Full wwPDB EM Validation Report

Oct 6, 2024 – 06:10 AM JST

PDB ID	:	7V85
EMDB ID	:	EMD-31790
Title	:	Cryo-EM structure of SARS-CoV-2 S-Kappa variant (B.1.617.1) in complex with Angiotensin-converting enzyme 2 (ACE2) ectodomain, two ACE2-bound form
Authors	:	Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Hsu, S.T.D.
Deposited on	:	2021-08-22
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

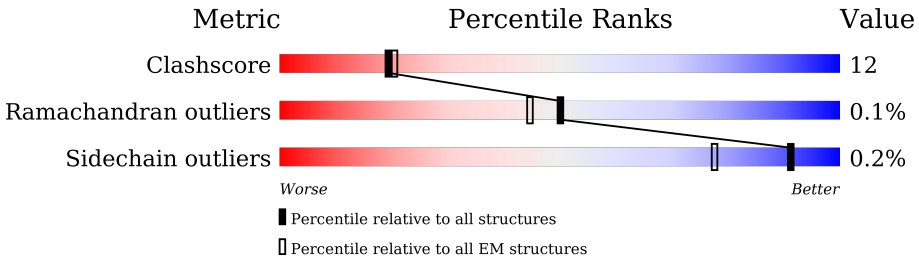
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1283	58% 22% 19%
1	B	1283	58% 23% 19%
1	C	1283	60% 20% 19%
2	F	861	46% 48% 22% 31%
2	H	861	36% 48% 21% 31%
3	D	2	50% 50%
3	E	2	50% 50%
3	G	2	100%

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Mol	Chain	Length	Quality of chain
3	I	2	100%
3	J	2	100%
3	K	2	100%
3	L	2	100%
3	M	2	100%
3	N	2	50% 50%
3	O	2	100%
3	P	2	100%
3	Q	2	50% 50%
3	R	2	50% 100%
3	S	2	100%
3	T	2	100%
3	U	2	100%
3	V	2	100%
3	W	2	100%
3	X	2	100%
3	Y	2	50% 50%
3	Z	2	100%
3	a	2	100%
3	b	2	100%
3	c	2	100%
3	d	2	100%
3	e	2	100%
3	f	2	100%
3	g	2	100%

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Mol	Chain	Length	Quality of chain
3	h	2	100%
3	i	2	100%
3	j	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	B	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	C	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		

There are 261 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASP	GLY	variant	UNP P0DTC2
A	154	LYS	GLU	engineered mutation	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	484	GLN	GLU	engineered mutation	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1071	HIS	GLN	engineered mutation	UNP P0DTC2
A	1101	ASP	HIS	engineered mutation	UNP P0DTC2
A	1209	GLU	-	expression tag	UNP P0DTC2
A	1210	PHE	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	ASP	-	expression tag	UNP P0DTC2
A	1245	ASN	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	ALA	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ILE	-	expression tag	UNP P0DTC2
A	1250	GLN	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	SER	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	ARG	-	expression tag	UNP P0DTC2
A	1255	PRO	-	expression tag	UNP P0DTC2
A	1256	LEU	-	expression tag	UNP P0DTC2
A	1257	GLU	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ARG	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	PRO	-	expression tag	UNP P0DTC2
A	1262	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	LEU	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLU	-	expression tag	UNP P0DTC2
A	1270	GLU	-	expression tag	UNP P0DTC2
A	1271	ASP	-	expression tag	UNP P0DTC2
A	1272	LEU	-	expression tag	UNP P0DTC2
A	1273	ASN	-	expression tag	UNP P0DTC2
A	1274	MET	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	THR	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	154	LYS	GLU	engineered mutation	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	484	GLN	GLU	engineered mutation	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1071	HIS	GLN	engineered mutation	UNP P0DTC2
B	1101	ASP	HIS	engineered mutation	UNP P0DTC2
B	1209	GLU	-	expression tag	UNP P0DTC2
B	1210	PHE	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	GLY	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	ASP	-	expression tag	UNP P0DTC2
B	1245	ASN	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	ALA	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ILE	-	expression tag	UNP P0DTC2
B	1250	GLN	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	SER	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	ARG	-	expression tag	UNP P0DTC2
B	1255	PRO	-	expression tag	UNP P0DTC2
B	1256	LEU	-	expression tag	UNP P0DTC2
B	1257	GLU	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	PRO	-	expression tag	UNP P0DTC2
B	1262	PHE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	LEU	-	expression tag	UNP P0DTC2
B	1267	ILE	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLU	-	expression tag	UNP P0DTC2
B	1270	GLU	-	expression tag	UNP P0DTC2
B	1271	ASP	-	expression tag	UNP P0DTC2
B	1272	LEU	-	expression tag	UNP P0DTC2
B	1273	ASN	-	expression tag	UNP P0DTC2
B	1274	MET	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	THR	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	HIS	-	expression tag	UNP P0DTC2
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	154	LYS	GLU	engineered mutation	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	484	GLN	GLU	engineered mutation	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1071	HIS	GLN	engineered mutation	UNP P0DTC2
C	1101	ASP	HIS	engineered mutation	UNP P0DTC2
C	1209	GLU	-	expression tag	UNP P0DTC2
C	1210	PHE	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	ASP	-	expression tag	UNP P0DTC2
C	1245	ASN	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	ALA	-	expression tag	UNP P0DTC2
C	1248	ASP	-	expression tag	UNP P0DTC2
C	1249	ILE	-	expression tag	UNP P0DTC2
C	1250	GLN	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	SER	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	ARG	-	expression tag	UNP P0DTC2
C	1255	PRO	-	expression tag	UNP P0DTC2
C	1256	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1257	GLU	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ARG	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	PRO	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	LEU	-	expression tag	UNP P0DTC2
C	1267	ILE	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLU	-	expression tag	UNP P0DTC2
C	1270	GLU	-	expression tag	UNP P0DTC2
C	1271	ASP	-	expression tag	UNP P0DTC2
C	1272	LEU	-	expression tag	UNP P0DTC2
C	1273	ASN	-	expression tag	UNP P0DTC2
C	1274	MET	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	THR	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	HIS	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2,Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	H	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		

- Molecule 3 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
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		

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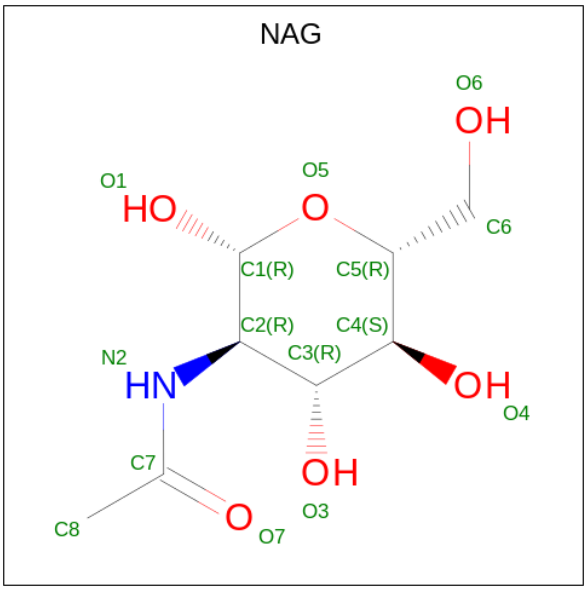
Mol	Chain	Residues	Atoms	AltConf	Trace
3	b	2	Total C N O 28 16 2 10	0	0
3	c	2	Total C N O 28 16 2 10	0	0
3	d	2	Total C N O 28 16 2 10	0	0
3	e	2	Total C N O 28 16 2 10	0	0
3	f	2	Total C N O 28 16 2 10	0	0
3	g	2	Total C N O 28 16 2 10	0	0
3	h	2	Total C N O 28 16 2 10	0	0
3	i	2	Total C N O 28 16 2 10	0	0
3	j	2	Total C N O 28 16 2 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

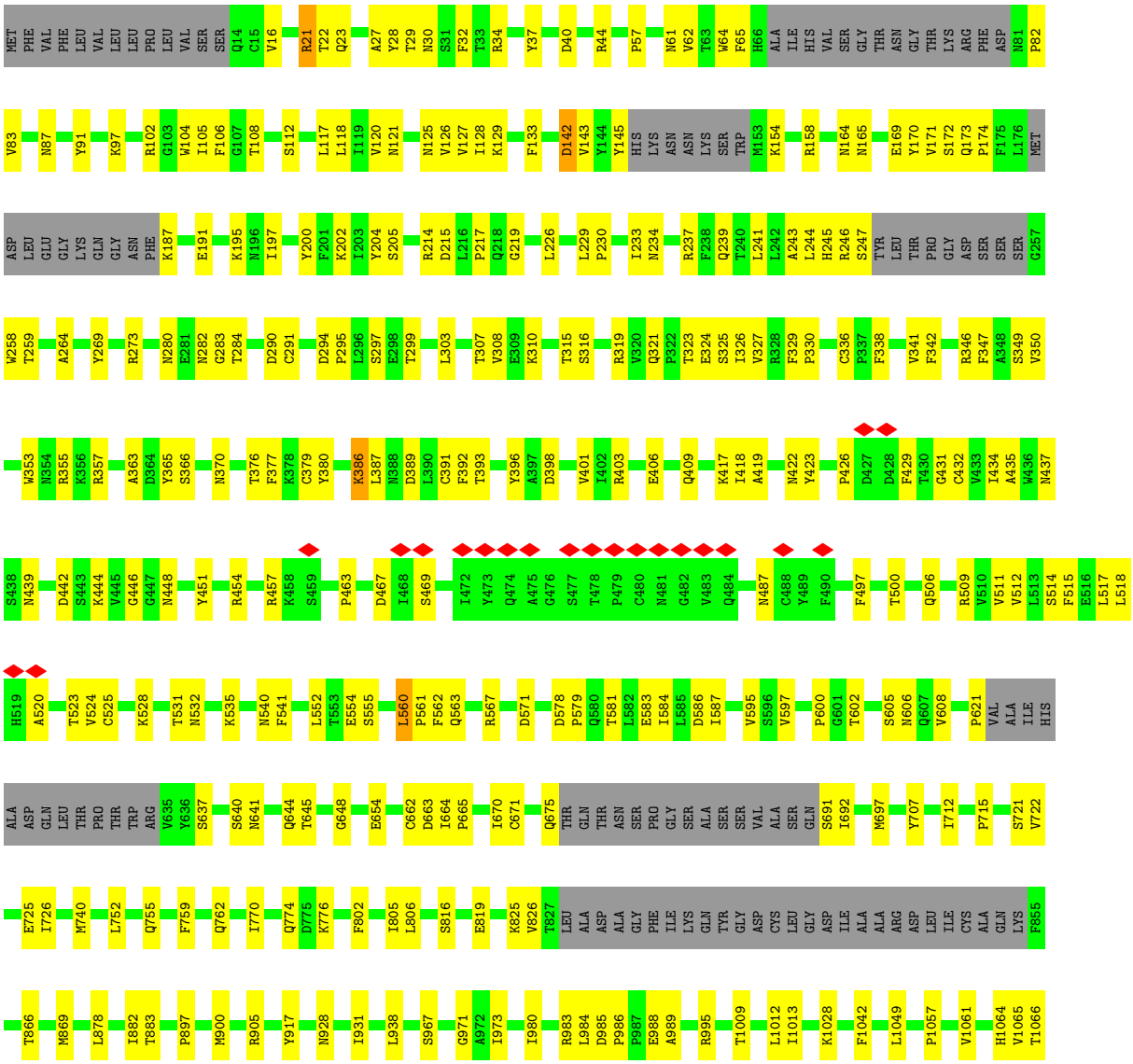
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4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

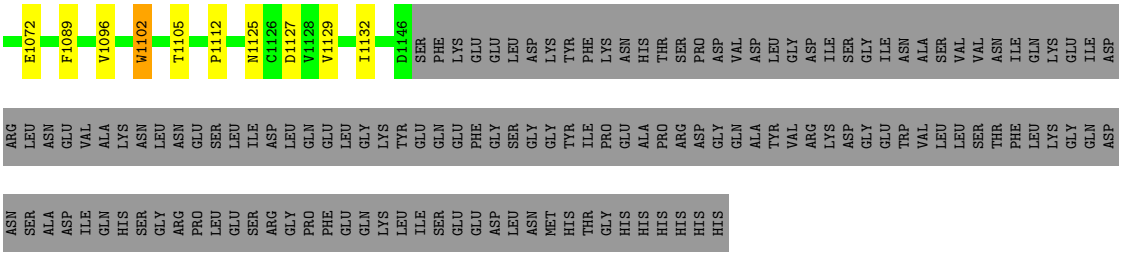
3 Residue-property plots (i)

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

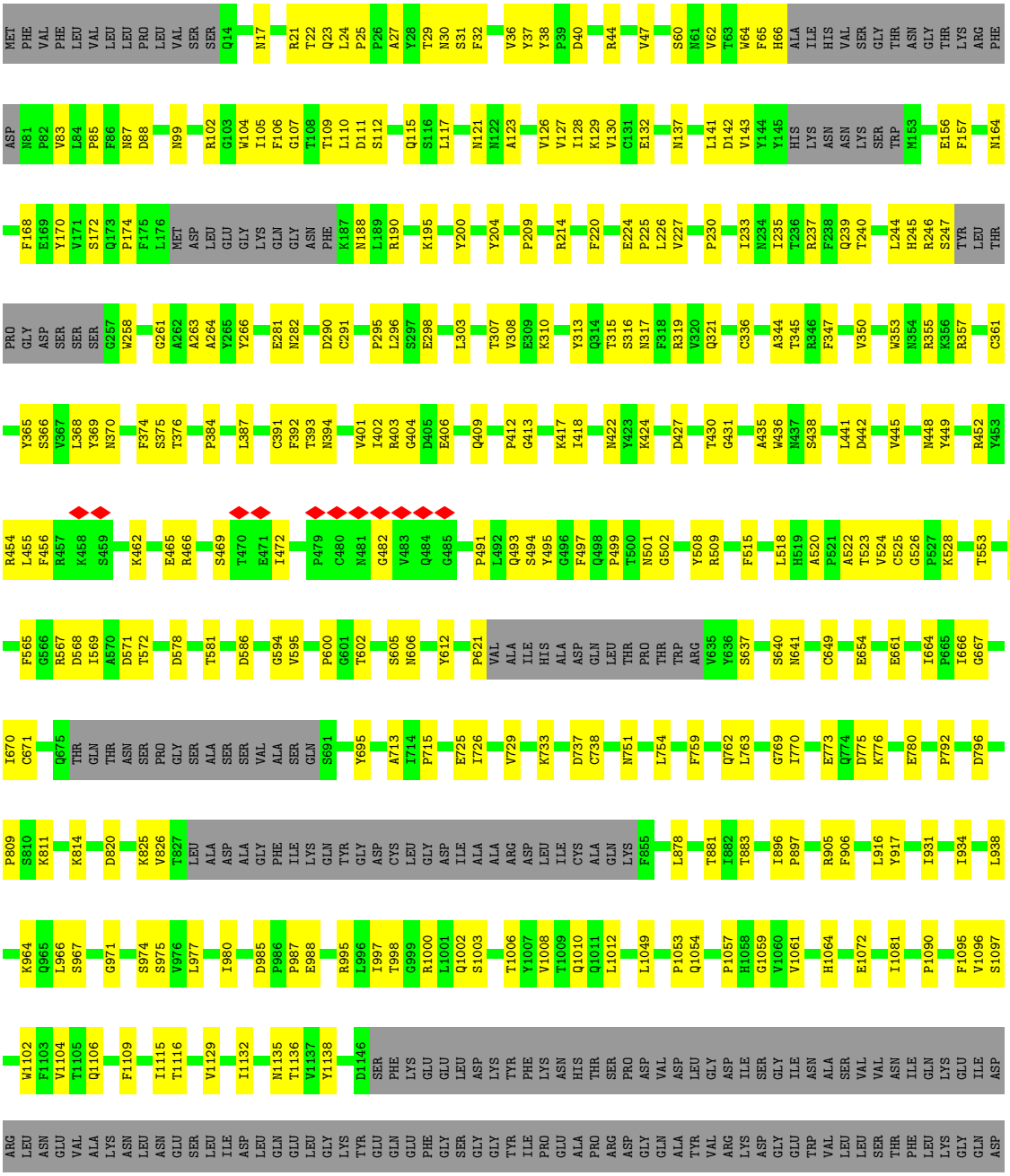
Chain A:

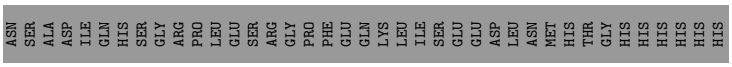




• Molecule 1: Spike glycoprotein

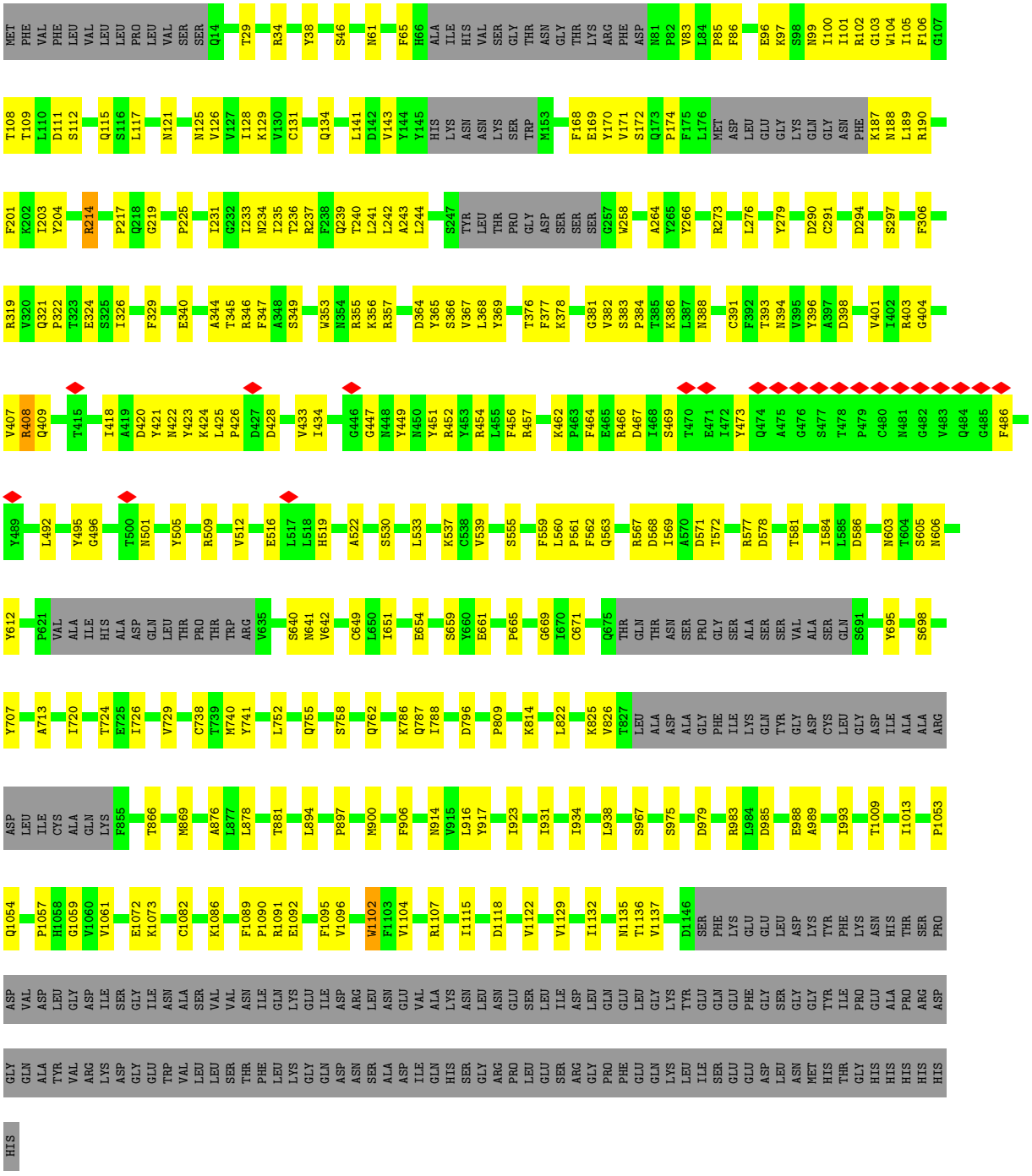
Chain B:





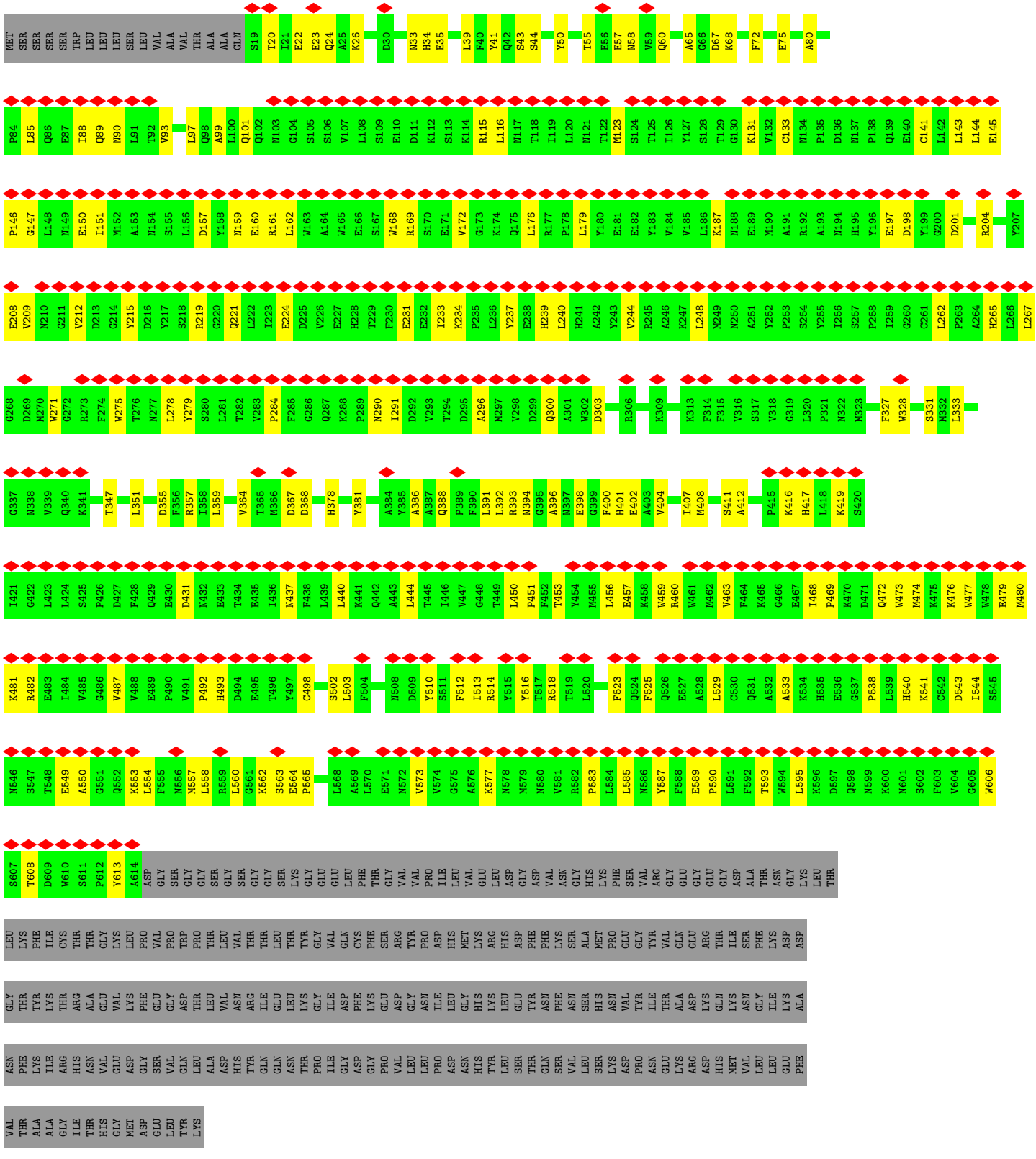
• Molecule 1: Spike glycoprotein

Chain C:



