full wwPDB EM Validation Report (i)

Dec 17, 2022 – 01:22 PM EST

PDB ID	:	7UZ7
EMDB ID	:	EMD-26881
Title	:	Structure of the SARS-CoV-2 S 6P trimer in complex with the mouse antibody Fab fragment, M8a-31
Authors	:	Fan, C.; Bjorkman, P.J.
Deposited on	:	2022-05-08
Resolution	:	2.90 Å(reported)
Based on initial model	:	7SC1

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 (i) 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 (1)) were used in the production of this report:

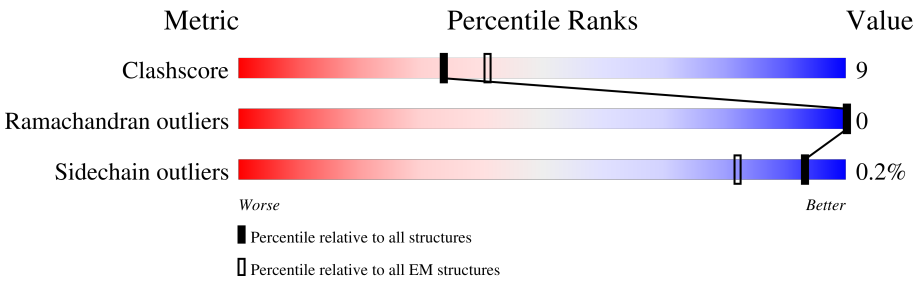
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.90 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	1256	13% 67% 18% 16%
1	B	1256	13% 66% 18% 16%
1	C	1256	12% 66% 18% 16%
2	H	228	42% 40% 11% 49%
2	M	228	42% 38% 13% 49%
2	P	228	40% 37% 13% 49%
3	L	220	38% 35% 16% 49%
3	N	220	39% 36% 15% 49%

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Mol	Chain	Length	Quality of chain
3	Q	220	38% 38% 13% 49%
4	D	2	100%
4	E	2	100%
4	F	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30552 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
			Total	C	N	O	S		
1	A	1059	8216	5243	1367	1569	37	0	0
1	B	1059	8216	5243	1367	1569	37	0	0
1	C	1059	8216	5243	1367	1569	37	0	0

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2

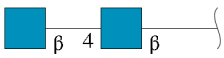
- Molecule 2 is a protein called M8a-31 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	116	894	562	153	176	3	0	0
2	M	116	894	562	153	176	3	0	0
2	P	116	894	562	153	176	3	0	0

- Molecule 3 is a protein called M8a-31 Fab light chain.

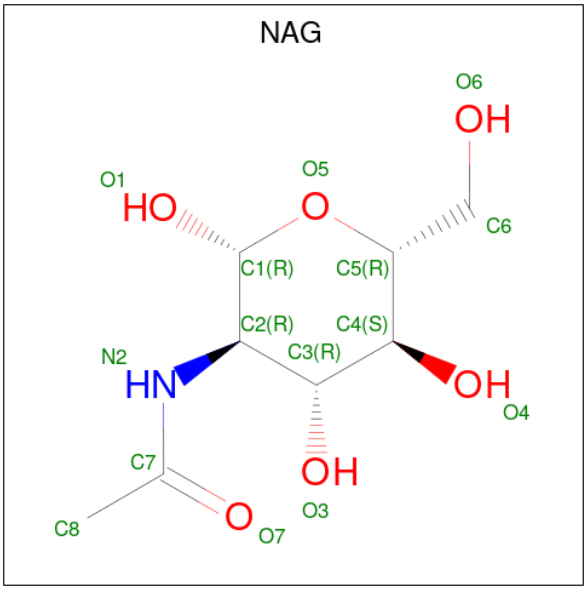
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	112	864	548	138	174	4	0	0
3	N	112	864	548	138	174	4	0	0
3	Q	112	864	548	138	174	4	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
			Total	C	N	O		
4	E	2	28	16	2	10	0	0
			Total	C	N	O		
4	F	2	28	16	2	10	0	0

- Molecule 5 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
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	A	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	B	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0

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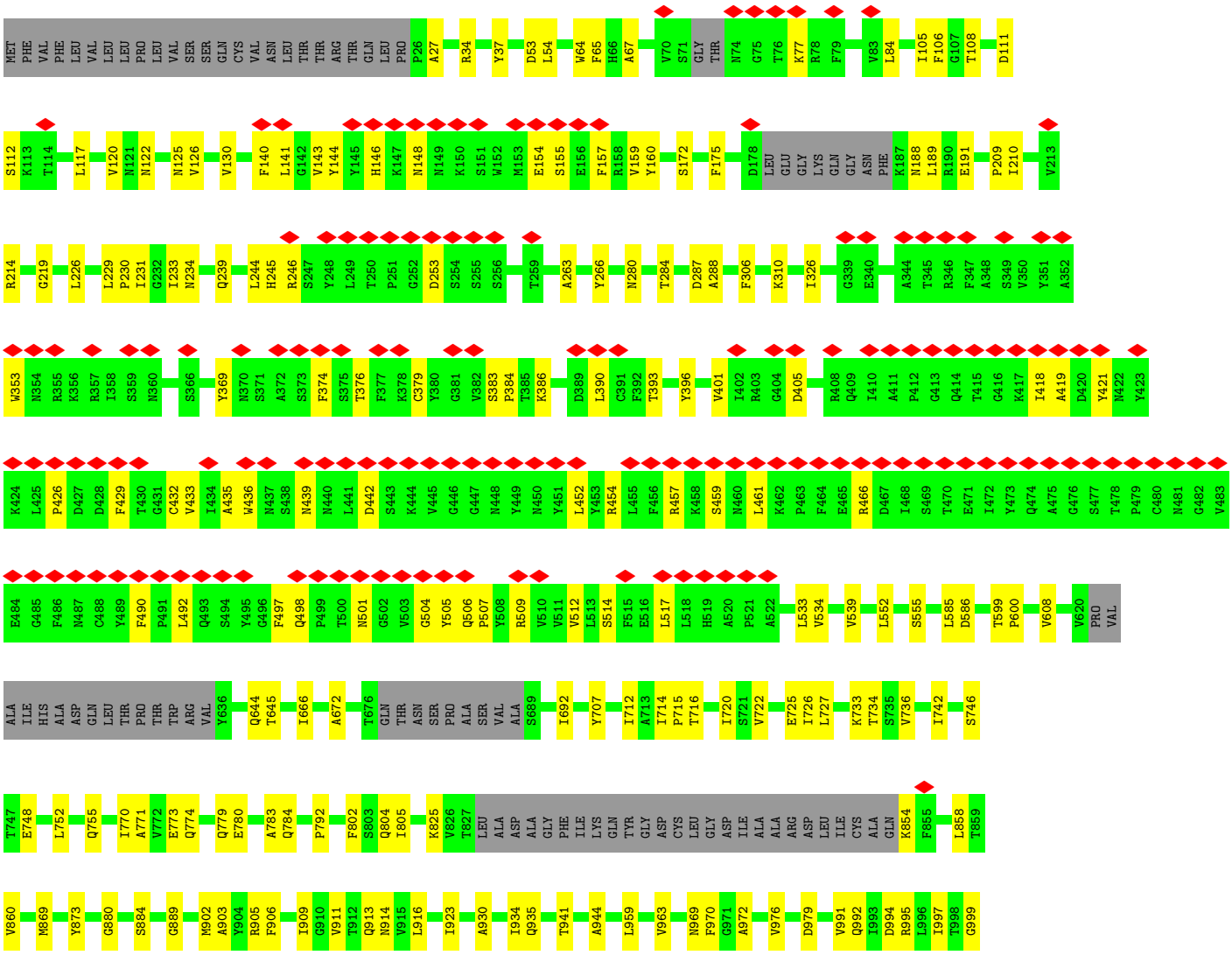
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0
			Total	C	N	O	
5	C	1	182	104	13	65	0

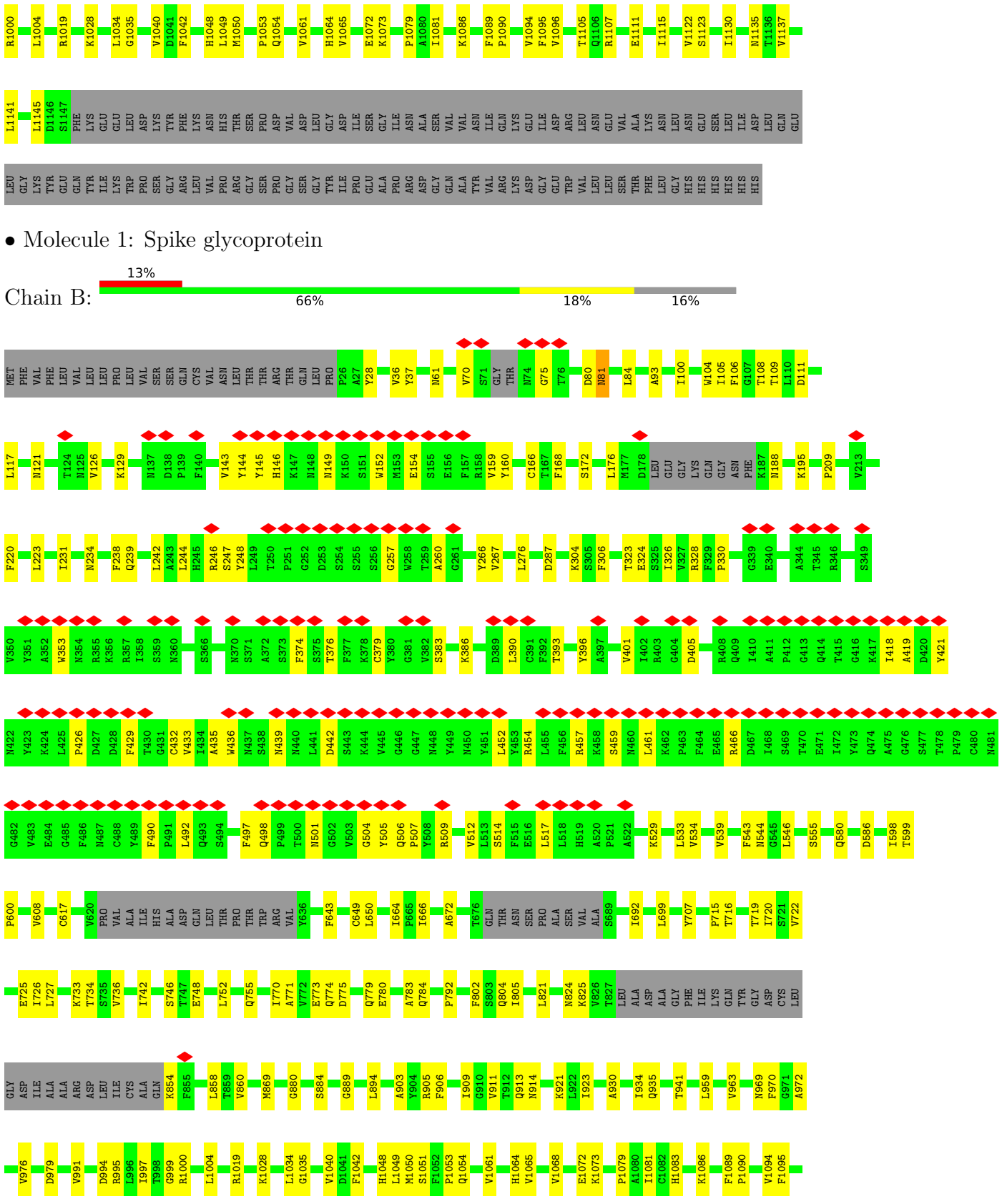
3 Residue-property plots (i)

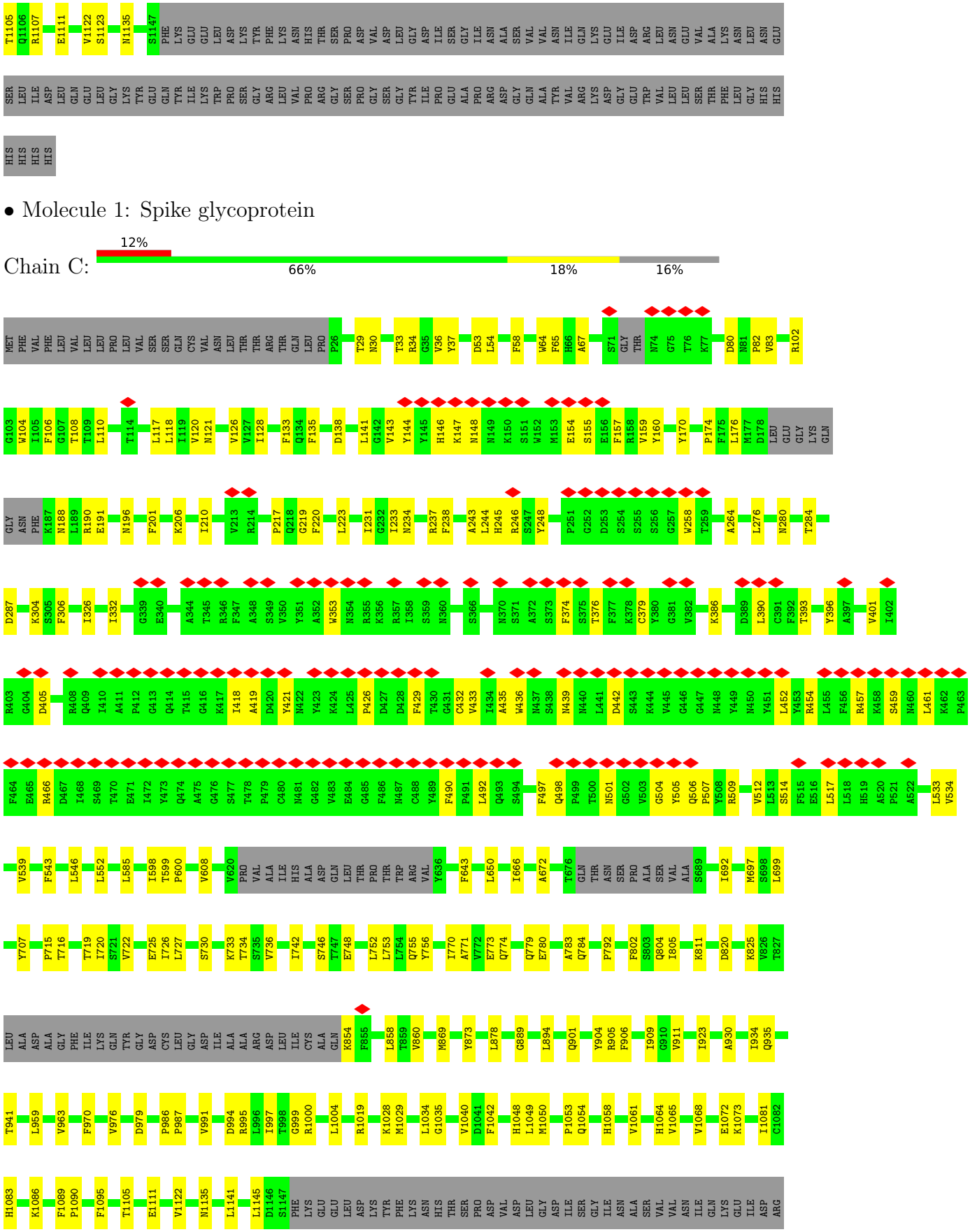
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 A: 13% 67% 18% 16%

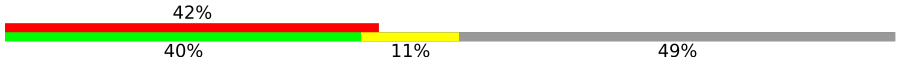


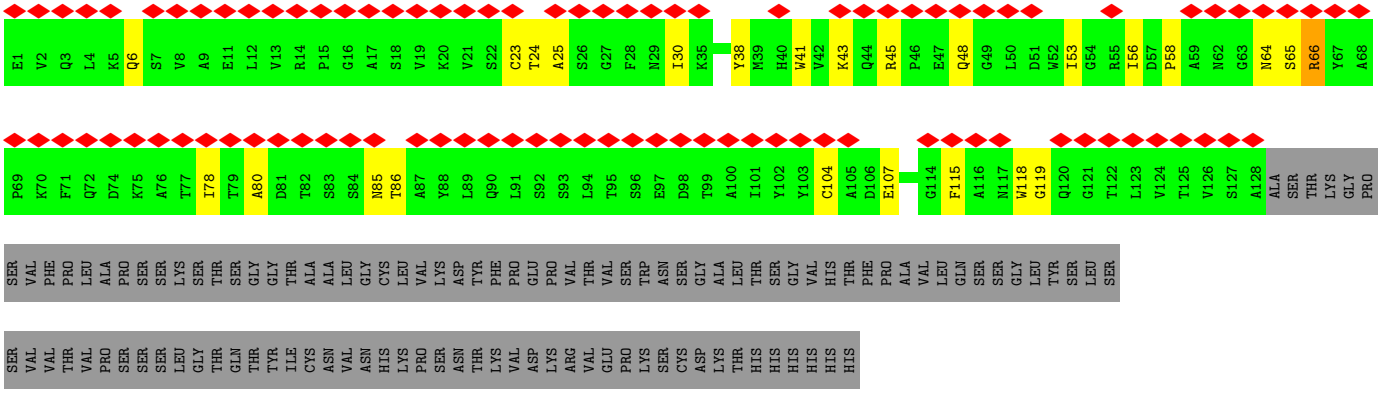

R1000 L1004 R1019 K1028 L1034 G1035 V1040 D1041 F1042 H1048 L1049 M1050 P1053 Q1054 V1061 H1064 V1065 E1072 K1073 P1079 A1080 I1081 K1086 F1089 P1090 V1094 F1095 V1096 T1105 Q1106 R1107 E1111 I1115 V1122 S1123 I1130 N1135 T1136 V1137
L1141 L1145 D1146 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU
LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO SER GLY ARG LEU VAL PRO ARG GLY SER PRO GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: Spike glycoprotein
Chain B:
13%
66%
18%
16%
MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO P26 A27 Y28 V36 Y37 N61 V70 S71 GLY THR N74 G75 T76 D80 N81 L84 A93 I100 W104 I105 F106 G107 T108 T109 L110 D111
L117 N121 T124 N125 V126 K129 N137 D138 P139 F140 V143 Y144 Y145 H146 K147 N148 N149 K150 S151 W152 M153 E154 S155 E156 F157 R158 V159 Y160 C166 T167 F168 S172 L176 M177 D178 LEU GLU GLY LYS GLN GLY ASN PHE K187 N188 K195 P209 V213
F220 L223 I231 N234 F238 Q239 L242 A243 L244 H245 R246 S247 Y248 L249 T250 P251 G252 D253 S254 S255 S256 G257 W258 T259 A260 G261 Y266 V267 L276 D287 K304 S305 F306 T323 E324 S325 I326 V327 R328 F329 P330 G339 E340 A344 T345 R346 S349
V350 Y351 A352 W353 N354 R355 K356 R357 I358 S359 N360 S366 N370 S371 A372 S373 F374 S375 T376 F377 K378 C379 Y380 G381 V382 S383 K386 D389 L390 C391 F392 T393 Y396 A397 V401 I402 R403 G404 D405 R408 Q409 I410 A411 P412 G413 Q414 T415 G416 K417 I418 A419 D420 Y421
N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 I434 A435 W436 N437 S438 N439 N440 L441 D442 S443 K444 V445 G446 G447 N448 Y449 N450 Y451 L452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 P463 F464 E465 R466 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 S477 T478 P479 C480 N481
G482 V483 E484 G485 F486 N487 C488 Y489 F490 P491 L492 Q493 S494 F497 Q498 P499 T500 N501 G502 V503 G504 Y505 Q506 P507 Y508 R509 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 K529 L533 V534 V539 F543 N544 G545 L546 S555 Q580 D586 I598 T599
P600 V608 G617 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL Y636 F643 G649 L650 I664 P665 I666 A672 T676 GLN THR ASN SER PRO ALA SER VAL ALA S689 I692 L699 Y707 P715 T716 T719 I720 S721 V722
E725 I726 L727 K733 T734 S735 V736 I742 S746 T747 E748 L752 Q755 I770 A771 V772 E773 Q774 D775 Q779 E780 A783 Q784 P792 F802 S803 Q804 I805 L821 N824 K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU
GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 F855 L858 T859 V860 M869 G880 S884 G889 L894 A903 Y904 R905 F906 I909 G910 V911 T912 Q913 N914 K921 L922 I923 A930 I934 Q935 T941 L959 V963 N969 F970 G971 A972
V976 D979 V991 D994 R995 L996 I997 T998 G999 R1000 L1004 R1019 K1028 L1034 G1035 V1040 D1041 F1042 H1048 L1049 M1050 S1051 F1052 P1053 Q1054 V1061 H1064 V1065 V1068 E1072 K1073 P1079 A1080 I1081 C1082 H1083 K1086 F1089 P1090 V1094 F1095


T1105 Q1106 R1107 E1111 V1122 S1123 N1135 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU
SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO SER GLY ARG LEU VAL PRO ARG GLY SER PRO GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY HIS HIS
HIS HIS HIS HIS
• Molecule 1: Spike glycoprotein
Chain C:
12%
66%
18%
16%
MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO P26 T29 N30 T33 R34 G35 V36 Y37 D53 L54 F58 W64 F65 H66 A67 S71 GLY THR N74 G75 T76 K77 D80 N81 P82 V83 R102
G103 W104 I105 F106 G107 T108 T109 L110 T114 L117 L118 T119 V120 N121 V126 V127 I128 F133 Q134 F135 D138 L141 G142 V143 Y144 Y145 H146 K147 N148 N149 K150 S151 W152 M153 E154 S155 E156 F157 R158 V159 Y160 Y170 P174 F175 L176 M177 D178 LEU GLU GLY LYS GLN
GLY ASN PHE K187 N188 L189 R190 E191 N196 F201 K206 I210 V213 R214 P217 Q218 G219 F220 L223 I231 G232 I233 N234 R237 F238 A243 L244 H245 R246 S247 Y248 P251 G252 D253 S254 S255 S256 G257 W258 T259 A264 L276 N280 T284
D287 K304 S305 F306 I326 I332 G339 E340 A344 T345 R346 F347 A348 S349 V350 Y351 A352 W353 N354 R355 K356 R357 I358 S359 N360 S366 N370 S371 A372 S373 F374 S375 T376 F377 K378 C379 Y380 G381 V382 K386 D389 L390 C391 F392 T393 Y396 A397 V401 I402
R403 G404 D405 R408 Q409 I410 A411 P412 G413 Q414 T415 G416 K417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 I434 A435 W436 N437 S438 N439 N440 L441 D442 S443 K444 V445 G446 G447 N448 Y449 N450 Y451 L452 Y453 R454 L455 F456 R457 K458 S459 M460 L461 K462 P463
F464 E465 R466 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 S477 T478 P479 C480 N481 G482 V483 E484 G485 F486 N487 C488 Y489 F490 P491 L492 Q493 S494 F497 Q498 P499 T500 N501 G502 V503 G504 Y505 Q506 P507 Y508 R509 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 L533 V534
V539 F543 L546 L552 L585 I598 T599 P600 V608 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL Y636 F643 L650 I666 A672 T676 GLN THR ASN SER PRO ALA SER VAL ALA S689 I692 M697 S698 L699
Y707 P715 T716 T719 I720 S721 V722 E725 I726 L727 S730 K733 T734 S735 V736 I742 S746 T747 E748 L752 L753 L754 Q755 Y756 I770 A771 V772 E773 Q774 Q779 E780 A783 Q784 P792 F802 S803 Q804 I805 K811 D820 K825 V826 T827
LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 F855 L858 T859 V860 M869 Y873 L878 G889 L894 Q901 Y904 R905 F906 I909 G910 V911 I923 A930 I934 Q935
T941 L959 V963 F970 V976 D979 P986 P987 V991 D994 R995 L996 I997 T998 G999 R1000 L1004 R1019 K1028 M1029 L1034 G1035 V1040 D1041 F1042 H1048 L1049 M1050 P1053 Q1054 H1058 V1061 H1064 V1065 V1068 E1072 K1073 I1081 G1082
H1083 K1086 F1089 P1090 F1095 T1105 E1111 V1122 N1135 L1141 L1145 D1146 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG

- Molecule 2: M8a-31 Fab heavy chain

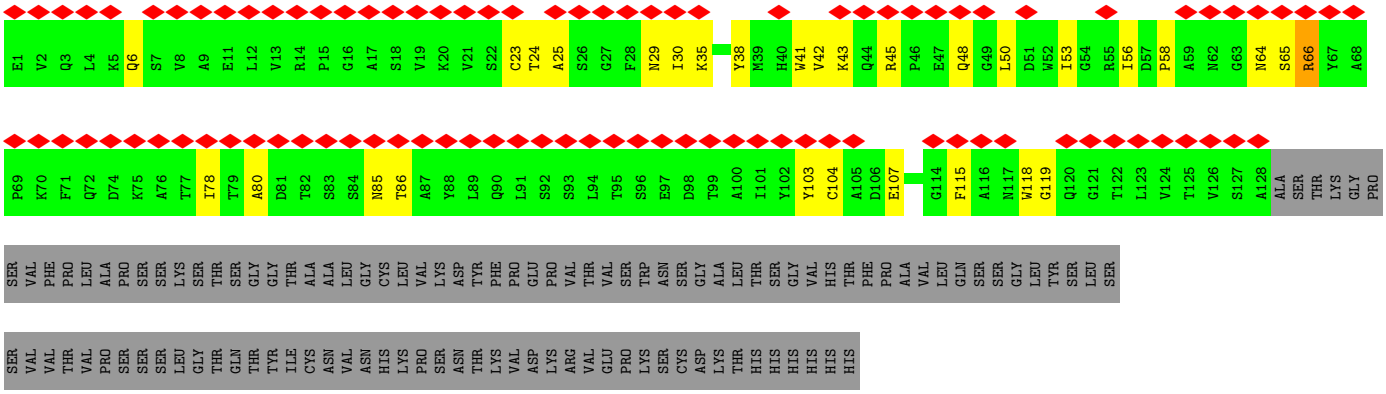
Chain H:





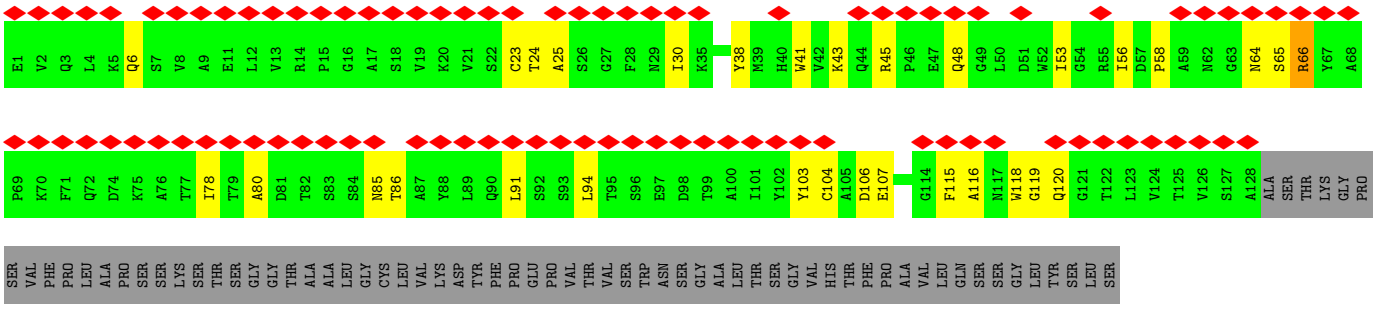
- Molecule 2: M8a-31 Fab heavy chain

Chain M:



- Molecule 2: M8a-31 Fab heavy chain

Chain P:



SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS ARG VAL GLU PRO LYS SER CYS ASP LYS THR HIS HIS HIS HIS HIS HIS

- Molecule 3: M8a-31 Fab light chain

Chain L:

D1 I2 V3 M4 T5 Q6 S7 P8 S9 S10 L11 T12 V13 T14 A15 G16 E17 K18 V19 T20 M21 S22 C23 K24 S25 S26 Q27 S28 L29 L30 N31 S32 Q35 K36 N37 Y38 L39 T40 W41 Y42 Q43 Q44 K45 V46 G47 Q48 P49 L53 I54 A57 S65 T66 R67 D68 P69 G70 V71

P72 D74 R75 F76 T77 G78 S79 G80 F83 G84 T85 D86 F87 T88 L89 T90 I91 S92 S93 V94 Q95 A96 E97 D98 L99 A100 Y103 C104 Q105 N106 D107 Y108 S109 Y114 P115 L116 T117 F118 G119 A120 G121 T122 K123 V124 E125 L126 LYS ARG THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO

PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU

THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

- Molecule 3: M8a-31 Fab light chain

Chain N:

D1 I2 V3 M4 T5 Q6 S7 P8 S9 S10 L11 T12 V13 T14 A15 G16 E17 K18 V19 T20 M21 S22 C23 K24 S25 S26 Q27 S28 L29 L30 N31 S32 Q35 K36 N37 Y38 L39 T40 W41 Y42 Q43 Q44 K45 V46 G47 Q48 P49 P50 K51 L52 L53 I54 A57 S65 T66 R67 D68 P69

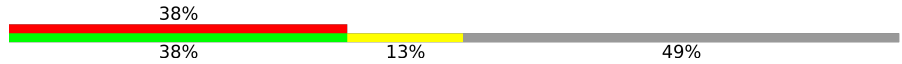
G70 V71 P72 D74 R75 F76 T77 G78 S79 G80 F83 G84 T85 D86 F87 T88 L89 T90 I91 S92 S93 V94 Q95 A96 E97 D98 L99 A100 Y103 C104 Q105 N106 D107 Y108 S109 Y114 P115 L116 T117 F118 G119 A120 G121 T122 K123 V124 E125 L126 LYS ARG THR VAL ALA ALA PRO SER VAL PHE ILE

PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER

THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

- Molecule 3: M8a-31 Fab light chain

Chain Q:



D1 I2 V3 M4 T5 Q6 S7 P8 S9 S10 L11 T12 V13 T14 A15 G16 E17 K18 V19 T20 M21 S22 C23 K24 S25 S26 Q27 S28 L29 L30 N31 S32 Q35 K36 N37 Y38 L39 T40 W41 Y42 Q43 Q44 K45 V46 G47 Q48 P49 L53 I54 A57 S65 T66 R67 D68 P69 G70 V71

P72 D74 R75 F76 T77 G78 S79 G80 F83 G84 T85 D86 F87 T88 L89 T90 I91 S92 S93 V94 Q95 A96 E97 D98 L99 A100 V101 Y102 Y103 C104 Q105 N106 S109 Y114 P115 L116 T117 A120 G121 T122 K123 V124 E125 L126 LYS ARG THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO PRO

SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR

LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1
NAG2

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

NAG1
NAG2

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	295711	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.299	Depositor
Minimum map value	-0.789	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	299.52002, 299.52002, 299.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.30	1/8411 (0.0%)	0.50	3/11461 (0.0%)
1	B	0.29	1/8411 (0.0%)	0.50	3/11461 (0.0%)
1	C	0.26	0/8411	0.47	0/11461
2	H	0.25	0/914	0.50	0/1244
2	M	0.25	0/914	0.50	0/1244
2	P	0.25	0/914	0.50	0/1244
3	L	0.25	0/884	0.51	0/1204
3	N	0.25	0/884	0.50	0/1204
3	Q	0.25	0/884	0.49	0/1204
All	All	0.28	2/30627 (0.0%)	0.49	6/41727 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1079	PRO	CG-CD	-12.17	1.10	1.50
1	B	1079	PRO	CG-CD	-10.94	1.14	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1079	PRO	N-CD-CG	-14.97	80.75	103.20
1	B	1079	PRO	N-CD-CG	-13.90	82.34	103.20
1	B	1079	PRO	CA-N-CD	-9.89	97.65	111.50
1	A	1079	PRO	CA-N-CD	-9.34	98.42	111.50
1	A	1079	PRO	CA-CB-CG	-7.71	89.34	104.00
1	B	1079	PRO	CA-CB-CG	-7.58	89.60	104.00

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	8216	0	7920	139	0
1	B	8216	0	7920	140	0
1	C	8216	0	7920	156	0
2	H	894	0	862	16	0
2	M	894	0	862	22	0
2	P	894	0	862	20	0
3	L	864	0	839	24	0
3	N	864	0	839	22	0
3	Q	864	0	839	20	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	182	0	169	1	0
5	B	182	0	169	0	0
5	C	182	0	169	1	0
All	All	30552	0	29445	540	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 9.