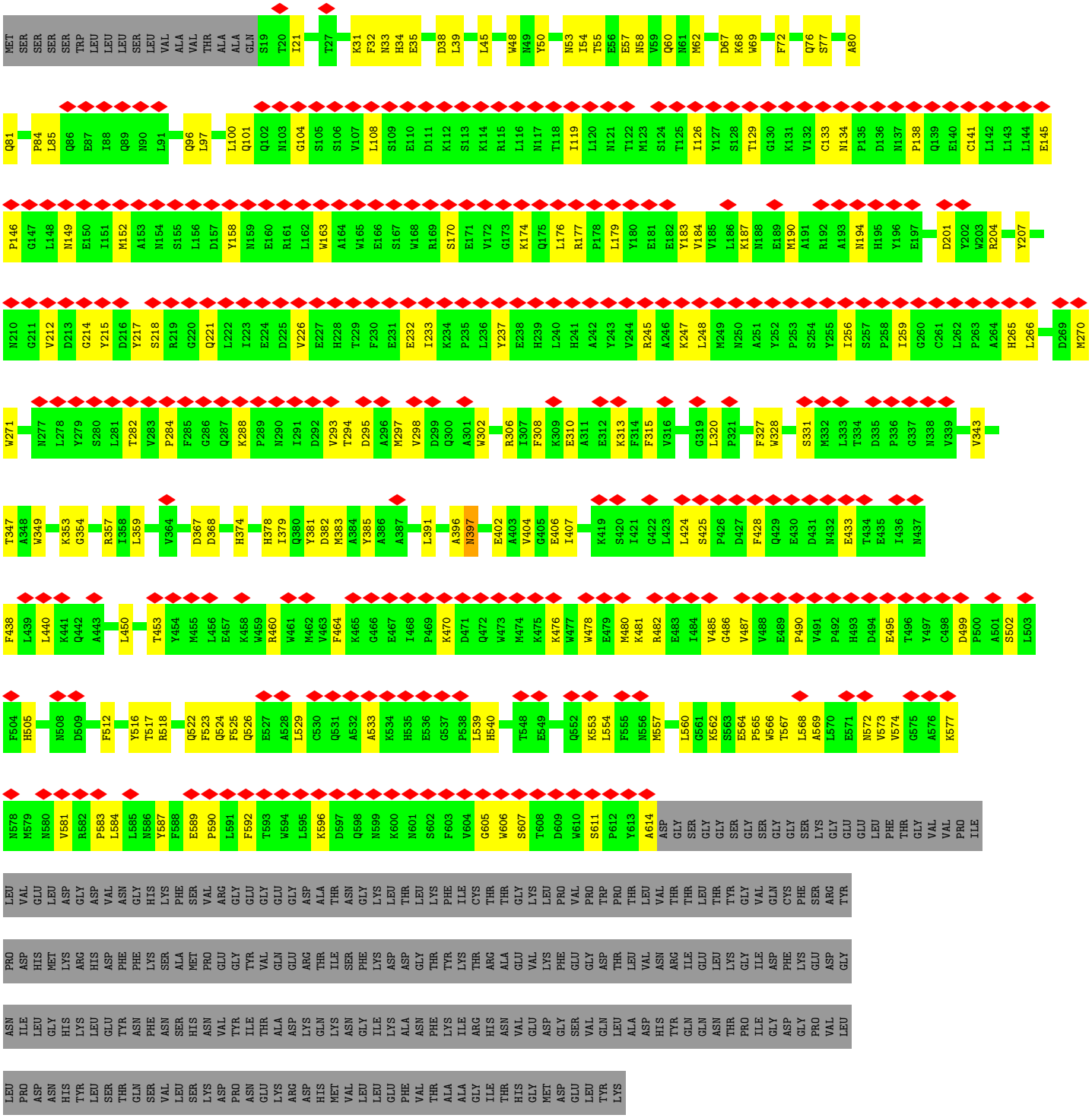
• Molecule 2: Angiotensin-converting enzyme 2,Green fluorescent protein

Chain F:



• Molecule 2: Angiotensin-converting enzyme 2,Green fluorescent protein

Chain H:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

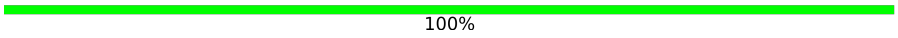
Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

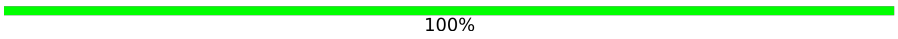
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



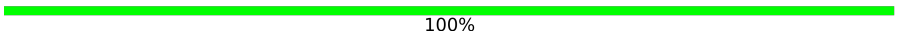
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



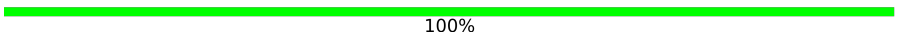
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



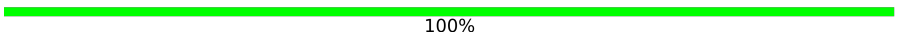
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



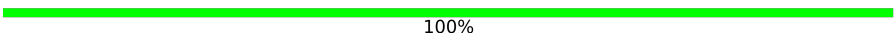
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

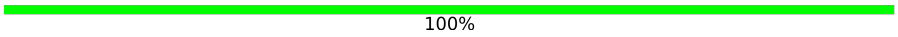


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

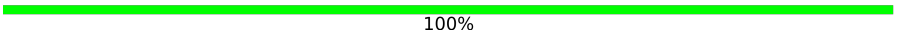
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

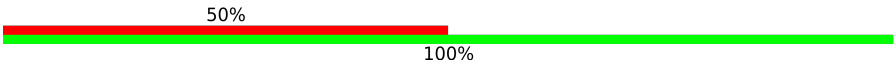


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

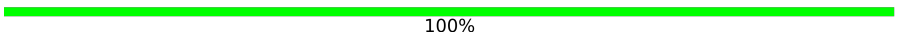
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



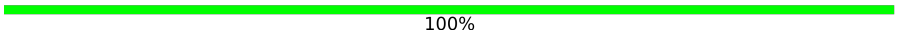
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



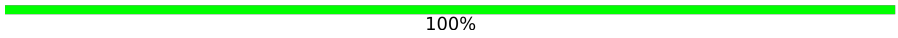
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



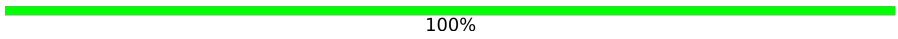
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



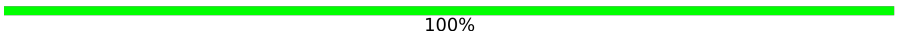
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



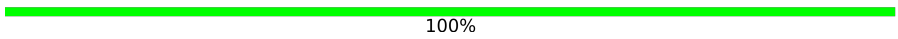
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

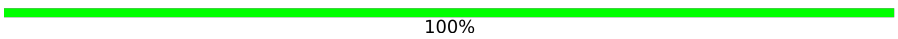


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

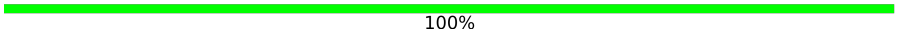
Chain Y:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

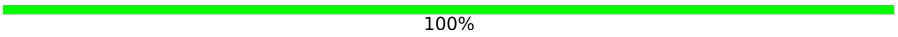
Chain Z:



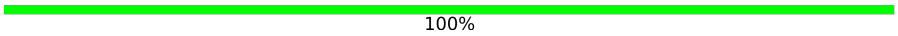
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

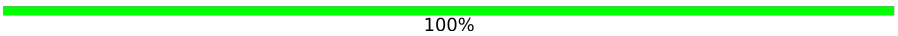
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

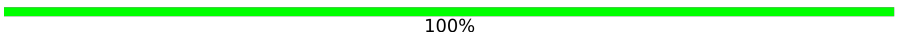
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

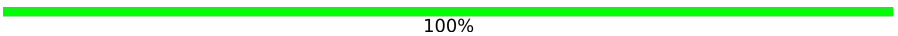
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

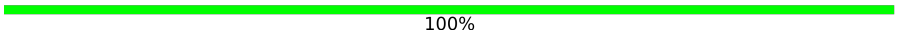
Chain e: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 

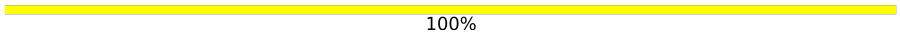
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



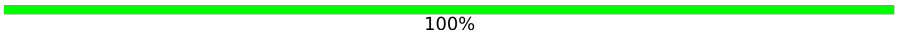
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



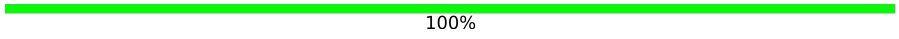
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66721	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 ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.614	Depositor
Minimum map value	-0.681	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/8295	0.52	1/11291 (0.0%)
1	B	0.33	0/8295	0.51	0/11291
1	C	0.33	0/8295	0.50	0/11291
2	F	0.24	0/4999	0.46	0/6792
2	H	0.24	0/4999	0.45	0/6792
All	All	0.31	0/34883	0.49	1/47457 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	560	LEU	CA-CB-CG	6.11	129.35	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8109	0	7900	223	0
1	B	8109	0	7900	200	0
1	C	8109	0	7903	194	0
2	F	4862	0	4639	140	0
2	H	4862	0	4639	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	25	1	0
3	E	28	0	25	1	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
3	i	28	0	25	0	0
3	j	28	0	25	0	0
4	A	56	0	52	3	0
4	B	56	0	52	1	0
4	C	70	0	65	3	0
All	All	35101	0	33925	858	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 12.