All (540) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.18	0.76
1:C:452:LEU:HD21	1:C:492:LEU:HB3	1.68	0.75
1:B:452:LEU:HD21	1:B:492:LEU:HB3	1.68	0.75
1:C:121:ASN:HD22	1:C:126:VAL:HG22	1.53	0.73
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.21	0.73
1:A:452:LEU:HD21	1:A:492:LEU:HB3	1.69	0.72
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.72	0.72
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.72	0.71
1:C:287:ASP:HB3	1:C:306:PHE:HE2	1.55	0.71
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.24	0.70
1:C:110:LEU:HD12	1:C:237:ARG:NH1	2.08	0.69
1:A:105:ILE:HB	1:A:239:GLN:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:GLU:O	1:A:784:GLN:NE2	2.26	0.69
1:C:780:GLU:O	1:C:784:GLN:NE2	2.26	0.69
1:A:65:PHE:HE2	1:A:84:LEU:HD21	1.58	0.69
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.20	0.69
3:Q:13:VAL:HG11	3:Q:19:VAL:HG12	1.76	0.68
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.28	0.67
1:B:780:GLU:O	1:B:784:GLN:NE2	2.25	0.67
2:M:104:CYS:H	2:M:119:GLY:H	1.42	0.67
3:Q:39:LEU:HD21	3:Q:104:CYS:HB2	1.76	0.67
2:P:104:CYS:H	2:P:119:GLY:H	1.43	0.67
1:B:287:ASP:HB3	1:B:306:PHE:HE2	1.59	0.66
1:A:214:ARG:O	1:A:266:TYR:OH	2.12	0.66
3:L:13:VAL:HG11	3:L:19:VAL:HG12	1.78	0.66
1:B:330:PRO:HD3	1:B:544:ASN:HD21	1.61	0.65
2:H:6:GLN:HA	2:H:23:CYS:HA	1.78	0.65
2:M:6:GLN:HA	2:M:23:CYS:HA	1.78	0.65
3:N:39:LEU:HD21	3:N:104:CYS:HB2	1.79	0.64
1:A:144:TYR:HB2	1:A:246:ARG:HD3	1.80	0.64
3:L:39:LEU:HD21	3:L:104:CYS:HB2	1.78	0.64
2:P:6:GLN:HA	2:P:23:CYS:HA	1.79	0.64
1:B:144:TYR:HB2	1:B:246:ARG:HD3	1.80	0.63
2:P:103:TYR:HB3	2:P:118:TRP:HB3	1.81	0.63
1:C:121:ASN:HB2	1:C:176:LEU:HD12	1.79	0.63
1:B:244:LEU:HD13	1:B:248:TYR:CE2	2.34	0.63
1:C:141:LEU:HB3	1:C:243:ALA:HA	1.80	0.63
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.80	0.63
1:A:498:GLN:H	1:A:501:ASN:HD21	1.47	0.62
1:C:498:GLN:H	1:C:501:ASN:HD21	1.47	0.62
1:C:102:ARG:HG2	1:C:141:LEU:HD22	1.81	0.62
2:P:56:ILE:HD12	2:P:80:ALA:HB2	1.82	0.62
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.64	0.62
1:A:143:VAL:HG13	1:A:245:HIS:HA	1.81	0.62
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.22	0.62
1:B:498:GLN:H	1:B:501:ASN:HD21	1.47	0.61
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.66	0.61
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.64	0.61
3:L:6:GLN:HE21	3:L:119:GLY:HA3	1.66	0.61
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.01	0.60
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.02	0.60
1:C:986:PRO:HG2	1:C:987:PRO:HD3	1.81	0.60
1:C:1105:THR:HG23	1:C:1111:GLU:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:56:ILE:HD12	2:M:80:ALA:HB2	1.83	0.60
3:Q:6:GLN:HE21	3:Q:122:THR:HG23	1.66	0.60
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.20	0.60
1:C:326:ILE:HD11	1:C:533:LEU:HA	1.82	0.59
1:C:176:LEU:HA	1:C:190:ARG:NH2	2.16	0.59
2:H:56:ILE:HD12	2:H:80:ALA:HB2	1.82	0.59
3:N:105:GLN:NE2	3:N:106:ASN:O	2.36	0.59
1:A:1105:THR:HG23	1:A:1111:GLU:H	1.67	0.59
3:N:13:VAL:HG11	3:N:19:VAL:HG12	1.84	0.59
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.26	0.59
1:B:100:ILE:HG22	1:B:242:LEU:HD12	1.84	0.59
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.02	0.58
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.85	0.58
3:Q:105:GLN:NE2	3:Q:106:ASN:O	2.37	0.58
1:C:104:TRP:HH2	1:C:176:LEU:HD21	1.69	0.58
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.86	0.58
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.35	0.58
1:B:1105:THR:HG23	1:B:1111:GLU:H	1.67	0.57
3:L:41:TRP:N	3:L:54:ILE:O	2.37	0.57
1:B:84:LEU:O	1:B:238:PHE:N	2.37	0.57
1:C:825:LYS:NZ	1:C:941:THR:O	2.32	0.57
3:L:105:GLN:NE2	3:L:106:ASN:O	2.37	0.57
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.85	0.57
1:C:102:ARG:HE	1:C:243:ALA:HB2	1.70	0.57
3:L:53:LEU:HD23	3:L:89:LEU:HD21	1.87	0.57
3:N:41:TRP:N	3:N:54:ILE:O	2.38	0.57
1:A:122:ASN:HB3	1:A:125:ASN:O	2.05	0.56
2:H:104:CYS:H	2:H:119:GLY:H	1.53	0.56
1:A:599:THR:HB	1:A:608:VAL:HG12	1.86	0.56
1:A:1048:HIS:NE2	1:A:1050:MET:O	2.37	0.56
1:A:34:ARG:NH2	1:A:191:GLU:OE1	2.38	0.56
2:H:25:ALA:O	2:H:85:ASN:ND2	2.39	0.56
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.70	0.56
1:C:976:VAL:HG13	1:C:979:ASP:HB2	1.88	0.56
1:A:108:THR:OG1	1:A:234:ASN:O	2.25	0.55
3:L:75:ARG:HG3	3:L:76:PHE:H	1.71	0.55
1:C:83:VAL:HG12	1:C:237:ARG:NH2	2.22	0.55
1:B:734:THR:HG22	1:B:860:VAL:HG22	1.89	0.55
1:A:287:ASP:OD1	1:A:288:ALA:N	2.39	0.55
1:A:67:ALA:HB3	1:A:263:ALA:HB1	1.89	0.55
2:M:25:ALA:O	2:M:85:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:A:231:ILE:HD12	1.88	0.55
1:B:188:ASN:HA	1:B:209:PRO:HA	1.88	0.55
1:C:210:ILE:HG21	1:C:217:PRO:HG3	1.88	0.55
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.89	0.55
3:N:75:ARG:HG3	3:N:76:PHE:H	1.70	0.55
2:H:115:PHE:O	2:H:118:TRP:NE1	2.40	0.55
3:Q:75:ARG:HG3	3:Q:76:PHE:H	1.72	0.55
5:A:1311:NAG:H83	5:A:1311:NAG:H3	1.88	0.55
1:B:276:LEU:HD11	1:B:304:LYS:HA	1.89	0.55
1:A:405:ASP:N	1:A:504:GLY:O	2.41	0.54
1:B:108:THR:OG1	1:B:234:ASN:O	2.24	0.54
1:A:976:VAL:HG13	1:A:979:ASP:HB2	1.88	0.54
3:N:53:LEU:HD23	3:N:89:LEU:HD21	1.88	0.54
2:P:115:PHE:O	2:P:118:TRP:NE1	2.41	0.54
1:B:70:VAL:HG13	1:B:75:GLY:HA2	1.90	0.54
3:N:2:ILE:HD12	3:N:106:ASN:HD22	1.71	0.54
2:P:25:ALA:O	2:P:85:ASN:ND2	2.40	0.54
3:Q:41:TRP:N	3:Q:54:ILE:O	2.40	0.54
1:C:143:VAL:HG12	1:C:154:GLU:HG2	1.89	0.54
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.25	0.54
1:A:326:ILE:HD11	1:A:533:LEU:HA	1.89	0.54
1:A:1086:LYS:HD3	1:A:1122:VAL:HG21	1.90	0.54
1:B:28:TYR:HD2	1:B:61:ASN:HB3	1.73	0.54
1:B:555:SER:HB2	1:B:586:ASP:HB2	1.90	0.54
3:Q:25:SER:OG	3:Q:84:GLY:O	2.25	0.54
1:B:1051:SER:OG	1:B:1064:HIS:ND1	2.35	0.54
1:B:643:PHE:O	1:B:650:LEU:N	2.38	0.53
1:C:376:THR:HB	1:C:435:ALA:HB3	1.90	0.53
1:C:34:ARG:NH1	1:C:219:GLY:O	2.42	0.53
1:C:598:ILE:HD12	1:C:650:LEU:HD11	1.89	0.53
2:P:30:ILE:HG22	2:P:58:PRO:HG3	1.91	0.53
1:A:231:ILE:HG22	1:A:233:ILE:HG12	1.91	0.53
2:M:64:ASN:OD1	2:M:66:ARG:NH1	2.41	0.53
2:P:6:GLN:O	2:P:120:GLN:NE2	2.36	0.53
1:B:976:VAL:HG13	1:B:979:ASP:HB2	1.90	0.53
1:C:405:ASP:N	1:C:504:GLY:O	2.41	0.53
3:Q:53:LEU:HD23	3:Q:89:LEU:HD21	1.90	0.53
1:A:736:VAL:HG22	1:A:858:LEU:HD13	1.90	0.53
1:B:326:ILE:HD11	1:B:533:LEU:HA	1.91	0.53
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.89	0.53
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HB	1:A:435:ALA:HB3	1.91	0.52
1:C:439:ASN:HB2	1:C:506:GLN:HB3	1.91	0.52
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.42	0.52
2:H:64:ASN:OD1	2:H:66:ARG:NH1	2.41	0.52
2:P:64:ASN:OD1	2:P:66:ARG:NH1	2.42	0.52
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.89	0.52
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.42	0.52
1:B:439:ASN:HB2	1:B:506:GLN:HB3	1.92	0.52
1:B:854:LYS:HD3	1:B:963:VAL:HG21	1.92	0.52
1:C:104:TRP:HD1	1:C:238:PHE:CE1	2.28	0.52
1:C:736:VAL:HG22	1:C:858:LEU:HD13	1.91	0.52
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.92	0.52
1:C:191:GLU:HG3	1:C:223:LEU:HD21	1.91	0.52
2:H:30:ILE:HG22	2:H:58:PRO:HG3	1.90	0.52
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.92	0.52
1:A:439:ASN:HB2	1:A:506:GLN:HB3	1.92	0.52
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.92	0.52
1:B:405:ASP:N	1:B:504:GLY:O	2.41	0.52
1:C:176:LEU:HA	1:C:190:ARG:HH22	1.75	0.52
1:B:736:VAL:HG22	1:B:858:LEU:HD13	1.91	0.52
1:B:825:LYS:NZ	1:B:941:THR:O	2.33	0.52
1:C:104:TRP:HD1	1:C:238:PHE:HE1	1.58	0.52
1:C:889:GLY:HA3	1:C:1034:LEU:HD23	1.92	0.52
3:N:74:ASP:OD1	3:N:74:ASP:N	2.43	0.52
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.42	0.52
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.92	0.52
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.92	0.52
1:A:914:ASN:HA	1:C:1089:PHE:HE2	1.75	0.51
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.92	0.51
1:C:643:PHE:O	1:C:650:LEU:N	2.41	0.51
1:B:734:THR:HG21	1:B:959:LEU:HD11	1.92	0.51
1:A:854:LYS:HD3	1:A:963:VAL:HG21	1.92	0.51
1:B:598:ILE:HD12	1:B:650:LEU:HD11	1.92	0.51
1:B:106:PHE:O	1:B:117:LEU:N	2.43	0.51
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.92	0.51
1:C:176:LEU:HD22	1:C:190:ARG:HH12	1.75	0.51
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.92	0.51
1:A:111:ASP:OD2	1:A:112:SER:N	2.44	0.51
1:A:914:ASN:HA	1:C:1089:PHE:CE2	2.46	0.51
1:B:70:VAL:HG21	1:B:260:ALA:H	1.75	0.51
3:N:75:ARG:HD3	3:N:91:ILE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:THR:HG22	1:A:860:VAL:HG22	1.93	0.51
1:A:1040:VAL:HG21	1:B:1035:GLY:HA3	1.93	0.51
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	1.93	0.51
1:C:83:VAL:HG12	1:C:237:ARG:HH21	1.75	0.51
1:B:376:THR:HB	1:B:435:ALA:HB3	1.92	0.50
1:C:734:THR:HG22	1:C:860:VAL:HG22	1.92	0.50
2:M:30:ILE:HG22	2:M:58:PRO:HG3	1.92	0.50
1:A:65:PHE:CE2	1:A:84:LEU:HD21	2.43	0.50
1:A:501:ASN:HB3	1:A:505:TYR:HB3	1.94	0.50
3:N:6:GLN:HE21	3:N:119:GLY:HA3	1.76	0.50
1:B:498:GLN:H	1:B:501:ASN:ND2	2.10	0.50
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.93	0.50
1:A:117:LEU:HD12	1:A:231:ILE:HG21	1.94	0.50
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.94	0.50
1:B:287:ASP:HB3	1:B:306:PHE:CE2	2.44	0.50
2:M:45:ARG:HH11	2:M:48:GLN:HG2	1.77	0.50
3:Q:99:LEU:HG	3:Q:125:GLU:HA	1.93	0.50
1:A:720:ILE:HG13	1:A:923:ILE:HG23	1.93	0.50
1:B:396:TYR:O	1:B:514:SER:N	2.42	0.50
1:C:110:LEU:HD22	1:C:135:PHE:CE2	2.46	0.50
1:C:854:LYS:HD3	1:C:963:VAL:HG21	1.94	0.50
1:A:64:TRP:CD1	1:A:266:TYR:HE1	2.29	0.50
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.92	0.50
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.93	0.50
1:B:501:ASN:HB3	1:B:505:TYR:HB3	1.94	0.50
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.44	0.50
3:Q:95:GLN:H	3:Q:98:ASP:HB2	1.77	0.50
1:C:133:PHE:HB2	1:C:135:PHE:CE2	2.47	0.50
1:C:143:VAL:HG22	1:C:245:HIS:HA	1.94	0.50
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.93	0.50
1:B:889:GLY:HA3	1:B:1034:LEU:HD23	1.94	0.49
1:C:396:TYR:HB2	1:C:514:SER:HB3	1.94	0.49
1:C:501:ASN:HB3	1:C:505:TYR:HB3	1.94	0.49
2:P:45:ARG:HH11	2:P:48:GLN:HG2	1.77	0.49
1:B:1086:LYS:HD3	1:B:1122:VAL:HG21	1.93	0.49
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.93	0.49
2:P:45:ARG:HD2	2:P:48:GLN:HG2	1.94	0.49
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.94	0.49
1:C:146:HIS:CE1	1:C:148:ASN:HB2	2.47	0.49
3:L:9:SER:HA	3:L:122:THR:HG22	1.94	0.49
2:M:29:ASN:HD21	2:M:35:LYS:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:103:TYR:HB3	2:M:118:TRP:HB3	1.93	0.49
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.94	0.49
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.26	0.49
2:H:45:ARG:HH11	2:H:48:GLN:HG2	1.77	0.49
2:M:45:ARG:HD2	2:M:48:GLN:HG2	1.94	0.49
1:A:644:GLN:NE2	1:A:645:THR:O	2.44	0.49
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.94	0.49
3:N:9:SER:HA	3:N:122:THR:HG22	1.95	0.49
1:A:159:VAL:HG23	1:A:160:TYR:CD2	2.48	0.49
1:C:188:ASN:HA	1:C:210:ILE:H	1.78	0.49
1:A:143:VAL:HA	1:A:154:GLU:HA	1.94	0.49
1:A:34:ARG:NH1	1:A:219:GLY:O	2.46	0.49
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.78	0.49
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.93	0.49
1:B:742:ILE:HD13	1:B:1000:ARG:HB3	1.95	0.49
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.48	0.49
1:C:37:TYR:OH	1:C:54:LEU:O	2.28	0.49
1:C:498:GLN:H	1:C:501:ASN:ND2	2.10	0.49
1:C:144:TYR:HD1	1:C:155:SER:HB3	1.77	0.49
3:N:42:TYR:HB2	3:N:103:TYR:HB2	1.95	0.49
1:A:141:LEU:HD12	1:A:157:PHE:HA	1.95	0.48
1:B:457:ARG:NH1	1:B:459:SER:O	2.47	0.48
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.35	0.48
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.39	0.48
1:C:994:ASP:HA	1:C:997:ILE:HG22	1.95	0.48
2:H:45:ARG:HD2	2:H:48:GLN:HG2	1.95	0.48
3:L:95:GLN:H	3:L:98:ASP:HB2	1.78	0.48
3:Q:42:TYR:HB2	3:Q:103:TYR:HB2	1.93	0.48
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.94	0.48
1:A:498:GLN:H	1:A:501:ASN:ND2	2.10	0.48
1:C:439:ASN:HA	1:C:507:PRO:HD2	1.95	0.48
2:M:115:PHE:O	2:M:118:TRP:NE1	2.45	0.48
1:C:716:THR:HG21	1:C:1073:LYS:HE3	1.96	0.48
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.34	0.48
1:C:1048:HIS:NE2	1:C:1050:MET:O	2.47	0.48
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.38	0.48
1:A:742:ILE:HD13	1:A:1000:ARG:HB3	1.95	0.48
1:B:145:TYR:H	1:B:246:ARG:NH1	2.11	0.48
1:B:159:VAL:HG23	1:B:160:TYR:CD2	2.48	0.48
1:C:29:THR:HG22	1:C:30:ASN:H	1.79	0.48
3:N:95:GLN:H	3:N:98:ASP:HB2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:HA	1:A:209:PRO:HA	1.96	0.48
1:C:742:ILE:HD13	1:C:1000:ARG:HB3	1.95	0.48
1:C:742:ILE:HG21	1:C:997:ILE:HG13	1.95	0.48
1:C:1086:LYS:HD3	1:C:1122:VAL:HG21	1.96	0.48
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.95	0.48
1:A:727:LEU:HD11	1:A:1028:LYS:HD2	1.95	0.48
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.49	0.48
1:B:247:SER:HB3	1:B:257:GLY:HA3	1.96	0.48
1:A:734:THR:HG21	1:A:959:LEU:HD11	1.96	0.48
3:L:42:TYR:HB2	3:L:103:TYR:HB2	1.96	0.48
1:B:746:SER:OG	1:B:748:GLU:OE1	2.32	0.48
2:H:24:THR:HG22	2:H:86:THR:HG22	1.96	0.48
1:C:457:ARG:NH1	1:C:459:SER:O	2.46	0.47
3:L:2:ILE:HD12	3:L:106:ASN:HD22	1.79	0.47
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.97	0.47
1:A:37:TYR:OH	1:A:54:LEU:O	2.28	0.47
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	1.96	0.47
1:C:742:ILE:HD11	1:C:1004:LEU:HD12	1.96	0.47
1:C:426:PRO:HG2	1:C:429:PHE:HB2	1.97	0.47
1:C:552:LEU:HD23	1:C:585:LEU:HD13	1.96	0.47
1:A:903:ALA:HB1	1:A:913:GLN:HB2	1.95	0.47
1:A:1089:PHE:CE2	1:A:1123:SER:HB2	2.50	0.47
1:B:168:PHE:CG	1:B:231:ILE:HD11	2.48	0.47
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.94	0.47
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.97	0.47
1:B:880:GLY:O	1:B:884:SER:OG	2.28	0.47
1:B:1089:PHE:CE2	1:B:1123:SER:HB2	2.50	0.47
1:C:37:TYR:OH	1:C:53:ASP:OD1	2.32	0.47
1:C:326:ILE:HD12	1:C:534:VAL:HG22	1.95	0.47
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.97	0.47
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.97	0.47
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.97	0.47
1:A:889:GLY:HA3	1:A:1034:LEU:HD23	1.95	0.47
1:B:779:GLN:O	1:B:783:ALA:HB3	2.15	0.47
1:C:108:THR:OG1	1:C:234:ASN:O	2.32	0.47
3:L:75:ARG:HD3	3:L:91:ILE:HA	1.97	0.47
1:A:120:VAL:HG11	1:A:141:LEU:HD22	1.95	0.47
1:B:146:HIS:HB3	1:B:149:ASN:HB2	1.97	0.47
1:B:439:ASN:HA	1:B:507:PRO:HD2	1.96	0.47
1:A:742:ILE:HD11	1:A:1004:LEU:HD12	1.97	0.47
1:C:930:ALA:O	1:C:934:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ILE:HG22	2:H:65:SER:HB3	1.97	0.47
3:L:25:SER:OG	3:L:84:GLY:O	2.32	0.47
2:M:56:ILE:HG22	2:M:65:SER:HB3	1.97	0.47
2:P:91:LEU:HB3	2:P:94:LEU:HD21	1.97	0.47
1:A:396:TYR:O	1:A:514:SER:N	2.42	0.46
1:B:143:VAL:HA	1:B:154:GLU:HA	1.97	0.46
1:B:716:THR:HG21	1:B:1073:LYS:HE3	1.97	0.46
1:B:742:ILE:HD11	1:B:1004:LEU:HD12	1.95	0.46
3:L:99:LEU:HG	3:L:125:GLU:HA	1.98	0.46
1:A:421:TYR:HA	1:A:461:LEU:HD13	1.98	0.46
1:B:930:ALA:O	1:B:934:ILE:HG12	2.16	0.46
1:A:779:GLN:O	1:A:783:ALA:HB3	2.15	0.46
1:B:421:TYR:HA	1:B:461:LEU:HD13	1.97	0.46
1:C:231:ILE:HG22	1:C:233:ILE:HG12	1.97	0.46
3:L:41:TRP:CE3	3:L:89:LEU:HD22	2.51	0.46
1:A:534:VAL:HG21	1:A:539:VAL:HG11	1.98	0.46
3:N:75:ARG:CG	3:N:76:PHE:H	2.26	0.46
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.97	0.46
1:B:752:LEU:O	1:B:755:GLN:HG2	2.16	0.46
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.97	0.46
2:M:24:THR:HG22	2:M:86:THR:HG22	1.97	0.46
1:A:77:LYS:HE3	1:A:253:ASP:HA	1.96	0.46
1:A:393:THR:HG23	1:A:517:LEU:HD23	1.97	0.46
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.97	0.46
1:A:439:ASN:HA	1:A:507:PRO:HD2	1.97	0.46
1:A:552:LEU:HD23	1:A:585:LEU:HD13	1.98	0.46
1:B:1094:VAL:N	1:B:1105:THR:O	2.47	0.46
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.51	0.46
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.46	0.46
1:A:746:SER:OG	1:A:748:GLU:OE1	2.32	0.46
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.98	0.46
1:A:280:ASN:OD1	1:A:284:THR:N	2.49	0.46
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.51	0.46
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.81	0.45
1:C:104:TRP:CH2	1:C:176:LEU:HD21	2.49	0.45
1:C:752:LEU:O	1:C:755:GLN:HG2	2.15	0.45
1:C:65:PHE:CE1	1:C:82:PRO:HG2	2.52	0.45
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.51	0.45
2:H:38:TYR:CE1	2:H:107:GLU:HG3	2.51	0.45
3:N:41:TRP:CE3	3:N:89:LEU:HD22	2.52	0.45
1:C:421:TYR:HA	1:C:461:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:GLY:O	1:A:884:SER:OG	2.30	0.45
1:A:902:MET:HB3	1:A:916:LEU:HD13	1.98	0.45
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.99	0.45
1:C:117:LEU:HB2	1:C:233:ILE:HD11	1.99	0.45
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.99	0.45
1:A:930:ALA:O	1:A:934:ILE:HG12	2.16	0.45
1:C:734:THR:HG21	1:C:959:LEU:HD11	1.98	0.45
1:A:37:TYR:OH	1:A:53:ASP:OD2	2.34	0.45
1:A:433:VAL:HG22	1:A:512:VAL:HG22	1.99	0.45
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.99	0.45
1:A:752:LEU:O	1:A:755:GLN:HG2	2.17	0.45
1:A:909:ILE:HG13	1:A:911:VAL:HG23	1.99	0.45
1:B:994:ASP:HA	1:B:997:ILE:HG22	1.98	0.45
1:C:36:VAL:HB	1:C:220:PHE:CE1	2.51	0.45
1:C:104:TRP:CD1	1:C:238:PHE:HE1	2.33	0.45
1:C:393:THR:HG23	1:C:517:LEU:HD23	1.98	0.45
1:C:779:GLN:O	1:C:783:ALA:HB3	2.17	0.45
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.50	0.45
1:A:716:THR:HG21	1:A:1073:LYS:HE3	1.98	0.45
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.52	0.45
2:P:56:ILE:HG22	2:P:65:SER:HB3	1.97	0.45
1:C:454:ARG:HE	1:C:457:ARG:HD2	1.82	0.45
1:C:909:ILE:HG13	1:C:911:VAL:HG23	1.98	0.45
2:P:38:TYR:CE1	2:P:107:GLU:HG3	2.52	0.45
1:C:1081:ILE:HG23	1:C:1135:ASN:HB3	1.99	0.45
3:N:114:TYR:HB3	3:N:115:PRO:HD3	1.99	0.45
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.29	0.45
2:M:38:TYR:CE1	2:M:107:GLU:HG3	2.52	0.45
2:P:24:THR:HG22	2:P:86:THR:HG22	1.98	0.45
1:A:742:ILE:HG21	1:A:997:ILE:HG13	2.00	0.44
1:B:905:ARG:CZ	1:B:1050:MET:HG2	2.47	0.44
1:C:143:VAL:HG12	1:C:154:GLU:HA	1.98	0.44
1:C:244:LEU:HD13	1:C:248:TYR:CD2	2.52	0.44
1:B:617:CYS:HB3	1:B:649:CYS:HB3	1.84	0.44
1:C:770:ILE:O	1:C:774:GLN:HG2	2.17	0.44
1:A:994:ASP:HA	1:A:997:ILE:HG22	1.98	0.44
1:B:454:ARG:HE	1:B:457:ARG:HD2	1.82	0.44
1:C:396:TYR:O	1:C:514:SER:N	2.42	0.44
1:C:784:GLN:HG3	1:C:1029:MET:HG2	2.00	0.44
3:Q:75:ARG:HD3	3:Q:91:ILE:HA	1.99	0.44
3:Q:75:ARG:CG	3:Q:76:PHE:H	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG22	1:B:172:SER:O	2.17	0.44
1:A:454:ARG:HE	1:A:457:ARG:HD2	1.83	0.44
1:A:457:ARG:NH1	1:A:459:SER:O	2.46	0.44
1:A:1115:ILE:HG22	1:A:1137:VAL:HA	2.00	0.44
3:Q:41:TRP:CE3	3:Q:89:LEU:HD22	2.53	0.44
1:B:105:ILE:HB	1:B:239:GLN:HB3	2.00	0.44
1:B:742:ILE:HG21	1:B:997:ILE:HG13	1.99	0.44
1:B:770:ILE:O	1:B:774:GLN:HG2	2.17	0.44
1:A:310:LYS:HG3	1:A:600:PRO:HA	2.00	0.44
1:B:244:LEU:HD13	1:B:248:TYR:CD2	2.53	0.44
1:B:386:LYS:HD2	2:M:38:TYR:HD1	1.83	0.44
1:C:128:ILE:HD12	1:C:170:TYR:HD2	1.82	0.44
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.82	0.44
1:A:146:HIS:CE1	1:A:148:ASN:HB2	2.53	0.44
2:M:56:ILE:HD13	2:M:78:ILE:HG22	2.00	0.44
3:N:41:TRP:CD1	3:N:89:LEU:HD13	2.52	0.44
1:B:991:VAL:O	1:B:995:ARG:HG2	2.18	0.44
1:C:746:SER:OG	1:C:748:GLU:OE1	2.34	0.44
1:A:369:TYR:OH	1:A:384:PRO:O	2.21	0.43
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.00	0.43
1:B:386:LYS:HE2	1:B:390:LEU:HD23	1.99	0.43
1:B:418:ILE:HG13	1:B:419:ALA:N	2.33	0.43
2:P:56:ILE:HD13	2:P:78:ILE:HG22	2.00	0.43
1:A:1081:ILE:HG23	1:A:1135:ASN:HB3	2.00	0.43
1:B:80:ASP:C	1:B:81:ASN:HD22	2.22	0.43
1:C:138:ASP:OD1	1:C:138:ASP:N	2.52	0.43
1:C:418:ILE:HG13	1:C:419:ALA:N	2.33	0.43
1:B:121:ASN:HD22	1:B:176:LEU:HB2	1.84	0.43
1:B:393:THR:HG23	1:B:517:LEU:HD23	2.00	0.43
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.99	0.43
1:A:770:ILE:O	1:A:774:GLN:HG2	2.18	0.43
1:B:93:ALA:O	1:B:266:TYR:N	2.50	0.43
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.99	0.43
1:C:220:PHE:CD2	1:C:287:ASP:HA	2.53	0.43
1:C:534:VAL:HG21	1:C:539:VAL:HG11	1.99	0.43
3:L:41:TRP:CD1	3:L:89:LEU:HD13	2.53	0.43
1:A:873:TYR:HE1	1:C:699:LEU:HB3	1.82	0.43
1:A:991:VAL:O	1:A:995:ARG:HG2	2.18	0.43
1:B:143:VAL:HG22	1:B:152:TRP:HE3	1.82	0.43
1:C:1141:LEU:HD23	1:C:1145:LEU:HG	2.00	0.43
2:H:56:ILE:HD13	2:H:78:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:41:TRP:CD1	3:Q:89:LEU:HD13	2.53	0.43
1:A:353:TRP:CE2	1:A:466:ARG:HB3	2.54	0.43
1:A:1141:LEU:HD23	1:A:1145:LEU:HG	2.00	0.43
1:C:33:THR:HA	1:C:58:PHE:CD1	2.53	0.43
1:C:386:LYS:HE2	1:C:390:LEU:HD23	2.00	0.43
1:C:991:VAL:O	1:C:995:ARG:HG2	2.19	0.43
3:L:75:ARG:CG	3:L:76:PHE:H	2.29	0.43
3:N:99:LEU:HG	3:N:125:GLU:HA	2.01	0.43
1:A:126:VAL:HG22	1:A:172:SER:O	2.19	0.43
1:A:970:PHE:CG	1:A:999:GLY:HA3	2.54	0.43
1:A:1094:VAL:HG23	1:A:1107:ARG:HG3	2.00	0.43
1:B:129:LYS:HE2	1:B:166:CYS:SG	2.59	0.43
1:B:903:ALA:HB1	1:B:913:GLN:HB2	2.01	0.43
1:C:353:TRP:CE2	1:C:466:ARG:HB3	2.54	0.43
3:L:114:TYR:HB3	3:L:115:PRO:HD3	1.99	0.43
2:P:43:LYS:HB3	2:P:53:ILE:HD11	2.00	0.43
3:Q:41:TRP:HB2	3:Q:54:ILE:HB	2.01	0.43
2:P:106:ASP:HB2	2:P:116:ALA:HB3	2.00	0.43
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.34	0.43
1:A:969:ASN:HB3	1:A:972:ALA:O	2.19	0.43
1:B:543:PHE:O	1:B:546:LEU:HD23	2.18	0.43
1:A:418:ILE:HG13	1:A:419:ALA:N	2.33	0.43
1:A:825:LYS:NZ	1:A:941:THR:O	2.34	0.43
1:B:353:TRP:CE2	1:B:466:ARG:HB3	2.54	0.43
3:Q:114:TYR:HB3	3:Q:115:PRO:HD3	2.01	0.43
1:C:386:LYS:HD2	2:P:38:TYR:HD1	1.84	0.42
1:C:118:LEU:HD21	1:C:120:VAL:HG23	2.01	0.42
1:C:753:LEU:HD13	1:C:997:ILE:HD11	2.01	0.42
1:A:144:TYR:CD1	1:A:155:SER:HB3	2.54	0.42
1:B:386:LYS:NZ	2:M:35:LYS:O	2.37	0.42
3:Q:43:GLN:HB2	3:Q:53:LEU:HD13	2.01	0.42
1:B:869:MET:HB3	1:B:869:MET:HE2	1.61	0.42
1:B:1081:ILE:HG23	1:B:1135:ASN:HB3	2.02	0.42
1:C:970:PHE:CG	1:C:999:GLY:HA3	2.55	0.42
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.84	0.42
1:A:1130:ILE:HD11	1:B:921:LYS:HE3	2.01	0.42
1:C:730:SER:O	1:C:1058:HIS:HB3	2.19	0.42
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	2.02	0.42
1:C:144:TYR:HA	1:C:246:ARG:HG3	2.02	0.42
1:B:529:LYS:HA	1:B:529:LYS:HD3	1.94	0.42
1:C:67:ALA:HA	1:C:80:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PHE:HZ	5:C:1312:NAG:HN2	1.66	0.42
3:L:45:LYS:HB2	3:L:48:GLN:NE2	2.35	0.42
1:B:970:PHE:CG	1:B:999:GLY:HA3	2.55	0.42
1:C:36:VAL:HB	1:C:220:PHE:HE1	1.85	0.42
1:C:276:LEU:HD11	1:C:304:LYS:HG3	2.01	0.42
1:C:901:GLN:O	1:C:904:TYR:HB2	2.19	0.42
1:A:130:VAL:HG21	1:A:231:ILE:HG23	2.00	0.42
1:A:175:PHE:CD2	1:A:226:LEU:HD21	2.55	0.42
1:A:386:LYS:HE2	1:A:390:LEU:HD23	2.01	0.42
1:A:733:LYS:HE3	1:A:771:ALA:HB1	2.01	0.42
1:C:543:PHE:O	1:C:546:LEU:HD23	2.19	0.42
1:C:878:LEU:HD11	1:C:1054:GLN:HE22	1.84	0.42
2:P:41:TRP:CD1	2:P:78:ILE:HG21	2.55	0.42
1:A:383:SER:HB2	2:H:107:GLU:OE2	2.20	0.42
1:C:599:THR:HB	1:C:608:VAL:HG12	2.02	0.42
3:N:45:LYS:HB2	3:N:48:GLN:NE2	2.35	0.42
1:A:140:PHE:CD1	1:A:244:LEU:HD12	2.55	0.41
3:L:38:TYR:HB2	3:L:108:TYR:HB2	2.02	0.41
2:M:38:TYR:HB2	2:M:56:ILE:O	2.20	0.41
1:A:229:LEU:HA	1:A:230:PRO:HD3	1.91	0.41
1:B:1083:HIS:O	1:B:1086:LYS:HG2	2.19	0.41
1:C:121:ASN:ND2	1:C:126:VAL:HG22	2.30	0.41
1:A:1073:LYS:HE3	1:A:1073:LYS:HB2	1.89	0.41
1:C:719:THR:N	1:C:1068:VAL:O	2.53	0.41
1:C:1083:HIS:O	1:C:1086:LYS:HG2	2.20	0.41
3:L:4:MET:HE1	3:L:25:SER:HB3	2.03	0.41
1:B:37:TYR:HB3	1:B:223:LEU:HB2	2.02	0.41
1:B:383:SER:HB2	2:M:107:GLU:OE2	2.21	0.41
1:B:598:ILE:HG23	1:B:664:ILE:HG21	2.01	0.41
1:C:206:LYS:HB3	1:C:223:LEU:HD23	2.01	0.41
1:C:379:CYS:HA	1:C:432:CYS:HA	2.02	0.41
2:M:42:VAL:HG21	2:M:50:LEU:HD21	2.03	0.41
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.55	0.41
1:B:733:LYS:HE3	1:B:771:ALA:HB1	2.02	0.41
1:C:244:LEU:HA	1:C:258:TRP:CH2	2.56	0.41
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.49	0.41
1:C:869:MET:HE2	1:C:869:MET:HB3	1.71	0.41
3:Q:41:TRP:CZ3	3:Q:104:CYS:HB3	2.55	0.41
1:A:1123:SER:HB3	1:B:914:ASN:CG	2.41	0.41
1:B:36:VAL:HB	1:B:220:PHE:CE1	2.56	0.41
1:B:719:THR:N	1:B:1068:VAL:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.56	0.41
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.56	0.41
1:C:733:LYS:HE3	1:C:771:ALA:HB1	2.02	0.41
1:A:379:CYS:HA	1:A:432:CYS:HA	2.02	0.41
1:A:991:VAL:HG13	1:A:992:GLN:HE21	1.86	0.41
1:B:93:ALA:HB3	1:B:266:TYR:HB2	2.02	0.41
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.36	0.41
1:B:969:ASN:HB3	1:B:972:ALA:O	2.21	0.41
2:H:41:TRP:CD1	2:H:78:ILE:HG21	2.56	0.41
3:L:24:LYS:HE3	3:L:24:LYS:HB3	1.95	0.41
3:L:43:GLN:HB2	3:L:53:LEU:HD13	2.03	0.41
3:N:38:TYR:HB2	3:N:108:TYR:HB2	2.03	0.41
3:Q:45:LYS:HB2	3:Q:48:GLN:NE2	2.35	0.41
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	2.03	0.41
3:L:41:TRP:HB2	3:L:54:ILE:HB	2.03	0.41
2:M:43:LYS:HB3	2:M:53:ILE:HD11	2.02	0.41
1:B:379:CYS:HA	1:B:432:CYS:HA	2.02	0.40
1:B:599:THR:HB	1:B:608:VAL:HG12	2.02	0.40
1:B:1094:VAL:HG23	1:B:1107:ARG:HG3	2.02	0.40
2:H:43:LYS:HB3	2:H:53:ILE:HD11	2.02	0.40
1:B:84:LEU:HD23	1:B:267:VAL:HG11	2.04	0.40
1:B:699:LEU:HD22	1:C:873:TYR:CE1	2.56	0.40
1:C:159:VAL:HG23	1:C:160:TYR:CD2	2.56	0.40
1:C:332:ILE:HG13	1:C:332:ILE:O	2.21	0.40
1:A:869:MET:HE1	1:C:697:MET:SD	2.61	0.40
1:B:328:ARG:HH21	1:B:580:GLN:HB2	1.87	0.40
1:C:196:ASN:OD1	1:C:201:PHE:HD1	2.04	0.40
1:A:825:LYS:HE2	1:A:944:ALA:HB3	2.04	0.40
1:A:906:PHE:CE2	1:A:916:LEU:HB2	2.56	0.40
1:B:104:TRP:HD1	1:B:238:PHE:CE1	2.38	0.40
1:B:821:LEU:HA	1:B:824:ASN:HB2	2.03	0.40
1:B:1048:HIS:NE2	1:B:1050:MET:O	2.54	0.40
1:C:280:ASN:OD1	1:C:284:THR:N	2.54	0.40
2:M:41:TRP:CD1	2:M:78:ILE:HG21	2.56	0.40
3:N:44:GLN:O	3:N:100:ALA:HB1	2.22	0.40
3:N:75:ARG:HG3	3:N:76:PHE:N	2.36	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	1047/1256 (83%)	1020 (97%)	27 (3%)	0	100	100
1	B	1047/1256 (83%)	1018 (97%)	29 (3%)	0	100	100
1	C	1047/1256 (83%)	1022 (98%)	25 (2%)	0	100	100
2	H	114/228 (50%)	106 (93%)	8 (7%)	0	100	100
2	M	114/228 (50%)	106 (93%)	8 (7%)	0	100	100
2	P	114/228 (50%)	105 (92%)	9 (8%)	0	100	100
3	L	110/220 (50%)	100 (91%)	10 (9%)	0	100	100
3	N	110/220 (50%)	100 (91%)	10 (9%)	0	100	100
3	Q	110/220 (50%)	101 (92%)	9 (8%)	0	100	100
All	All	3813/5112 (75%)	3678 (96%)	135 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	908/1096 (83%)	908 (100%)	0	100	100
1	B	908/1096 (83%)	907 (100%)	1 (0%)	93	98
1	C	908/1096 (83%)	907 (100%)	1 (0%)	93	98
2	H	95/193 (49%)	94 (99%)	1 (1%)	73	92
2	M	95/193 (49%)	94 (99%)	1 (1%)	73	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	95/193 (49%)	94 (99%)	1 (1%)	73	92
3	L	98/195 (50%)	98 (100%)	0	100	100
3	N	98/195 (50%)	98 (100%)	0	100	100
3	Q	98/195 (50%)	98 (100%)	0	100	100
All	All	3303/4452 (74%)	3298 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	ASN
1	C	147	LYS
2	H	66	ARG
2	M	66	ARG
2	P	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	501	ASN
1	B	501	ASN
1	C	121	ASN
1	C	501	ASN
3	L	6	GLN
3	N	6	GLN