All (858) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.55	0.89
2:F:529:LEU:O	2:F:533:ALA:HB2	1.72	0.89
1:A:27:ALA:HB3	1:A:64:TRP:O	1.76	0.84
1:A:315:THR:HG22	1:A:316:SER:H	1.43	0.83
1:B:245:HIS:HE2	1:B:247:SER:HG	1.24	0.83
1:A:28:TYR:HB3	1:A:61:ASN:HD21	1.45	0.81
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.62	0.81
1:B:315:THR:HG22	1:B:316:SER:H	1.46	0.81
1:A:984:LEU:HD21	1:A:988:GLU:HG2	1.64	0.79
1:B:725:GLU:OE2	1:B:1064:HIS:NE2	2.11	0.79
1:A:34:ARG:HH22	1:A:219:GLY:H	1.28	0.78
1:B:518:LEU:HD12	1:B:520:ALA:H	1.47	0.78
1:A:205:SER:H	1:A:226:LEU:HD23	1.49	0.78
2:H:248:LEU:HB3	2:H:256:ILE:HG13	1.65	0.77
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.67	0.76
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.68	0.76
1:B:412:PRO:HB3	1:B:427:ASP:HA	1.68	0.76
1:C:34:ARG:HH22	1:C:219:GLY:H	1.32	0.75
1:C:346:ARG:NH2	1:C:451:TYR:OH	2.20	0.74
1:B:99:ASN:O	1:B:102:ARG:NH2	2.21	0.74
1:C:65:PHE:O	1:C:264:ALA:HA	1.88	0.73
1:C:452:ARG:HG2	1:C:492:LEU:HB3	1.70	0.72
2:F:209:VAL:HG11	2:F:565:PRO:HB3	1.70	0.72
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.71	0.71
2:H:560:LEU:HD13	2:H:564:GLU:HG3	1.71	0.71
1:A:560:LEU:HD12	1:A:561:PRO:HD2	1.72	0.71
1:A:826:VAL:HG11	1:A:1057:PRO:HG2	1.72	0.70
1:A:740:MET:SD	1:C:319:ARG:NH1	2.64	0.70
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.72	0.70
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.71	0.70
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.73	0.70
2:H:80:ALA:HB1	2:H:101:GLN:HG2	1.72	0.70
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.73	0.70
2:F:474:MET:HE2	2:F:498:CYS:HA	1.73	0.70
1:B:393:THR:HB	1:B:522:ALA:HA	1.73	0.70
1:C:454:ARG:NH2	1:C:469:SER:O	2.25	0.70
1:A:403:ARG:HB3	1:A:406:GLU:HG3	1.75	0.69
1:A:125:ASN:HA	1:A:174:PRO:HD3	1.75	0.69
1:A:346:ARG:NH1	1:A:442:ASP:OD1	2.24	0.69
1:A:518:LEU:HD12	1:A:520:ALA:H	1.57	0.69
1:C:355:ARG:HH22	1:C:464:PHE:HE1	1.41	0.69
2:H:476:LYS:NZ	2:H:480:MET:SD	2.65	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:GLU:OE2	1:A:1064:HIS:NE2	2.23	0.69
1:B:344:ALA:O	1:B:509:ARG:NH1	2.22	0.68
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.24	0.68
1:A:442:ASP:O	1:A:448:ASN:ND2	2.26	0.68
1:A:108:THR:O	1:A:237:ARG:NH1	2.26	0.68
1:C:809:PRO:O	1:C:814:LYS:NZ	2.26	0.68
1:C:560:LEU:HD23	1:C:562:PHE:HE1	1.59	0.68
1:A:65:PHE:O	1:A:264:ALA:HA	1.95	0.67
1:B:214:ARG:NH1	1:B:266:TYR:OH	2.27	0.67
1:B:565:PHE:HE2	1:B:567:ARG:HH21	1.42	0.67
1:C:724:THR:HG23	1:C:934:ILE:HD11	1.75	0.67
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.76	0.67
1:A:645:THR:HG21	1:A:670:ILE:HD13	1.77	0.66
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.77	0.66
1:A:280:ASN:OD1	1:A:284:THR:N	2.20	0.66
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.77	0.66
1:C:34:ARG:HH21	1:C:217:PRO:HG2	1.60	0.66
2:F:479:GLU:HA	2:F:482:ARG:HD3	1.78	0.66
2:H:482:ARG:HH22	2:H:611:SER:HB2	1.59	0.66
1:B:345:THR:O	1:B:509:ARG:NH2	2.29	0.65
2:F:402:GLU:OE1	2:F:518:ARG:NH1	2.29	0.65
2:H:271:TRP:NE1	2:H:502:SER:O	2.27	0.65
1:A:878:LEU:O	1:A:882:ILE:HG12	1.96	0.65
1:B:170:TYR:HE1	1:B:172:SER:HB2	1.60	0.65
2:F:231:GLU:O	2:F:234:LYS:NZ	2.29	0.65
2:F:553:LYS:HG2	2:F:573:VAL:HG22	1.77	0.65
2:F:407:ILE:HD11	2:F:525:PHE:HD2	1.61	0.65
1:B:132:GLU:HB2	1:B:164:ASN:HB2	1.79	0.65
2:F:85:LEU:HD13	2:F:97:LEU:HD23	1.78	0.65
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.29	0.65
1:B:438:SER:HB3	1:B:441:LEU:HB2	1.78	0.65
1:B:568:ASP:OD1	1:B:572:THR:OG1	2.14	0.65
1:B:641:ASN:HD21	1:B:654:GLU:HG3	1.60	0.65
1:C:117:LEU:HD13	1:C:235:ILE:HD11	1.79	0.65
1:B:25:PRO:HD2	1:B:66:HIS:HB3	1.79	0.64
1:C:349:SER:OG	1:C:452:ARG:O	2.14	0.64
2:F:523:PHE:HB3	2:F:583:PRO:HB2	1.78	0.64
2:F:408:MET:HA	2:F:411:SER:HB3	1.79	0.64
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.78	0.64
1:B:809:PRO:O	1:B:814:LYS:NZ	2.28	0.64
1:B:1129:VAL:HB	1:B:1132:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:THR:O	1:C:509:ARG:NH2	2.30	0.64
2:H:404:VAL:HA	2:H:407:ILE:HD12	1.79	0.64
2:H:402:GLU:HB3	2:H:518:ARG:HH11	1.63	0.64
2:H:53:ASN:O	2:H:58:ASN:ND2	2.31	0.64
1:A:971:GLY:O	1:A:995:ARG:NH2	2.30	0.63
2:H:215:TYR:O	2:H:567:THR:OG1	2.14	0.63
2:H:284:PRO:HG3	2:H:440:LEU:HD13	1.80	0.63
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.79	0.63
1:C:1104:VAL:HG13	1:C:1115:ILE:HG12	1.80	0.63
1:C:106:PHE:HD2	1:C:235:ILE:HG21	1.63	0.63
2:H:564:GLU:HB3	2:H:568:LEU:HD22	1.79	0.63
2:F:147:GLY:H	2:F:150:GLU:HB3	1.60	0.63
1:C:34:ARG:NH1	1:C:219:GLY:O	2.29	0.63
2:F:529:LEU:O	2:F:533:ALA:CB	2.47	0.63
1:B:826:VAL:HG11	1:B:1057:PRO:HG2	1.80	0.62
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.17	0.62
1:B:123:ALA:HB3	4:B:2002:NAG:H82	1.79	0.62
2:F:161:ARG:NH1	2:F:265:HIS:O	2.33	0.62
1:A:143:VAL:HG23	1:A:154:LYS:HB3	1.81	0.62
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.80	0.62
1:C:433:VAL:HG23	1:C:512:VAL:HG12	1.82	0.62
1:B:246:ARG:HH12	1:B:258:TRP:HE3	1.45	0.62
1:C:99:ASN:O	1:C:102:ARG:NH2	2.31	0.62
2:H:396:ALA:HA	2:H:562:LYS:HG3	1.81	0.62
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.82	0.62
1:C:369:TYR:HE2	1:C:384:PRO:HB2	1.63	0.62
2:F:248:LEU:HD11	2:F:278:LEU:HD21	1.80	0.62
2:H:237:TYR:OH	2:H:485:VAL:O	2.16	0.62
1:A:1125:ASN:ND2	1:A:1127:ASP:OD2	2.32	0.62
1:A:662:CYS:HB2	1:A:697:MET:HG3	1.82	0.61
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.64	0.61
1:A:34:ARG:NH1	1:A:219:GLY:O	2.33	0.61
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.82	0.61
2:H:96:GLN:HB3	2:H:391:LEU:HD13	1.82	0.61
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.24	0.61
2:H:553:LYS:NZ	2:H:572:ASN:O	2.33	0.61
1:A:319:ARG:NH2	1:B:737:ASP:OD2	2.34	0.61
1:B:501:ASN:ND2	2:H:353:LYS:O	2.34	0.61
2:F:201:ASP:OD1	2:F:204:ARG:NH2	2.31	0.61
1:A:555:SER:OG	1:A:584:ILE:O	2.15	0.60
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:ARG:HG3	1:C:382:VAL:HG13	1.83	0.60
1:B:393:THR:HA	1:B:523:THR:HG22	1.84	0.60
1:C:61:ASN:HB3	4:C:2001:NAG:HN2	1.65	0.60
1:C:86:PHE:N	1:C:236:THR:O	2.31	0.60
2:H:407:ILE:HD11	2:H:525:PHE:HD2	1.67	0.60
1:B:971:GLY:O	1:B:995:ARG:NH1	2.35	0.60
2:H:201:ASP:OD1	2:H:204:ARG:NH2	2.31	0.60
2:H:481:LYS:HG2	2:H:487:VAL:HB	1.82	0.60
2:H:529:LEU:O	2:H:533:ALA:HB2	2.02	0.60
1:A:319:ARG:O	1:A:321:GLN:NE2	2.31	0.60
1:A:560:LEU:HB3	1:A:563:GLN:OE1	2.01	0.60
1:B:452:ARG:HH11	1:B:494:SER:HB2	1.66	0.60
1:C:421:TYR:HD1	1:C:457:ARG:HB2	1.66	0.60
1:C:989:ALA:O	1:C:993:ILE:HG12	2.01	0.60
2:F:468:ILE:HG21	2:F:476:LYS:HE2	1.83	0.60
1:B:776:LYS:NZ	1:B:780:GLU:OE1	2.35	0.60
2:H:232:GLU:HB2	2:H:581:VAL:HG11	1.84	0.60
2:H:381:TYR:HB2	2:H:404:VAL:HG11	1.84	0.60
1:A:409:GLN:HB3	1:A:419:ALA:HB2	1.83	0.60
1:A:454:ARG:NH2	1:A:469:SER:O	2.35	0.60
1:A:1096:VAL:O	1:A:1102:TRP:HA	2.02	0.59
1:B:392:PHE:O	1:B:523:THR:N	2.33	0.59
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.35	0.59
2:F:85:LEU:HD12	2:F:88:ILE:HD13	1.83	0.59
1:C:641:ASN:HD21	1:C:654:GLU:HG3	1.67	0.59
2:H:214:GLY:O	2:H:577:LYS:NZ	2.35	0.59
1:C:105:ILE:HG12	1:C:241:LEU:HD21	1.84	0.59
2:H:367:ASP:OD1	2:H:368:ASP:N	2.35	0.59
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.27	0.59
2:H:460:ARG:NH2	2:H:505:HIS:O	2.35	0.59
1:C:516:GLU:OE1	1:C:519:HIS:N	2.35	0.59
2:H:378:HIS:HE1	2:H:402:GLU:HA	1.68	0.59
1:C:106:PHE:HB3	1:C:235:ILE:HD12	1.84	0.59
1:A:640:SER:OG	1:A:641:ASN:OD1	2.20	0.59
1:C:357:ARG:NH1	1:C:396:TYR:OH	2.36	0.59
2:F:239:HIS:CD2	2:F:595:LEU:HB3	2.36	0.59
1:C:567:ARG:NH1	1:C:571:ASP:OD1	2.36	0.59
1:B:115:GLN:HA	1:B:132:GLU:HG2	1.85	0.58
2:F:208:GLU:OE2	2:F:219:ARG:NH1	2.36	0.58
1:B:1096:VAL:O	1:B:1102:TRP:HA	2.04	0.58
1:C:290:ASP:OD1	1:C:291:CYS:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:412:ALA:O	2:F:417:HIS:ND1	2.36	0.58
1:A:29:THR:OG1	1:A:215:ASP:OD2	2.21	0.58
1:A:245:HIS:HB3	1:A:259:THR:HB	1.86	0.58
1:C:340:GLU:OE1	1:C:356:LYS:NZ	2.36	0.58
1:B:375:SER:HB3	1:B:436:TRP:HA	1.85	0.58
1:A:429:PHE:CE2	1:A:431:GLY:HA3	2.39	0.58
2:H:177:ARG:NH2	2:H:470:LYS:O	2.37	0.58
1:B:553:THR:OG1	1:B:586:ASP:OD1	2.18	0.58
1:C:401:VAL:HG22	1:C:509:ARG:HD3	1.85	0.58
2:H:397:ASN:C	2:H:397:ASN:HD22	2.07	0.58
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.39	0.57
1:C:353:TRP:O	1:C:466:ARG:NH1	2.36	0.57
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.34	0.57
2:H:58:ASN:O	2:H:62:MET:HE2	2.04	0.57
1:C:418:ILE:HG23	1:C:422:ASN:HD22	1.68	0.57
1:A:87:ASN:HB2	1:A:269:TYR:HD2	1.69	0.57
1:A:245:HIS:NE2	1:A:247:SER:OG	2.35	0.57
1:A:567:ARG:NH2	1:A:571:ASP:OD1	2.37	0.57
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.23	0.57
2:F:176:LEU:HD13	2:F:179:LEU:HD12	1.86	0.57
2:H:77:SER:O	2:H:81:GLN:NE2	2.33	0.57
2:H:382:ASP:OD1	2:H:385:TYR:OH	2.21	0.57
1:B:303:LEU:HD12	1:B:308:VAL:HG23	1.85	0.57
1:A:825:LYS:NZ	1:A:938:LEU:O	2.38	0.57
2:F:378:HIS:HE1	2:F:402:GLU:HA	1.70	0.57
2:H:294:THR:HA	2:H:297:MET:HG3	1.87	0.57
1:A:621:PRO:HB3	1:A:637:SER:HB2	1.86	0.57
1:C:1115:ILE:HG22	1:C:1137:VAL:HG23	1.86	0.57
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.35	0.56
1:C:29:THR:O	1:C:61:ASN:HA	2.05	0.56
1:B:121:ASN:HA	1:B:126:VAL:HG12	1.86	0.56
1:B:737:ASP:OD1	1:B:738:CYS:N	2.39	0.56
1:C:661:GLU:O	1:C:695:TYR:OH	2.14	0.56
2:H:379:ILE:O	2:H:383:MET:HG2	2.05	0.56
1:B:21:ARG:NH1	1:B:23:GLN:OE1	2.39	0.56
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.87	0.56
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.71	0.56
1:C:496:GLY:O	1:C:501:ASN:ND2	2.33	0.56
1:B:168:PHE:HE1	1:B:170:TYR:HB2	1.70	0.56
1:A:983:ARG:NH1	1:C:381:GLY:O	2.39	0.56
2:H:184:VAL:HG22	2:H:464:PHE:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:457:GLU:HG2	2:F:513:ILE:HD13	1.87	0.56
2:H:55:THR:HG23	2:H:58:ASN:H	1.70	0.56
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.88	0.56
2:F:271:TRP:NE1	2:F:502:SER:O	2.34	0.56
2:H:177:ARG:HH12	2:H:495:GLU:HG3	1.70	0.56
1:A:316:SER:O	1:A:595:VAL:HG22	2.06	0.56
1:C:97:LYS:HE3	1:C:187:LYS:N	2.21	0.56
1:C:640:SER:OG	1:C:641:ASN:N	2.39	0.56
1:B:493:GLN:OE1	2:H:31:LYS:NZ	2.34	0.55
1:A:83:VAL:HG11	1:A:237:ARG:HH21	1.70	0.55
1:A:105:ILE:HD11	1:A:241:LEU:HG	1.88	0.55
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.39	0.55
1:B:825:LYS:NZ	1:B:938:LEU:O	2.39	0.55
1:C:108:THR:O	1:C:237:ARG:NH1	2.39	0.55
1:C:568:ASP:OD1	1:C:569:ILE:N	2.39	0.55
1:C:568:ASP:OD1	1:C:572:THR:OG1	2.24	0.55
1:C:826:VAL:HG11	1:C:1057:PRO:HG2	1.88	0.55
3:D:2:NAG:H3	3:D:2:NAG:H83	1.88	0.55
1:C:560:LEU:HG	1:C:561:PRO:HD2	1.87	0.55
1:C:640:SER:OG	1:C:641:ASN:OD1	2.23	0.55
2:H:21:ILE:HG21	2:H:84:PRO:HD2	1.87	0.55
1:C:96:GLU:O	1:C:190:ARG:NH1	2.39	0.55
1:A:164:ASN:HB2	3:E:1:NAG:H82	1.87	0.55
1:A:392:PHE:HD1	1:A:517:LEU:HD13	1.70	0.55
1:C:104:TRP:HB3	1:C:106:PHE:HE1	1.71	0.55
1:B:336:CYS:HA	1:B:361:CYS:HB2	1.88	0.55
1:B:567:ARG:NH1	1:B:571:ASP:OD2	2.40	0.55
2:H:54:ILE:HD11	2:H:343:VAL:H	1.71	0.55
4:A:2004:NAG:H83	4:A:2004:NAG:H3	1.89	0.55
2:F:44:SER:HB3	2:F:351:LEU:HD22	1.88	0.55
1:A:280:ASN:HD21	1:A:282:ASN:HB2	1.70	0.55
1:B:896:ILE:HD12	1:B:897:PRO:HD2	1.89	0.55
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.89	0.55
1:B:526:GLY:O	1:B:528:LYS:NZ	2.38	0.55
1:B:974:SER:OG	1:B:975:SER:N	2.39	0.55
2:H:35:GLU:HG3	2:H:72:PHE:HE2	1.72	0.55
1:A:290:ASP:OD1	1:A:291:CYS:N	2.40	0.54
1:B:661:GLU:O	1:B:695:TYR:OH	2.22	0.54
1:C:383:SER:HB3	1:C:386:LYS:HD2	1.88	0.54
2:F:367:ASP:OD1	2:F:368:ASP:N	2.38	0.54
2:H:425:SER:HB2	2:H:428:PHE:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:NH2	1:A:217:PRO:O	2.40	0.54
1:A:444:LYS:HG2	1:A:446:GLY:H	1.73	0.54
1:A:988:GLU:OE1	1:A:988:GLU:N	2.40	0.54
2:F:22:GLU:HG2	2:F:89:GLN:HG3	1.89	0.54
2:F:590:PRO:HA	2:F:593:THR:HG22	1.89	0.54
2:H:97:LEU:HA	2:H:100:LEU:HB2	1.90	0.54
1:B:317:ASN:HA	1:B:594:GLY:HA2	1.89	0.54
1:A:308:VAL:H	1:A:602:THR:HG22	1.73	0.54
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.23	0.54
1:B:319:ARG:O	1:B:321:GLN:NE2	2.39	0.54
1:B:640:SER:OG	1:B:641:ASN:N	2.41	0.54
1:C:141:LEU:HD23	1:C:243:ALA:HB2	1.89	0.54
2:H:104:GLY:O	2:H:194:ASN:ND2	2.41	0.54
1:A:329:PHE:HD2	1:A:528:LYS:HB2	1.73	0.54
1:B:239:GLN:HG3	1:B:240:THR:H	1.72	0.54
1:B:376:THR:N	1:B:435:ALA:O	2.38	0.54
2:F:75:GLU:N	2:F:75:GLU:OE1	2.40	0.54
2:F:143:LEU:HD12	2:F:144:LEU:H	1.73	0.54
2:F:453:THR:HG21	2:F:516:TYR:HB2	1.90	0.54
2:H:245:ARG:NH1	2:H:605:GLY:O	2.40	0.54
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.31	0.53
1:A:233:ILE:HG22	1:A:234:ASN:H	1.74	0.53
1:B:605:SER:OG	1:B:606:ASN:N	2.41	0.53
1:A:112:SER:HB3	1:A:164:ASN:ND2	2.24	0.53
1:A:128:ILE:HD13	1:A:170:TYR:HD1	1.73	0.53
1:A:129:LYS:HD3	1:A:169:GLU:HG3	1.90	0.53
1:A:967:SER:O	1:A:967:SER:OG	2.27	0.53
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.43	0.53
2:F:67:ASP:OD1	2:F:68:LYS:N	2.41	0.53
2:F:411:SER:OG	2:F:543:ASP:OD1	2.26	0.53
2:F:416:LYS:HA	2:F:419:LYS:HD2	1.90	0.53
2:H:478:TRP:NE1	2:H:499:ASP:OD2	2.41	0.53
1:B:22:THR:OG1	1:B:261:GLY:O	2.27	0.53
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.89	0.53
1:C:559:PHE:CD2	1:C:584:ILE:HG12	2.43	0.53
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.89	0.53
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.91	0.53
1:C:408:ARG:NH1	1:C:409:GLN:HG2	2.24	0.53
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.90	0.53
1:A:342:PHE:CE1	1:A:511:VAL:HG11	2.44	0.53
1:A:567:ARG:NE	1:A:571:ASP:OD2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:O	1:C:386:LYS:NZ	2.42	0.53
2:H:270:MET:HB3	2:H:271:TRP:CE3	2.45	0.53
2:F:172:VAL:O	2:F:176:LEU:HD23	2.09	0.52
1:A:376:THR:HB	1:A:435:ALA:HB3	1.91	0.52
1:B:1000:ARG:O	1:B:1003:SER:OG	2.25	0.52
1:C:324:GLU:H	1:C:539:VAL:HG12	1.75	0.52
1:A:605:SER:OG	1:A:606:ASN:N	2.42	0.52
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.91	0.52
1:B:368:LEU:HA	1:B:374:PHE:HE2	1.74	0.52
1:B:105:ILE:HG22	1:B:110:LEU:HD22	1.90	0.52
1:B:376:THR:HB	1:B:435:ALA:HB3	1.90	0.52
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.30	0.52
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.92	0.52
1:B:117:LEU:HD11	1:B:233:ILE:HG13	1.90	0.52
2:F:147:GLY:O	2:F:151:ILE:N	2.34	0.52
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.91	0.52
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.42	0.52
1:C:1082:CYS:SG	1:C:1132:ILE:HD12	2.48	0.52
2:H:48:TRP:HZ3	2:H:359:LEU:HB2	1.74	0.52
1:A:323:THR:OG1	1:A:324:GLU:OE1	2.19	0.52
1:B:430:THR:OG1	1:B:515:PHE:O	2.28	0.52
1:C:516:GLU:HB2	1:C:519:HIS:ND1	2.24	0.52
1:A:712:ILE:HD11	1:A:1096:VAL:HG12	1.90	0.52
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.91	0.52
1:B:290:ASP:OD1	1:B:291:CYS:N	2.42	0.52
1:C:642:VAL:HG13	1:C:651:ILE:HG13	1.90	0.52
2:H:233:ILE:HD13	2:H:450:LEU:HD12	1.91	0.52
1:A:707:TYR:HD1	1:B:883:THR:HG23	1.74	0.52
1:B:621:PRO:HB3	1:B:637:SER:HB2	1.91	0.52
1:C:456:PHE:HB3	1:C:473:TYR:CG	2.45	0.52
2:F:271:TRP:CZ2	2:F:503:LEU:HA	2.45	0.52
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.92	0.51
2:H:170:SER:HA	2:H:174:LYS:HG3	1.92	0.51
1:A:398:ASP:O	1:A:511:VAL:HA	2.10	0.51
1:C:788:ILE:HG23	1:C:876:ALA:HB2	1.91	0.51
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.92	0.51
2:F:279:TYR:HD1	2:F:444:LEU:HD12	1.76	0.51
2:H:226:VAL:HG13	2:H:516:TYR:CZ	2.45	0.51
2:H:565:PRO:O	2:H:569:ALA:N	2.39	0.51
1:A:83:VAL:HA	1:A:239:GLN:HE22	1.76	0.51
1:A:170:TYR:HE1	1:A:172:SER:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:538:PRO:HB2	2:F:540:HIS:CD2	2.46	0.51
1:A:983:ARG:HD2	1:C:382:VAL:HG22	1.92	0.51
1:A:34:ARG:HH21	1:A:217:PRO:HG2	1.75	0.51
1:B:751:ASN:HA	1:B:754:LEU:HD12	1.92	0.51
2:F:482:ARG:O	2:F:606:TRP:NE1	2.43	0.51
1:A:379:CYS:CB	1:A:432:CYS:HA	2.39	0.51
1:B:462:LYS:HB2	1:B:465:GLU:HB2	1.93	0.51
2:H:158:TYR:CE2	2:H:266:LEU:HD11	2.46	0.51
1:A:640:SER:OG	1:A:641:ASN:N	2.42	0.51
1:B:83:VAL:HG11	1:B:237:ARG:HD2	1.93	0.51
1:B:319:ARG:NE	1:C:740:MET:SD	2.84	0.51
1:C:129:LYS:HG2	1:C:169:GLU:HG3	1.92	0.51
2:F:392:LEU:HD13	2:F:563:SER:HA	1.91	0.50
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.19	0.50
1:B:127:VAL:HG13	1:B:129:LYS:HZ3	1.77	0.50
1:B:1104:VAL:HG13	1:B:1115:ILE:HG12	1.93	0.50
1:C:357:ARG:HG3	1:C:396:TYR:HE1	1.76	0.50
2:F:396:ALA:HB3	2:F:400:PHE:HE2	1.77	0.50
1:B:796:ASP:OD1	1:B:796:ASP:N	2.42	0.50
1:C:988:GLU:OE1	1:C:988:GLU:N	2.45	0.50
1:A:675:GLN:N	1:A:691:SER:O	2.37	0.50
1:B:366:SER:O	1:B:370:ASN:ND2	2.44	0.50
1:C:421:TYR:CD1	1:C:457:ARG:HB2	2.46	0.50
1:A:97:LYS:HD2	1:A:187:LYS:HB3	1.94	0.50
1:B:409:GLN:OE1	1:B:417:LYS:N	2.39	0.50
2:F:492:PRO:HG3	2:F:613:TYR:CZ	2.47	0.50
2:H:33:ASN:OD1	2:H:34:HIS:N	2.44	0.50
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.93	0.50
1:A:641:ASN:HD21	1:A:654:GLU:HG3	1.76	0.50
1:C:866:THR:HG22	1:C:869:MET:HG3	1.93	0.50
1:C:501:ASN:HB3	1:C:505:TYR:HB2	1.93	0.49
2:F:394:ASN:HB2	2:F:562:LYS:HE3	1.94	0.49
1:A:21:ARG:HH11	1:A:22:THR:H	1.59	0.49
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.76	0.49
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.92	0.49
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.78	0.49
2:H:126:ILE:HG21	2:H:176:LEU:HD21	1.94	0.49
1:B:281:GLU:HG3	1:B:282:ASN:OD1	2.12	0.49
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.49
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.44	0.49
1:C:404:GLY:O	1:C:407:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:OD1	1:A:294:ASP:N	2.44	0.49
1:A:707:TYR:CD1	1:B:883:THR:HG23	2.48	0.49
2:H:176:LEU:HD13	2:H:179:LEU:HD12	1.94	0.49
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.78	0.49
1:A:586:ASP:OD1	1:A:587:ILE:N	2.45	0.49
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.47	0.49
1:C:578:ASP:N	1:C:578:ASP:OD1	2.45	0.49
1:A:104:TRP:HB3	1:A:106:PHE:CE2	2.48	0.49
1:A:816:SER:N	1:A:819:GLU:OE1	2.35	0.49
1:B:667:GLY:O	1:B:670:ILE:HG12	2.12	0.49
2:F:303:ASP:HA	2:F:364:VAL:HG22	1.93	0.49
1:A:105:ILE:HD13	1:A:239:GLN:HB2	1.94	0.49
1:B:1090:PRO:HD3	1:B:1095:PHE:HE1	1.77	0.49
1:C:366:SER:N	1:C:388:ASN:OD1	2.45	0.49
1:B:350:VAL:O	1:B:353:TRP:HD1	1.96	0.49
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.31	0.49
2:F:97:LEU:HG	2:F:101:GLN:HG3	1.95	0.49
1:A:883:THR:HG23	1:C:707:TYR:HD1	1.78	0.49
2:F:398:GLU:OE1	2:F:514:ARG:NH2	2.43	0.49
1:A:330:PRO:HA	1:A:579:PRO:HB2	1.95	0.48
1:A:644:GLN:NE2	1:A:648:GLY:O	2.45	0.48
1:B:30:ASN:HB3	1:B:32:PHE:CZ	2.48	0.48
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.76	0.48
2:F:481:LYS:HG2	2:F:487:VAL:HB	1.94	0.48
2:H:382:ASP:HA	2:H:385:TYR:CZ	2.48	0.48
1:C:324:GLU:OE1	1:C:537:LYS:NZ	2.43	0.48
2:F:386:ALA:O	2:F:393:ARG:NE	2.46	0.48
2:H:50:TYR:HB2	2:H:58:ASN:HB3	1.95	0.48
2:H:302:TRP:CD1	2:H:306:ARG:HG2	2.48	0.48
1:A:353:TRP:HH2	1:A:355:ARG:HH21	1.61	0.48
2:F:97:LEU:O	2:F:101:GLN:N	2.39	0.48
2:F:157:ASP:HB3	2:F:160:GLU:HG2	1.94	0.48
1:B:17:ASN:HB3	1:B:137:ASN:HD21	1.78	0.48
1:B:245:HIS:CD2	1:B:247:SER:HG	2.28	0.48
2:F:209:VAL:HG21	2:F:565:PRO:HG3	1.96	0.48
2:H:481:LYS:O	2:H:486:GLY:N	2.37	0.48
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.94	0.48
1:C:577:ARG:HB2	1:C:584:ILE:HG13	1.94	0.48
1:A:439:ASN:HB2	1:A:506:GLN:HB3	1.96	0.48
1:A:752:LEU:O	1:A:755:GLN:HG2	2.14	0.48
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.96	0.48
2:F:476:LYS:O	2:F:480:MET:HG3	2.13	0.48
1:B:295:PRO:HA	1:B:298:GLU:OE2	2.14	0.48
1:A:145:TYR:CG	1:A:154:LYS:HE2	2.48	0.48
1:A:759:PHE:HA	1:A:762:GLN:NE2	2.29	0.48
1:B:442:ASP:O	1:B:448:ASN:ND2	2.45	0.48
1:B:985:ASP:HB3	1:B:988:GLU:OE1	2.13	0.48
2:F:459:TRP:CD1	2:F:477:TRP:HB2	2.49	0.48
1:C:85:PRO:HA	1:C:237:ARG:HA	1.96	0.48
2:F:99:ALA:HB3	2:F:391:LEU:HD13	1.96	0.48
2:H:288:LYS:HG3	2:H:433:GLU:HB3	1.96	0.48
2:H:327:PHE:HD1	2:H:357:ARG:HA	1.79	0.48
2:H:347:THR:OG1	2:H:349:TRP:NE1	2.47	0.48
1:A:327:VAL:N	1:A:531:THR:OG1	2.43	0.48