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)

6 monosaccharides 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	D	1	1,4	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	D	2	4	14,14,15	0.21	0	17,19,21	0.50	0
4	NAG	E	1	1,4	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	E	2	4	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	F	1	1,4	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.51	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	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

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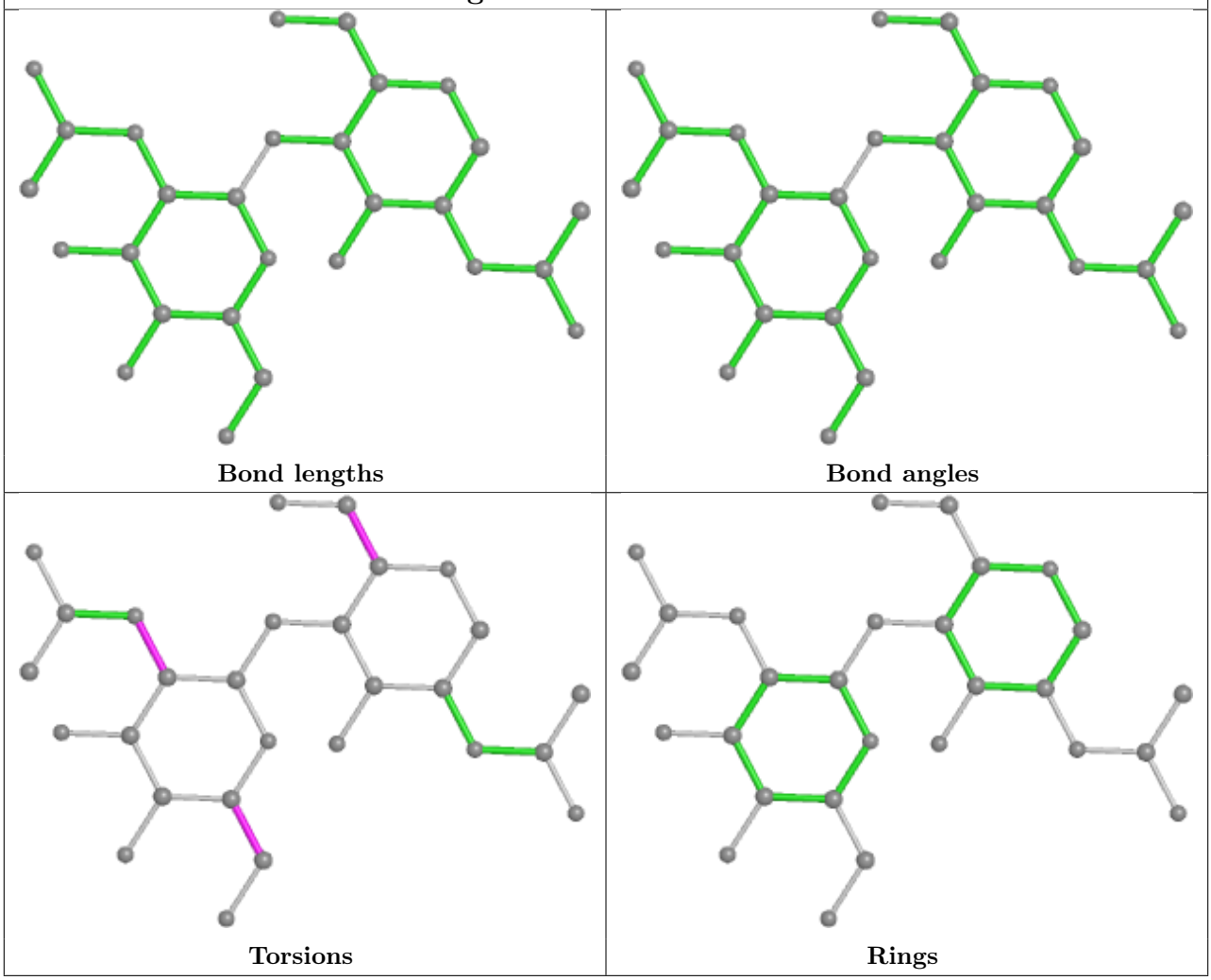
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6

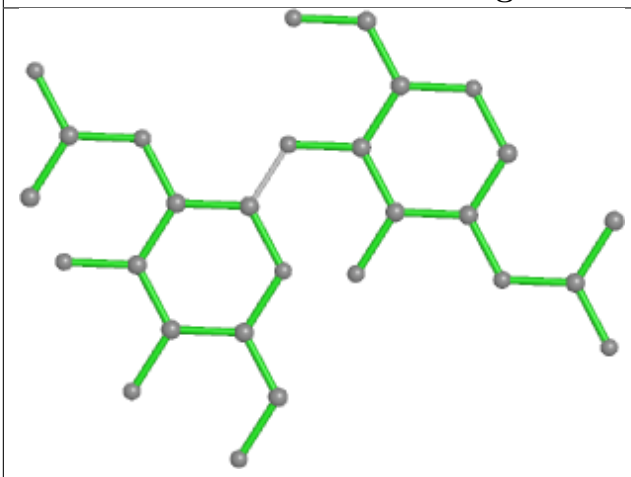
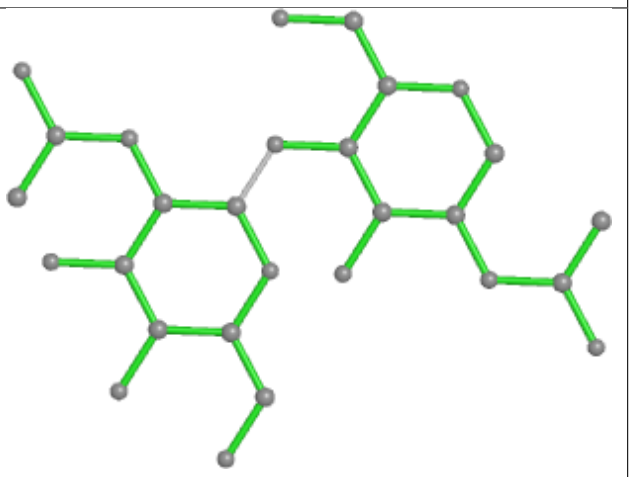
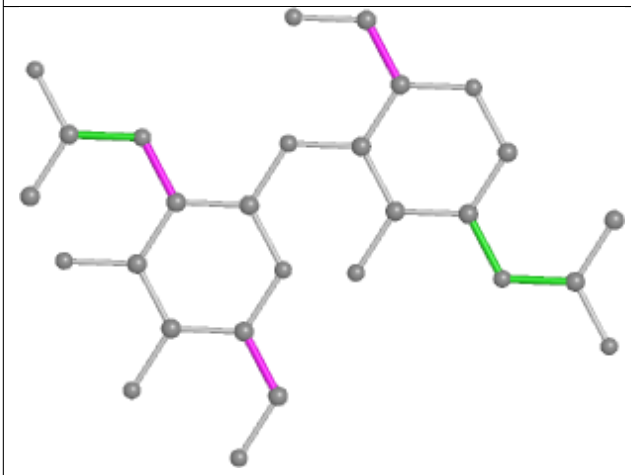
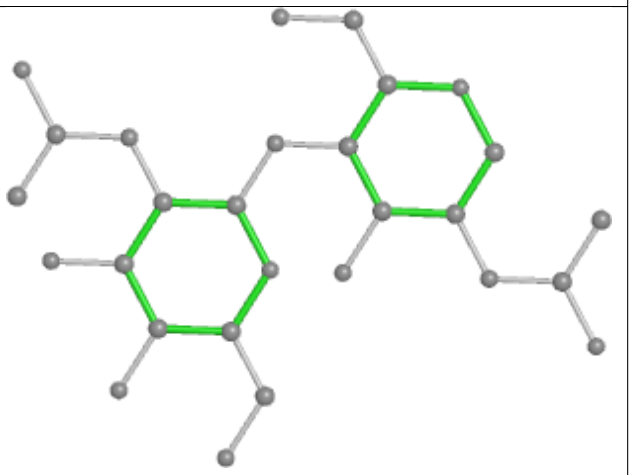
There are no ring outliers.

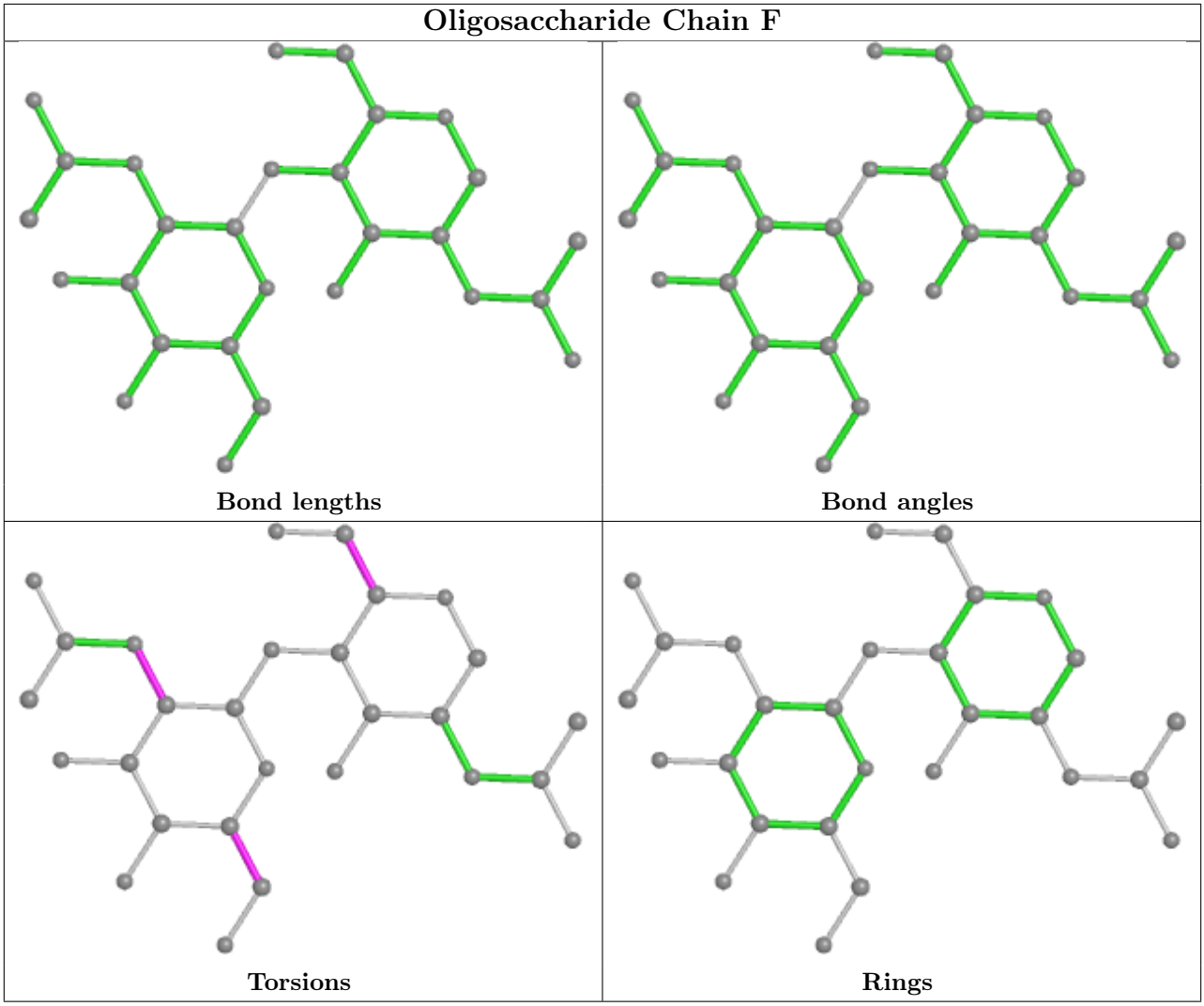
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D



Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.6 Ligand geometry (i)

39 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	$\#\|Z\| > 2$
5	NAG	C	1310	1	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	B	1306	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	C	1313	1	14,14,15	0.38	0	17,19,21	0.37	0
5	NAG	B	1311	1	14,14,15	0.27	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	1.24	1 (5%)
5	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	A	1310	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	A	1313	1	14,14,15	0.57	0	17,19,21	0.64	1 (5%)
5	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	C	1311	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	C	1306	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	A	1309	1	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	B	1308	1	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	A	1307	1	14,14,15	0.27	0	17,19,21	1.23	1 (5%)
5	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.38	0
5	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	1.21	1 (5%)
5	NAG	B	1305	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	A	1312	1	14,14,15	0.45	0	17,19,21	0.50	0
5	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	A	1306	1	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	B	1304	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	C	1312	1	14,14,15	0.35	0	17,19,21	0.43	0
5	NAG	A	1311	1	14,14,15	0.39	0	17,19,21	1.25	1 (5%)
5	NAG	B	1310	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	B	1313	1	14,14,15	0.28	0	17,19,21	0.52	0
5	NAG	B	1312	1	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	C	1304	1	14,14,15	0.27	0	17,19,21	0.56	0
5	NAG	C	1309	1	14,14,15	0.25	0	17,19,21	0.40	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
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1312	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1312	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1313	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1311	NAG	C2-N2-C7	4.31	129.04	122.90
5	C	1307	NAG	C2-N2-C7	3.67	128.12	122.90
5	B	1307	NAG	C2-N2-C7	3.53	127.93	122.90
5	A	1307	NAG	C2-N2-C7	3.44	127.80	122.90
5	A	1313	NAG	C1-O5-C5	2.16	115.11	112.19

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1308	NAG	O5-C5-C6-O6
5	A	1307	NAG	C8-C7-N2-C2
5	A	1307	NAG	O7-C7-N2-C2
5	B	1307	NAG	C8-C7-N2-C2
5	B	1307	NAG	O7-C7-N2-C2
5	C	1307	NAG	O7-C7-N2-C2
5	A	1308	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	B	1312	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	C	1307	NAG	C8-C7-N2-C2
5	A	1305	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1310	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	C	1312	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	C	1311	NAG	O5-C5-C6-O6
5	A	1312	NAG	C4-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	B	1312	NAG	O5-C5-C6-O6
5	A	1312	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	C	1311	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	C	1312	NAG	C4-C5-C6-O6
5	A	1311	NAG	C8-C7-N2-C2
5	A	1311	NAG	O7-C7-N2-C2
5	C	1313	NAG	C8-C7-N2-C2
5	C	1313	NAG	O7-C7-N2-C2
5	C	1310	NAG	C4-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	A	1307	NAG	C1-C2-N2-C7
5	B	1307	NAG	C1-C2-N2-C7
5	C	1307	NAG	C1-C2-N2-C7
5	B	1313	NAG	O5-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6

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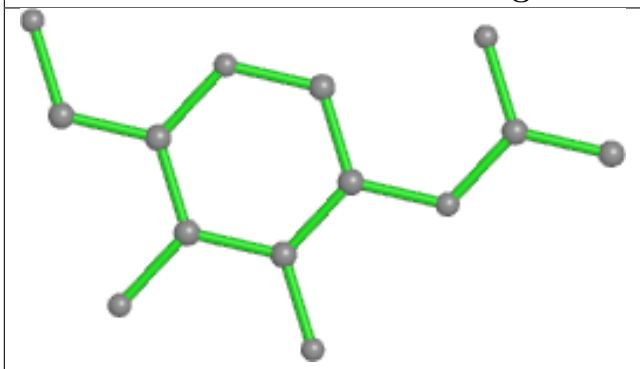
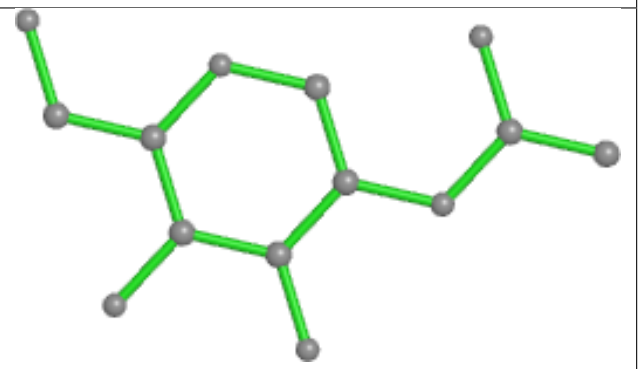
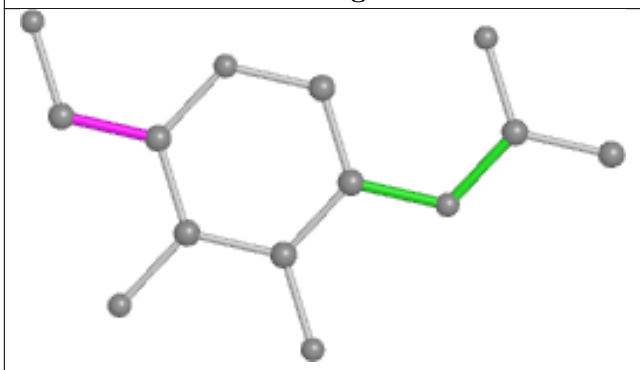
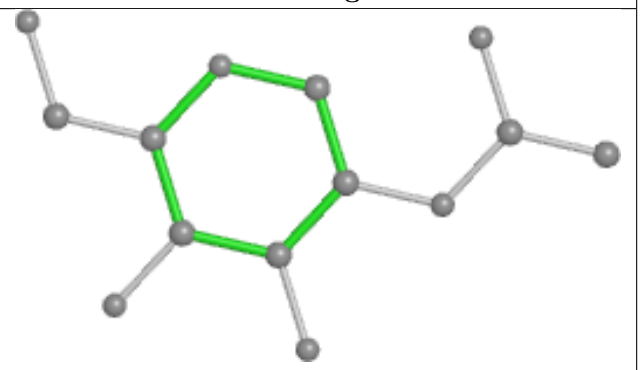
Mol	Chain	Res	Type	Atoms
5	C	1309	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	B	1313	NAG	C4-C5-C6-O6
5	A	1312	NAG	C3-C2-N2-C7
5	B	1313	NAG	C3-C2-N2-C7
5	C	1312	NAG	C3-C2-N2-C7
5	C	1304	NAG	C4-C5-C6-O6
5	A	1311	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1312	NAG	1	0
5	A	1311	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 C 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

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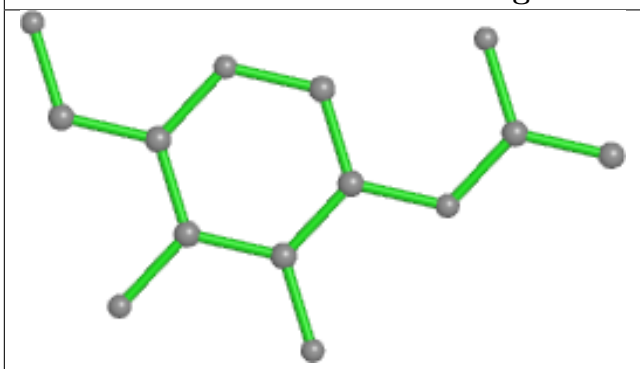
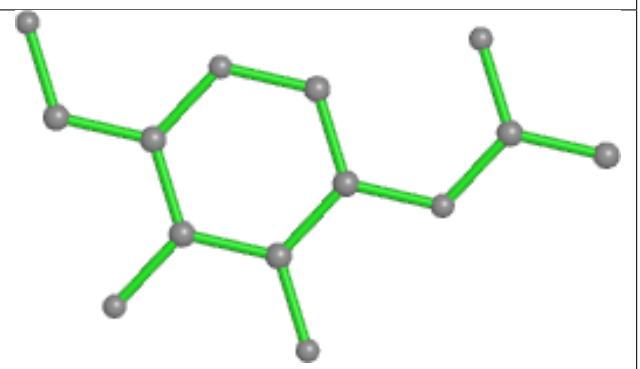
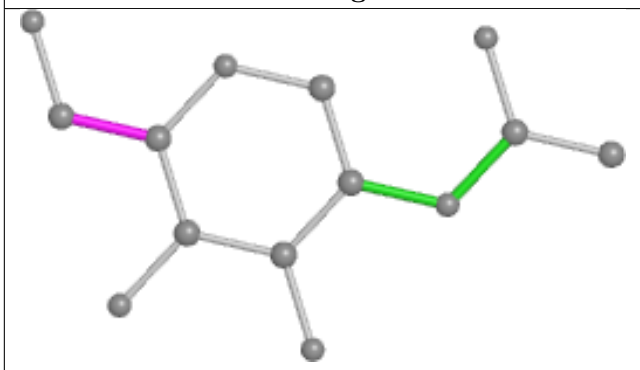
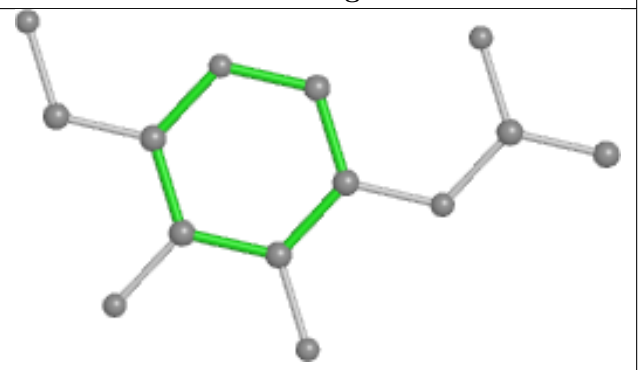
 Bond lengths	 Bond angles
 Torsions	 Rings

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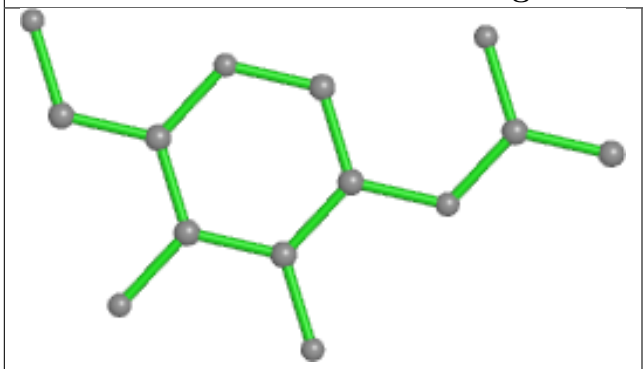

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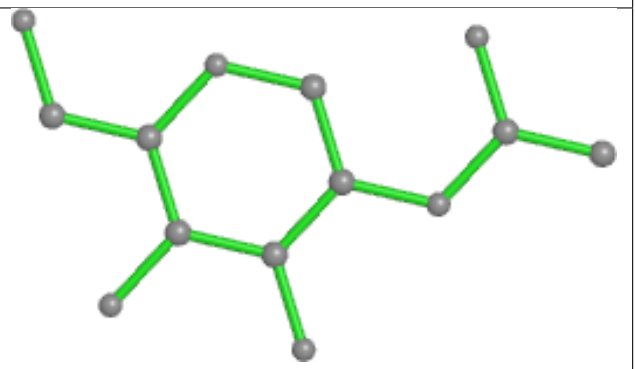

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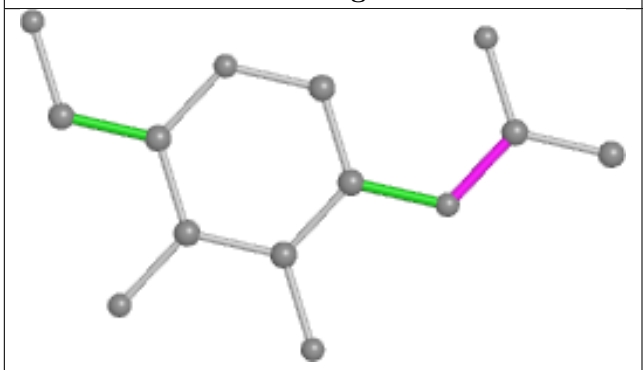

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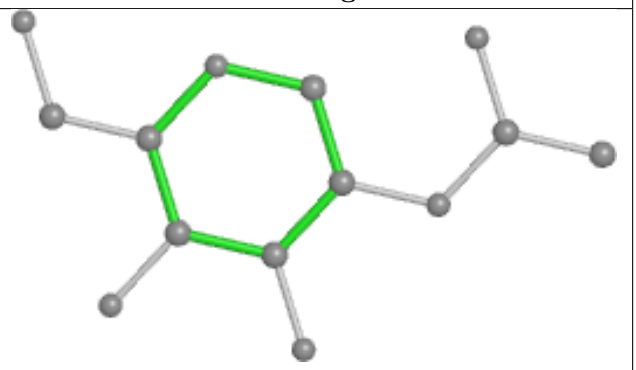
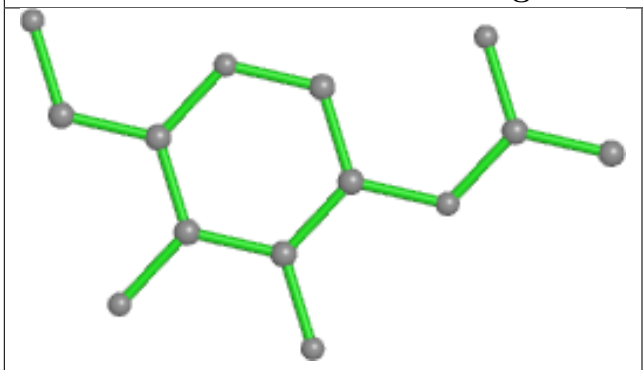


Rings

Ligand NAG B 1311



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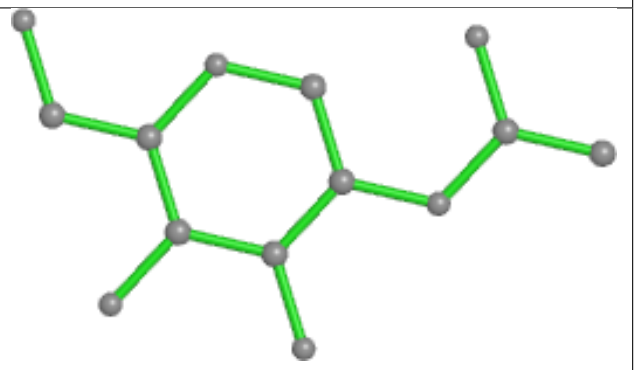

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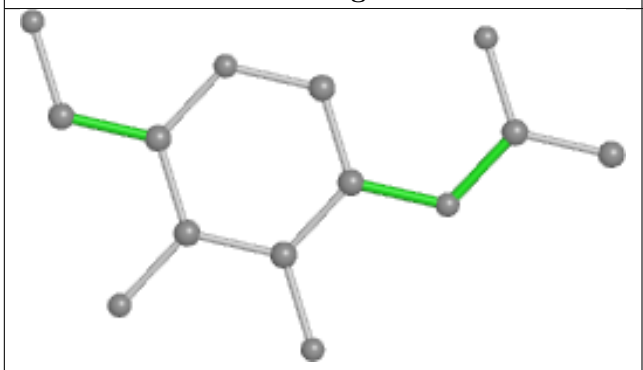
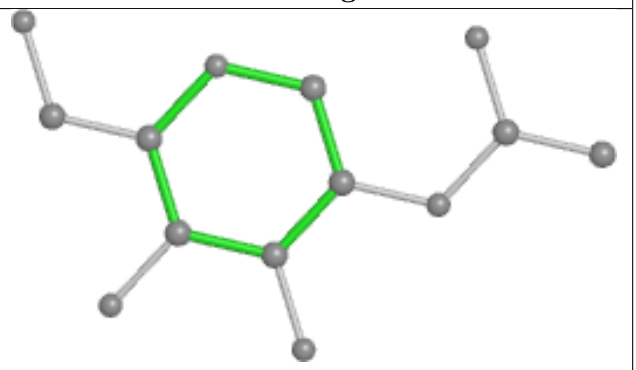


Torsions



Rings

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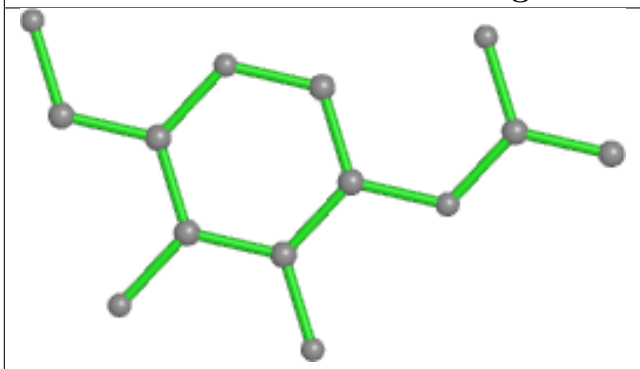
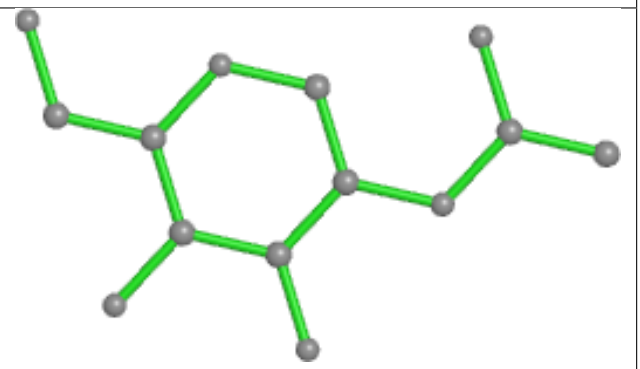
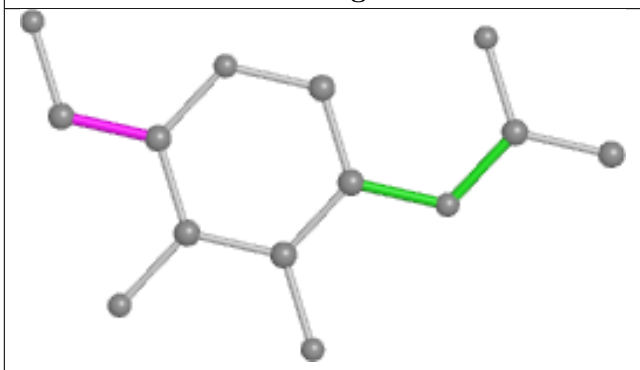
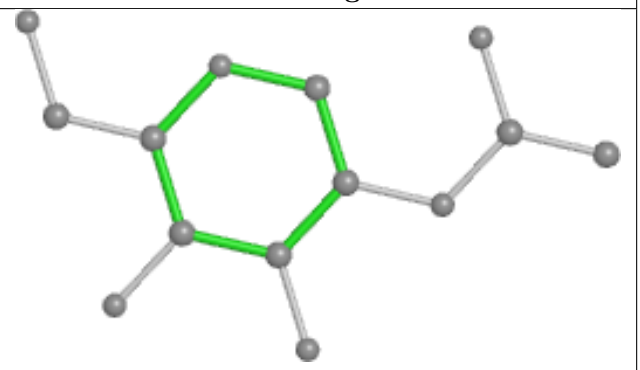
 Bond lengths	 Bond angles
 Torsions	 Rings

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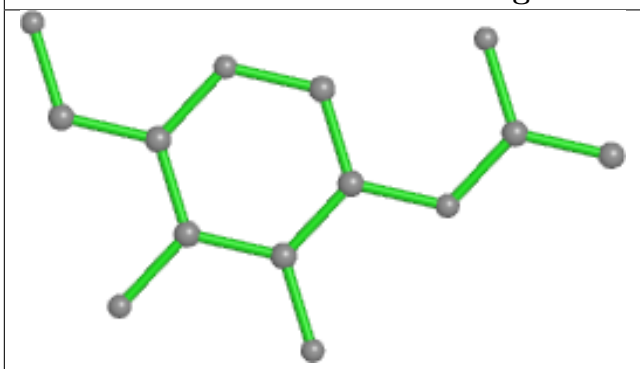
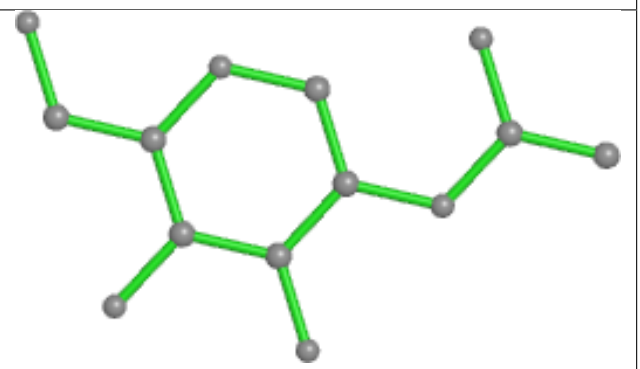
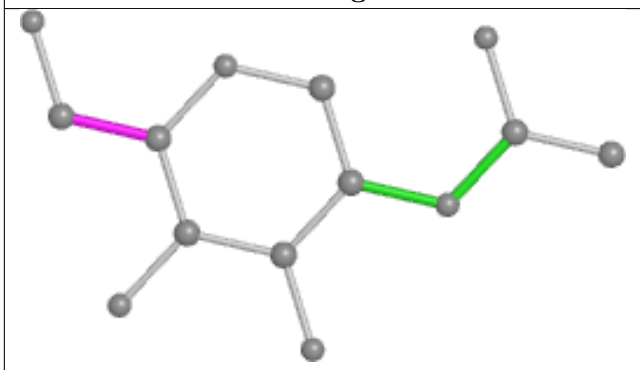
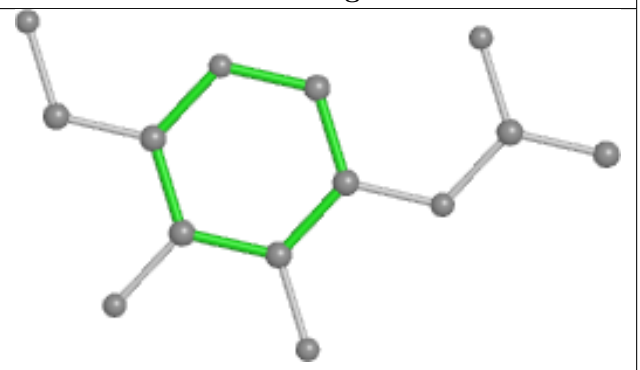
 Bond lengths	 Bond angles
 Torsions	 Rings

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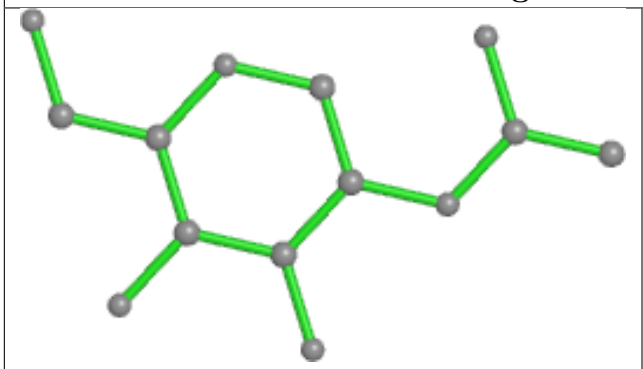
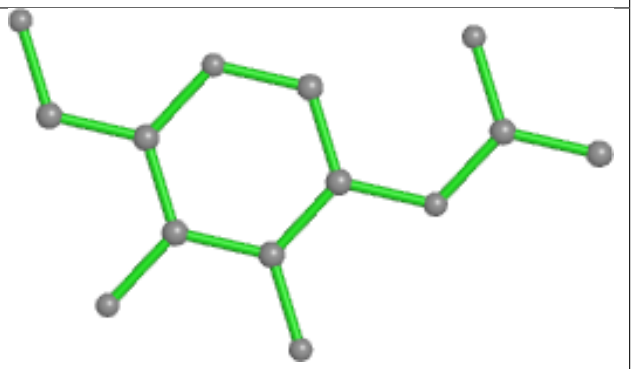
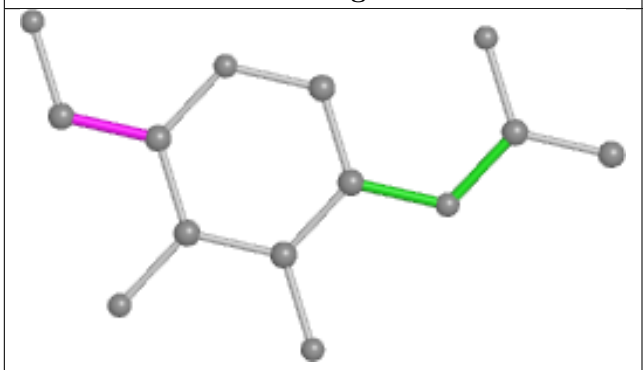
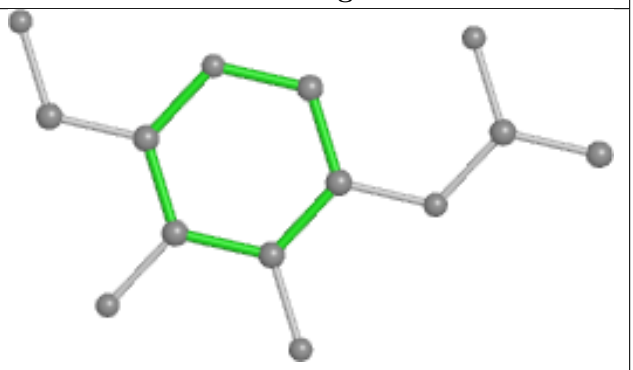
 Bond lengths	 Bond angles
 Torsions	 Rings

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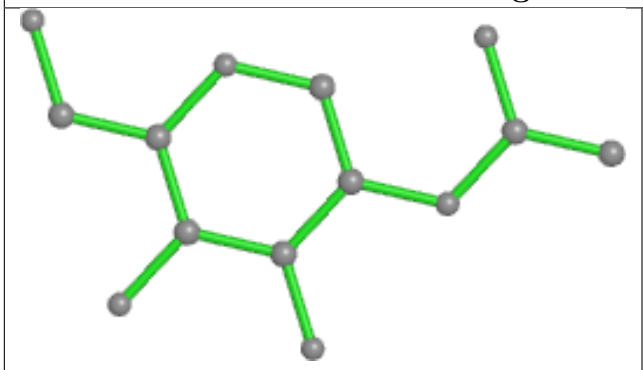
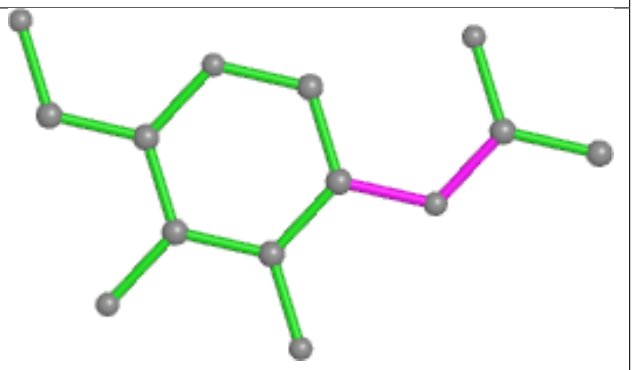
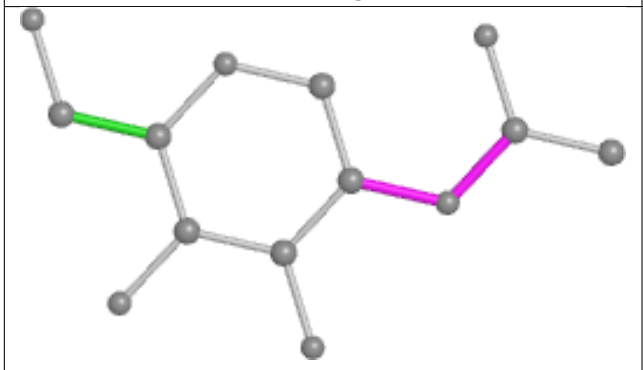
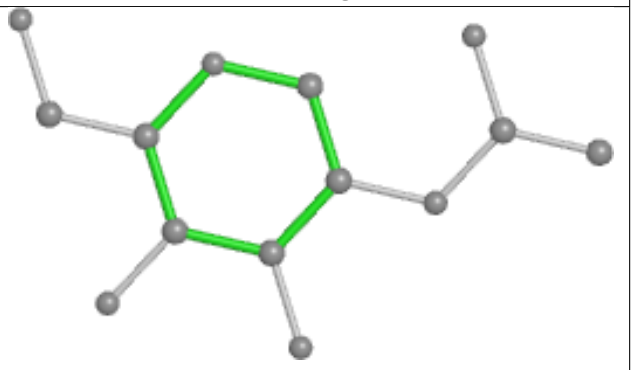
 Bond lengths	 Bond angles
 Torsions	 Rings

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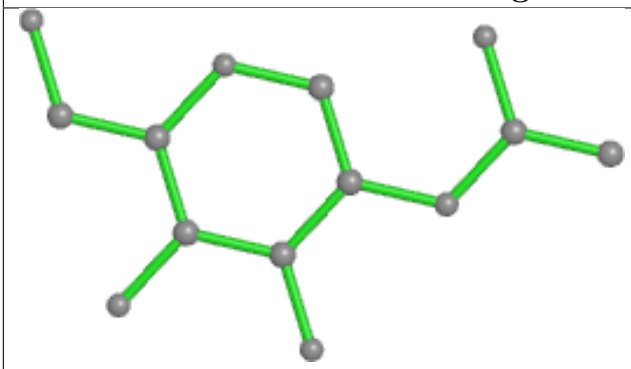
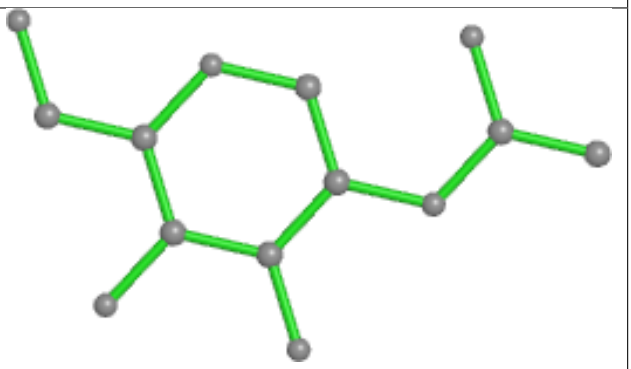
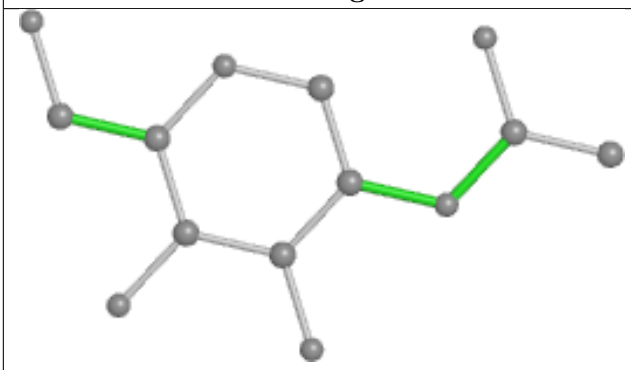
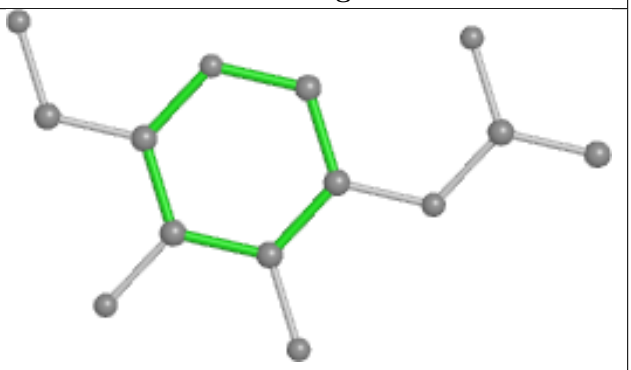
 Bond lengths	 Bond angles
 Torsions	 Rings

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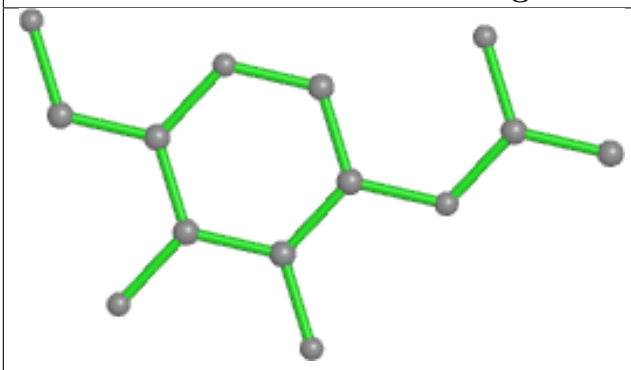
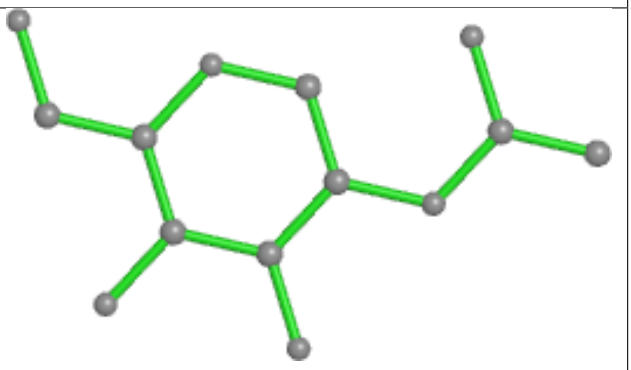
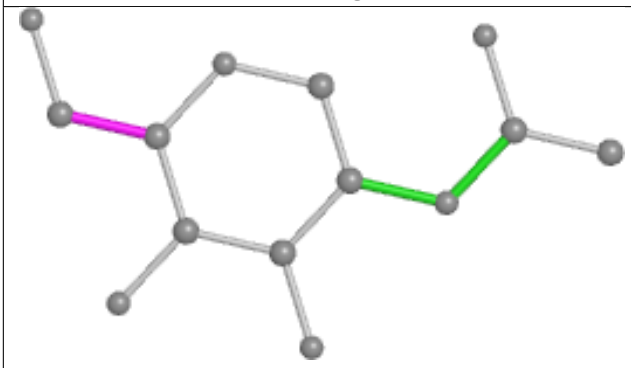
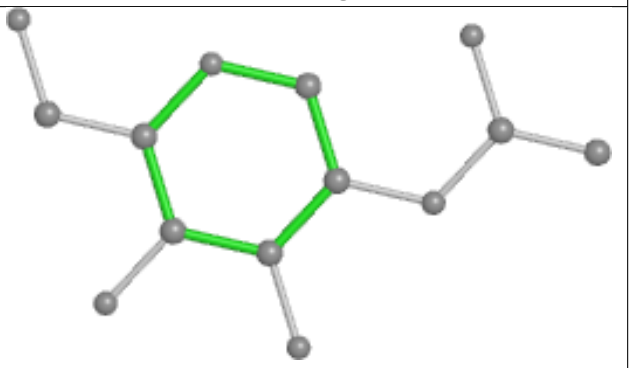
 Bond lengths	 Bond angles
 Torsions	 Rings

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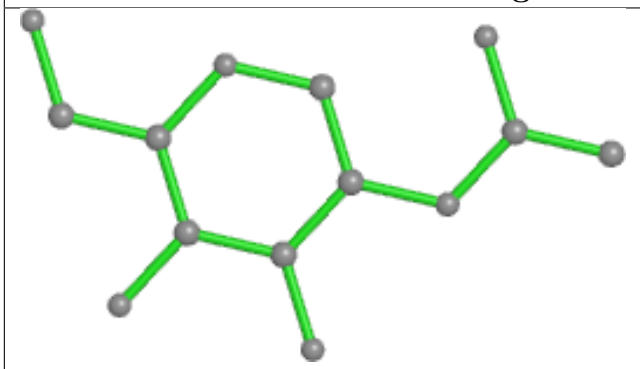
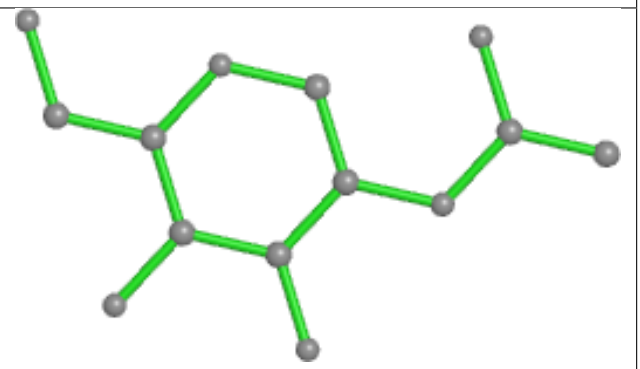
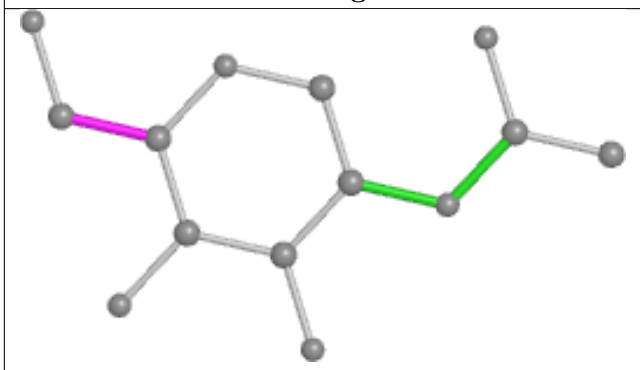
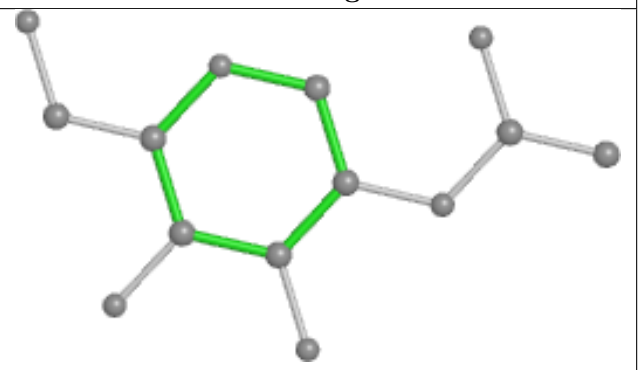
 Bond lengths	 Bond angles
 Torsions	 Rings