1:A:366:SER:O	1:A:370:ASN:ND2	2.47	0.48
1:A:233:ILE:HG22	1:A:234:ASN:N	2.28	0.47
1:A:338:PHE:CE2	1:A:363:ALA:HB1	2.49	0.47
1:B:977:LEU:HA	1:B:980:ILE:HD12	1.96	0.47
1:C:603:ASN:HD22	4:C:2004:NAG:H83	1.79	0.47
1:A:127:VAL:HG22	1:A:171:VAL:HG22	1.96	0.47
1:A:61:ASN:HB2	4:A:2001:NAG:H2	1.96	0.47
1:B:44:ARG:HB3	1:B:47:VAL:HG11	1.97	0.47
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.49	0.47
1:C:125:ASN:ND2	1:C:172:SER:O	2.48	0.47
2:H:402:GLU:HB2	2:H:518:ARG:HG3	1.96	0.47
2:H:207:TYR:HH	2:H:517:THR:HG1	1.62	0.47
1:A:57:PRO:HG3	1:A:273:ARG:HE	1.79	0.47
1:B:578:ASP:OD1	1:B:578:ASP:N	2.48	0.47
1:C:244:LEU:HD13	1:C:258:TRP:HB3	1.96	0.47
1:C:738:CYS:O	1:C:741:TYR:N	2.47	0.47
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.95	0.47
1:B:307:THR:HA	1:B:602:THR:HG21	1.96	0.47
1:B:578:ASP:OD2	1:B:581:THR:HB	2.15	0.47
1:A:307:THR:HA	1:A:602:THR:HG21	1.97	0.47
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.96	0.47
1:B:188:ASN:HA	1:B:209:PRO:HA	1.95	0.47
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.50	0.47
1:C:188:ASN:HB3	1:C:190:ARG:CZ	2.45	0.47
1:C:201:PHE:CD2	1:C:203:ILE:HD11	2.49	0.47
1:C:454:ARG:NH1	1:C:467:ASP:OD2	2.48	0.47
2:F:279:TYR:OH	2:F:437:ASN:OD1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:327:PHE:O	2:F:331:SER:OG	2.32	0.47
2:F:469:PRO:HD2	2:F:472:GLN:HB2	1.96	0.47
2:F:540:HIS:CE1	2:F:541:LYS:HG3	2.49	0.47
2:F:540:HIS:HA	2:F:587:TYR:CZ	2.49	0.47
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.45	0.47
1:B:170:TYR:CE1	1:B:172:SER:HB2	2.46	0.47
1:B:402:ILE:HD12	1:B:406:GLU:HB2	1.97	0.47
1:B:472:ILE:HG21	1:B:482:GLY:H	1.79	0.47
1:C:101:ILE:HD13	1:C:242:LEU:HD11	1.96	0.47
1:C:567:ARG:HD3	1:C:571:ASP:HA	1.96	0.47
2:F:131:LYS:HB3	2:F:141:CYS:HB3	1.97	0.47
2:F:456:LEU:HD23	2:F:512:PHE:CD2	2.50	0.47
2:F:463:VAL:HG12	2:F:468:ILE:HD11	1.95	0.47
2:F:233:ILE:HG22	2:F:585:LEU:HD21	1.95	0.47
2:F:267:LEU:HD13	2:F:275:TRP:HE1	1.80	0.47
2:H:226:VAL:O	2:H:516:TYR:OH	2.33	0.47
1:A:869:MET:HE1	1:C:669:GLY:HA2	1.96	0.46
1:B:985:ASP:CG	1:B:987:PRO:HD2	2.35	0.46
1:C:329:PHE:H	1:C:530:SER:HB2	1.80	0.46
1:C:560:LEU:O	1:C:562:PHE:N	2.48	0.46
2:F:328:TRP:HA	2:F:333:LEU:HD11	1.97	0.46
2:H:611:SER:HB3	2:H:614:ALA:HB3	1.97	0.46
1:A:392:PHE:O	1:A:523:THR:N	2.41	0.46
1:C:447:GLY:HA3	1:C:449:TYR:CZ	2.50	0.46
2:H:108:LEU:HD21	2:H:190:MET:SD	2.55	0.46
1:A:487:ASN:ND2	2:F:24:GLN:OE1	2.45	0.46
1:B:418:ILE:HA	1:B:422:ASN:ND2	2.31	0.46
1:B:567:ARG:HD3	1:B:571:ASP:HA	1.97	0.46
2:H:529:LEU:O	2:H:533:ALA:CB	2.63	0.46
1:A:347:PHE:HB2	1:A:401:VAL:HG23	1.95	0.46
1:A:418:ILE:HB	1:A:422:ASN:HB2	1.97	0.46
1:B:353:TRP:CZ2	1:B:466:ARG:HB2	2.50	0.46
1:C:117:LEU:HD11	1:C:233:ILE:HG12	1.97	0.46
1:C:377:PHE:HD1	1:C:434:ILE:HG13	1.80	0.46
1:A:349:SER:HB3	1:A:451:TYR:HD1	1.81	0.46
1:A:691:SER:OG	1:A:692:ILE:N	2.48	0.46
1:B:445:VAL:HG23	1:B:499:PRO:HG3	1.98	0.46
2:F:221:GLN:O	2:F:224:GLU:HG3	2.14	0.46
2:H:108:LEU:HD11	2:H:190:MET:SD	2.55	0.46
1:B:404:GLY:HA2	1:B:508:TYR:CG	2.51	0.46
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:ASP:OD2	2:F:357:ARG:NH2	2.49	0.46
2:H:295:ASP:HA	2:H:298:VAL:HG22	1.98	0.46
1:B:106:PHE:HD2	1:B:235:ILE:HG21	1.80	0.46
2:F:396:ALA:HA	2:F:562:LYS:HG3	1.97	0.46
2:H:97:LEU:HG	2:H:101:GLN:HG3	1.98	0.46
2:H:526:GLN:HG3	2:H:539:LEU:HD11	1.98	0.46
1:A:28:TYR:HB3	1:A:61:ASN:ND2	2.22	0.46
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.97	0.46
1:B:65:PHE:O	1:B:264:ALA:HA	2.15	0.46
1:B:308:VAL:H	1:B:602:THR:HG22	1.81	0.46
1:B:369:TYR:CE1	1:B:384:PRO:HB2	2.51	0.46
2:F:133:CYS:HA	2:F:141:CYS:HA	1.97	0.46
2:F:239:HIS:NE2	2:F:595:LEU:O	2.41	0.46
2:F:396:ALA:HB3	2:F:400:PHE:CE2	2.50	0.46
2:F:453:THR:HA	2:F:512:PHE:HE2	1.81	0.46
2:H:133:CYS:HB3	2:H:138:PRO:HA	1.96	0.46
2:H:581:VAL:HG23	2:H:584:LEU:HD12	1.98	0.46
1:A:197:ILE:HB	1:A:202:LYS:HZ1	1.81	0.46
1:A:202:LYS:HB3	1:A:204:TYR:CE1	2.50	0.46
1:A:985:ASP:OD1	1:A:986:PRO:HD2	2.16	0.46
1:B:417:LYS:HA	1:B:417:LYS:HD3	1.70	0.46
1:C:34:ARG:HH22	1:C:219:GLY:N	2.08	0.46
2:F:33:ASN:OD1	2:F:34:HIS:N	2.49	0.46
1:A:380:TYR:HB3	1:C:486:PHE:HE2	1.81	0.46
1:A:664:ILE:O	1:A:671:CYS:HB2	2.16	0.46
1:A:866:THR:H	1:A:869:MET:HE3	1.80	0.46
1:B:560:LEU:O	1:B:562:PHE:N	2.49	0.46
1:C:61:ASN:HB3	4:C:2001:NAG:N2	2.30	0.46
1:C:204:TYR:CD1	1:C:225:PRO:HA	2.50	0.46
1:A:417:LYS:HA	1:A:417:LYS:HD3	1.82	0.45
1:B:31:SER:HB3	1:B:60:SER:N	2.31	0.45
1:B:245:HIS:O	1:B:258:TRP:HA	2.16	0.45
1:B:316:SER:O	1:B:595:VAL:HG22	2.16	0.45
1:B:612:TYR:HB2	1:B:649:CYS:SG	2.55	0.45
2:F:57:GLU:HA	2:F:60:GLN:NE2	2.31	0.45
2:H:72:PHE:O	2:H:76:GLN:HG2	2.16	0.45
1:C:128:ILE:HD13	1:C:170:TYR:HD2	1.81	0.45
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.51	0.45
2:F:39:LEU:HD12	2:F:39:LEU:HA	1.83	0.45
2:F:55:THR:HG23	2:F:58:ASN:H	1.81	0.45
2:F:159:ASN:HA	2:F:162:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:402:GLU:HB3	2:F:518:ARG:HH11	1.81	0.45
2:H:218:SER:OG	2:H:221:GLN:HB2	2.16	0.45
1:A:118:LEU:HD21	1:A:120:VAL:HG13	1.97	0.45
1:B:27:ALA:HB3	1:B:64:TRP:CE3	2.50	0.45
1:B:998:THR:O	1:B:1002:GLN:OE1	2.33	0.45
1:C:103:GLY:N	1:C:241:LEU:HB2	2.31	0.45
1:C:533:LEU:HD23	1:C:533:LEU:H	1.81	0.45
1:C:967:SER:O	1:C:967:SER:OG	2.29	0.45
2:F:35:GLU:HG3	2:F:72:PHE:CZ	2.52	0.45
2:H:39:LEU:HD21	2:H:69:TRP:HA	1.98	0.45
2:H:217:TYR:CG	2:H:566:TRP:HZ2	2.34	0.45
1:B:406:GLU:O	1:B:409:GLN:HB2	2.17	0.45
1:B:413:GLY:N	1:B:427:ASP:OD1	2.50	0.45
1:C:825:LYS:HE3	1:C:938:LEU:O	2.17	0.45
2:F:116:LEU:HD21	2:F:187:LYS:NZ	2.31	0.45
2:H:67:ASP:OD1	2:H:68:LYS:N	2.49	0.45
1:B:107:GLY:H	1:B:235:ILE:HG23	1.81	0.45
1:C:376:THR:HG23	1:C:378:LYS:HD3	1.99	0.45
1:C:931:ILE:O	1:C:934:ILE:HG22	2.16	0.45
2:F:26:LYS:HE3	2:F:93:VAL:HG21	1.98	0.45
2:F:407:ILE:HD11	2:F:525:PHE:CD2	2.48	0.45
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.99	0.45
1:A:341:VAL:HG13	1:A:342:PHE:CD1	2.51	0.45
1:A:541:PHE:CD2	1:A:552:LEU:HD11	2.52	0.45
1:C:605:SER:OG	1:C:606:ASN:N	2.49	0.45
1:C:1096:VAL:O	1:C:1102:TRP:HA	2.17	0.45
2:F:347:THR:OG1	2:F:359:LEU:HB3	2.16	0.45
2:F:381:TYR:CD2	2:F:401:HIS:HA	2.51	0.45
2:F:560:LEU:HD22	2:F:564:GLU:HG3	1.99	0.45
2:H:57:GLU:HA	2:H:60:GLN:NE2	2.31	0.45
1:B:104:TRP:HB3	1:B:106:PHE:HE1	1.82	0.45
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.82	0.45
1:C:758:SER:O	1:C:762:GLN:NE2	2.23	0.45
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.17	0.45
2:F:43:SER:HA	2:F:65:ALA:HB1	1.98	0.45
1:A:126:VAL:N	1:A:172:SER:O	2.50	0.45
1:A:392:PHE:CD2	1:A:515:PHE:HB3	2.52	0.45
1:A:578:ASP:OD1	1:A:583:GLU:N	2.29	0.45
2:F:123:MET:SD	2:F:176:LEU:HD12	2.57	0.45
2:F:20:THR:HG22	2:F:23:GLU:HG2	1.99	0.45
1:A:102:ARG:HG3	1:A:243:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HG2	1:A:133:PHE:CZ	2.52	0.44
1:A:246:ARG:NH1	1:A:258:TRP:HB3	2.32	0.44
1:A:487:ASN:OD1	2:F:24:GLN:HB3	2.17	0.44
1:A:883:THR:HG23	1:C:707:TYR:CD1	2.51	0.44
1:B:357:ARG:HB2	1:B:394:ASN:OD1	2.17	0.44
1:B:422:ASN:ND2	1:B:454:ARG:HB3	2.32	0.44
1:C:100:ILE:HG22	1:C:242:LEU:HD12	2.00	0.44
1:C:563:GLN:O	1:C:577:ARG:NH1	2.51	0.44
2:F:22:GLU:HG3	2:F:88:ILE:HG23	1.99	0.44
2:F:145:GLU:HB2	2:F:146:PRO:HD2	1.99	0.44
2:F:378:HIS:HD1	2:F:401:HIS:CE1	2.35	0.44
2:H:438:PHE:HE2	2:H:540:HIS:HB2	1.82	0.44
1:A:21:ARG:HG2	1:A:23:GLN:H	1.80	0.44
1:B:24:LEU:HD21	1:B:263:ALA:HB3	2.00	0.44
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.18	0.44
1:C:878:LEU:HA	1:C:881:THR:HG22	2.00	0.44
2:F:240:LEU:O	2:F:244:VAL:HG23	2.17	0.44
2:H:315:PHE:HD2	2:H:320:LEU:HD12	1.81	0.44
2:H:407:ILE:HD11	2:H:525:PHE:CD2	2.50	0.44
2:F:577:LYS:H	2:F:577:LYS:HG2	1.62	0.44
1:A:40:ASP:OD2	1:A:44:ARG:NH2	2.32	0.44
1:A:280:ASN:OD1	1:A:283:GLY:N	2.50	0.44
1:A:663:ASP:OD1	1:A:664:ILE:N	2.51	0.44
1:B:38:TYR:HD2	1:B:224:GLU:HA	1.83	0.44
1:B:141:LEU:HD12	1:B:157:PHE:HD1	1.82	0.44
1:C:326:ILE:HG12	1:C:533:LEU:HA	1.98	0.44
1:C:612:TYR:HB2	1:C:649:CYS:SG	2.57	0.44
1:C:822:LEU:O	1:C:826:VAL:HG12	2.17	0.44
1:A:392:PHE:O	1:A:524:VAL:N	2.50	0.44
1:B:449:TYR:OH	2:H:38:ASP:OD2	2.16	0.44
1:B:878:LEU:HA	1:B:881:THR:HG22	1.99	0.44
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.20	0.44
1:C:420:ASP:OD1	1:C:420:ASP:N	2.41	0.44
2:F:115:ARG:HD2	2:F:115:ARG:HA	1.81	0.44
2:F:453:THR:HA	2:F:512:PHE:CE2	2.53	0.44
2:H:482:ARG:O	2:H:606:TRP:NE1	2.39	0.44
2:H:524:GLN:HB3	2:H:574:VAL:HG11	1.99	0.44
2:H:589:GLU:HB3	2:H:590:PRO:HD3	2.00	0.44
1:A:973:ILE:HD11	1:A:980:ILE:HD12	2.00	0.44
1:B:455:LEU:HD22	1:B:493:GLN:HG3	1.98	0.44
1:C:294:ASP:O	1:C:297:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.52	0.44
2:F:168:TRP:HD1	2:F:169:ARG:NH1	2.15	0.44
2:F:296:ALA:O	2:F:300:GLN:N	2.51	0.44
2:F:381:TYR:CD1	2:F:558:LEU:HD22	2.53	0.44
2:H:310:GLU:HA	2:H:313:LYS:HE2	1.99	0.44
1:A:82:PRO:O	1:A:239:GLN:NE2	2.49	0.44
1:A:665:PRO:HA	1:A:671:CYS:HB3	1.98	0.44
1:B:29:THR:HG23	1:B:62:VAL:HG13	2.00	0.44
1:C:462:LYS:HA	1:C:462:LYS:HD3	1.71	0.44
2:F:212:VAL:HG13	2:F:215:TYR:HB2	1.98	0.44
2:H:126:ILE:HA	2:H:129:THR:HG22	2.00	0.44
1:A:326:ILE:HD12	1:A:532:ASN:O	2.17	0.44
1:A:578:ASP:OD2	1:A:581:THR:HB	2.18	0.44
1:B:204:TYR:CD1	1:B:225:PRO:HA	2.53	0.44
2:F:187:LYS:HD3	2:F:187:LYS:HA	1.77	0.44
1:B:769:GLY:O	1:B:773:GLU:HG2	2.18	0.43
1:B:988:GLU:OE1	1:B:988:GLU:N	2.48	0.43
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.40	0.43
1:C:103:GLY:H	1:C:241:LEU:HB2	1.83	0.43
1:C:106:PHE:CD2	1:C:235:ILE:HG21	2.50	0.43
2:F:474:MET:SD	2:F:474:MET:N	2.91	0.43
2:F:482:ARG:NH2	2:F:608:THR:O	2.41	0.43
1:B:85:PRO:HA	1:B:237:ARG:HA	2.00	0.43
1:B:1116:THR:HA	1:B:1138:TYR:O	2.18	0.43
1:C:214:ARG:HH22	1:C:266:TYR:HE2	1.64	0.43
1:C:214:ARG:NH2	1:C:266:TYR:HE2	2.16	0.43
1:A:315:THR:HG22	1:A:316:SER:N	2.21	0.43
1:A:377:PHE:CD1	1:A:434:ILE:HD12	2.54	0.43
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.99	0.43
1:C:979:ASP:O	1:C:983:ARG:HG2	2.18	0.43
2:F:476:LYS:HB3	2:F:476:LYS:HE3	1.82	0.43
1:A:641:ASN:OD1	1:A:641:ASN:N	2.51	0.43
1:B:664:ILE:O	1:B:671:CYS:HB2	2.19	0.43
1:C:239:GLN:HG3	1:C:240:THR:H	1.83	0.43
1:C:424:LYS:NZ	1:C:425:LEU:O	2.48	0.43
1:C:713:ALA:HA	1:C:1073:LYS:O	2.17	0.43
2:F:35:GLU:HG3	2:F:72:PHE:HZ	1.83	0.43
1:A:61:ASN:OD1	1:A:62:VAL:N	2.52	0.43
1:A:170:TYR:CE1	1:A:172:SER:HB2	2.53	0.43
1:A:386:LYS:HD2	1:A:386:LYS:O	2.18	0.43
1:B:142:ASP:OD1	1:B:244:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:SER:OG	1:B:641:ASN:OD1	2.37	0.43
1:C:555:SER:OG	1:C:584:ILE:O	2.33	0.43
2:F:168:TRP:HD1	2:F:169:ARG:HH11	1.66	0.43
2:F:549:GLU:HG2	2:F:550:ALA:N	2.34	0.43
2:H:293:VAL:HG11	2:H:424:LEU:HD23	2.00	0.43
1:A:40:ASP:OD1	1:A:40:ASP:N	2.51	0.43
1:A:97:LYS:HZ2	1:A:187:LYS:N	2.16	0.43
1:C:188:ASN:OD1	1:C:189:LEU:N	2.52	0.43
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.51	0.43
2:H:265:HIS:CE1	2:H:490:PRO:HB3	2.54	0.43
1:A:329:PHE:CD2	1:A:528:LYS:HB2	2.52	0.43
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.87	0.43
1:B:967:SER:HA	1:B:975:SER:OG	2.19	0.43
1:C:126:VAL:HG22	1:C:172:SER:O	2.19	0.43
1:C:752:LEU:O	1:C:755:GLN:HG2	2.19	0.43
2:F:80:ALA:O	2:F:101:GLN:HG2	2.19	0.43
2:F:271:TRP:CD2	2:F:503:LEU:HD13	2.54	0.43
2:F:554:LEU:O	2:F:558:LEU:HG	2.18	0.43
1:B:303:LEU:HD11	1:B:313:TYR:CE2	2.54	0.43
1:B:966:LEU:HD23	1:B:966:LEU:HA	1.89	0.43
1:C:143:VAL:HG12	1:C:244:LEU:O	2.19	0.43
1:C:464:PHE:HD2	1:C:464:PHE:O	2.02	0.43
1:C:578:ASP:OD2	1:C:581:THR:HB	2.19	0.43
2:F:20:THR:O	2:F:24:GLN:HG3	2.19	0.43
2:F:290:ASN:OD1	2:F:291:ILE:N	2.52	0.43
2:H:470:LYS:HB2	2:H:470:LYS:HE3	1.65	0.43
1:A:29:THR:OG1	1:A:30:ASN:N	2.51	0.43
1:A:299:THR:OG1	1:A:597:VAL:HG21	2.19	0.43
1:A:325:SER:HA	1:A:540:ASN:OD1	2.19	0.43
1:A:721:SER:OG	1:A:1066:THR:OG1	2.36	0.43
1:B:129:LYS:HA	1:B:129:LYS:HD3	1.73	0.43
1:C:276:LEU:HD23	1:C:306:PHE:HE1	1.84	0.43
1:A:770:ILE:O	1:A:774:GLN:HG2	2.19	0.43
1:C:391:CYS:SG	1:C:522:ALA:HB1	2.59	0.43
1:C:426:PRO:HB2	1:C:428:ASP:OD1	2.19	0.43
1:A:500:THR:OG1	2:F:41:TYR:OH	2.26	0.42
1:A:535:LYS:NZ	1:A:554:GLU:HG2	2.33	0.42
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.49	0.42
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.89	0.42
1:C:34:ARG:HA	1:C:34:ARG:HD3	1.83	0.42
1:C:393:THR:OG1	1:C:516:GLU:OE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:TYR:CE1	2:F:451:PRO:HG2	2.54	0.42
2:H:308:PHE:HB3	2:H:328:TRP:HZ3	1.84	0.42
1:A:422:ASN:OD1	1:A:454:ARG:N	2.39	0.42
1:C:46:SER:HA	1:C:279:TYR:O	2.19	0.42
2:F:444:LEU:HD23	2:F:444:LEU:HA	1.89	0.42
2:H:259:ILE:HG13	2:H:607:SER:HB3	2.00	0.42
2:H:565:PRO:HD2	2:H:568:LEU:HD13	2.01	0.42
1:C:38:TYR:HB2	1:C:225:PRO:HD3	2.01	0.42
1:C:665:PRO:HA	1:C:671:CYS:HB3	2.00	0.42
1:C:1092:GLU:OE2	1:C:1107:ARG:NE	2.52	0.42
2:F:381:TYR:HB2	2:F:404:VAL:HG11	2.01	0.42
1:A:246:ARG:CZ	1:A:258:TRP:HB3	2.49	0.42
1:A:426:PRO:HD3	1:A:463:PRO:HB3	2.01	0.42
1:B:188:ASN:OD1	1:B:190:ARG:NH1	2.52	0.42
1:B:931:ILE:O	1:B:934:ILE:HG22	2.18	0.42
2:F:39:LEU:HD21	2:F:68:LYS:HG2	2.01	0.42
2:F:89:GLN:O	2:F:90:ASN:OD1	2.36	0.42
2:H:524:GLN:HG2	2:H:583:PRO:HG2	2.01	0.42
1:B:666:ILE:HB	1:B:670:ILE:O	2.18	0.42
1:C:641:ASN:N	1:C:641:ASN:OD1	2.53	0.42
2:H:247:LYS:HG3	2:H:282:THR:HA	2.01	0.42
2:H:397:ASN:C	2:H:397:ASN:ND2	2.72	0.42
2:H:592:PHE:O	2:H:596:LYS:HG3	2.19	0.42
1:A:61:ASN:HB2	4:A:2001:NAG:H83	2.00	0.42
1:A:1089:PHE:HE2	1:B:917:TYR:HD2	1.68	0.42
1:B:441:LEU:HB3	1:B:509:ARG:NH2	2.34	0.42
1:B:1081:ILE:HG23	1:B:1135:ASN:HB3	2.02	0.42
1:C:364:ASP:O	1:C:367:VAL:HG22	2.20	0.42
2:F:262:LEU:HD23	2:F:262:LEU:H	1.84	0.42
2:F:431:ASP:OD1	2:F:431:ASP:N	2.52	0.42
2:H:553:LYS:HD3	2:H:573:VAL:HA	2.02	0.42
1:C:121:ASN:HA	1:C:126:VAL:HG12	2.01	0.42
2:F:331:SER:HB3	2:F:357:ARG:HG2	2.00	0.42
2:H:149:ASN:HA	2:H:152:MET:HE2	2.02	0.42
1:A:125:ASN:OD1	1:A:173:GLN:HA	2.19	0.42
1:A:448:ASN:HB3	1:A:497:PHE:HB2	2.01	0.42
1:B:36:VAL:HG21	1:B:220:PHE:HE1	1.85	0.42
1:B:112:SER:HB3	1:B:164:ASN:OD1	2.20	0.42
1:B:315:THR:HG22	1:B:316:SER:N	2.24	0.42
1:C:897:PRO:HG2	1:C:900:MET:SD	2.60	0.42
1:C:1091:ARG:NE	1:C:1118:ASP:O	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:388:GLN:O	2:F:393:ARG:NE	2.52	0.42
2:H:374:HIS:CE1	2:H:406:GLU:HG2	2.55	0.42
2:H:379:ILE:O	2:H:383:MET:HE2	2.20	0.42
1:A:142:ASP:OD1	1:A:244:LEU:HB2	2.19	0.42
1:B:353:TRP:HH2	1:B:355:ARG:HH21	1.66	0.42
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	2.02	0.42
1:C:398:ASP:HB2	1:C:512:VAL:HG22	2.02	0.42
1:C:464:PHE:O	1:C:464:PHE:CD2	2.73	0.42
2:F:197:GLU:HG2	2:F:198:ASP:N	2.35	0.42
2:H:97:LEU:HA	2:H:97:LEU:HD12	1.93	0.42
2:H:315:PHE:CD2	2:H:320:LEU:HD12	2.53	0.42
1:A:357:ARG:HG2	1:A:396:TYR:HE1	1.85	0.42
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.02	0.42
1:B:40:ASP:OD1	1:B:40:ASP:N	2.52	0.42
1:B:374:PHE:HA	1:B:436:TRP:HB3	2.01	0.42
1:B:403:ARG:HB2	1:B:495:TYR:CE1	2.55	0.42
1:C:125:ASN:OD1	1:C:171:VAL:HG13	2.20	0.42
1:C:409:GLN:NE2	1:C:418:ILE:HG12	2.35	0.42
2:F:450:LEU:HB2	2:F:451:PRO:HD3	2.02	0.42
2:H:45:LEU:HD12	2:H:45:LEU:HA	1.94	0.42
2:H:522:GLN:HG3	2:H:523:PHE:N	2.35	0.42
1:A:200:TYR:HA	1:A:229:LEU:O	2.20	0.41
1:A:398:ASP:HB2	1:A:512:VAL:HG22	2.01	0.41
1:A:917:TYR:HD2	1:C:1089:PHE:HE2	1.67	0.41
1:B:456:PHE:HB2	1:B:491:PRO:HA	2.02	0.41
1:C:233:ILE:HG22	1:C:234:ASN:H	1.85	0.41
1:C:985:ASP:N	1:C:985:ASP:OD1	2.46	0.41
1:A:16:VAL:HG12	1:A:158:ARG:NH2	2.35	0.41
1:A:30:ASN:HB3	1:A:32:PHE:CE2	2.55	0.41
1:A:336:CYS:HB3	1:A:363:ALA:HA	2.01	0.41
1:A:983:ARG:O	1:C:383:SER:N	2.37	0.41
1:B:29:THR:OG1	1:B:30:ASN:N	2.53	0.41
1:B:975:SER:OG	1:B:975:SER:O	2.36	0.41
2:F:284:PRO:HD3	2:F:440:LEU:HD22	2.02	0.41
2:H:62:MET:HE3	2:H:62:MET:HB2	2.00	0.41
2:H:119:ILE:HG21	2:H:183:TYR:HB2	2.01	0.41
1:A:164:ASN:OD1	1:A:165:ASN:N	2.54	0.41
1:A:290:ASP:O	1:A:297:SER:HB3	2.21	0.41
1:B:997:ILE:HG13	1:B:998:THR:N	2.36	0.41
1:C:938:LEU:HD12	1:C:938:LEU:HA	1.90	0.41
2:F:402:GLU:HB3	2:F:518:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:468:ILE:HD12	2:F:473:TRP:HD1	1.85	0.41
2:H:539:LEU:HG	2:H:587:TYR:CD2	2.55	0.41
1:A:776:LYS:HB2	1:A:776:LYS:HE3	1.87	0.41
1:B:143:VAL:HA	1:B:156:GLU:HB3	2.02	0.41
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.55	0.41
1:C:115:GLN:OE1	1:C:131:CYS:N	2.54	0.41
1:C:577:ARG:HH21	1:C:584:ILE:HD11	1.85	0.41
1:A:205:SER:HB3	1:A:226:LEU:HG	2.02	0.41
1:A:640:SER:HG	1:A:641:ASN:N	2.18	0.41
1:B:369:TYR:HE1	1:B:384:PRO:HB2	1.84	0.41
1:B:759:PHE:HA	1:B:762:GLN:NE2	2.35	0.41
1:C:112:SER:N	1:C:134:GLN:OE1	2.34	0.41
1:C:214:ARG:HH11	1:C:214:ARG:C	2.23	0.41
2:F:50:TYR:HD1	2:F:58:ASN:HB3	1.85	0.41
2:F:239:HIS:HE2	2:F:595:LEU:C	2.21	0.41
2:F:460:ARG:HH11	2:F:512:PHE:HB2	1.86	0.41
1:B:938:LEU:HD12	1:B:938:LEU:HA	1.83	0.41
1:C:975:SER:O	1:C:975:SER:OG	2.37	0.41
2:H:217:TYR:CE2	2:H:221:GLN:HB3	2.56	0.41
1:B:424:LYS:HB3	1:B:462:LYS:O	2.21	0.41
2:H:212:VAL:HG13	2:H:215:TYR:HB2	2.02	0.41
2:H:557:MET:HG2	2:H:573:VAL:HG23	2.01	0.41
1:A:342:PHE:HE1	1:A:511:VAL:HG11	1.84	0.41
1:B:200:TYR:CD1	1:B:230:PRO:HA	2.56	0.41
2:F:492:PRO:O	2:F:493:HIS:ND1	2.54	0.41
2:F:589:GLU:HB3	2:F:590:PRO:HD3	2.01	0.41
2:H:331:SER:HB3	2:H:357:ARG:HG2	2.03	0.41
1:A:128:ILE:HD13	1:A:170:TYR:CD1	2.55	0.41
1:A:200:TYR:CD1	1:A:230:PRO:HA	2.56	0.41
1:A:386:LYS:HD3	1:A:389:ASP:HB3	2.01	0.41
1:A:1129:VAL:HB	1:A:1132:ILE:HG12	2.02	0.41
1:B:560:LEU:HD12	1:B:561:PRO:HD2	2.03	0.41
1:C:560:LEU:CG	1:C:561:PRO:HD2	2.50	0.41
1:C:796:ASP:OD1	1:C:796:ASP:N	2.52	0.41
2:H:85:LEU:HD13	2:H:97:LEU:HD23	2.02	0.41
2:H:134:ASN:HA	2:H:163:TRP:HZ2	1.86	0.41
1:A:310:LYS:HG2	1:A:664:ILE:HD11	2.04	0.41
1:A:365:TYR:CG	1:A:387:LEU:HB3	2.56	0.41
1:A:552:LEU:HA	1:A:586:ASP:O	2.21	0.41
1:A:560:LEU:O	1:A:562:PHE:N	2.54	0.41
1:B:568:ASP:OD1	1:B:569:ILE:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:VAL:HG13	1:C:917:TYR:HB3	2.02	0.41
1:C:403:ARG:HB2	1:C:495:TYR:CE1	2.56	0.41
1:C:720:ILE:HD12	1:C:923:ILE:HG23	2.02	0.41
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	2.03	0.41
2:F:378:HIS:CE1	2:F:402:GLU:HA	2.53	0.41
2:H:32:PHE:HA	2:H:35:GLU:HG2	2.02	0.41
2:H:133:CYS:SG	2:H:141:CYS:N	2.94	0.41
2:H:145:GLU:HB2	2:H:146:PRO:HD2	2.03	0.41
1:A:350:VAL:HG21	1:A:418:ILE:HD12	2.02	0.40
1:A:897:PRO:HG2	1:A:900:MET:HG3	2.02	0.40
1:B:357:ARG:HH21	1:B:394:ASN:ND2	2.19	0.40
1:B:454:ARG:NH2	1:B:469:SER:O	2.54	0.40
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.03	0.40
1:C:1129:VAL:HB	1:C:1132:ILE:HG23	2.03	0.40
2:F:237:TYR:CZ	2:F:451:PRO:HG2	2.56	0.40
2:F:529:LEU:HD23	2:F:544:ILE:HD13	2.03	0.40
2:F:557:MET:SD	2:F:558:LEU:HD23	2.61	0.40
2:H:554:LEU:HD12	2:H:554:LEU:HA	1.94	0.40
1:A:578:ASP:OD1	1:A:578:ASP:N	2.55	0.40
1:C:231:ILE:HG22	1:C:233:ILE:HD11	2.03	0.40
1:C:422:ASN:OD1	1:C:454:ARG:HB3	2.22	0.40
2:F:460:ARG:NH1	2:F:510:TYR:O	2.53	0.40
2:H:187:LYS:HA	2:H:187:LYS:HD3	1.91	0.40
1:A:752:LEU:HA	1:A:752:LEU:HD23	1.90	0.40
1:A:928:ASN:O	1:A:931:ILE:HG22	2.22	0.40
1:A:1009:THR:O	1:A:1013:ILE:HG12	2.21	0.40
1:B:117:LEU:HG	1:B:130:VAL:HG22	2.04	0.40
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	2.03	0.40
1:C:967:SER:HA	1:C:975:SER:OG	2.21	0.40
1:B:502:GLY:H	2:H:354:GLY:HA3	1.86	0.40
2:H:453:THR:HG23	2:H:512:PHE:CD2	2.56	0.40
2:H:460:ARG:NH1	2:H:512:PHE:HB2	2.36	0.40
1:A:121:ASN:HA	1:A:126:VAL:HG12	2.02	0.40
1:A:326:ILE:HD13	1:A:326:ILE:HA	1.88	0.40
1:B:87:ASN:HB3	1:B:88:ASP:H	1.80	0.40
1:C:321:GLN:HA	1:C:322:PRO:HD3	1.98	0.40
1:C:659:SER:HB2	1:C:698:SER:HB2	2.03	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	1022/1283 (80%)	947 (93%)	72 (7%)	3 (0%)	37 66
1	B	1022/1283 (80%)	948 (93%)	74 (7%)	0	100 100
1	C	1022/1283 (80%)	947 (93%)	74 (7%)	1 (0%)	48 76
2	F	594/861 (69%)	565 (95%)	29 (5%)	0	100 100
2	H	594/861 (69%)	556 (94%)	38 (6%)	0	100 100
All	All	4254/5571 (76%)	3963 (93%)	287 (7%)	4 (0%)	50 76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1102	TRP
1	C	1102	TRP
1	A	214	ARG
1	A	142	ASP

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	907/1116 (81%)	905 (100%)	2 (0%)	92 95
1	B	907/1116 (81%)	906 (100%)	1 (0%)	92 96
1	C	907/1116 (81%)	903 (100%)	4 (0%)	89 93
2	F	526/752 (70%)	526 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	526/752 (70%)	525 (100%)	1 (0%)	92 95
All	All	3773/4852 (78%)	3765 (100%)	8 (0%)	91 95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	386	LYS
1	B	964	LYS
1	C	214	ARG
1	C	394	ASN
1	C	408	ARG
1	C	914	ASN
2	H	397	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1106	GLN
2	F	540	HIS
2	H	401	HIS

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)

62 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	$\#\|Z\| > 2$
3	NAG	D	1	1,3	14,14,15	0.60	1 (7%)	17,19,21	0.58	0
3	NAG	D	2	3	14,14,15	0.40	0	17,19,21	1.24	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	NAG	G	1	1,3	14,14,15	0.35	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.18	0	17,19,21	0.51	0
3	NAG	I	1	1,3	14,14,15	0.29	0	17,19,21	0.42	0
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.52	0
3	NAG	J	1	1,3	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	K	1	1,3	14,14,15	0.41	0	17,19,21	0.40	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	L	1	1,3	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	M	1	1,3	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	M	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	N	1	1,3	14,14,15	1.30	1 (7%)	17,19,21	1.22	1 (5%)
3	NAG	N	2	3	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	O	1	1,3	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	O	2	3	14,14,15	0.17	0	17,19,21	0.46	0
3	NAG	P	1	1,3	14,14,15	0.19	0	17,19,21	0.37	0
3	NAG	P	2	3	14,14,15	0.31	0	17,19,21	0.38	0
3	NAG	Q	1	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.73	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	R	1	1,3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	R	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	S	1	1,3	14,14,15	0.35	0	17,19,21	0.54	0
3	NAG	S	2	3	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	T	1	1,3	14,14,15	0.32	0	17,19,21	0.40	0
3	NAG	T	2	3	14,14,15	0.20	0	17,19,21	0.47	0
3	NAG	U	1	1,3	14,14,15	0.20	0	17,19,21	0.51	0
3	NAG	U	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	V	1	1,3	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	V	2	3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	W	1	1,3	14,14,15	0.40	0	17,19,21	0.47	0
3	NAG	W	2	3	14,14,15	0.17	0	17,19,21	0.45	0
3	NAG	X	1	1,3	14,14,15	0.32	0	17,19,21	0.42	0
3	NAG	X	2	3	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	Y	1	1,3	14,14,15	1.11	1 (7%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	Y	2	3	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	Z	1	1,3	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	Z	2	3	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	a	1	1,3	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	a	2	3	14,14,15	0.18	0	17,19,21	0.45	0
3	NAG	b	1	1,3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	b	2	3	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	c	1	1,3	14,14,15	0.23	0	17,19,21	0.35	0
3	NAG	c	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	d	1	1,3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	d	2	3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	e	1	1,3	14,14,15	0.34	0	17,19,21	0.47	0
3	NAG	e	2	3	14,14,15	0.18	0	17,19,21	0.45	0
3	NAG	f	1	1,3	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	f	2	3	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	g	1	1,3	14,14,15	0.31	0	17,19,21	0.41	0
3	NAG	g	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	h	1	1,3	14,14,15	0.43	0	17,19,21	0.91	1 (5%)
3	NAG	h	2	3	14,14,15	0.17	0	17,19,21	0.64	1 (5%)
3	NAG	i	1	1,3	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	i	2	3	14,14,15	0.16	0	17,19,21	0.41	0
3	NAG	j	1	1,3	14,14,15	0.17	0	17,19,21	0.49	0
3	NAG	j	2	3	14,14,15	0.18	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	5/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	a	2	3	-	0/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	g	2	3	-	0/6/23/26	0/1/1/1
3	NAG	h	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	h	2	3	-	0/6/23/26	0/1/1/1
3	NAG	i	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	0/6/23/26	0/1/1/1
3	NAG	j	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O5-C1	-4.47	1.36	1.43
3	Y	1	NAG	O5-C1	-3.65	1.37	1.43
3	Q	1	NAG	O5-C1	-2.17	1.40	1.43
3	D	1	NAG	O5-C1	-2.11	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	C2-N2-C7	4.26	128.97	122.90
3	N	1	NAG	C3-C4-C5	3.36	116.24	110.24
3	Y	1	NAG	C3-C4-C5	2.67	115.00	110.24
3	h	1	NAG	C1-O5-C5	2.47	115.54	112.19
3	h	2	NAG	C1-O5-C5	2.09	115.03	112.19
3	D	2	NAG	C1-C2-N2	2.07	114.02	110.49

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	f	1	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2
3	W	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C3-C2-N2-C7
3	N	1	NAG	C3-C2-N2-C7
3	S	1	NAG	C3-C2-N2-C7
3	Y	1	NAG	C3-C2-N2-C7
3	e	1	NAG	C3-C2-N2-C7
3	M	2	NAG	C4-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7

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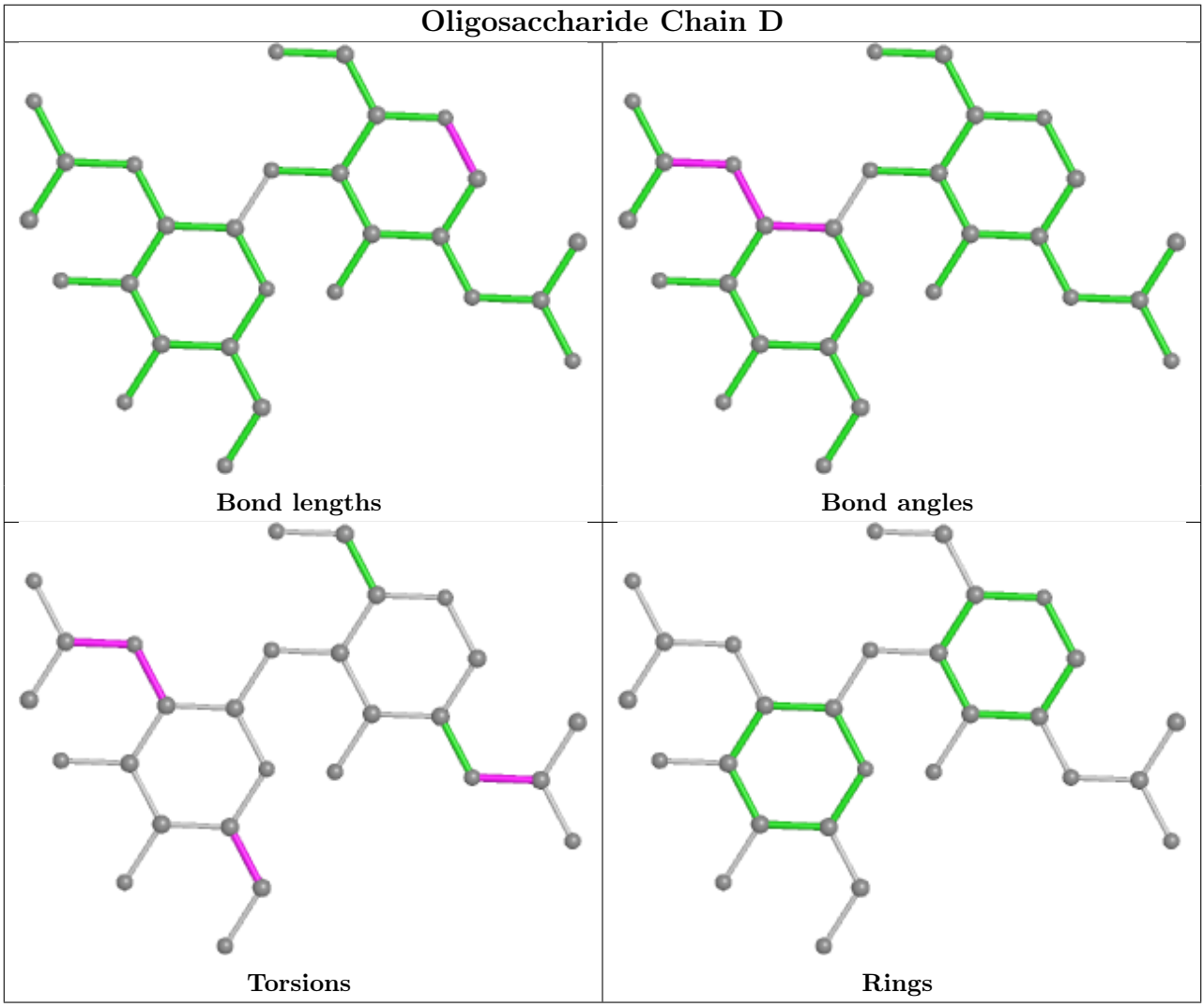
Mol	Chain	Res	Type	Atoms
3	h	1	NAG	C3-C2-N2-C7
3	g	1	NAG	C1-C2-N2-C7

There are no ring outliers.

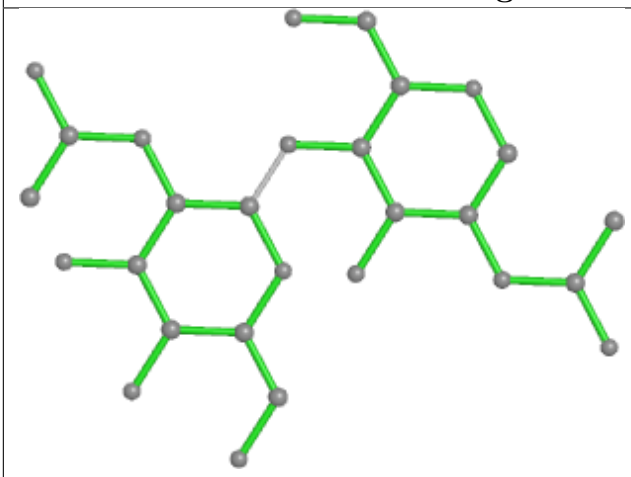
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	E	1	NAG	1	0

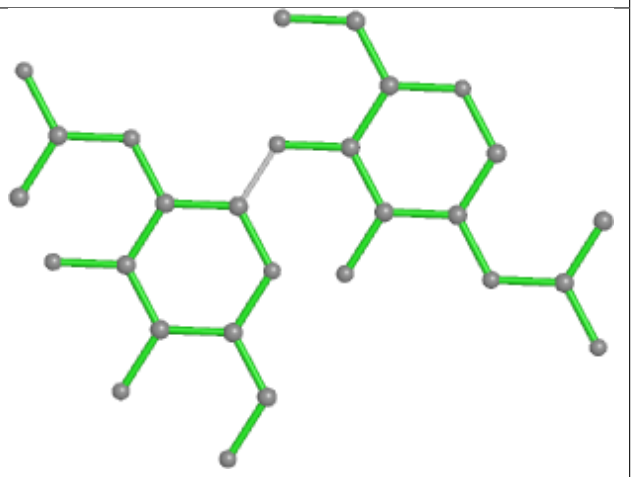
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