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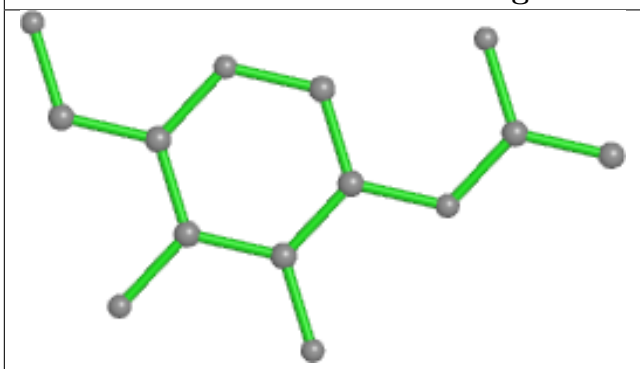
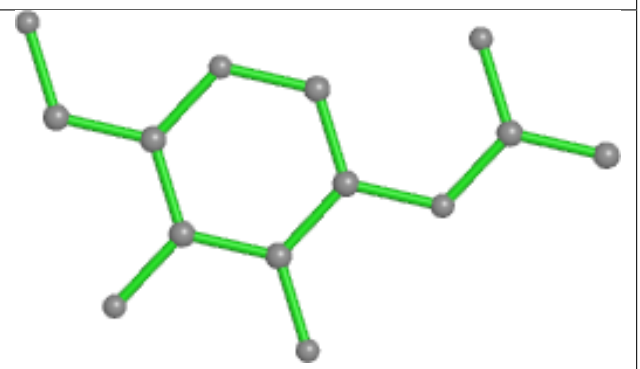
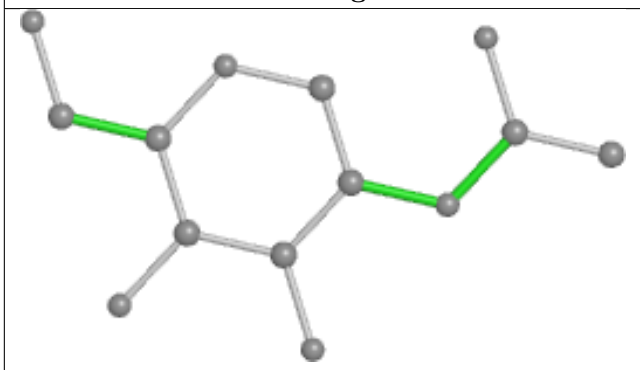
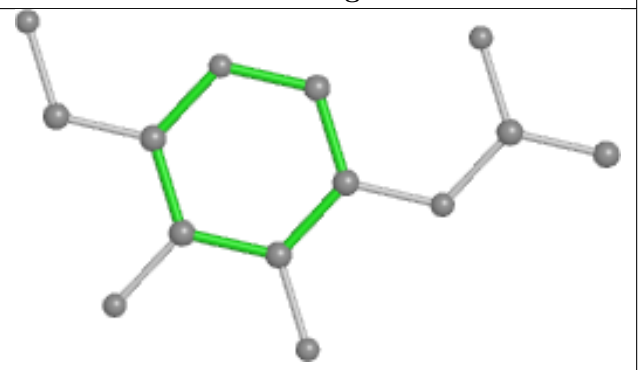
 Bond lengths	 Bond angles
 Torsions	 Rings

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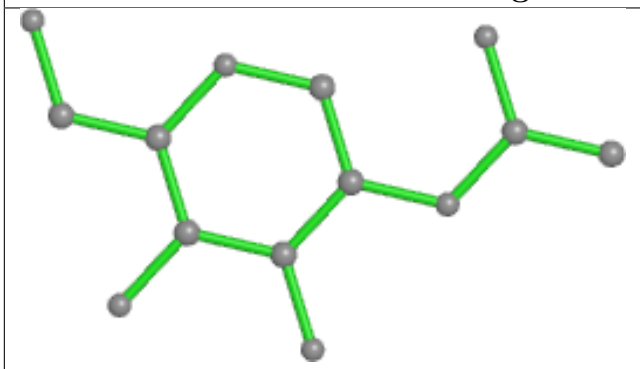
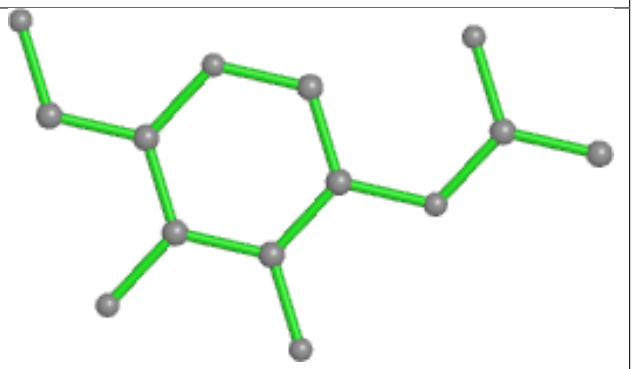
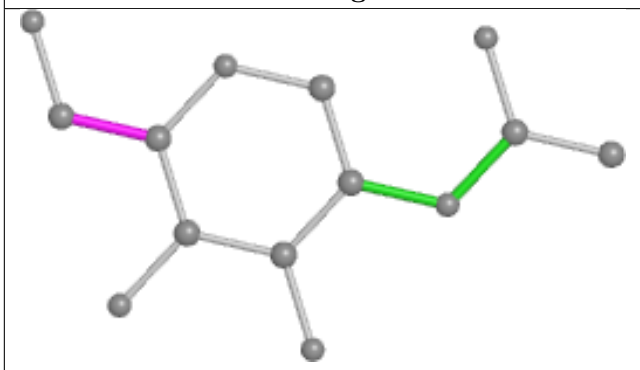
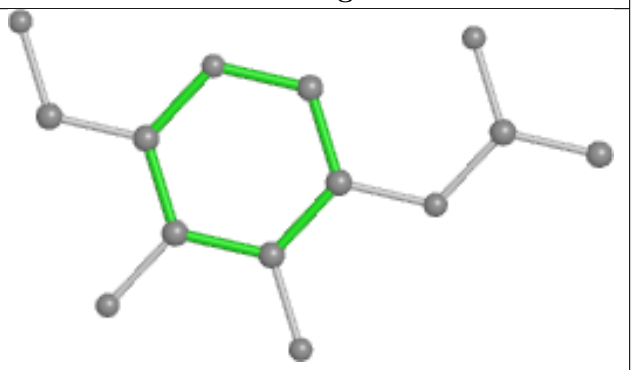
 Bond lengths	 Bond angles
 Torsions	 Rings

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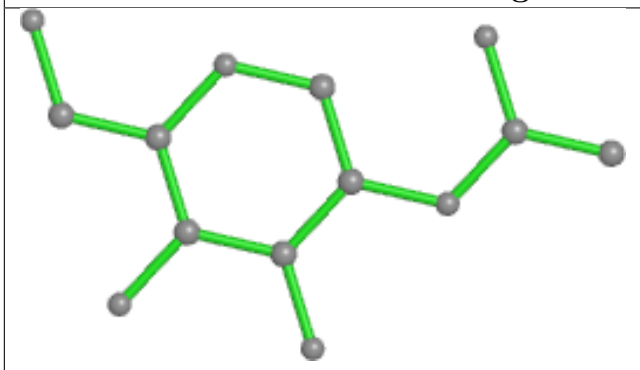
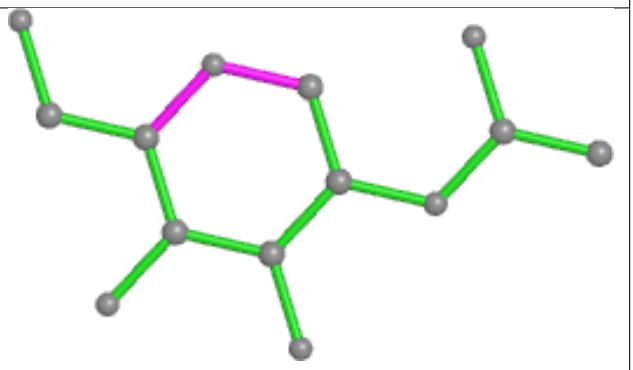
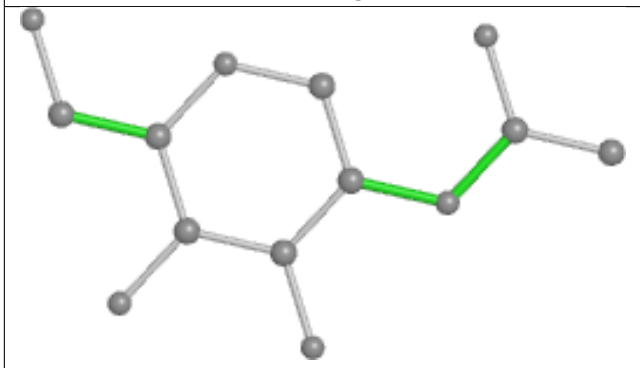
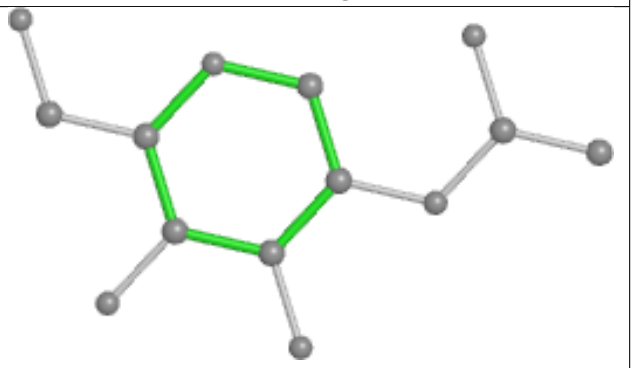
 Bond lengths	 Bond angles
 Torsions	 Rings

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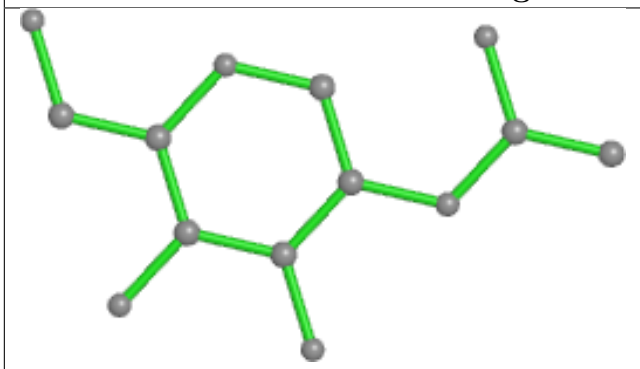
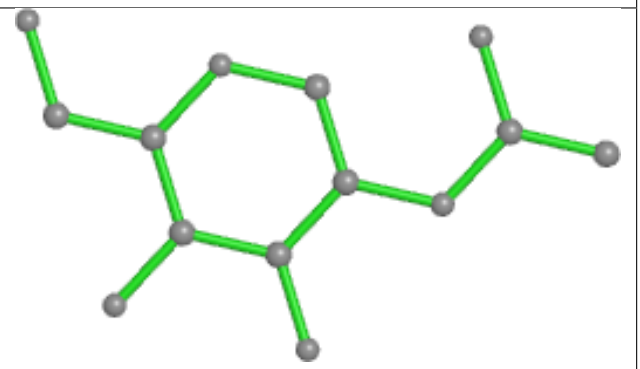
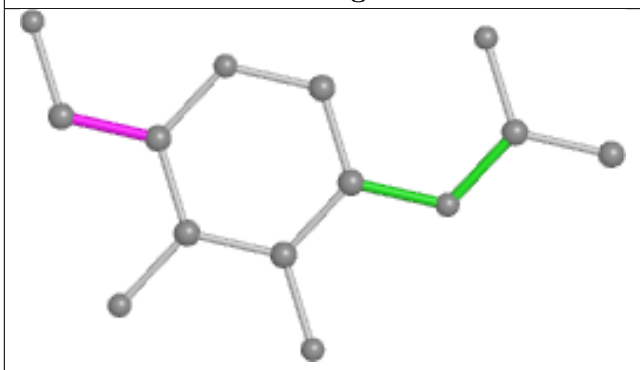
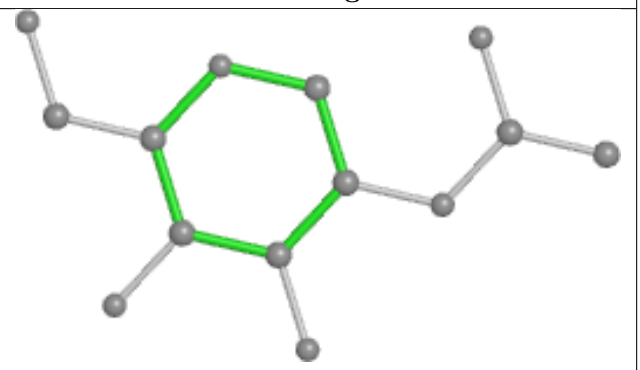
 Bond lengths	 Bond angles
 Torsions	 Rings

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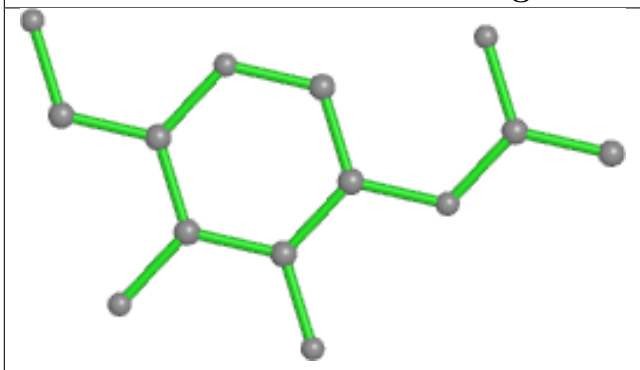
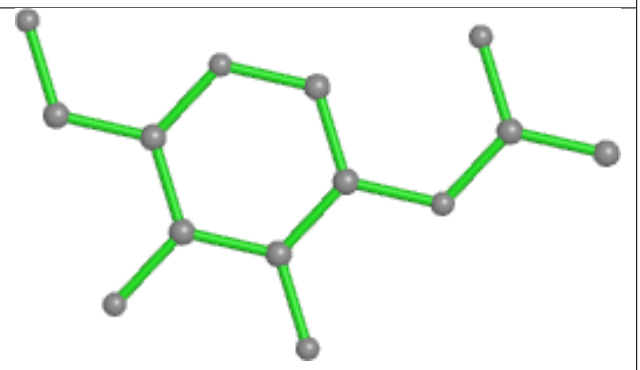
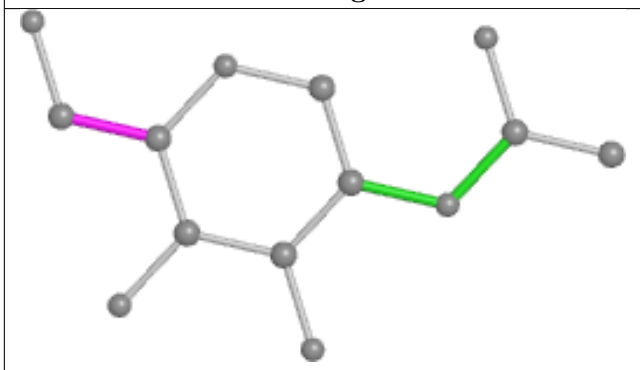
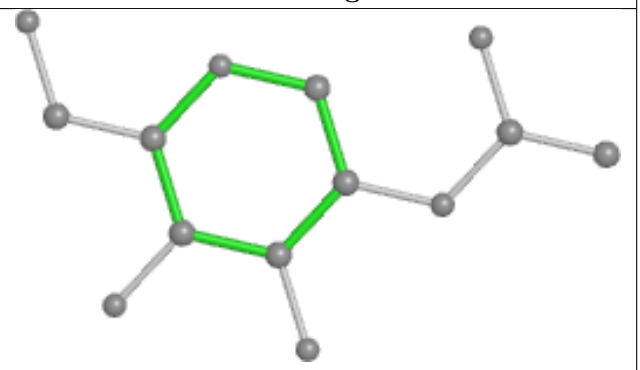
 Bond lengths	 Bond angles
 Torsions	 Rings

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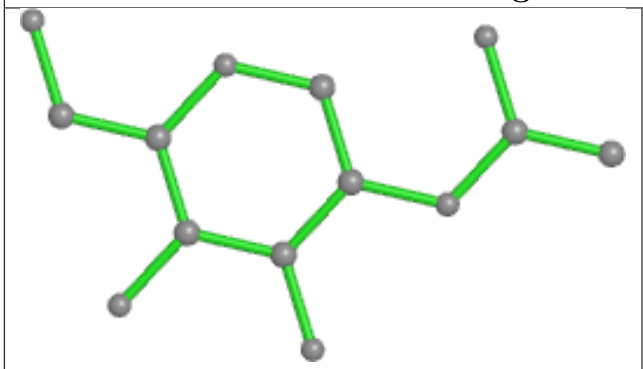
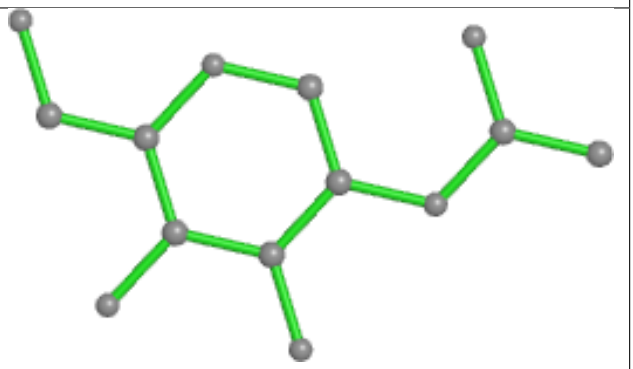
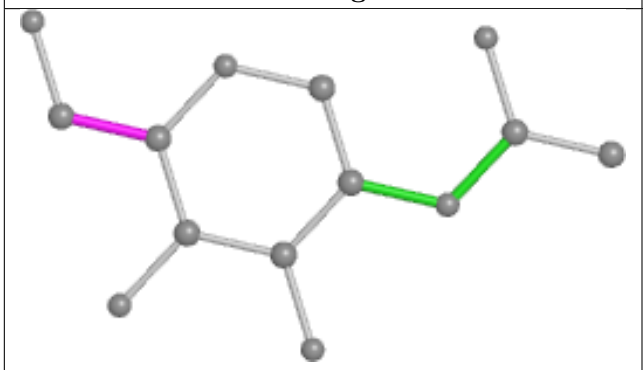
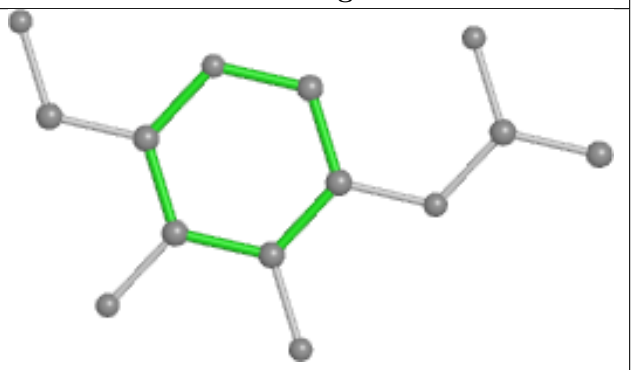
 Bond lengths	 Bond angles
 Torsions	 Rings

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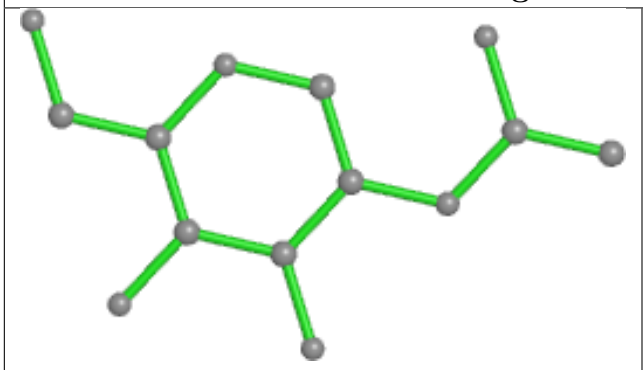
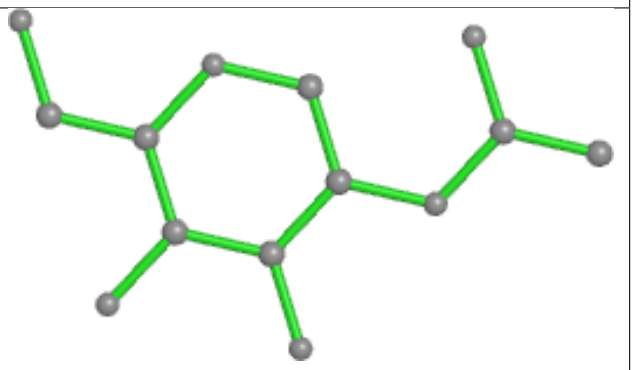
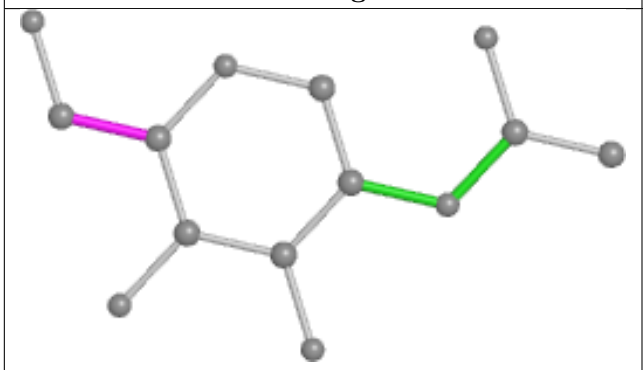
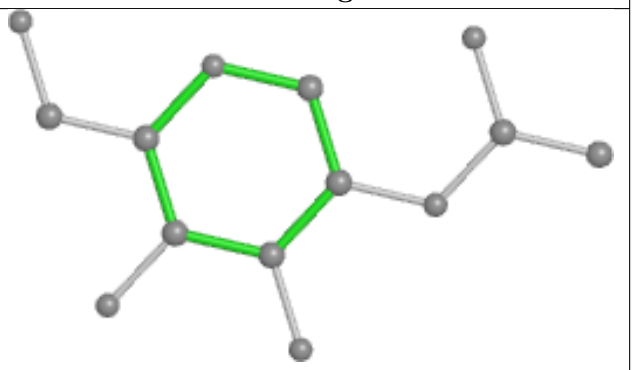
 Bond lengths	 Bond angles
 Torsions	 Rings

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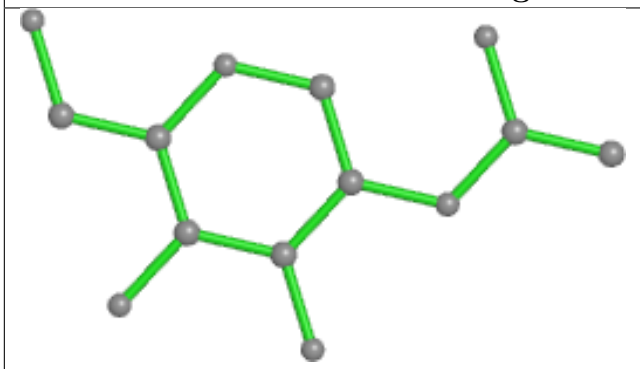
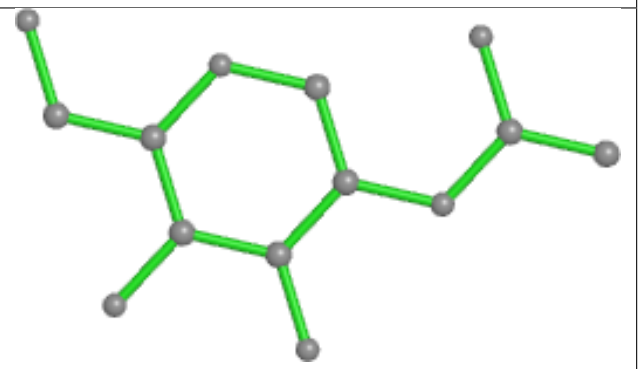
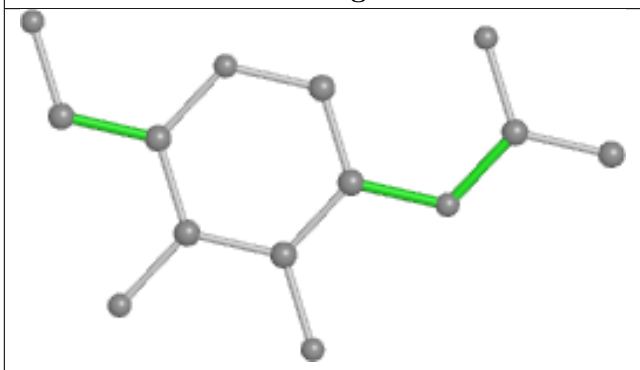
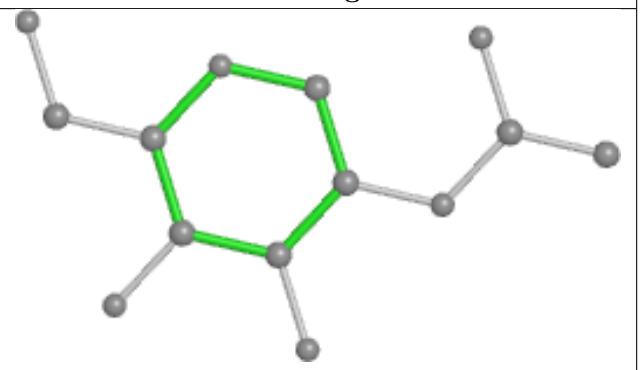
 Bond lengths	 Bond angles
 Torsions	 Rings

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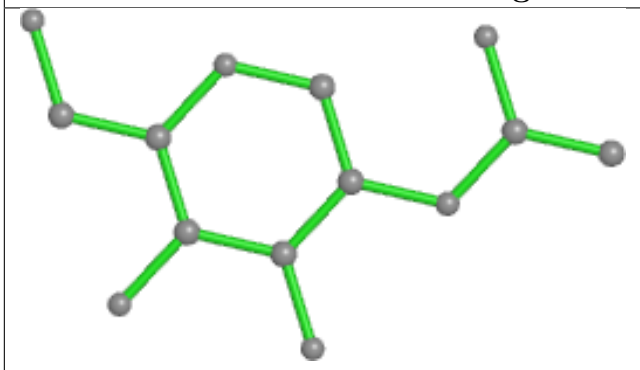
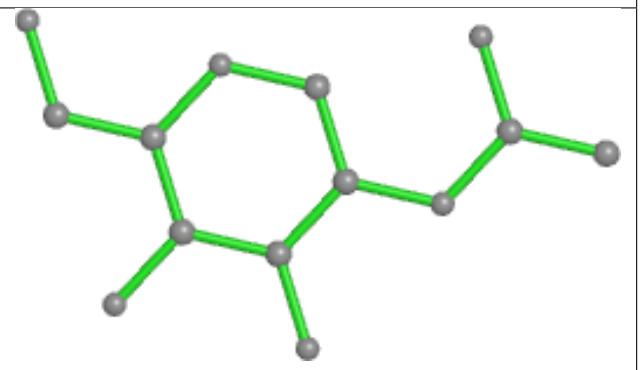
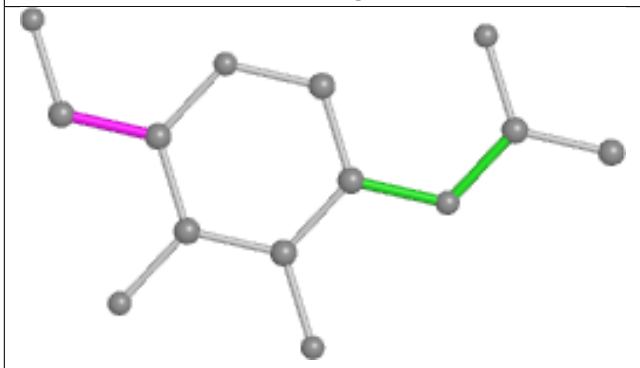
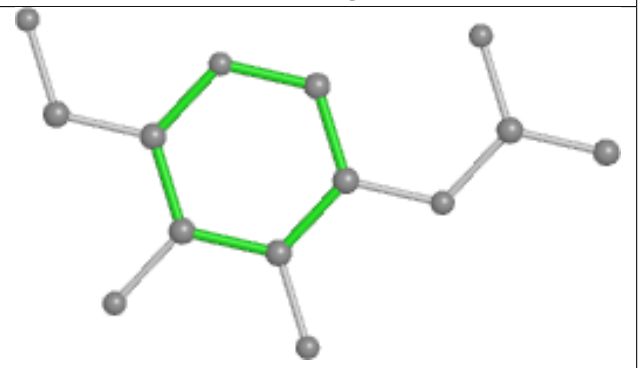
 Bond lengths	 Bond angles
 Torsions	 Rings

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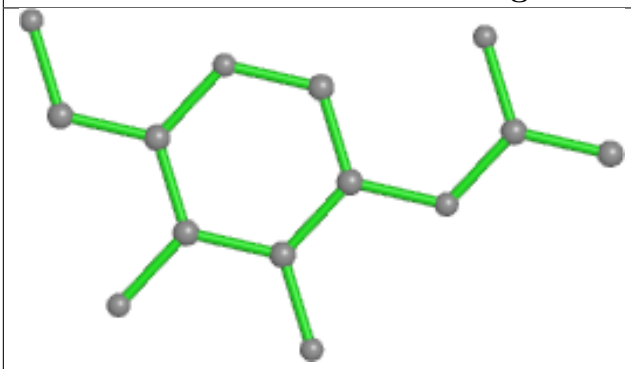
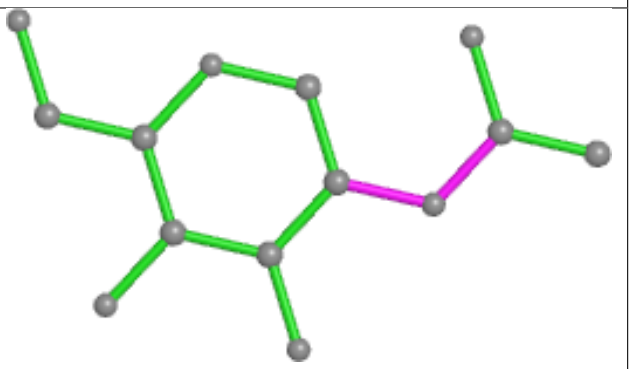
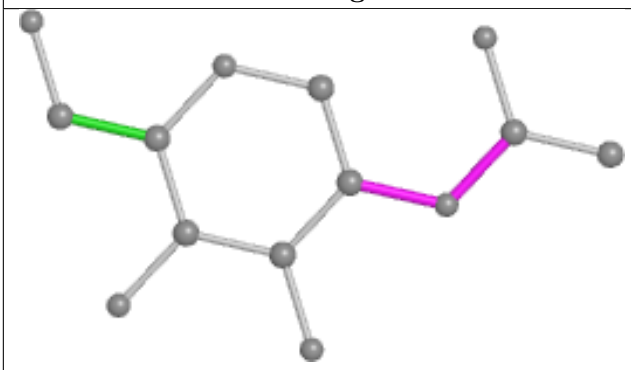
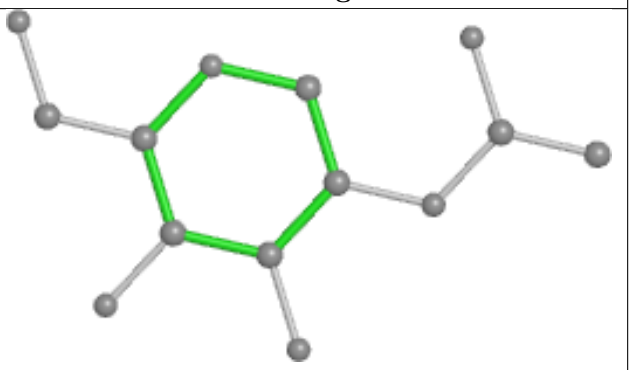
 Bond lengths	 Bond angles
 Torsions	 Rings

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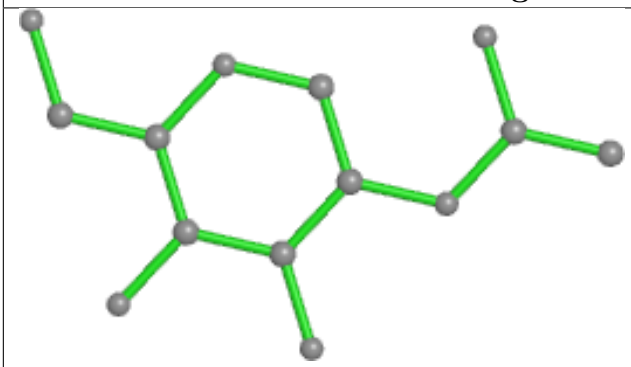
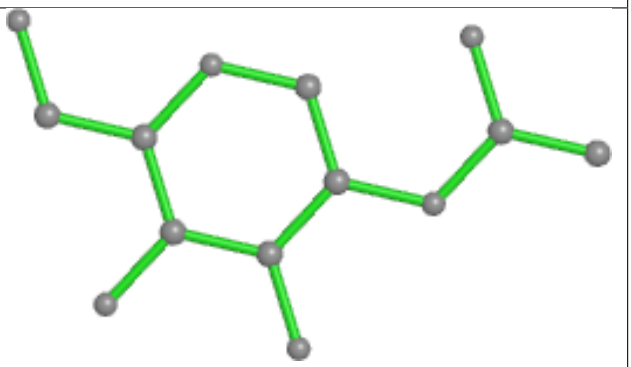
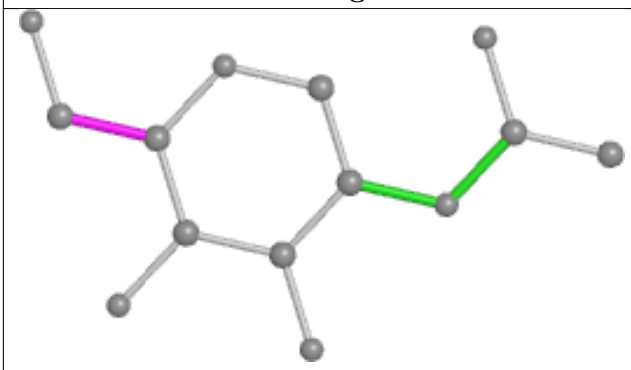
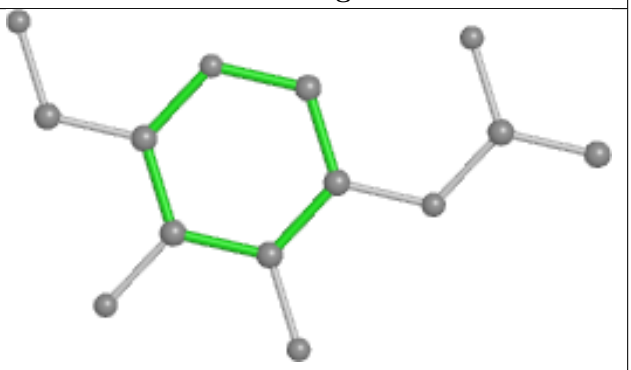
 Bond lengths	 Bond angles
 Torsions	 Rings

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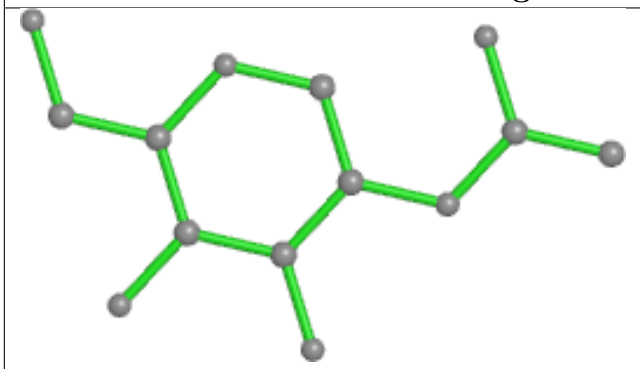
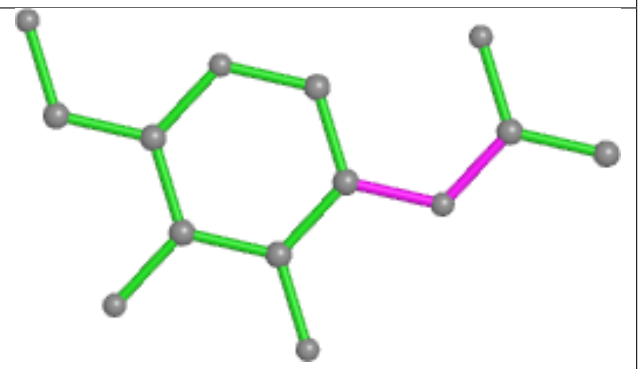
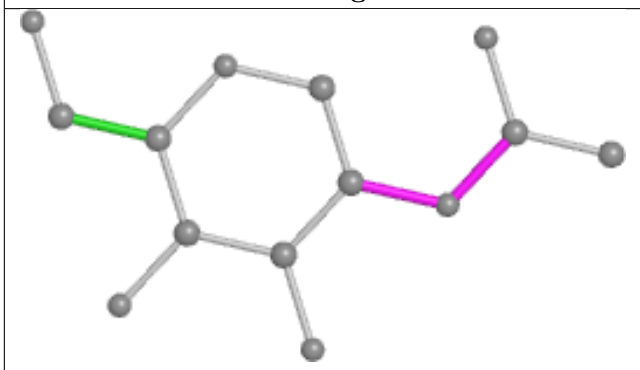
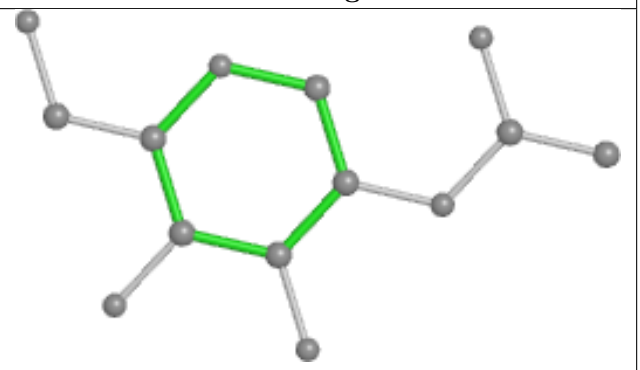
 Bond lengths	 Bond angles
 Torsions	 Rings

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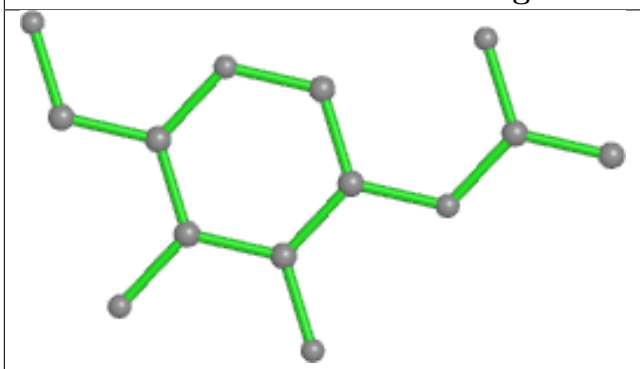
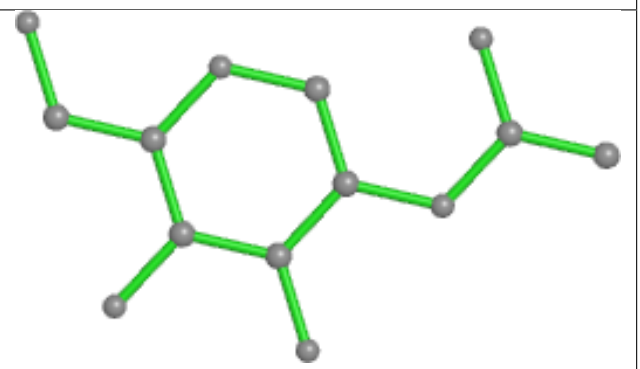
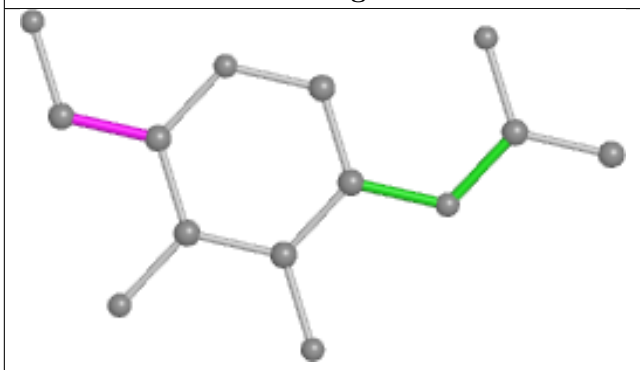
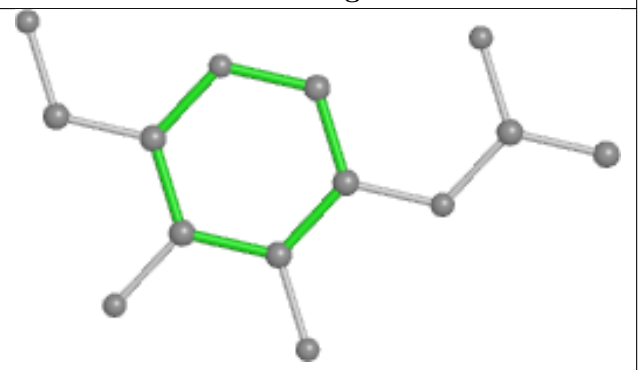
 Bond lengths	 Bond angles
 Torsions	 Rings

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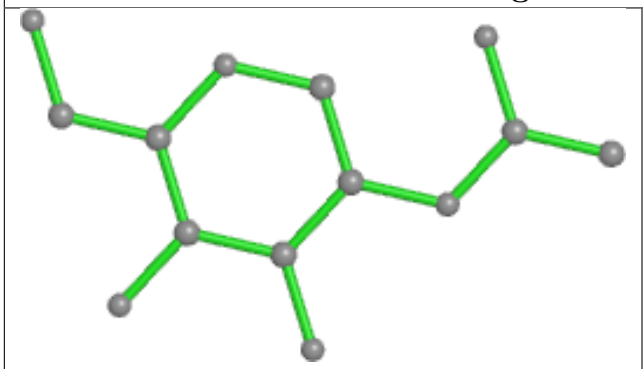
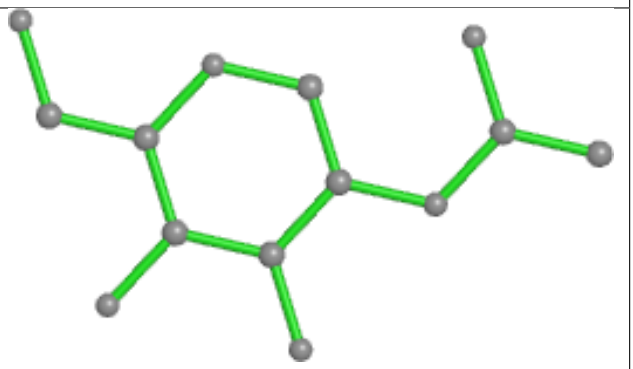
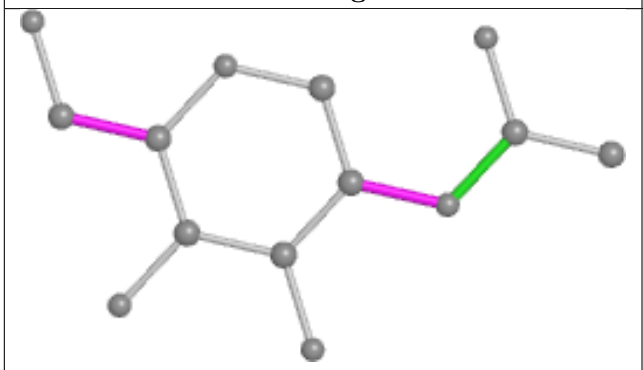
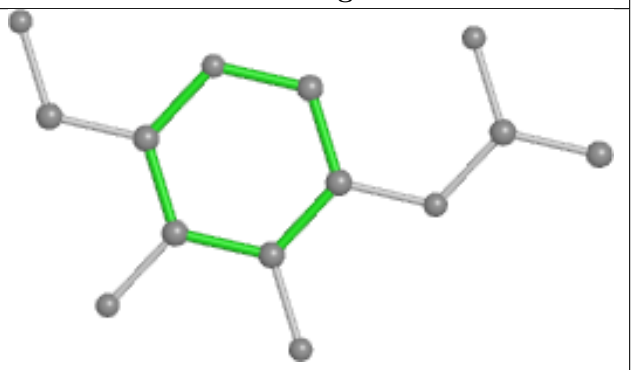
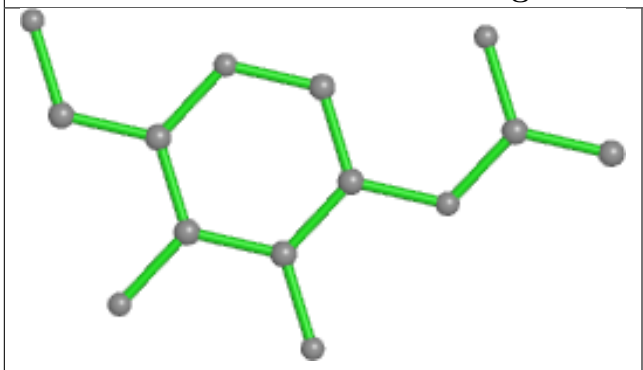
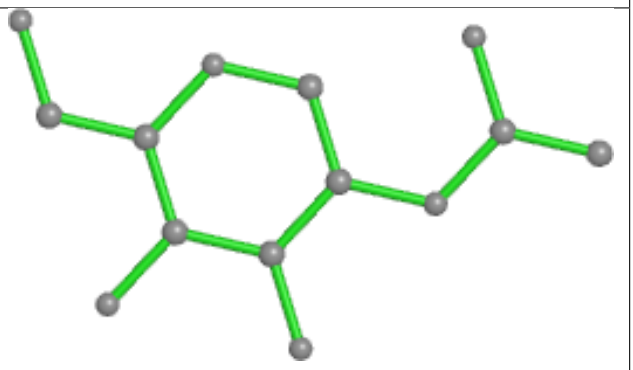
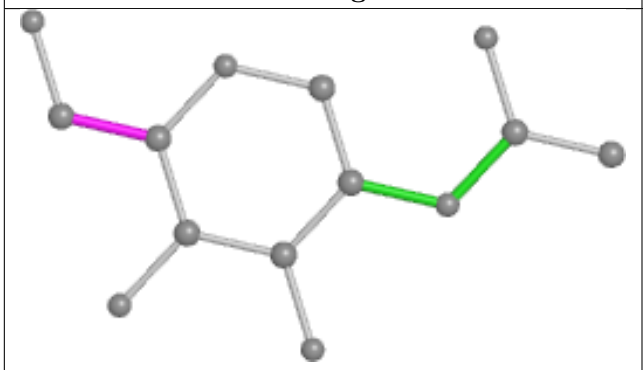
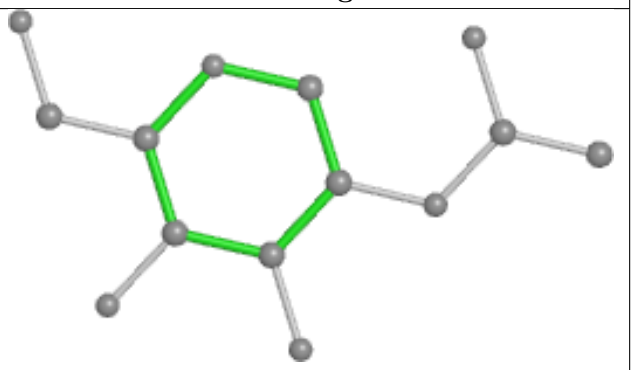
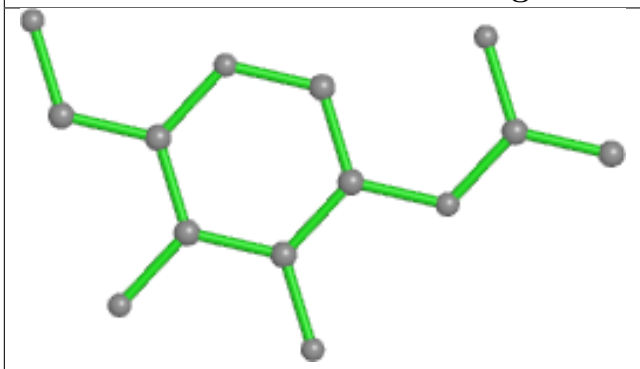
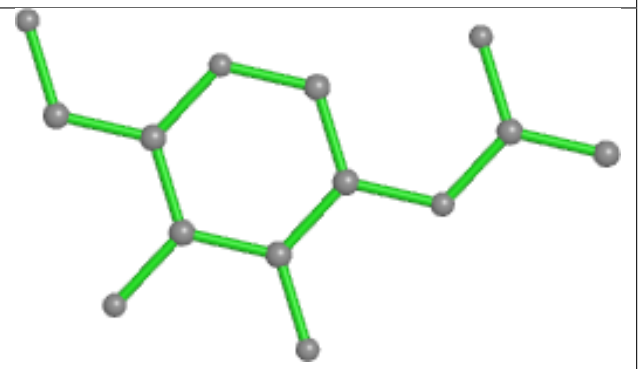
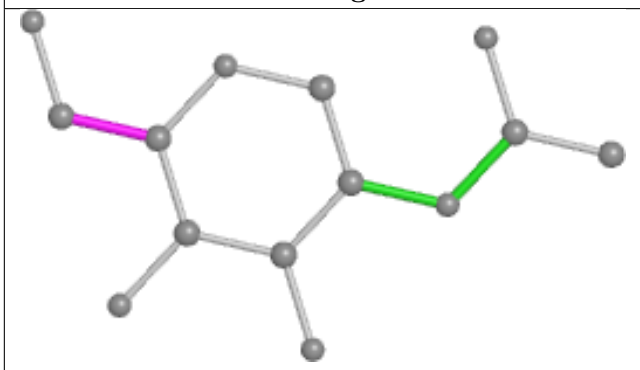
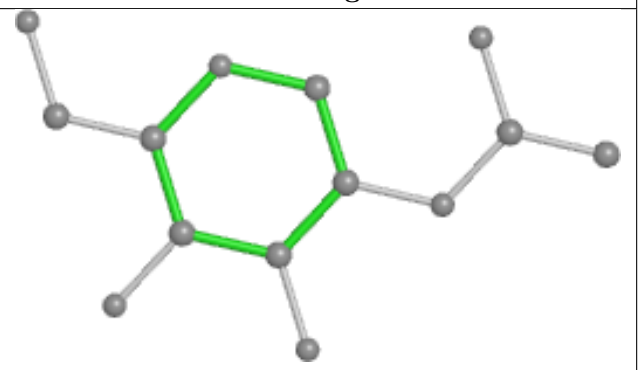
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

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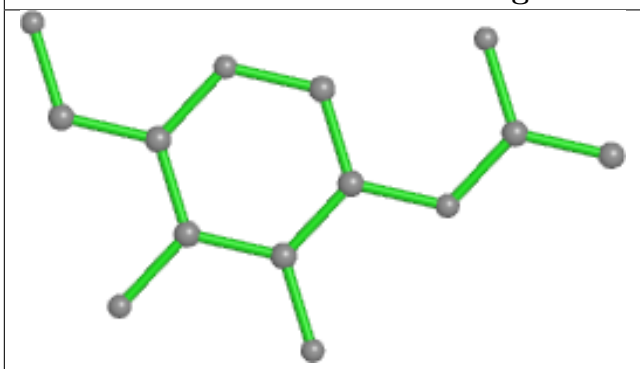
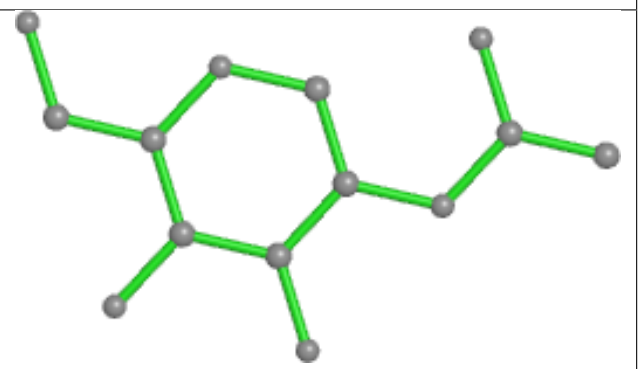
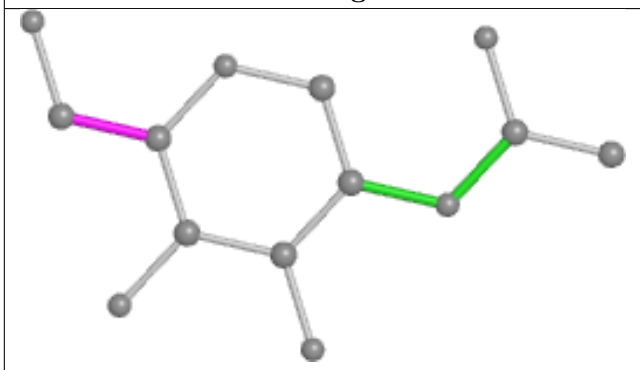
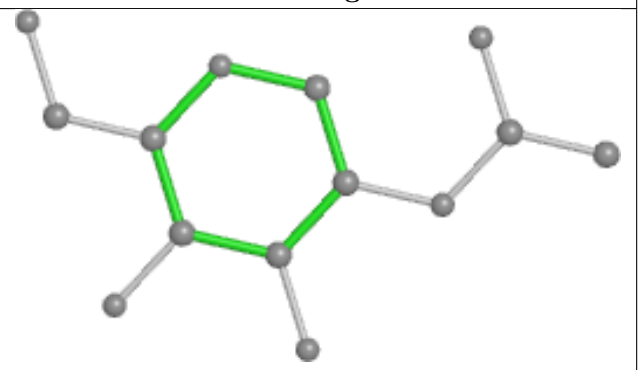
 Bond lengths	 Bond angles
 Torsions	 Rings

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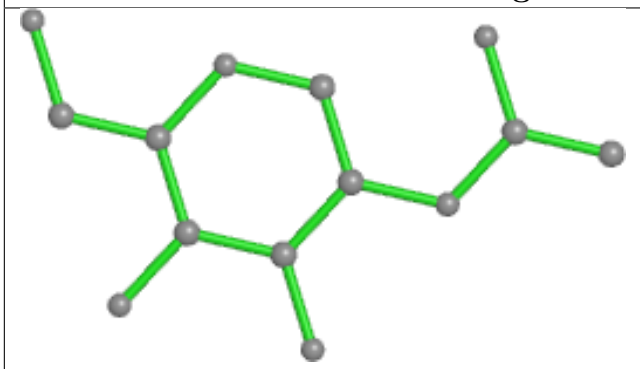
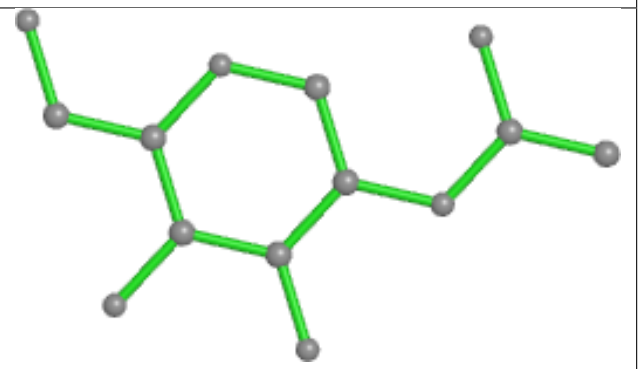
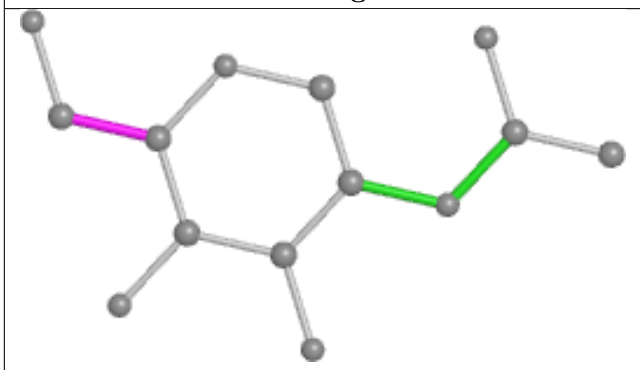
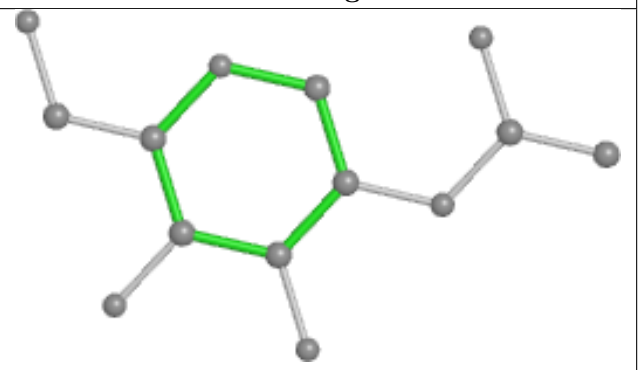
 Bond lengths	 Bond angles
 Torsions	 Rings

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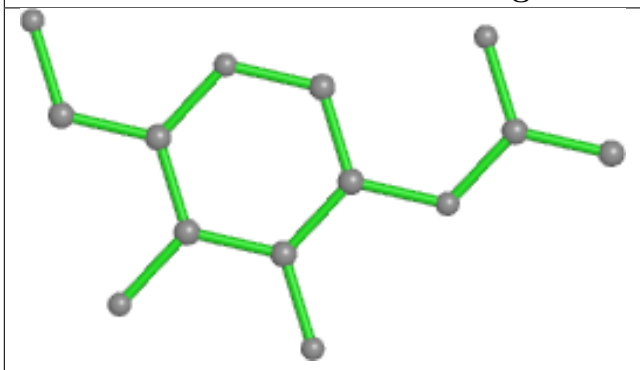
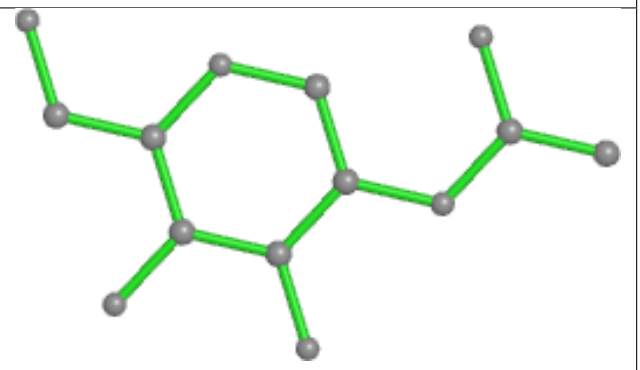
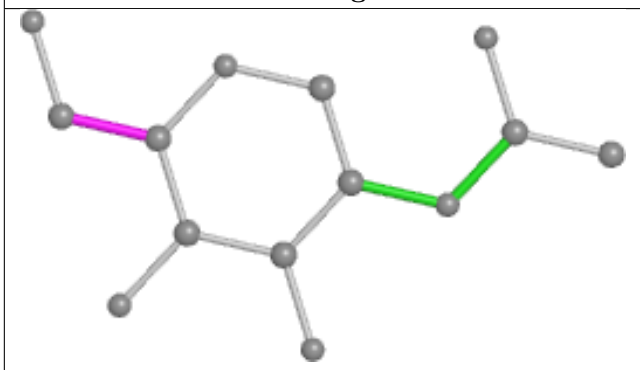
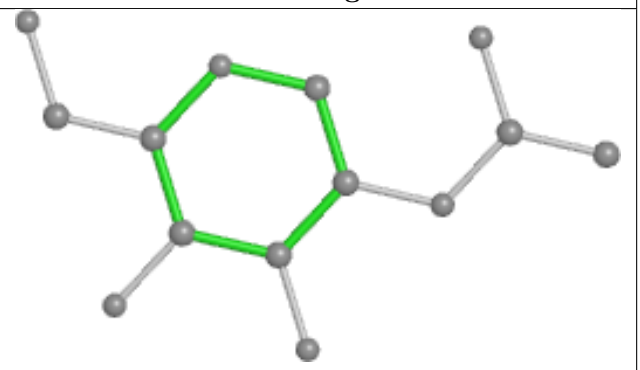
 Bond lengths	 Bond angles
 Torsions	 Rings