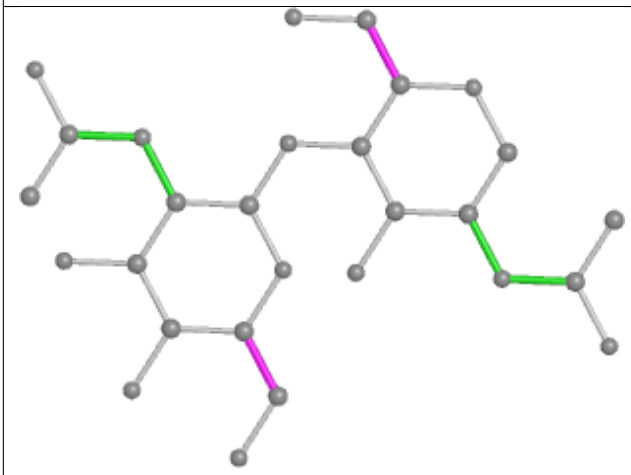
Oligosaccharide Chain E



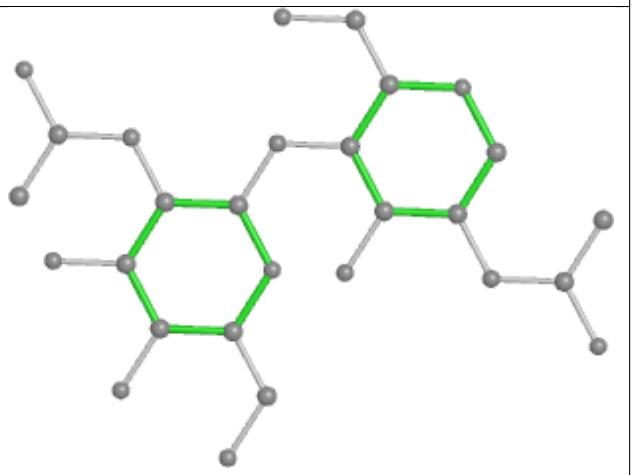
Bond lengths



Bond angles

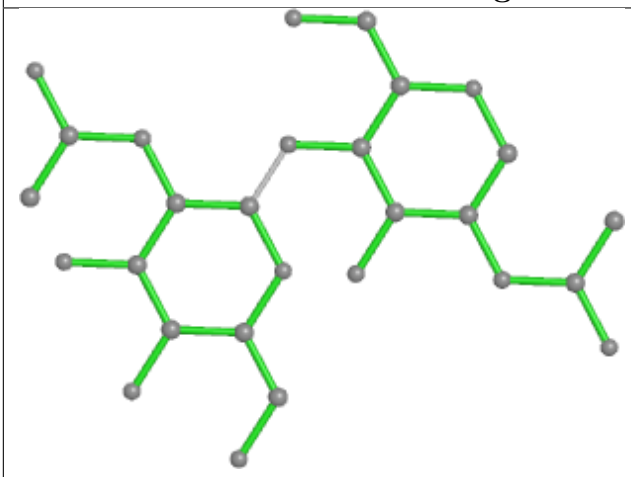


Torsions

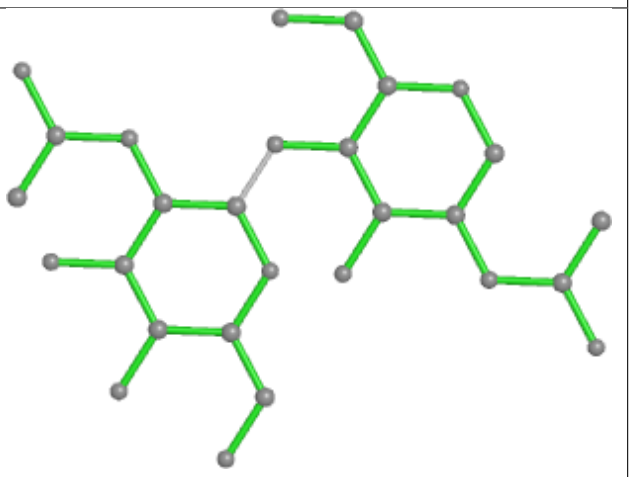


Rings

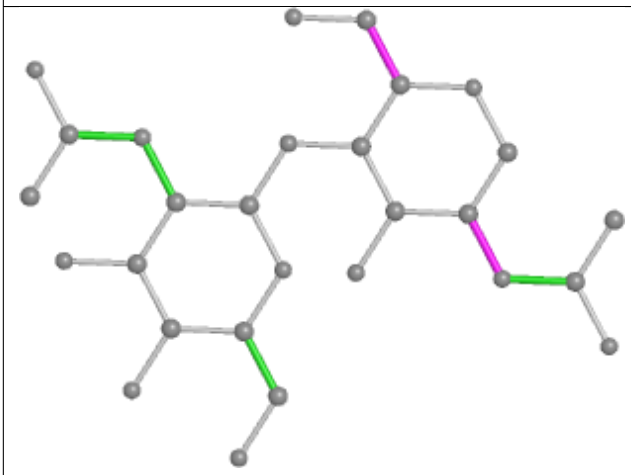
Oligosaccharide Chain G



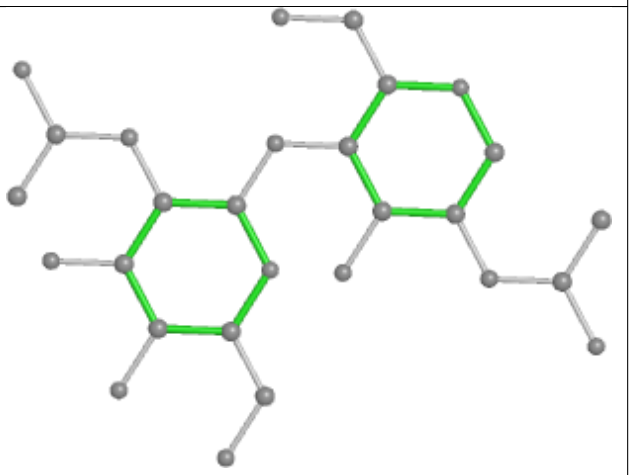
Bond lengths



Bond angles

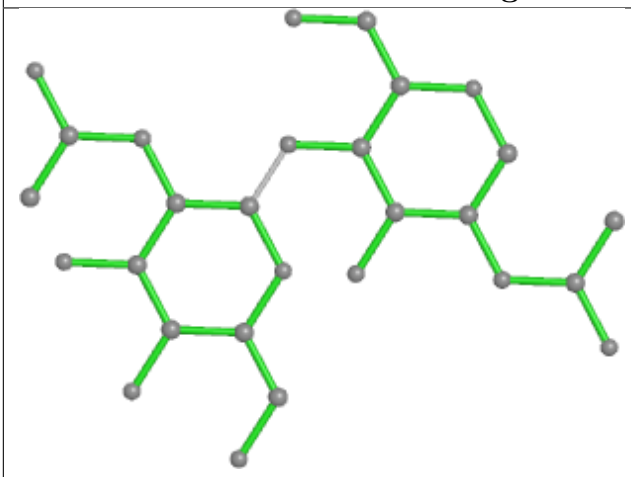


Torsions

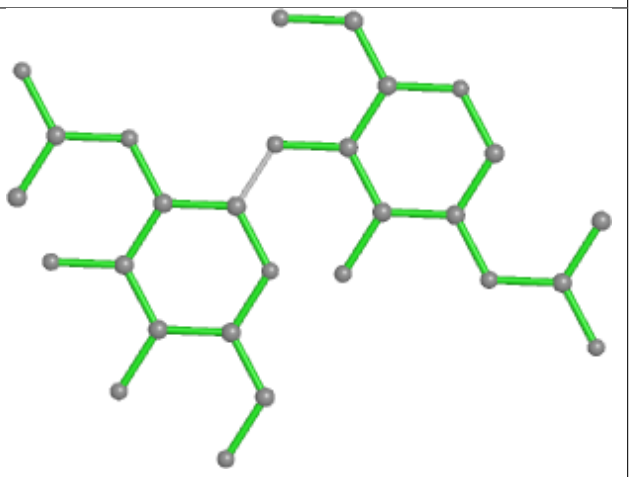


Rings

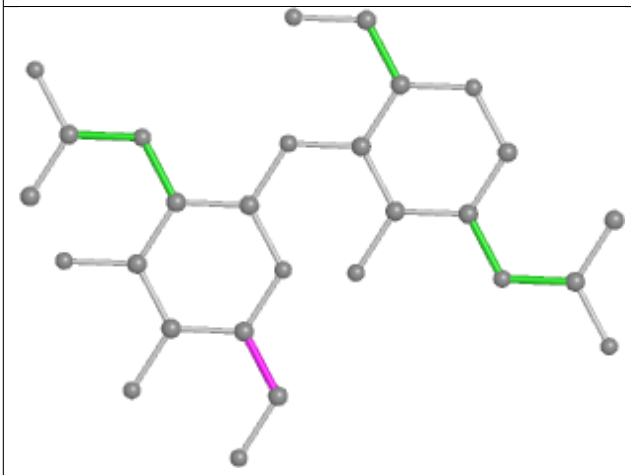
Oligosaccharide Chain I



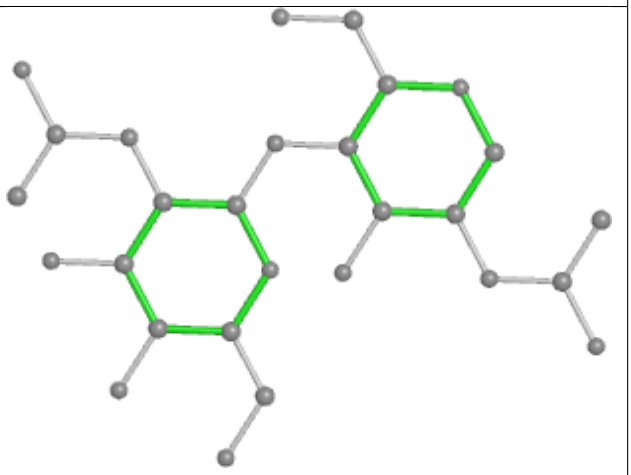
Bond lengths



Bond angles

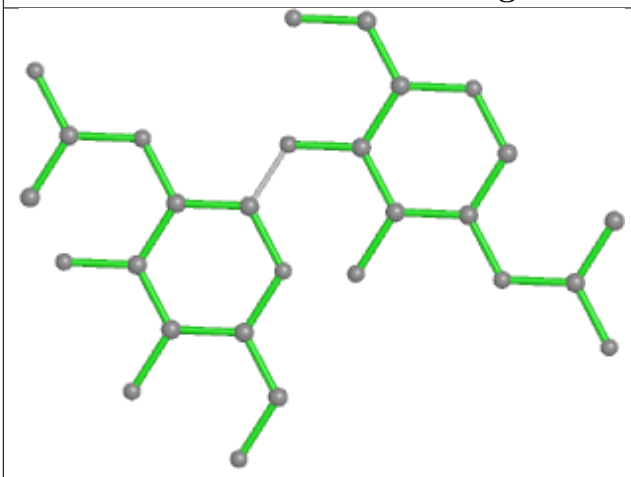


Torsions

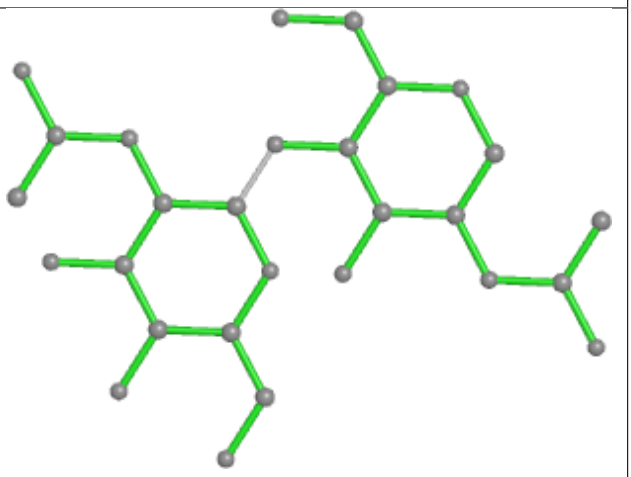


Rings

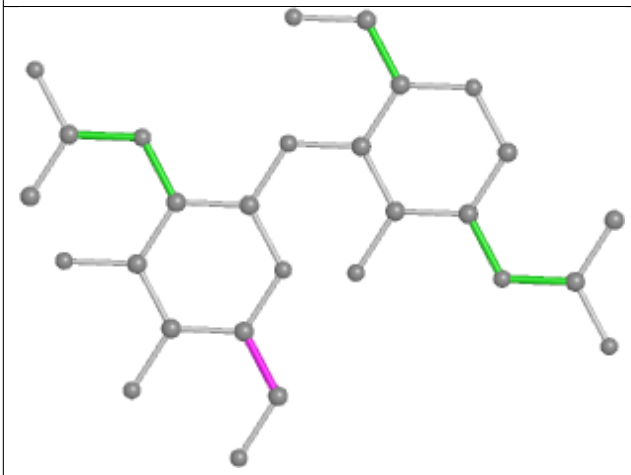
Oligosaccharide Chain J



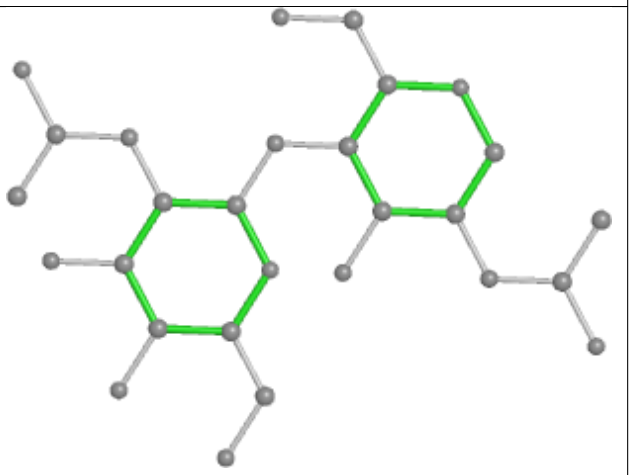
Bond lengths



Bond angles

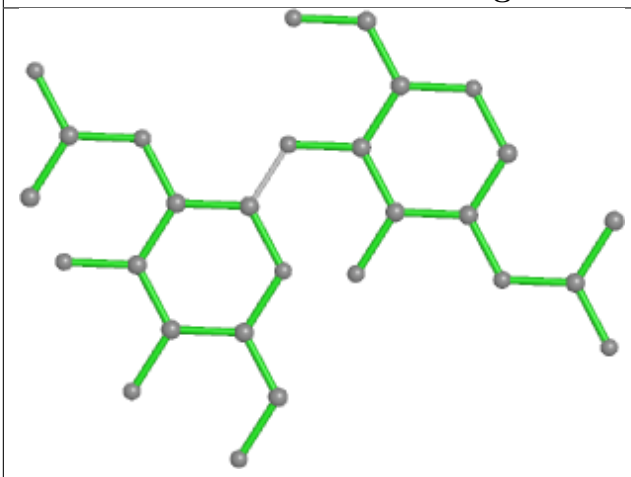


Torsions

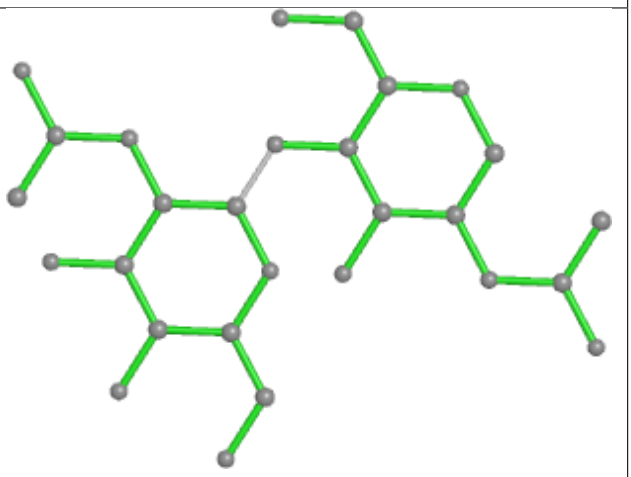


Rings

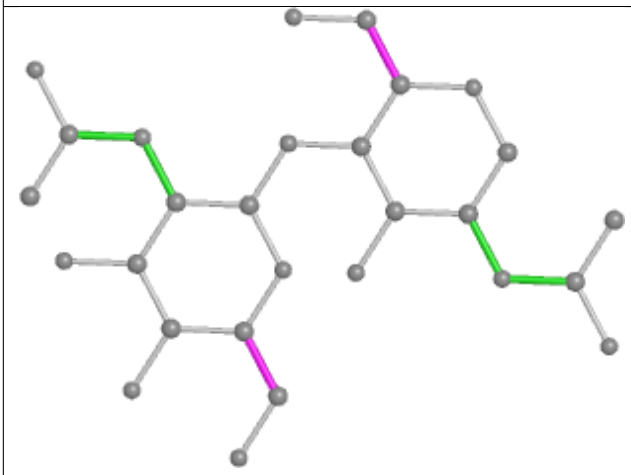
Oligosaccharide Chain K



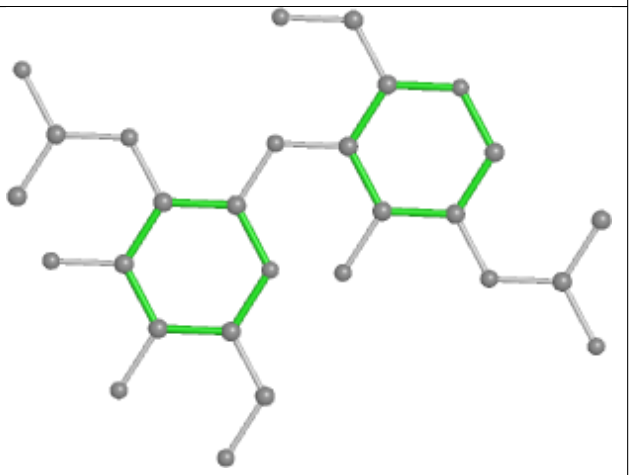
Bond lengths



Bond angles

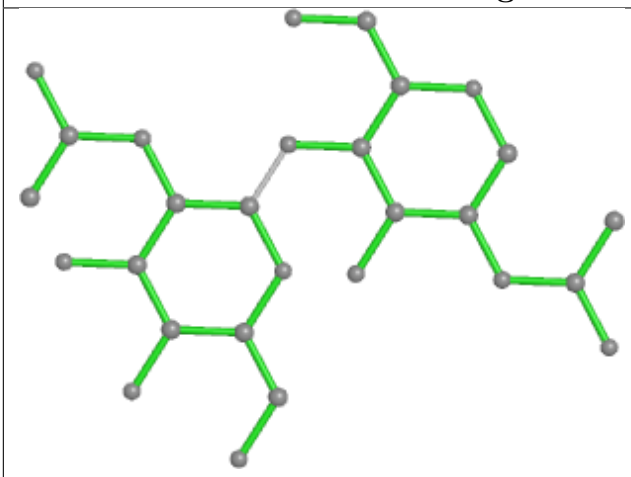


Torsions

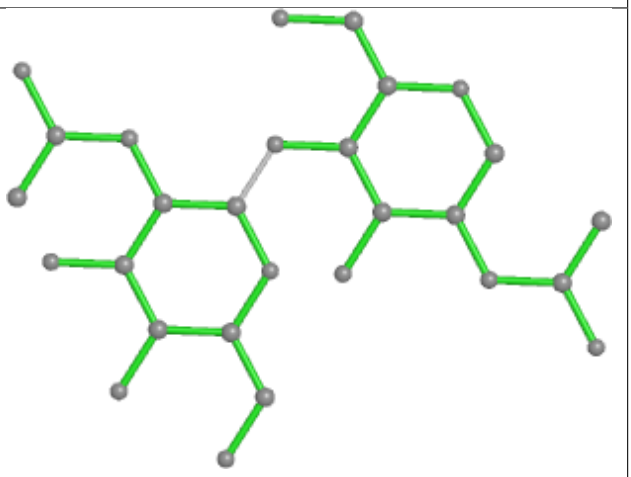


Rings

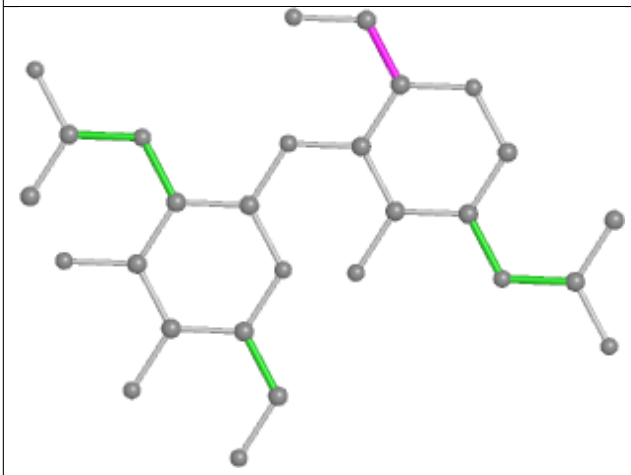
Oligosaccharide Chain L



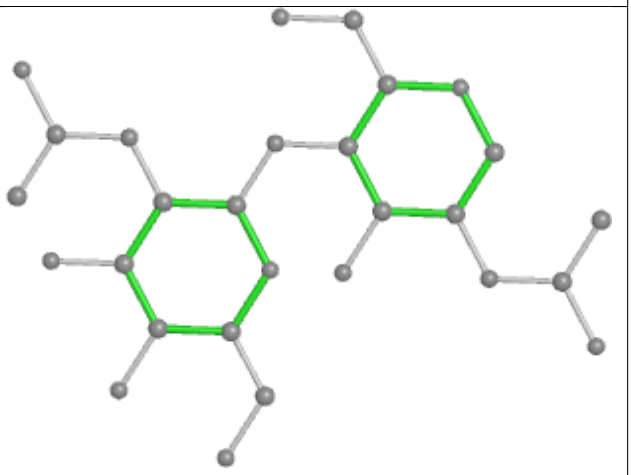
Bond lengths



Bond angles

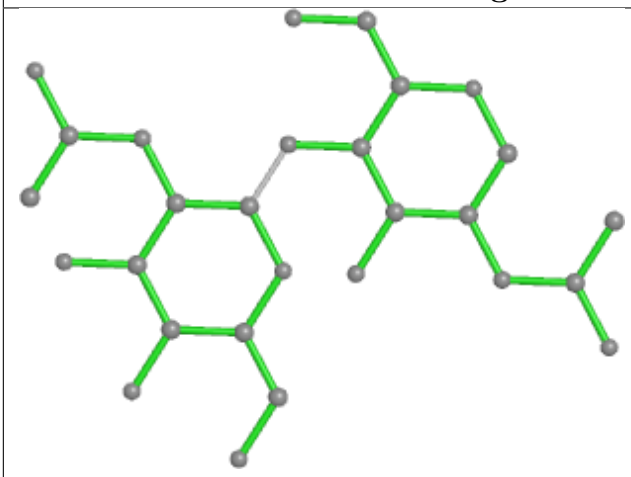


Torsions



Rings

Oligosaccharide Chain M



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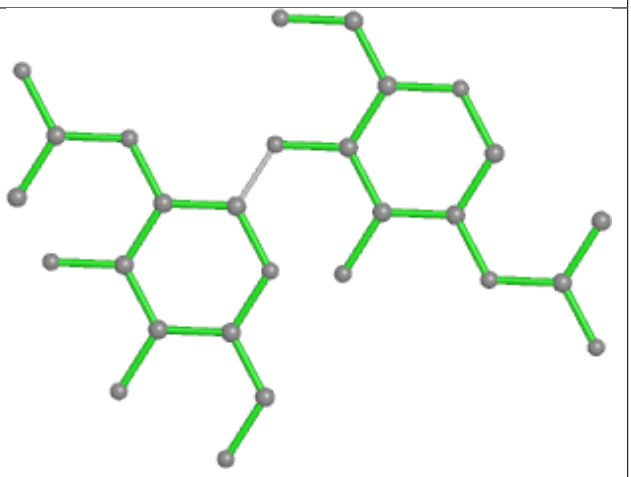

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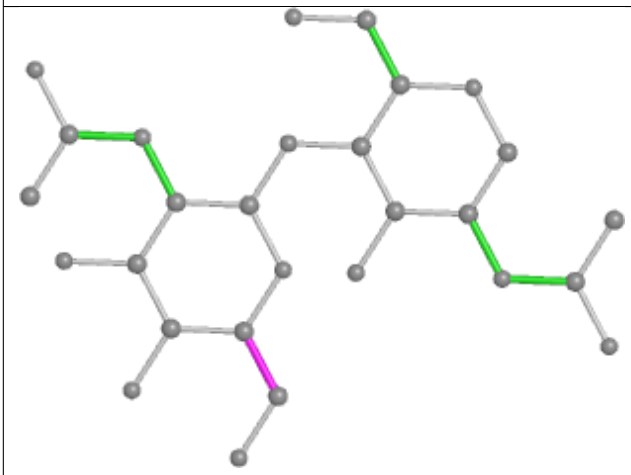

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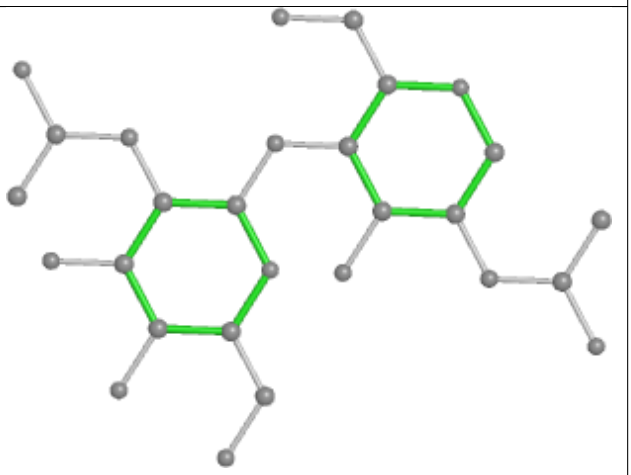
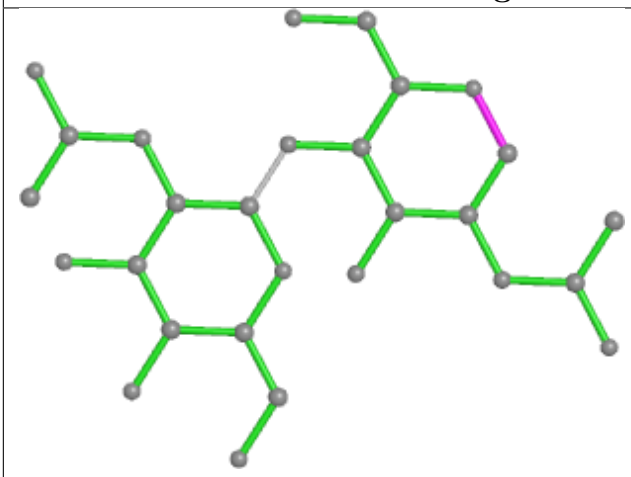
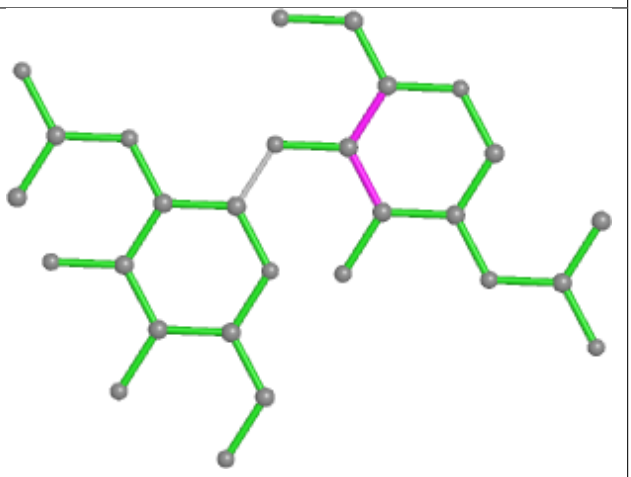


Rings

Oligosaccharide Chain N	
	
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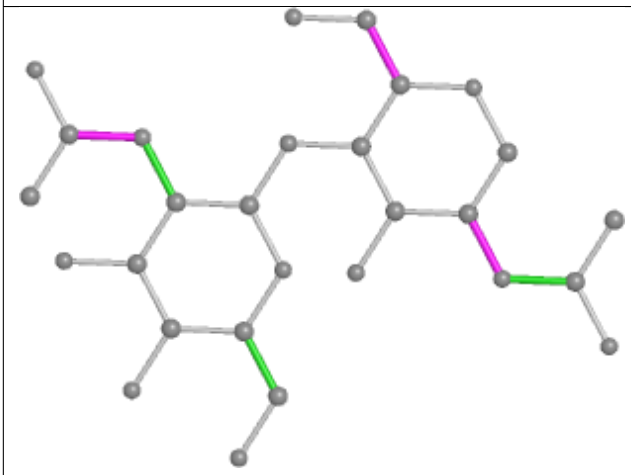
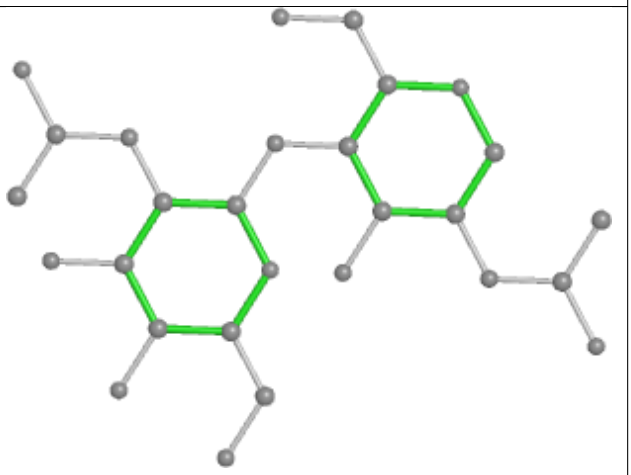
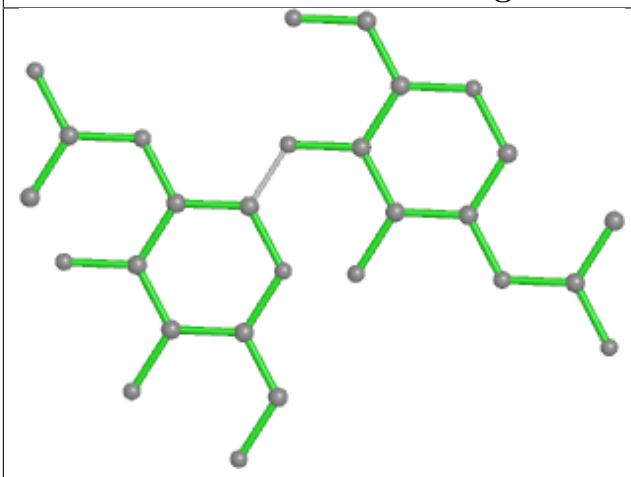
	
Torsions	**Rings**

Oligosaccharide Chain O



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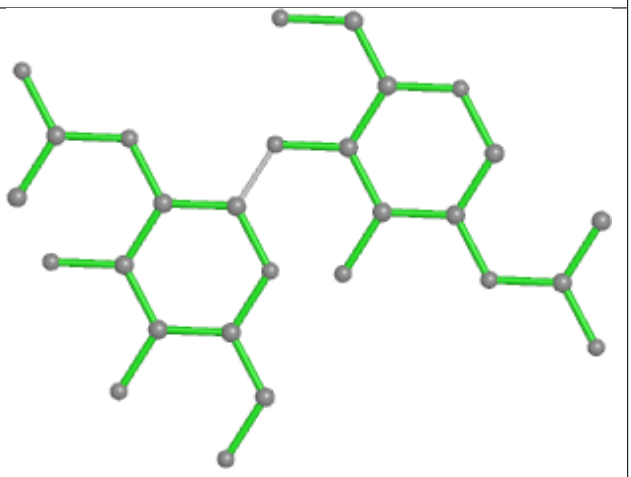

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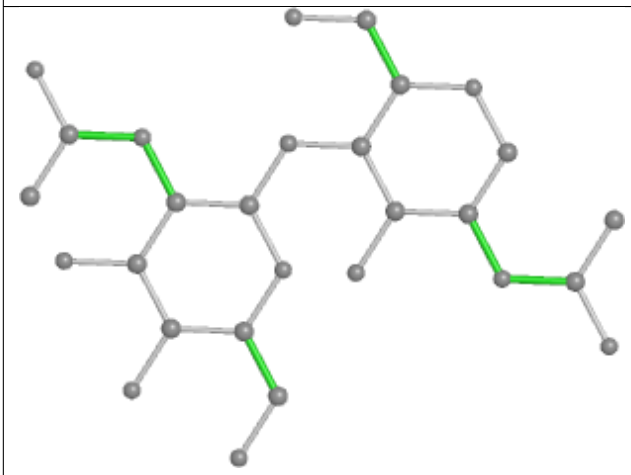

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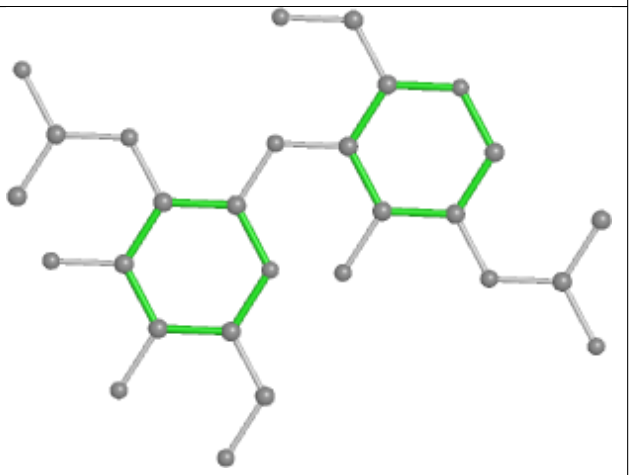
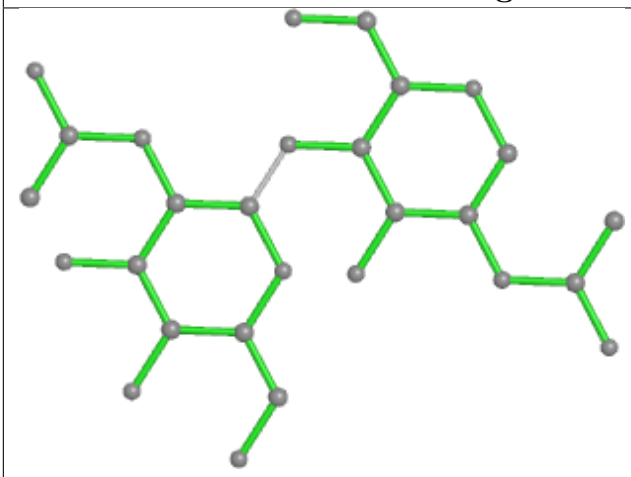