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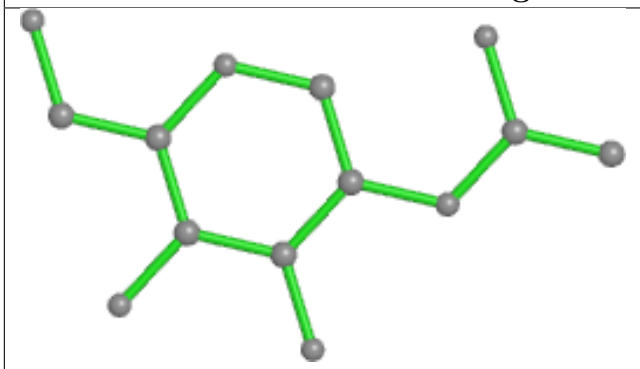
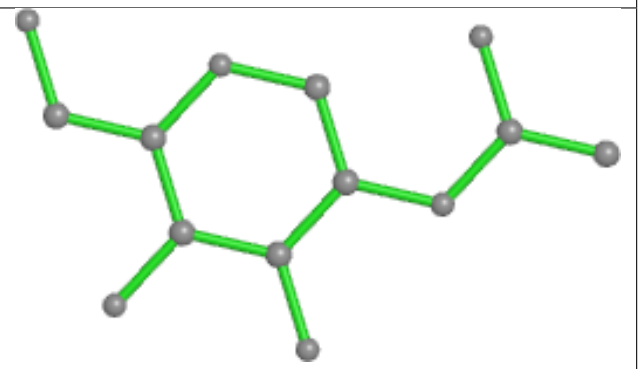
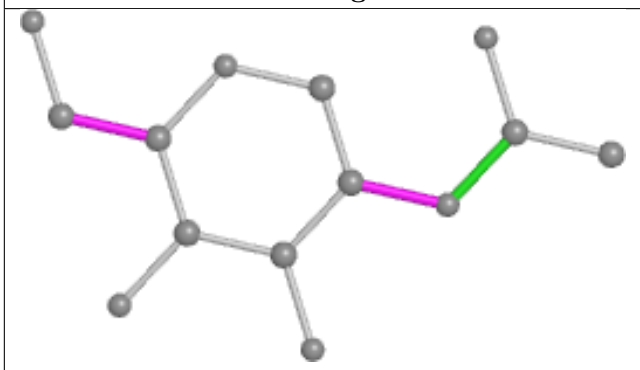
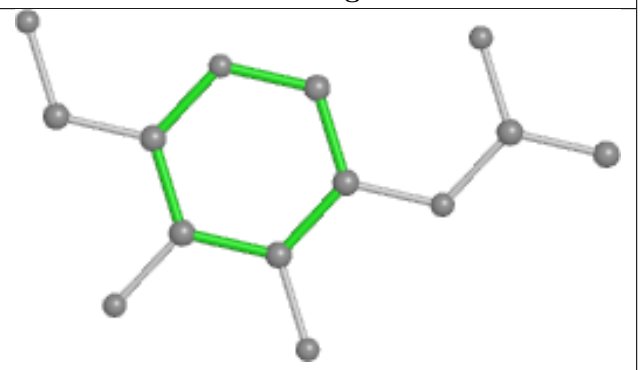
 Bond lengths	 Bond angles
 Torsions	 Rings

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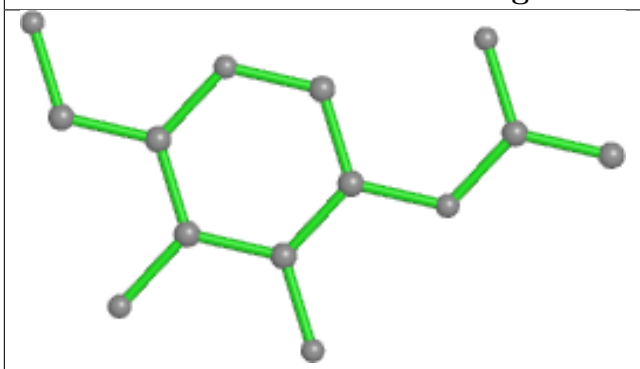
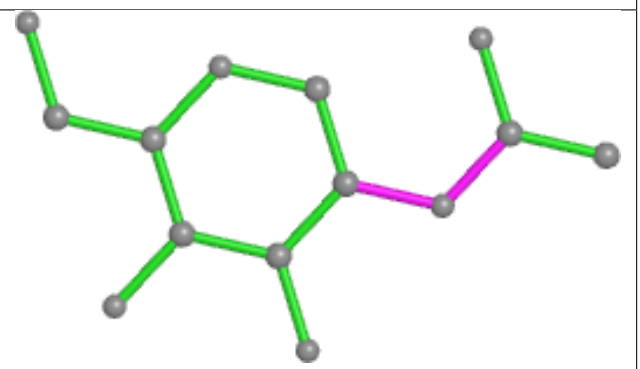
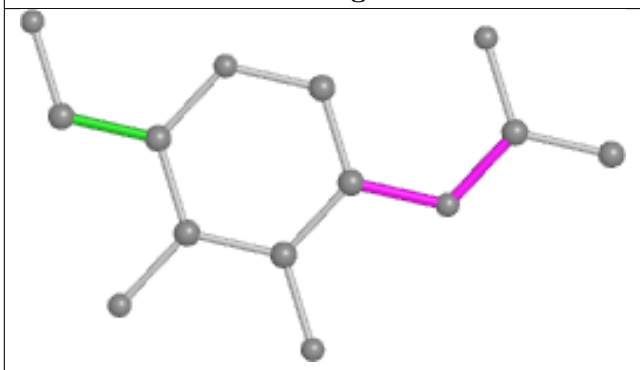
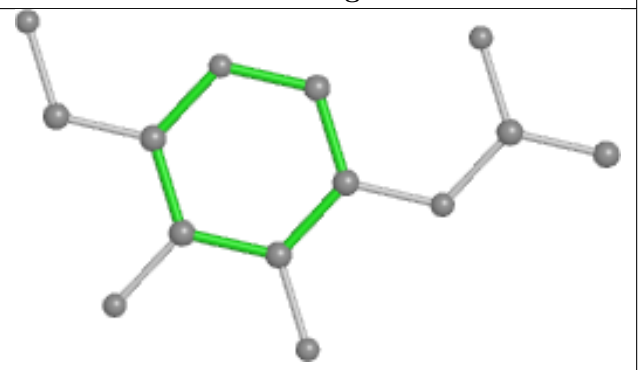
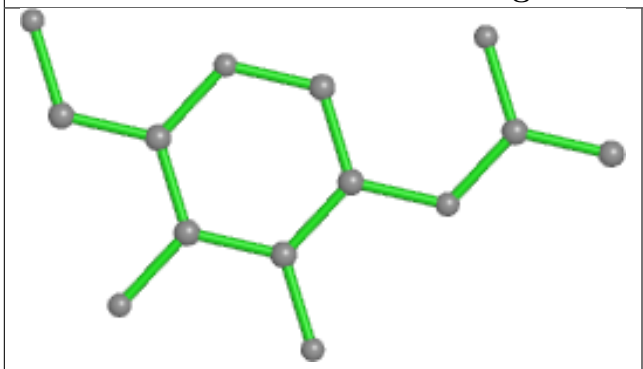
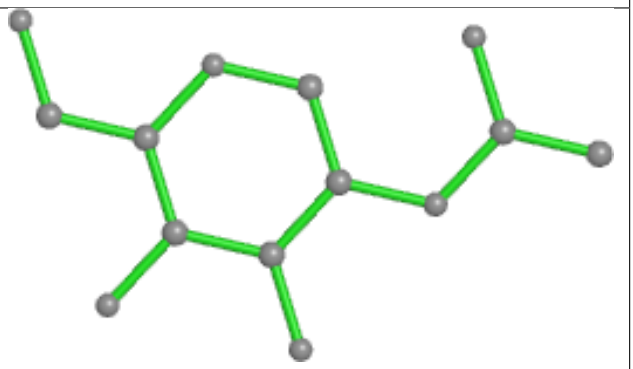
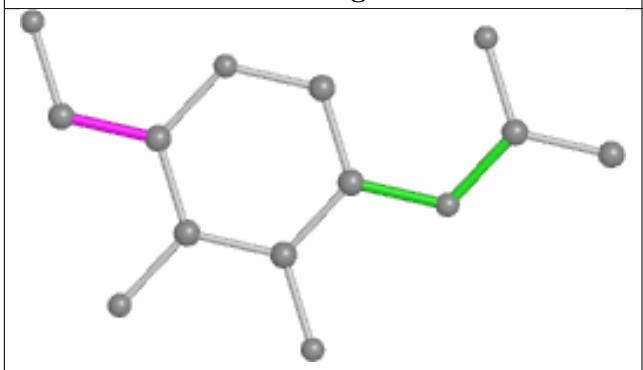
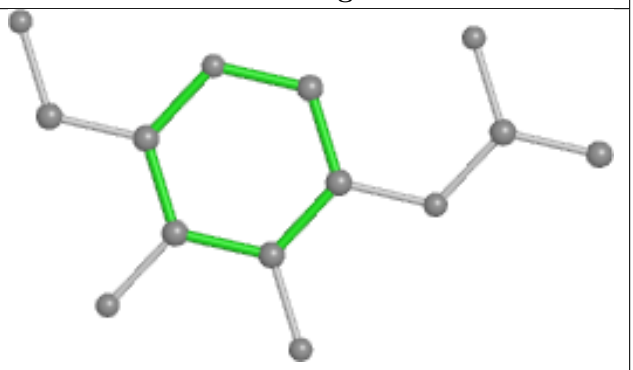
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

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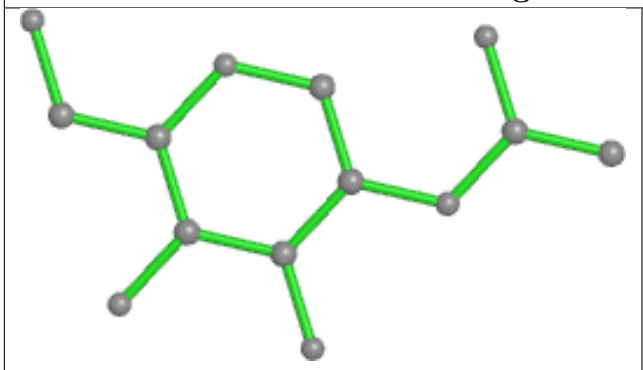
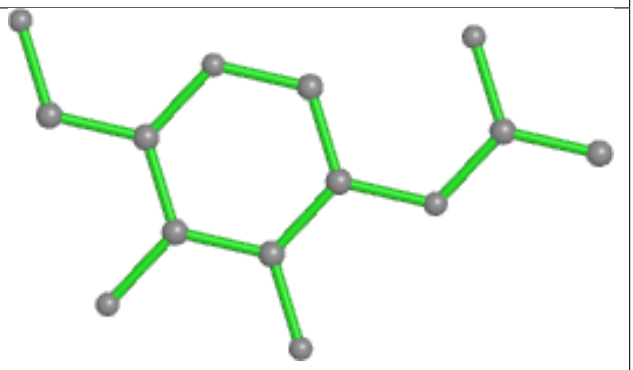
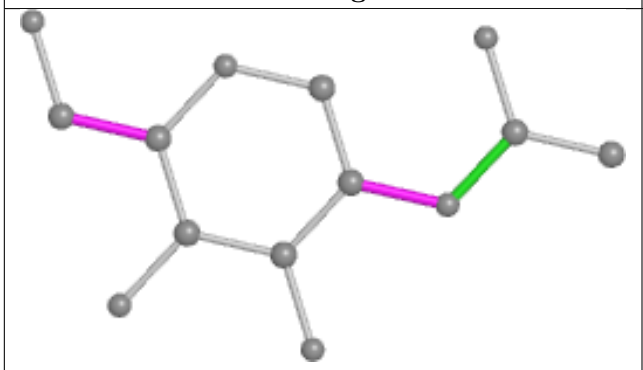
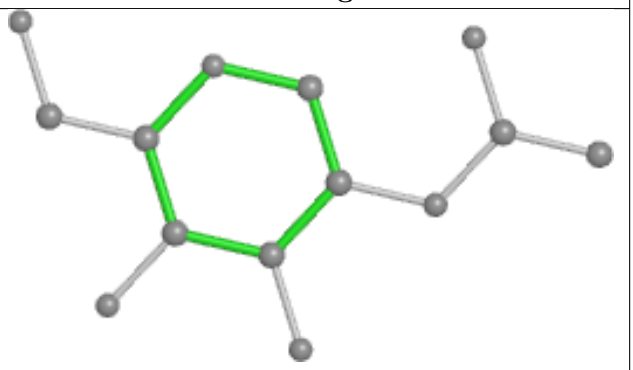
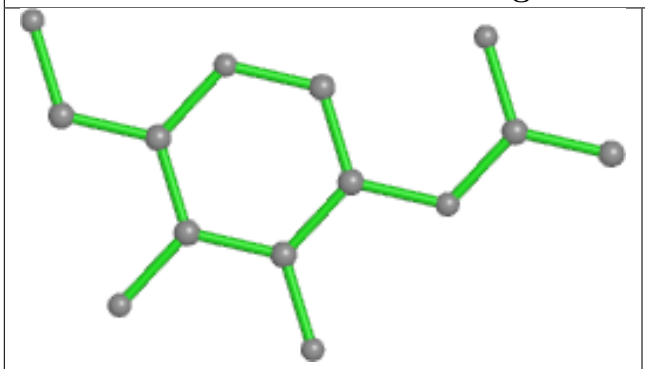
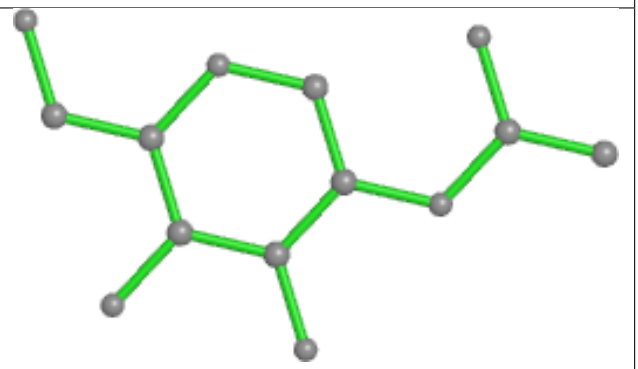
 Bond lengths	 Bond angles
 Torsions	 Rings

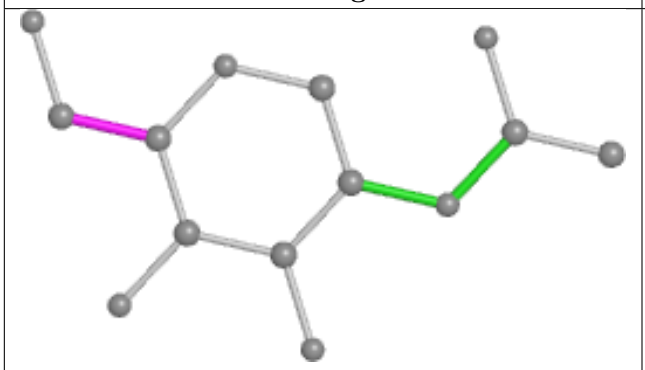
Ligand NAG B 1312



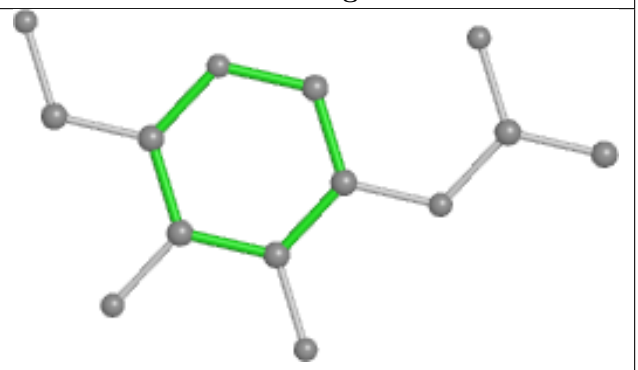
Bond lengths



Bond angles

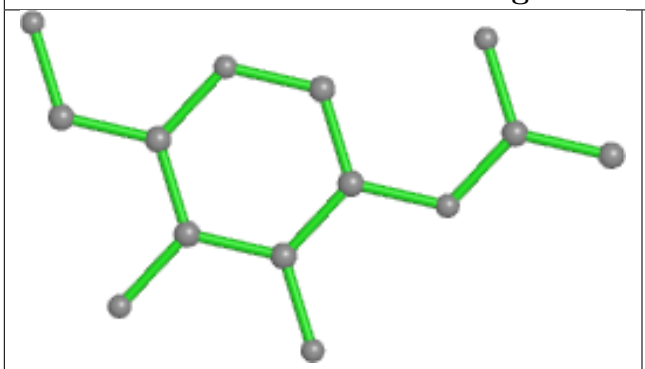


Torsions

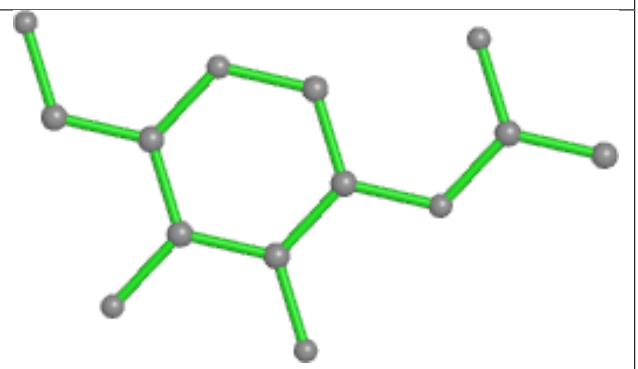


Rings

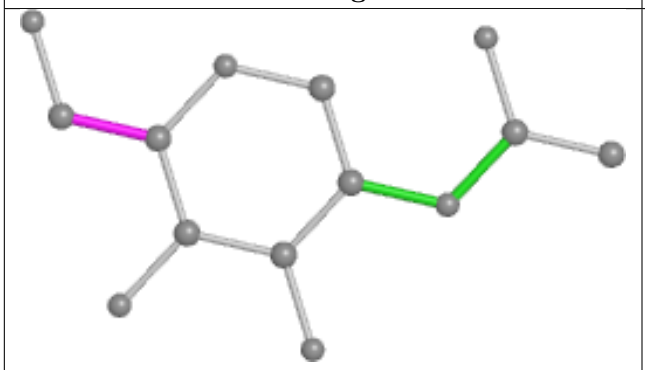
Ligand NAG A 1302



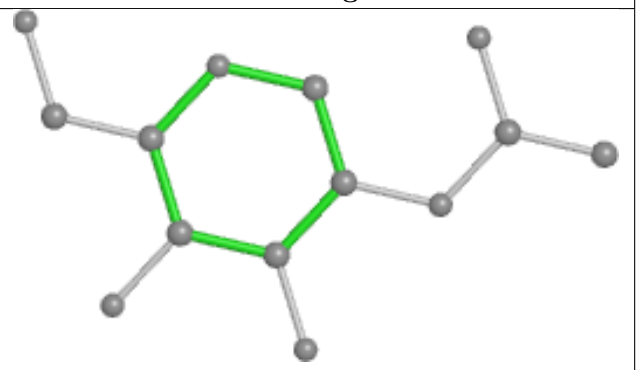
Bond lengths



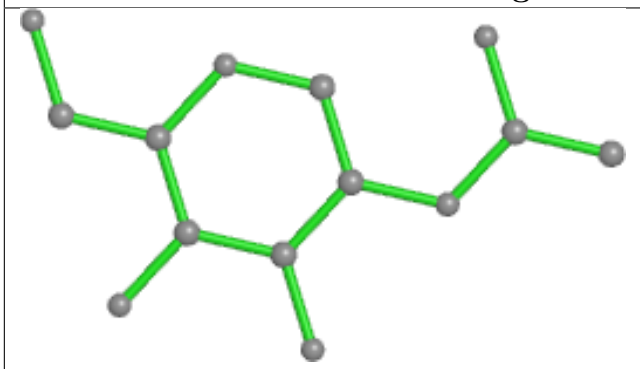
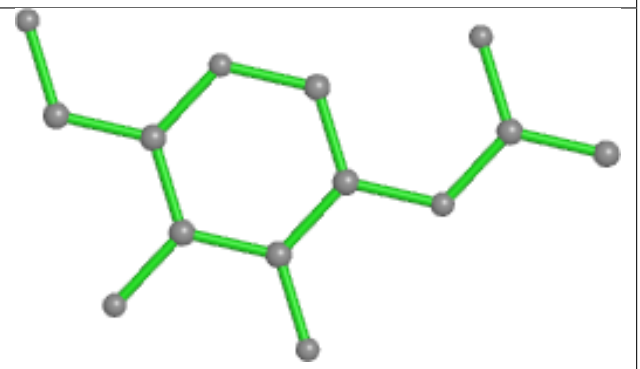
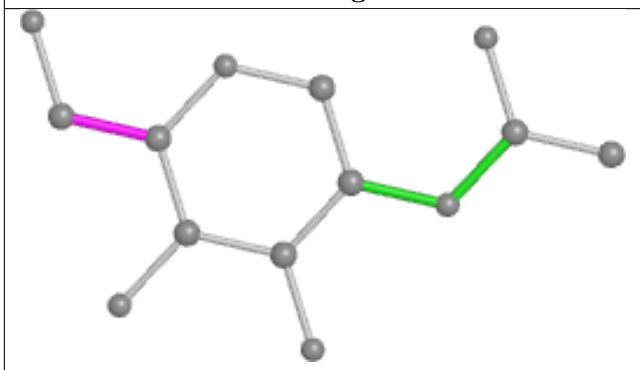
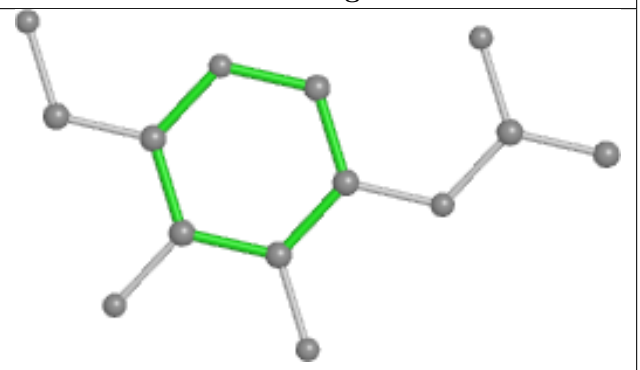
Bond angles

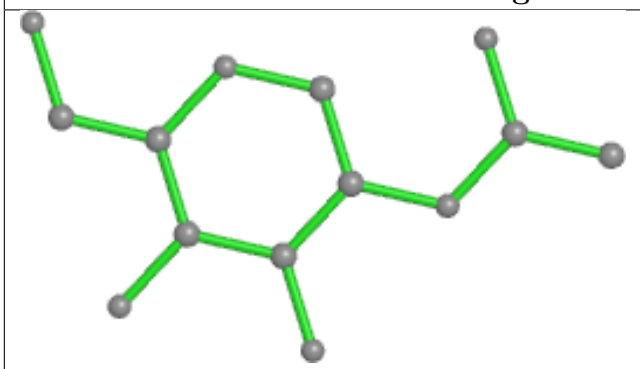
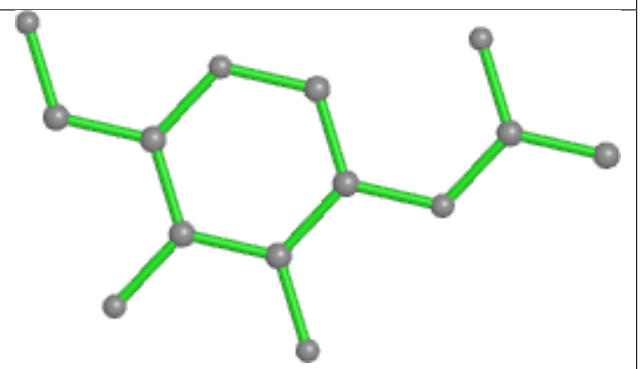
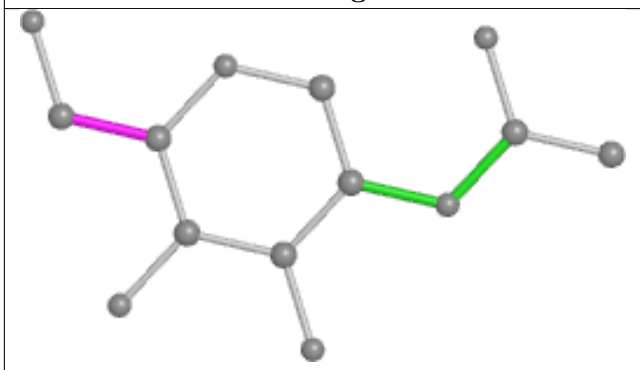
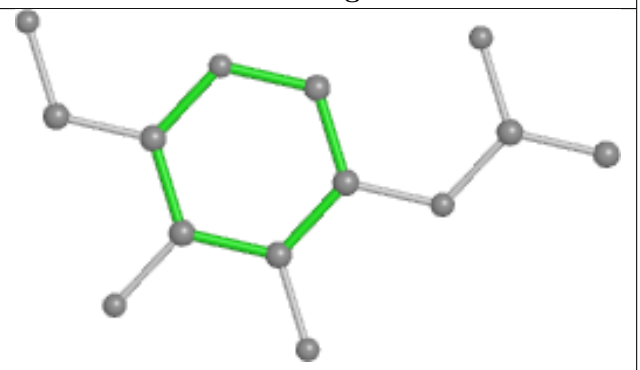


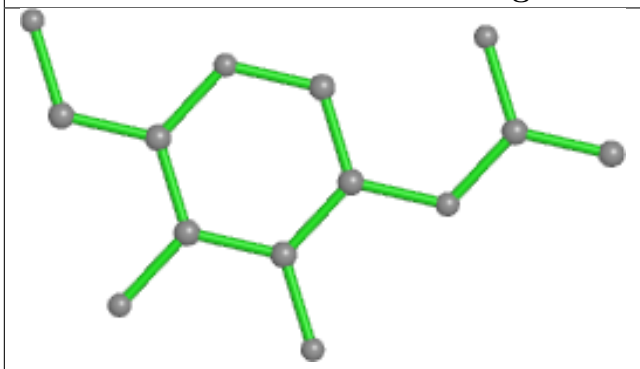
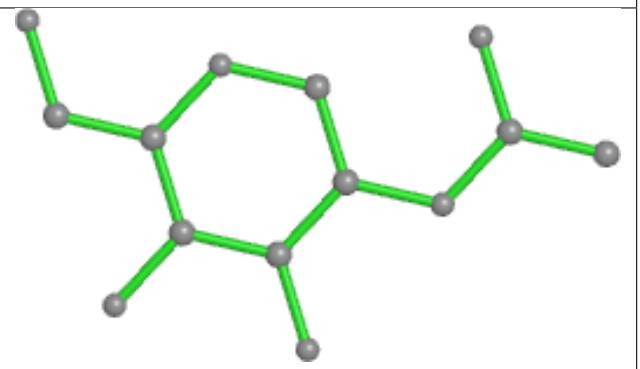
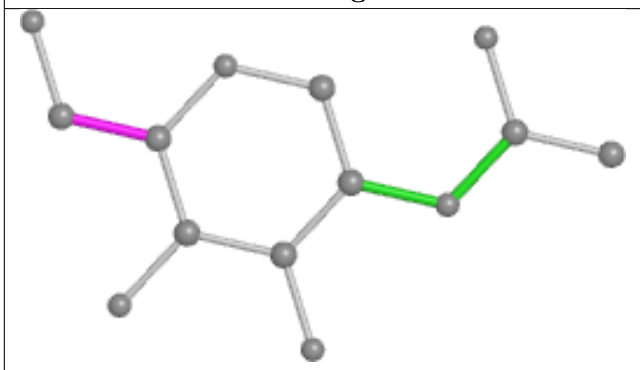
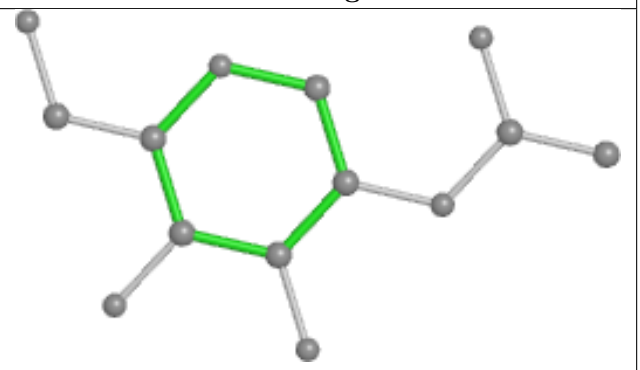
Torsions



Rings

Ligand NAG C 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1309	
 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.

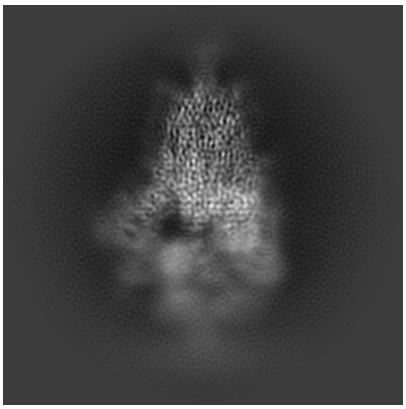
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26881. These allow visual inspection of the internal detail of the map and identification of artifacts.