Rings

Oligosaccharide Chain P



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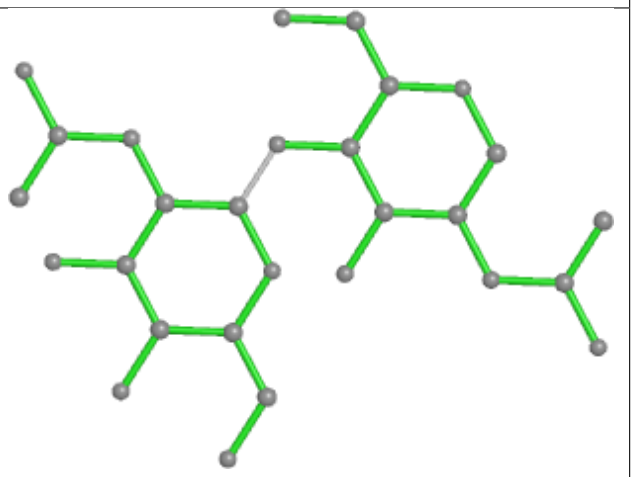

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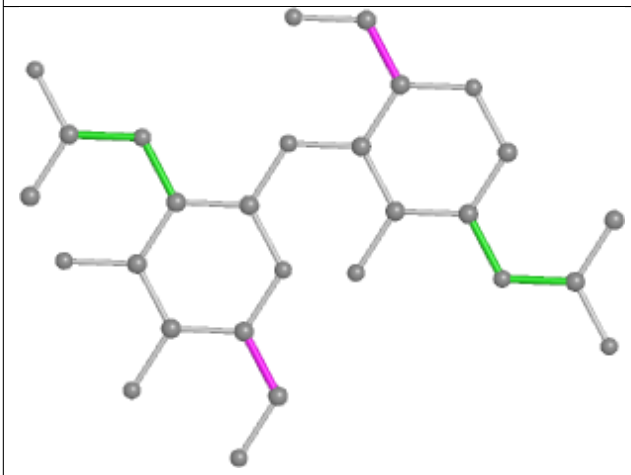

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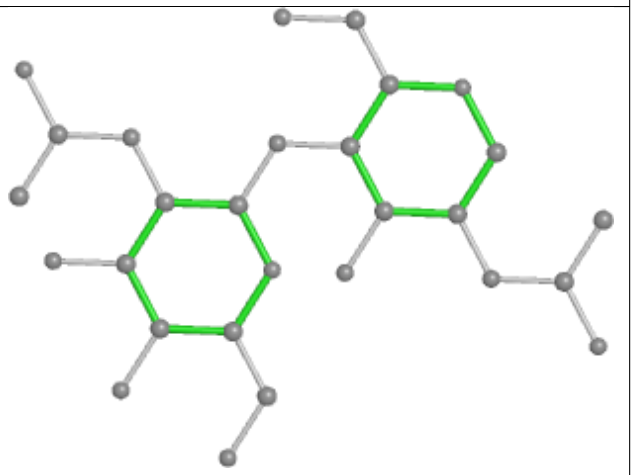
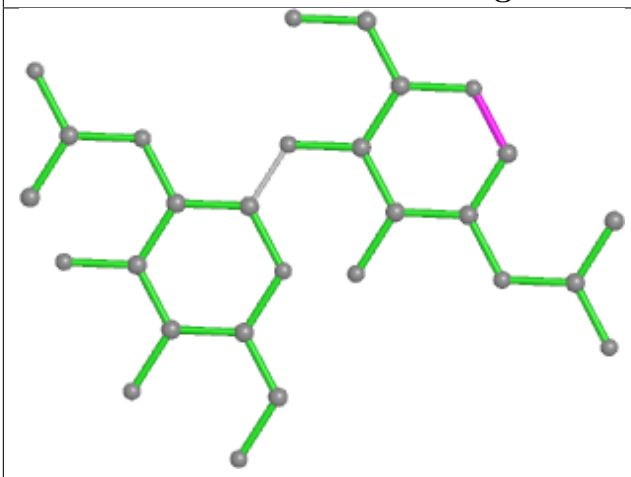


Rings

Oligosaccharide Chain Q



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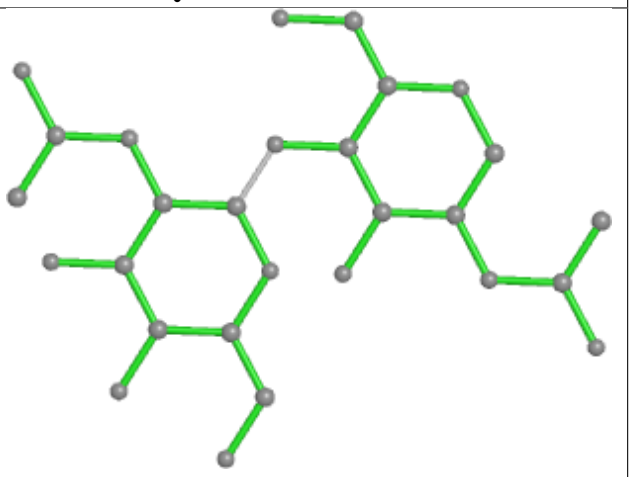

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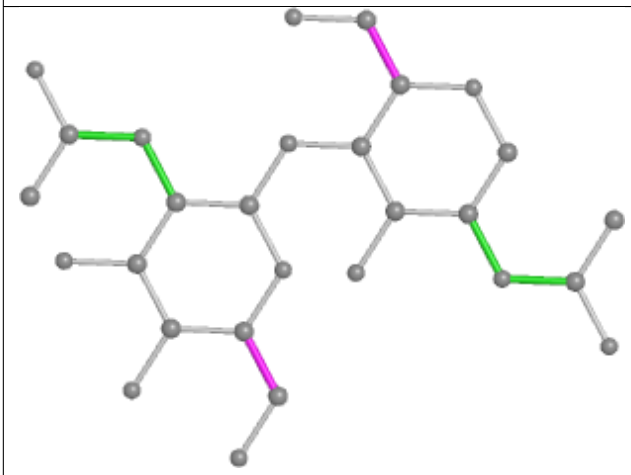

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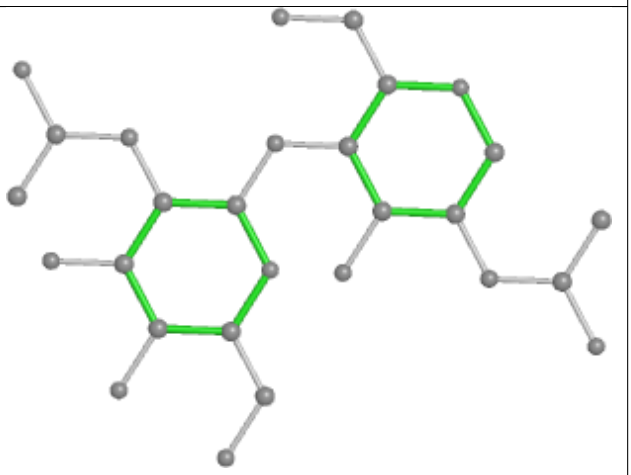
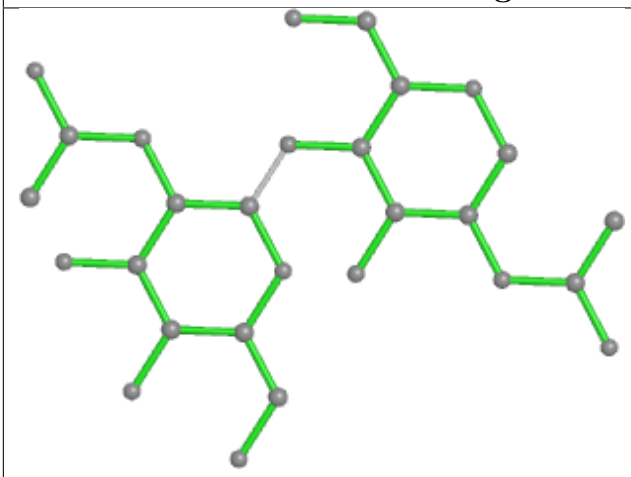


Rings

Oligosaccharide Chain R



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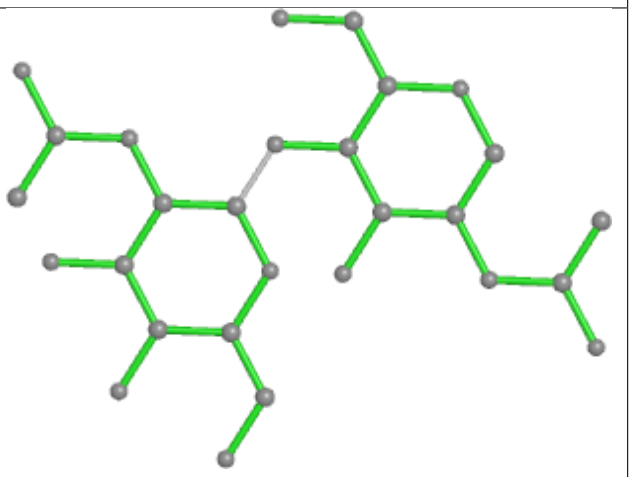

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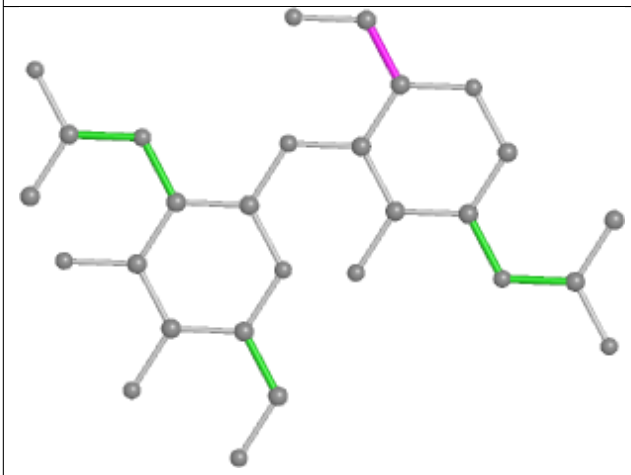

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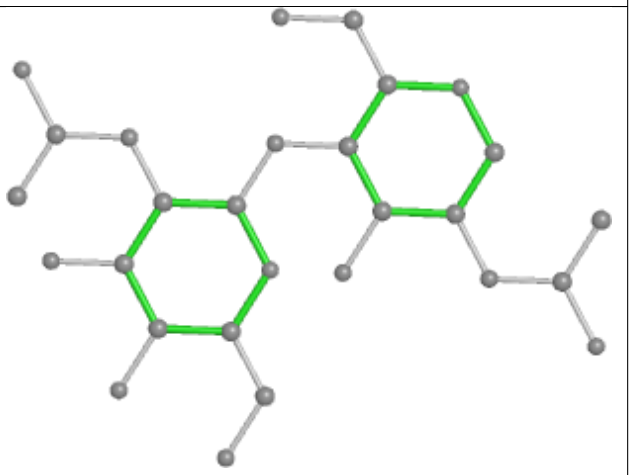
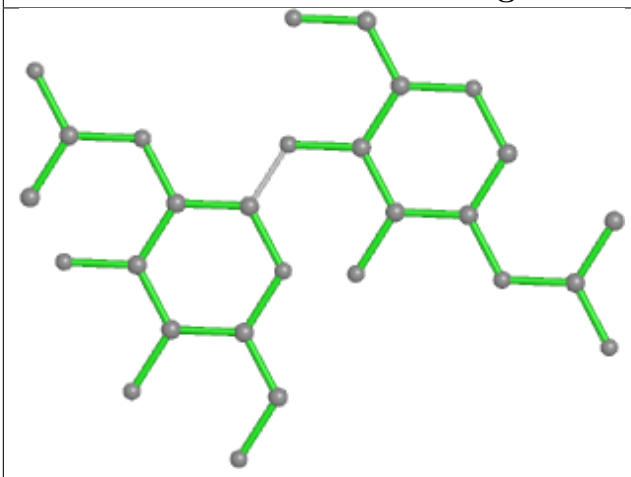


Rings

Oligosaccharide Chain S



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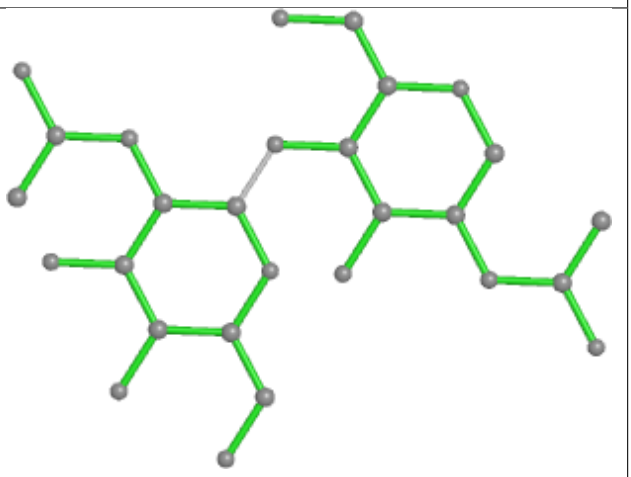

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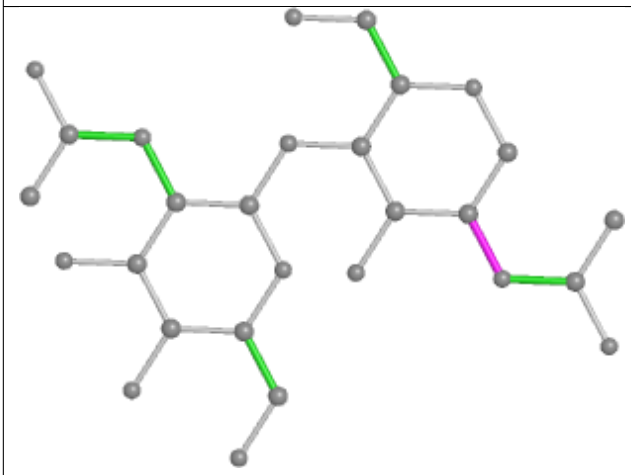

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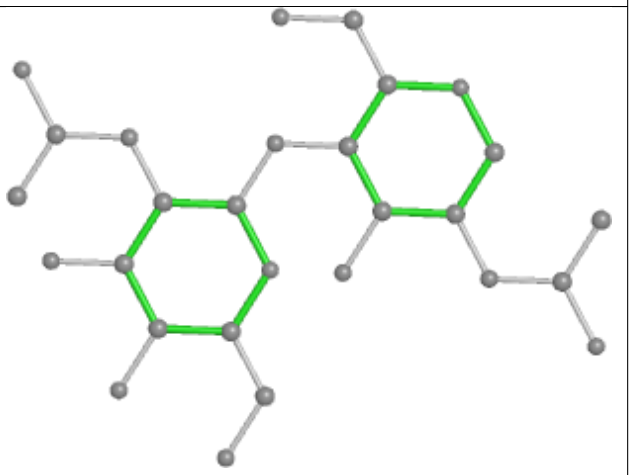
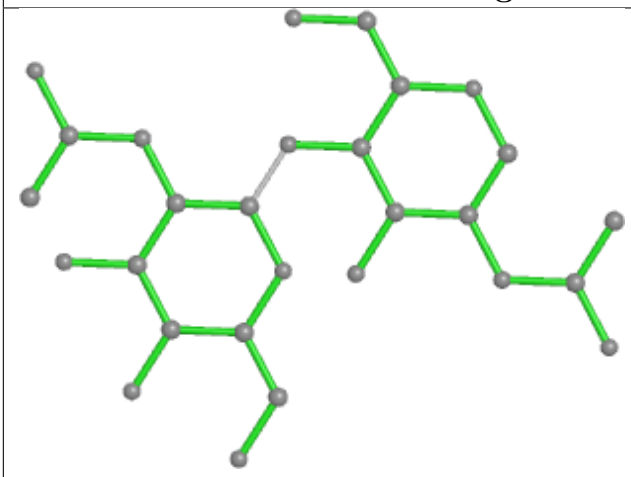


Rings

Oligosaccharide Chain T



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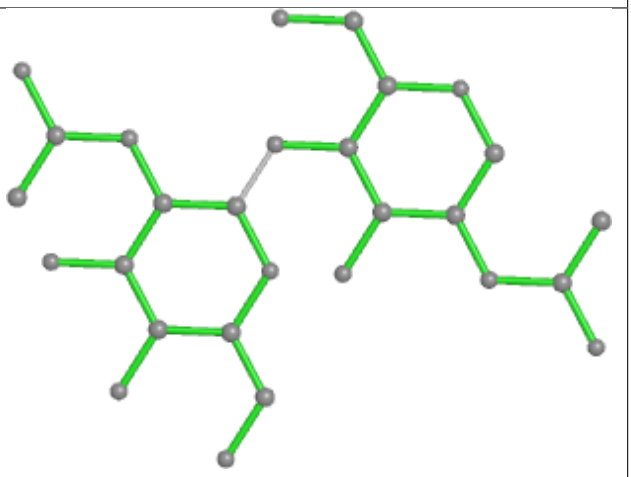

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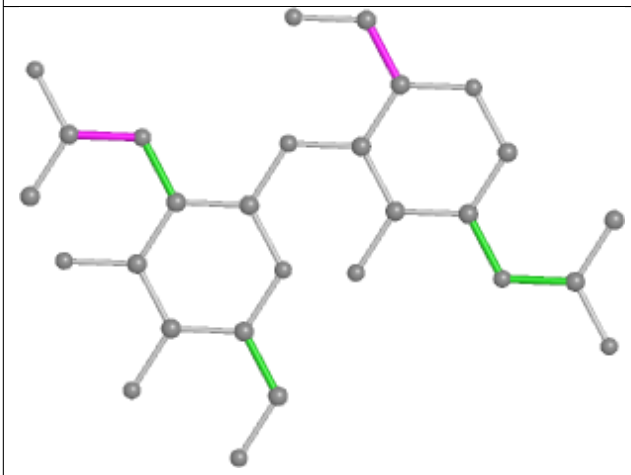

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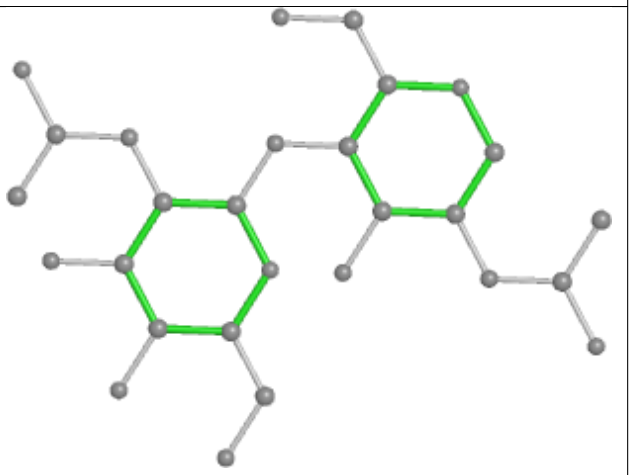
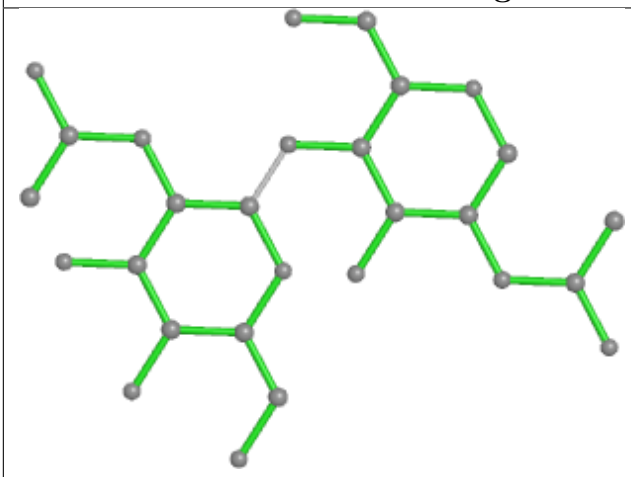


Rings

Oligosaccharide Chain U



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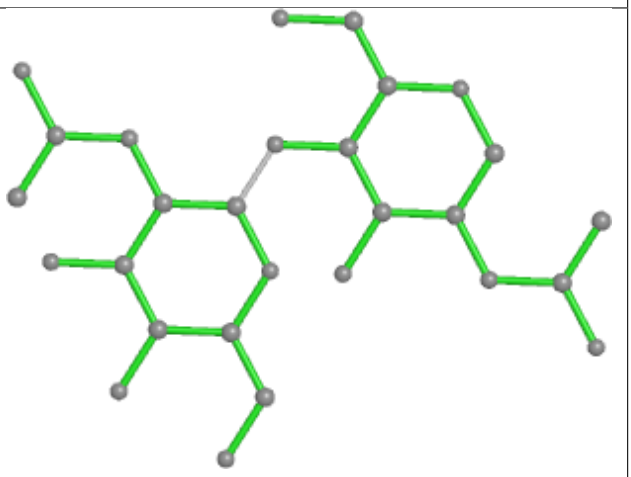

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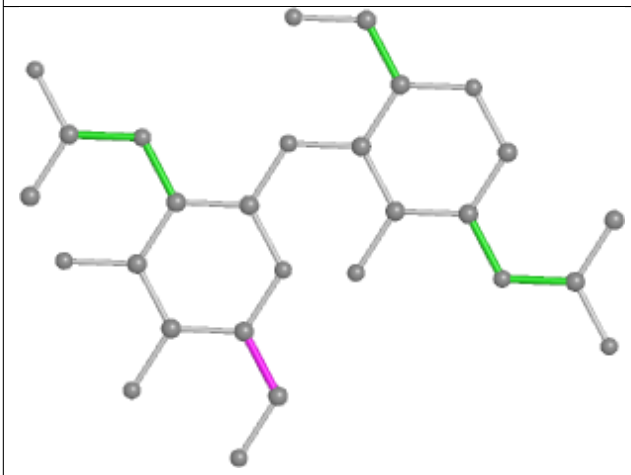

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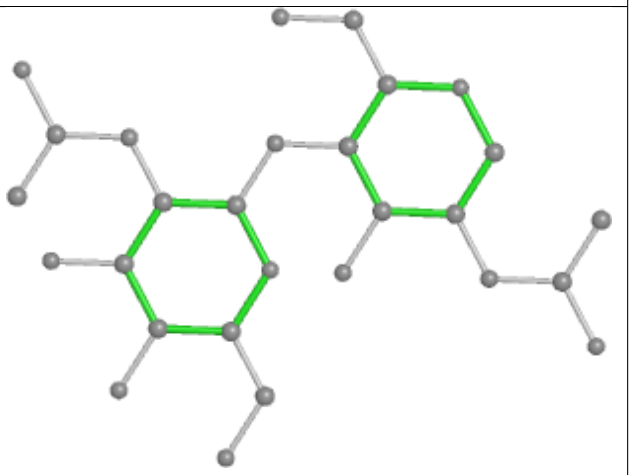
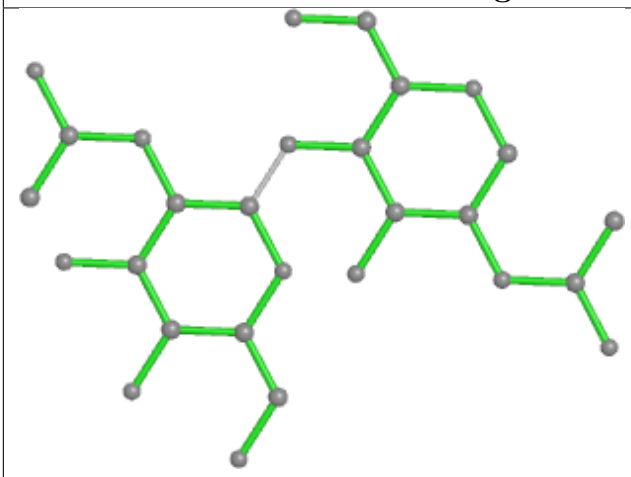


Rings

Oligosaccharide Chain V



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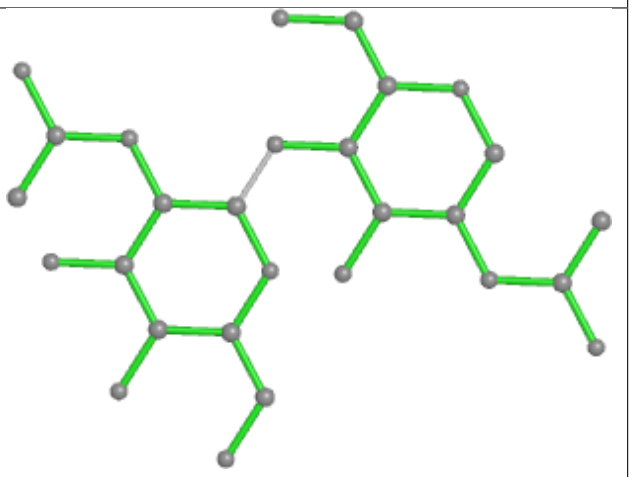