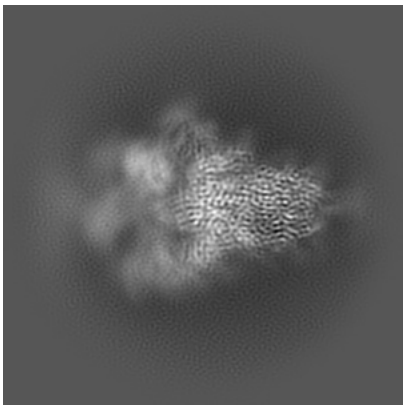
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

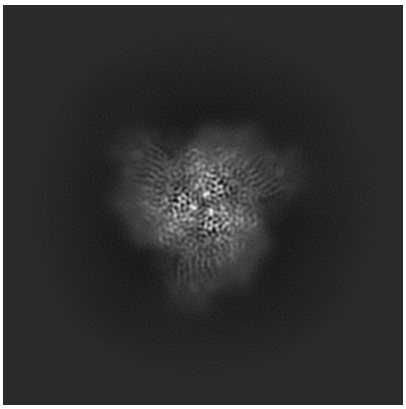
6.1.1 Primary map



X

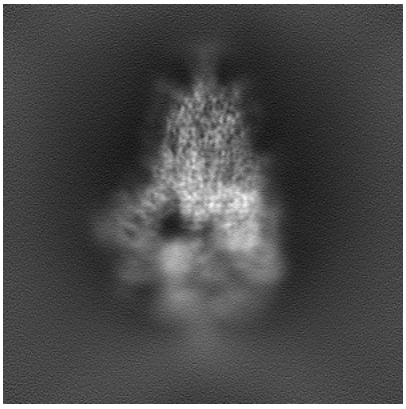


Y

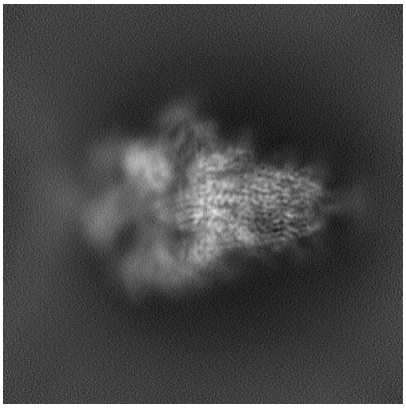


Z

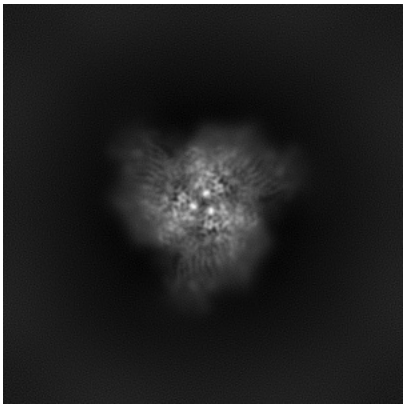
6.1.2 Raw map



X



Y

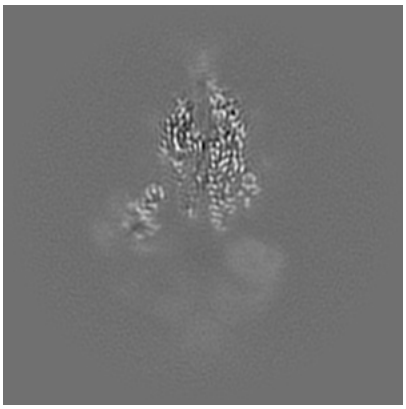


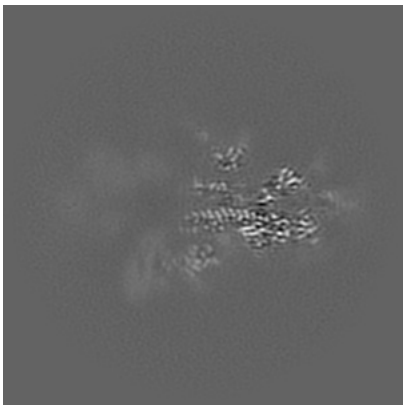
Z

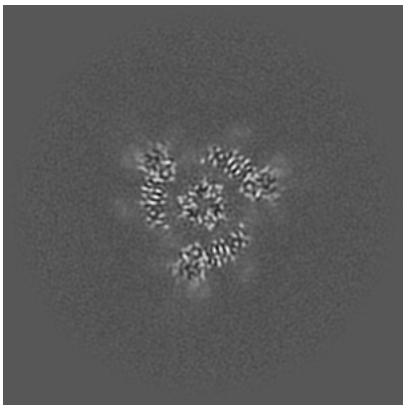
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

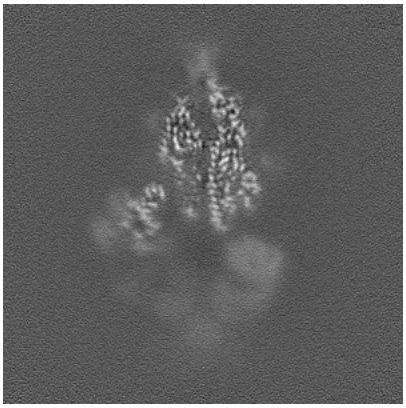
6.2.1 Primary map

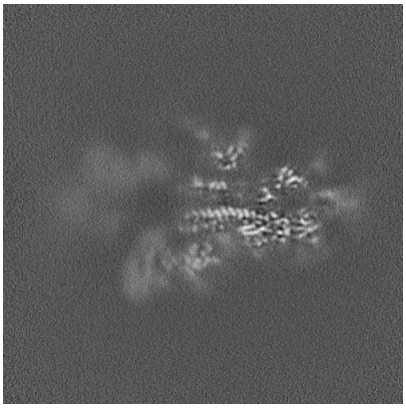

X Index: 180

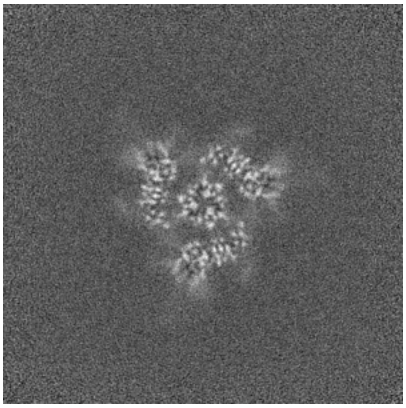

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

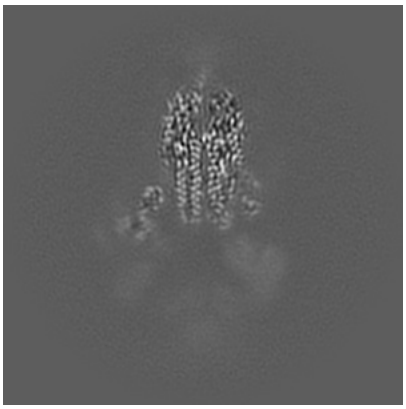

Y Index: 180

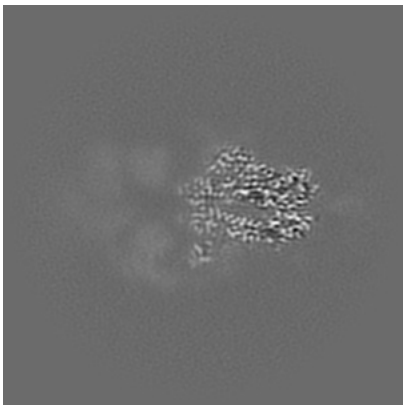

Z Index: 180

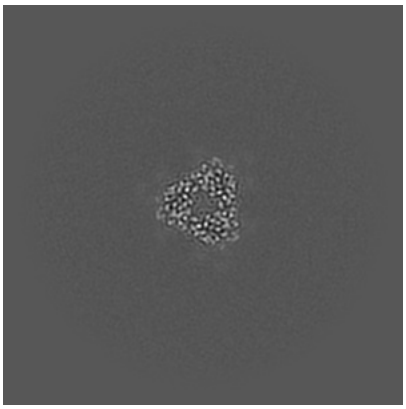
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

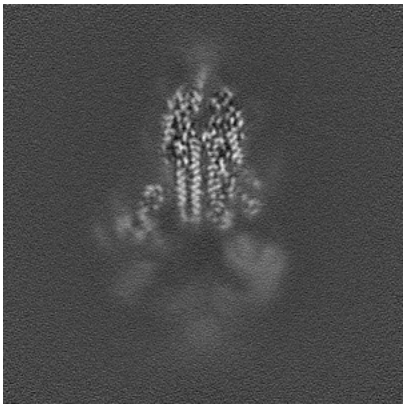
6.3.1 Primary map

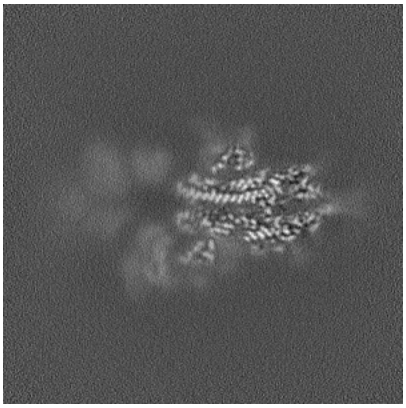

X Index: 186

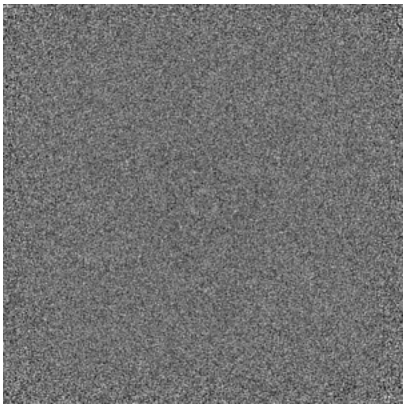

Y Index: 167


Z Index: 247

6.3.2 Raw map


X Index: 186

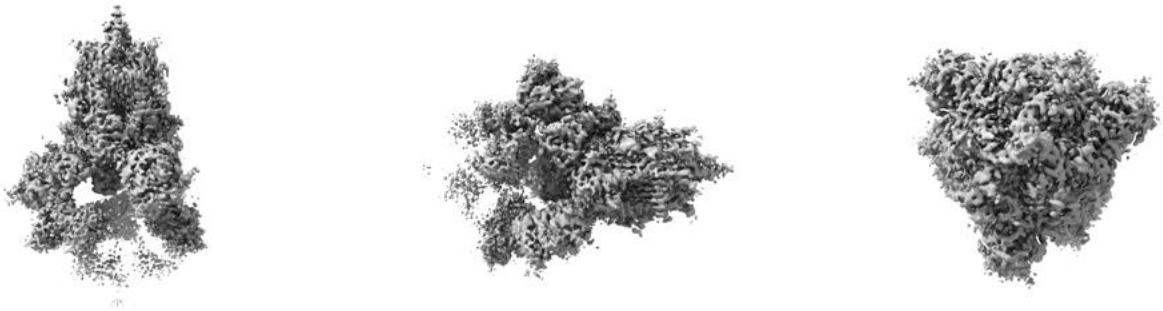

Y Index: 172


Z Index: 0

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

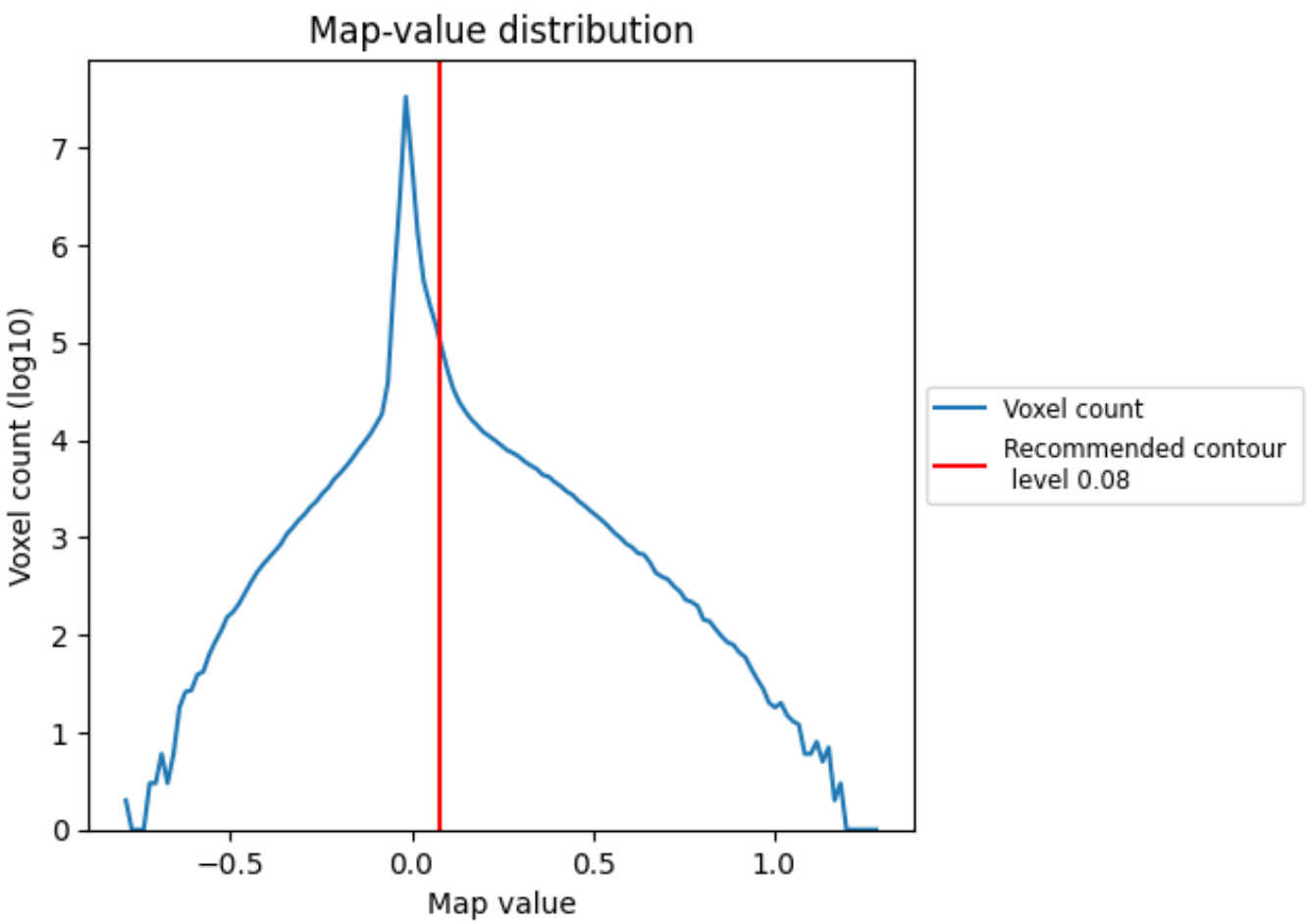
6.5 Mask visualisation (i)

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

7 Map analysis (i)

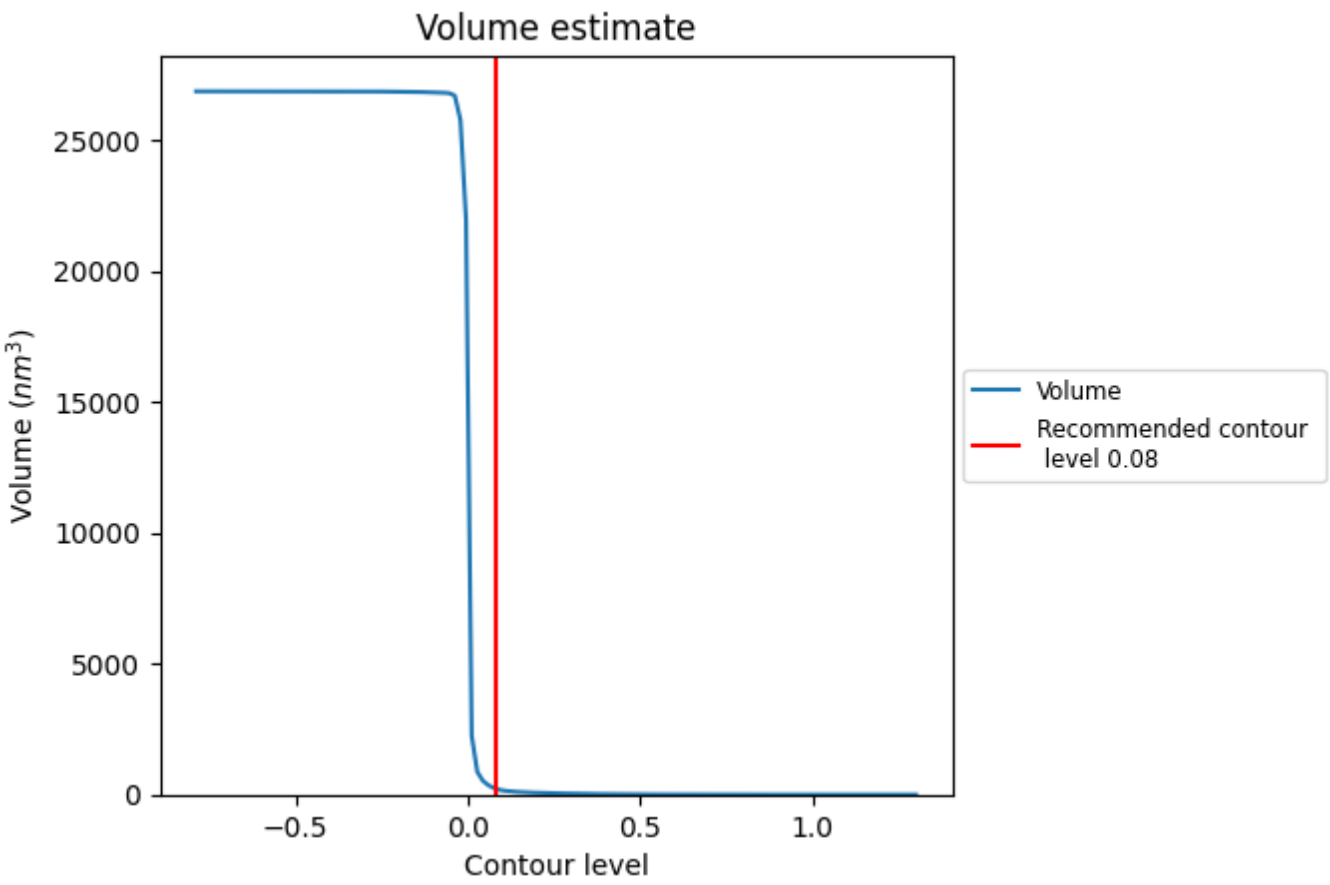
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

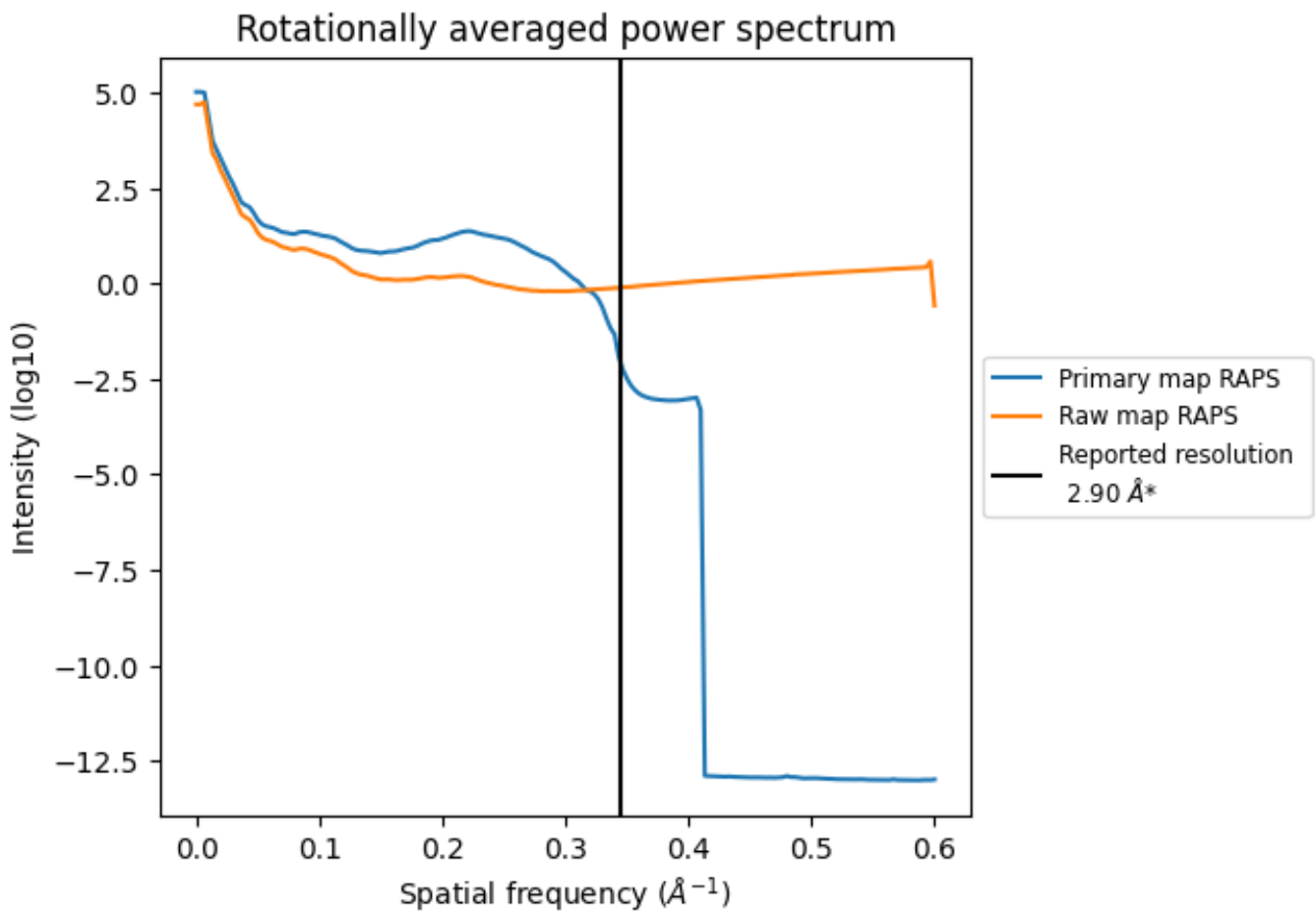
7.2 Volume estimate (i)



The volume at the recommended contour level is 228 nm^3; this corresponds to an approximate mass of 206 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)

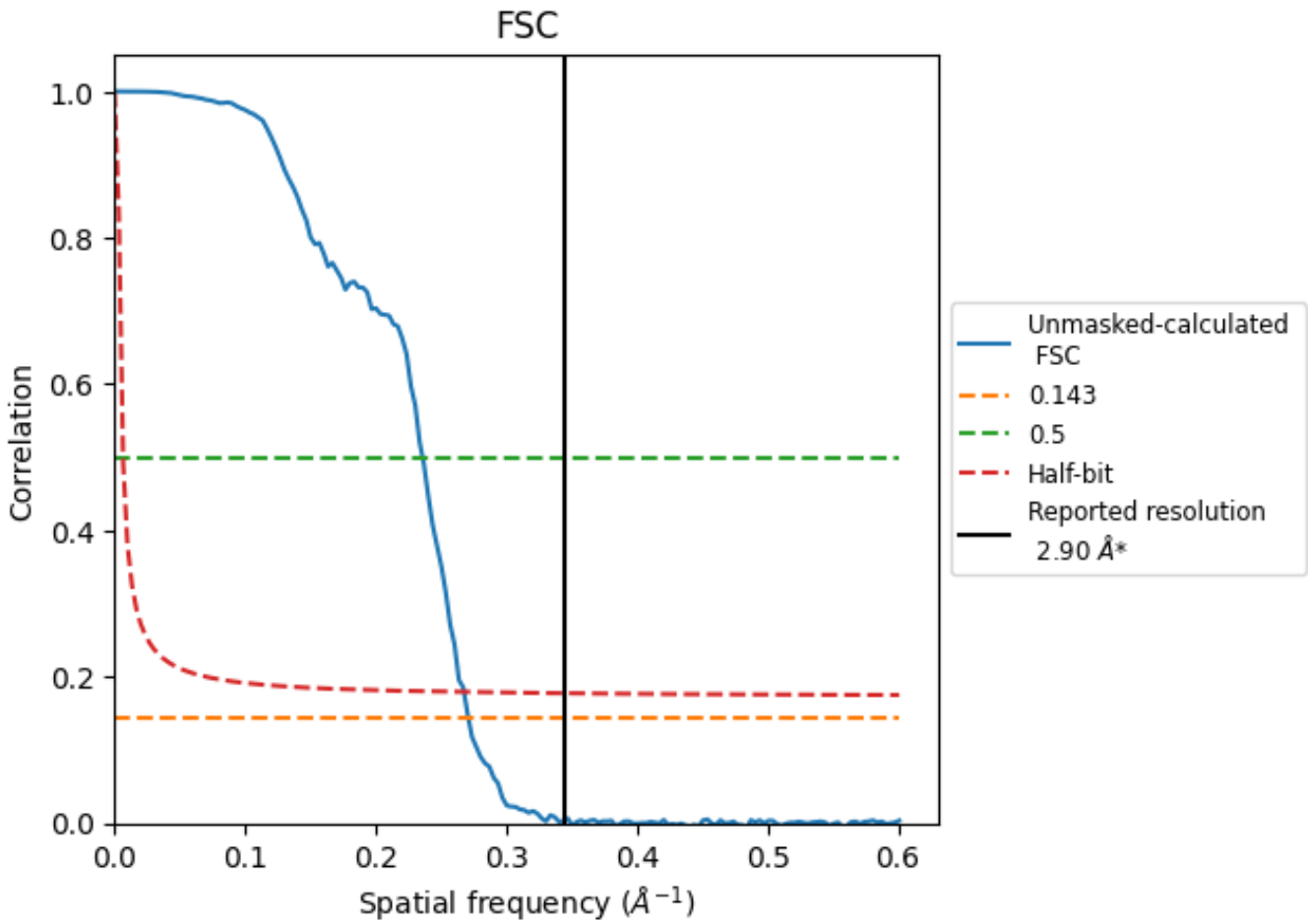


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

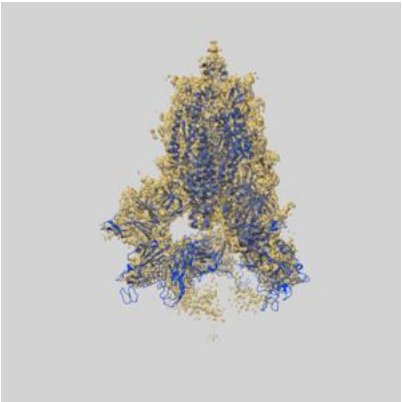
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.24	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.69 differs from the reported value 2.9 by more than 10 %

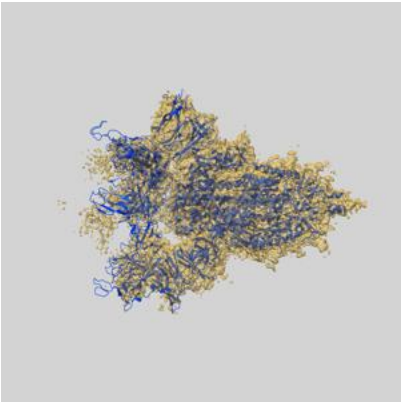
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26881 and PDB model 7UZ7. Per-residue inclusion information can be found in section 3 on page 12.

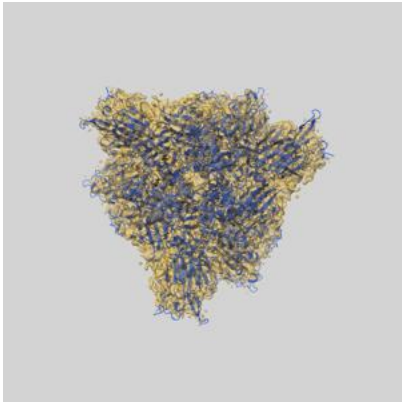
9.1 Map-model overlay (i)



X



Y



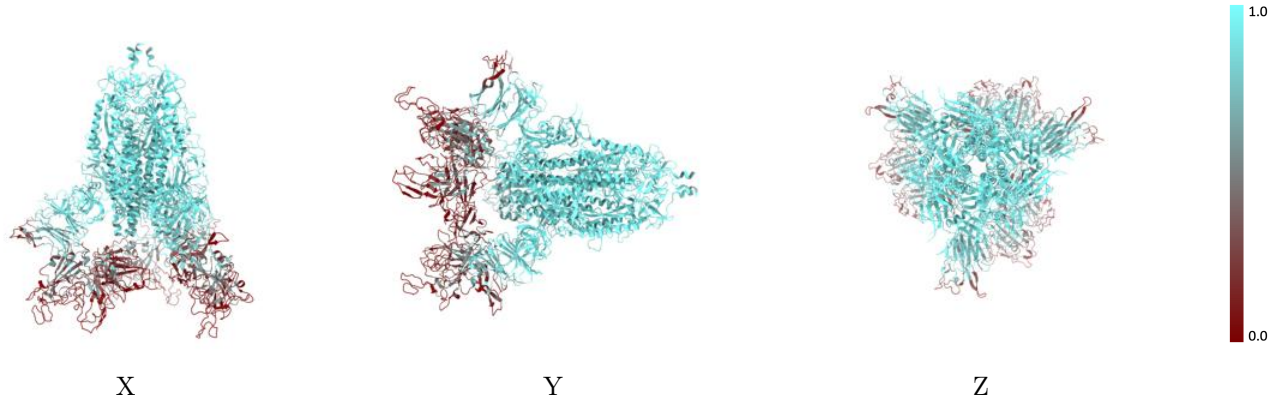
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

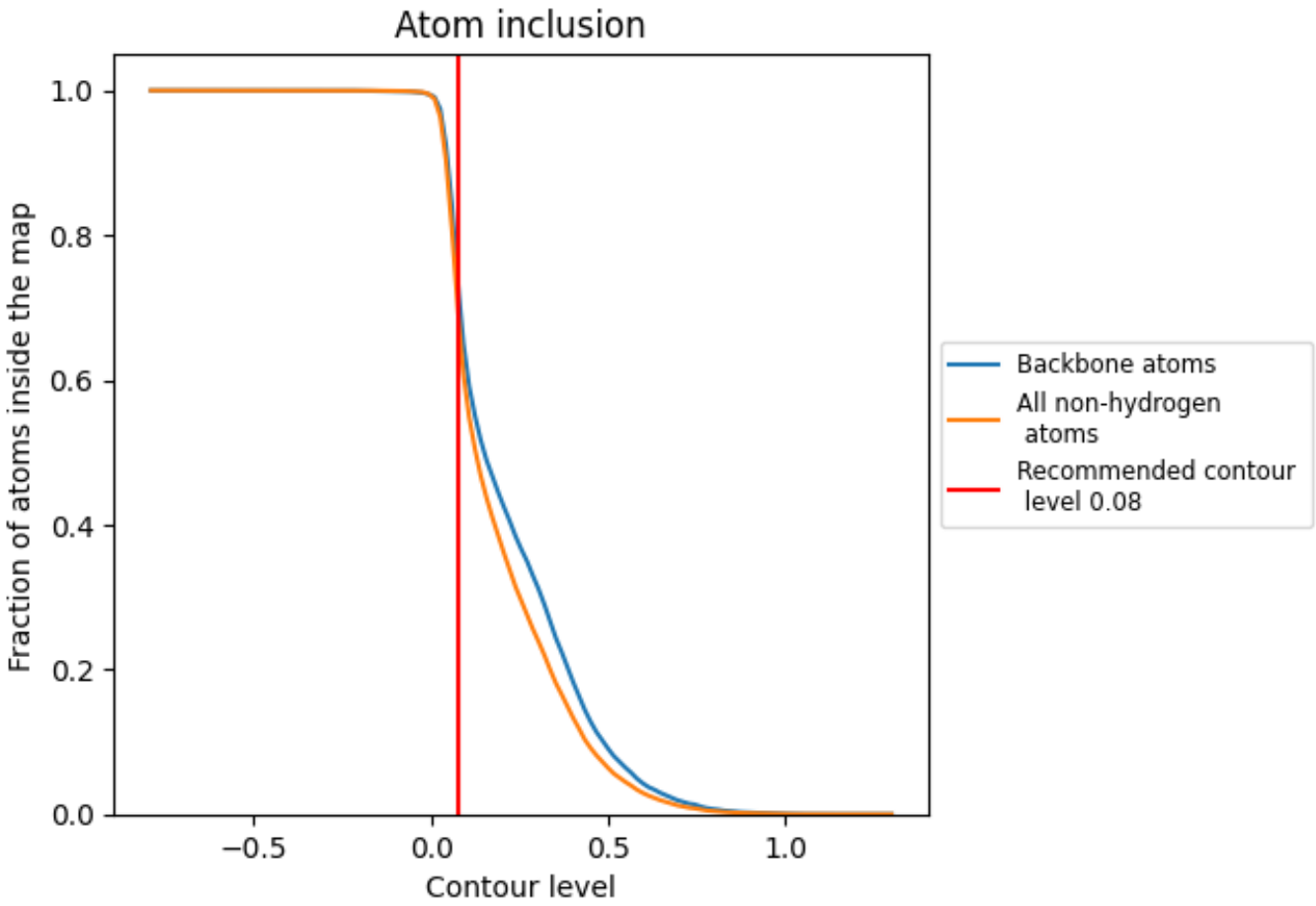
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6758	0.3600
A	0.7682	0.4190
B	0.7665	0.4180
C	0.7744	0.4200
D	0.8571	0.5180
E	0.8571	0.5030
F	0.8571	0.4990
H	0.2189	0.0680
L	0.2280	0.0890
M	0.2155	0.0690
N	0.2280	0.0900
P	0.2189	0.0650
Q	0.2303	0.0940