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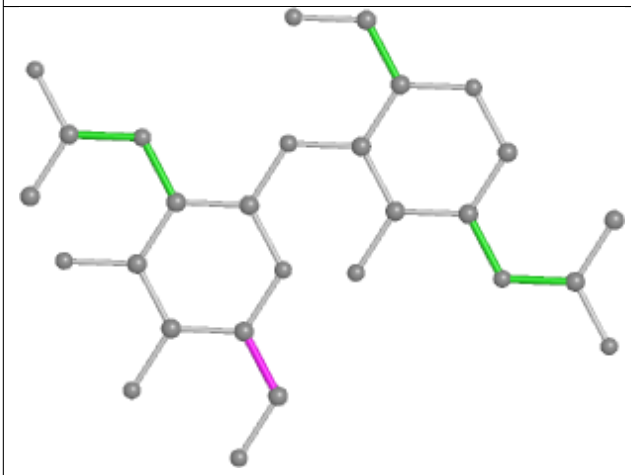

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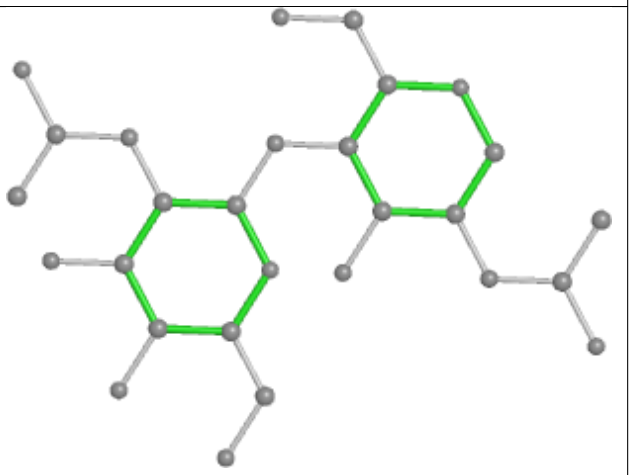
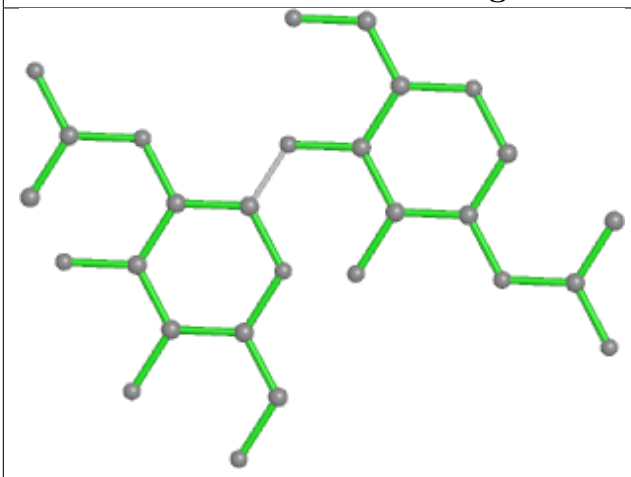


Rings

Oligosaccharide Chain W



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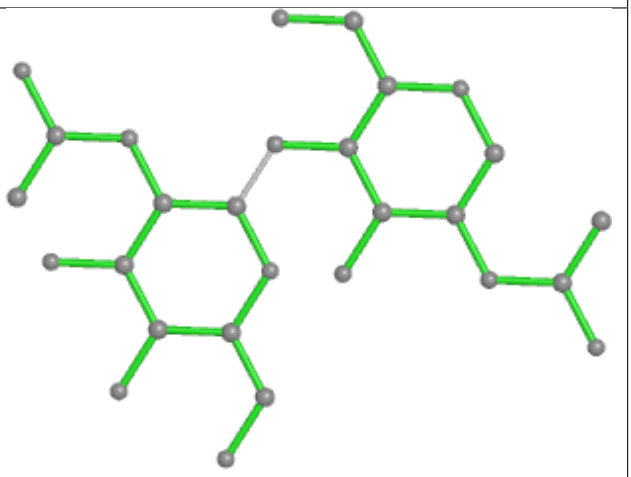
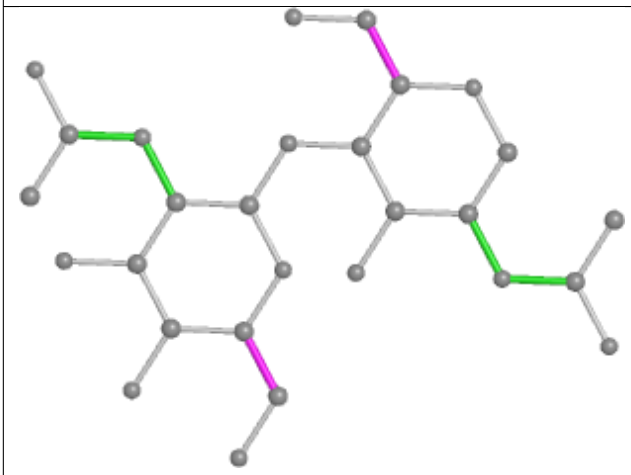


Bond angles



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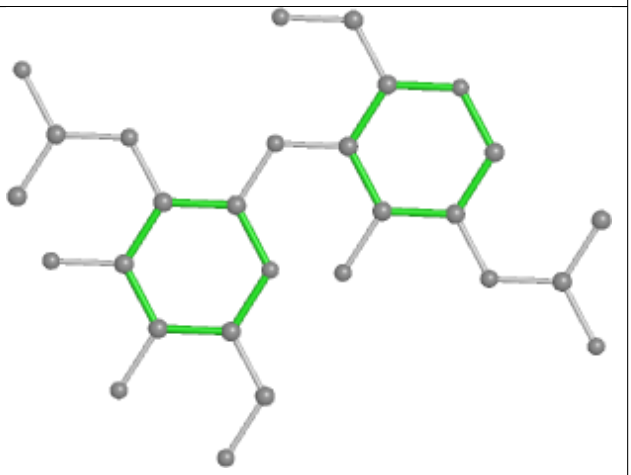
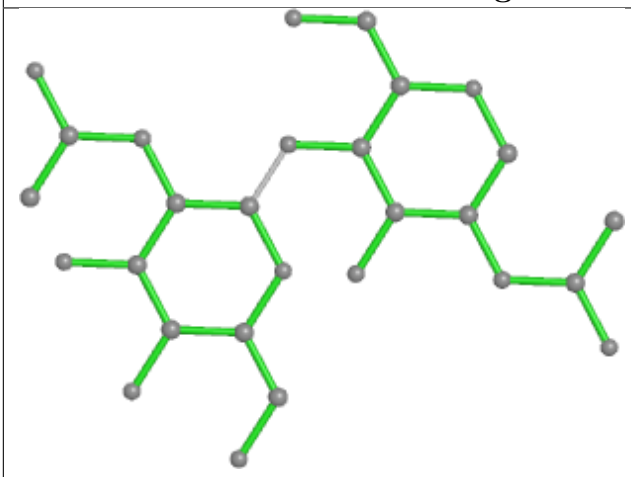


Rings

Oligosaccharide Chain X



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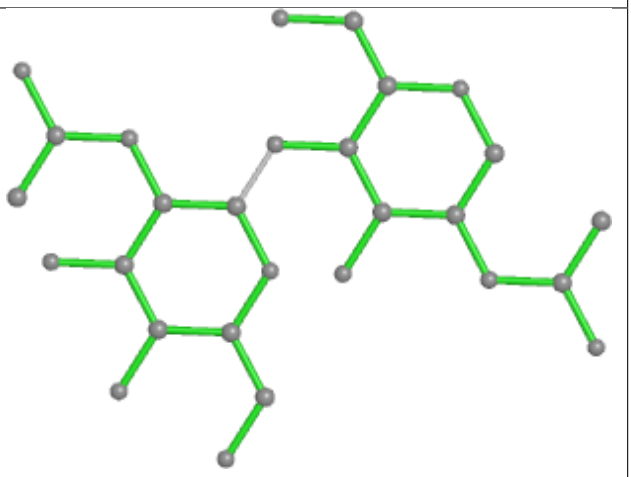
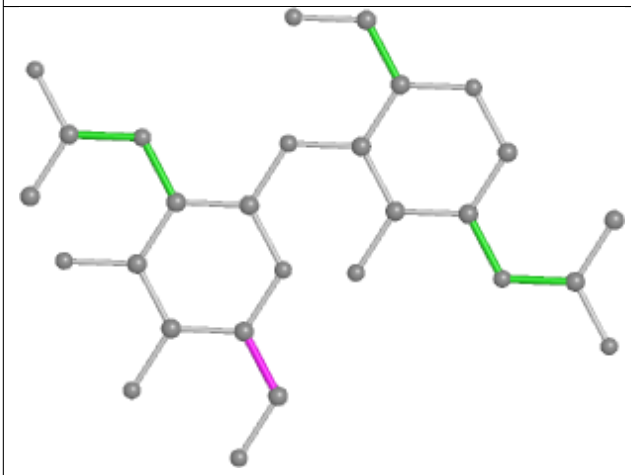


Bond angles



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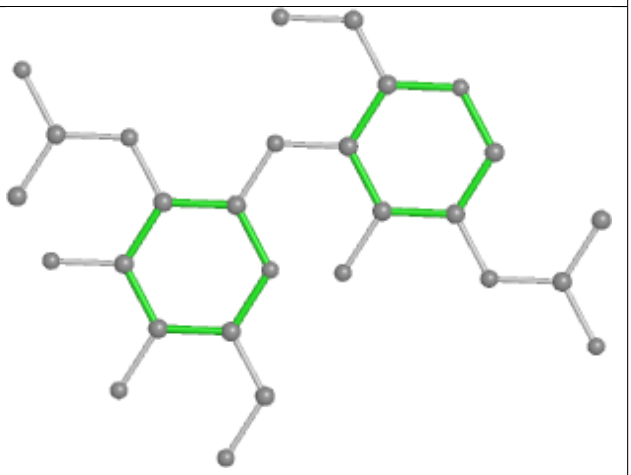
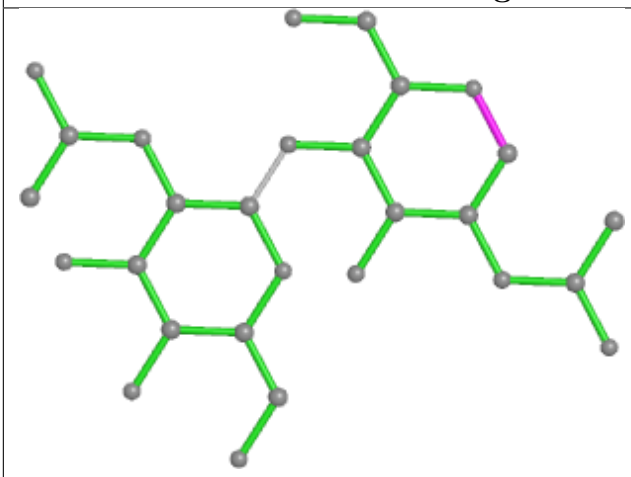


Rings

Oligosaccharide Chain Y



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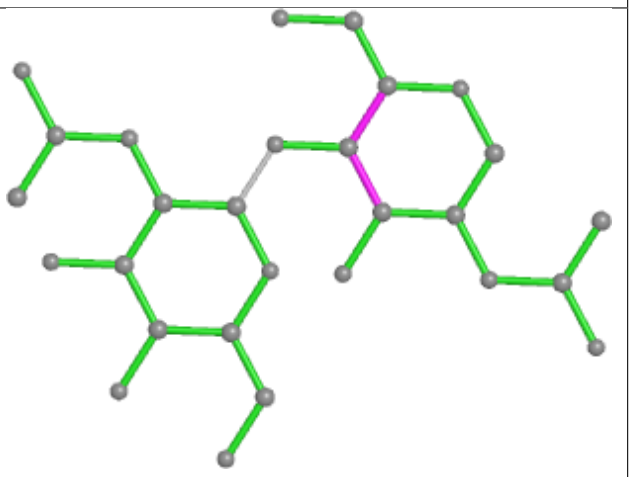
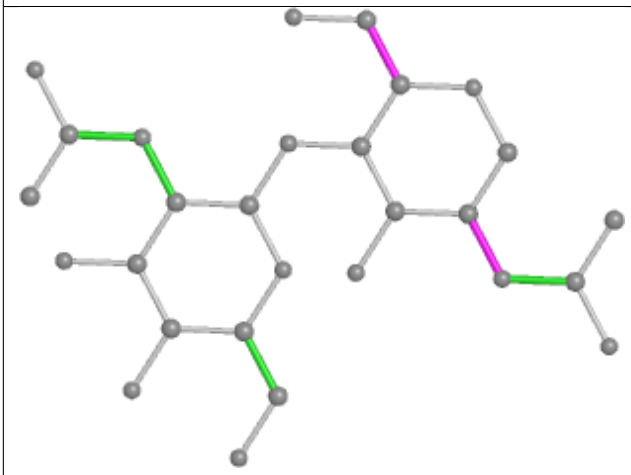


Bond angles



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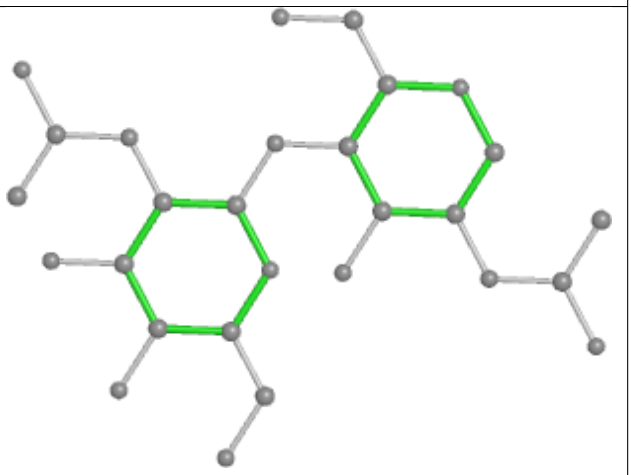
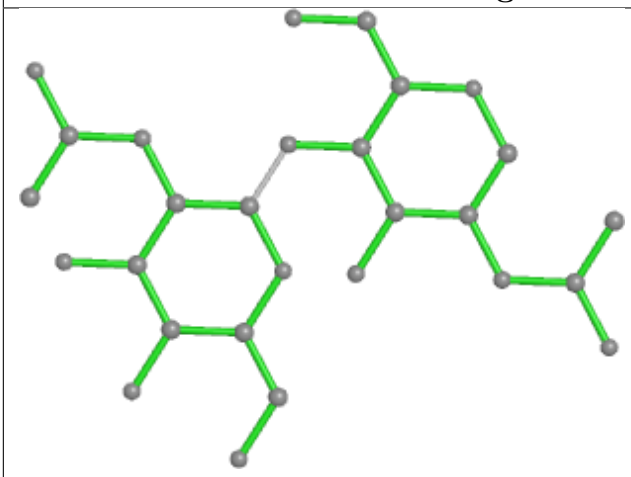
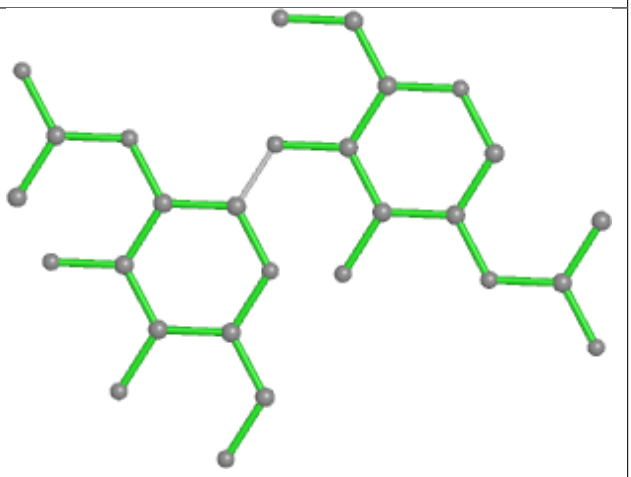


Rings

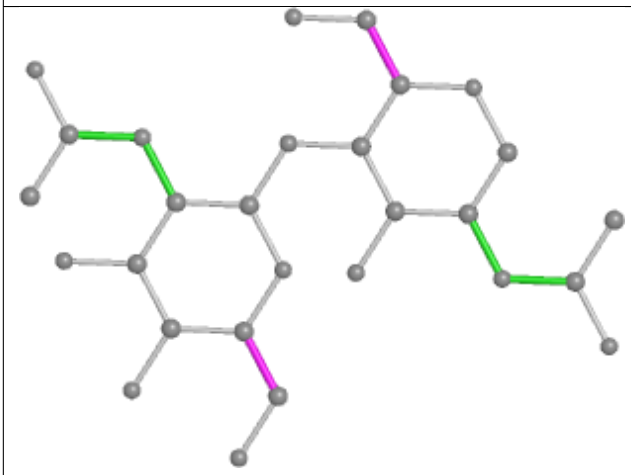
Oligosaccharide Chain Z



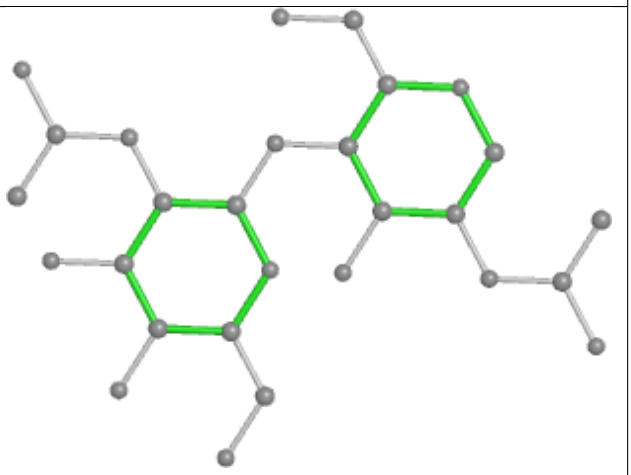
Bond lengths



Bond angles

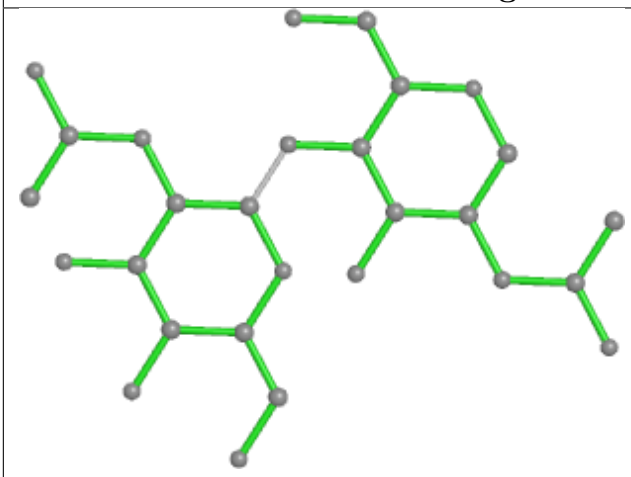


Torsions

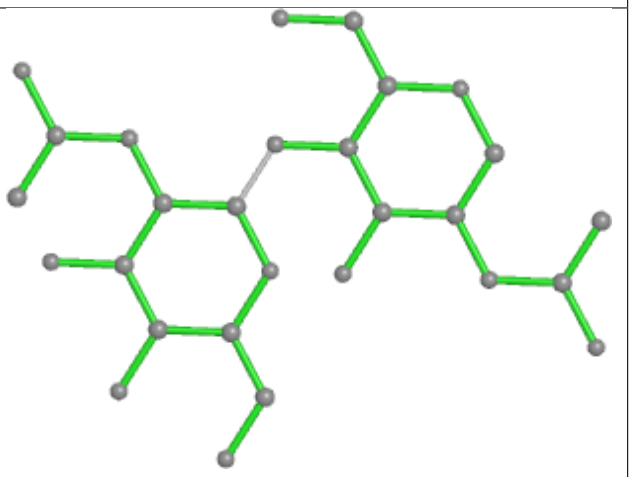


Rings

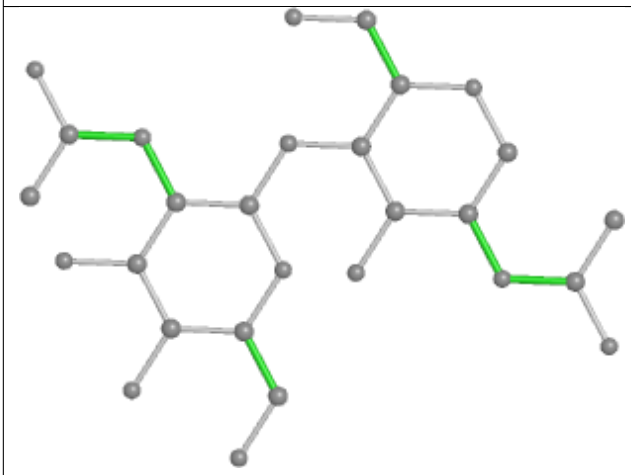
Oligosaccharide Chain a



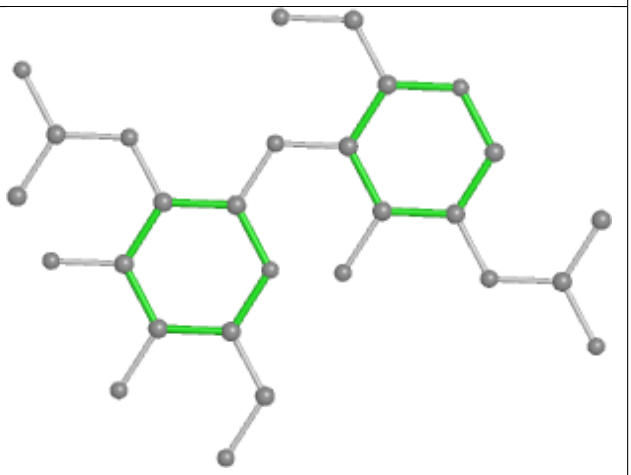
Bond lengths



Bond angles

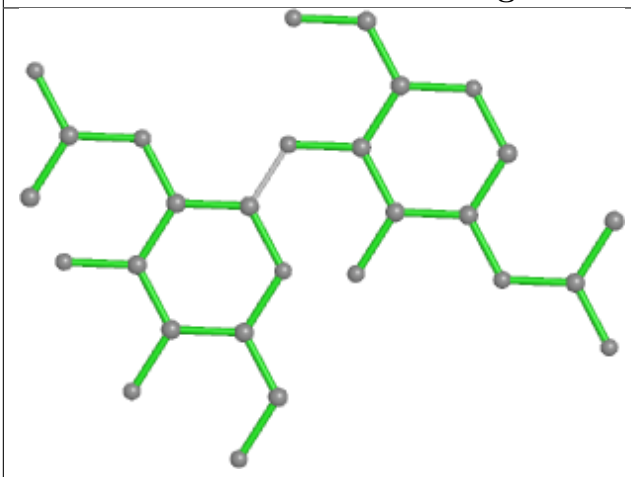


Torsions

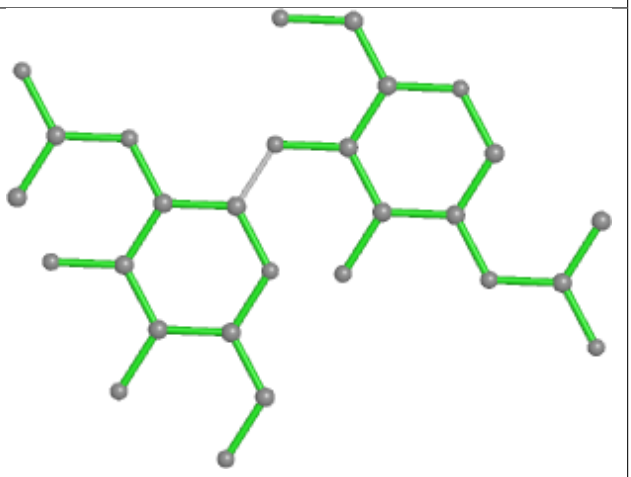


Rings

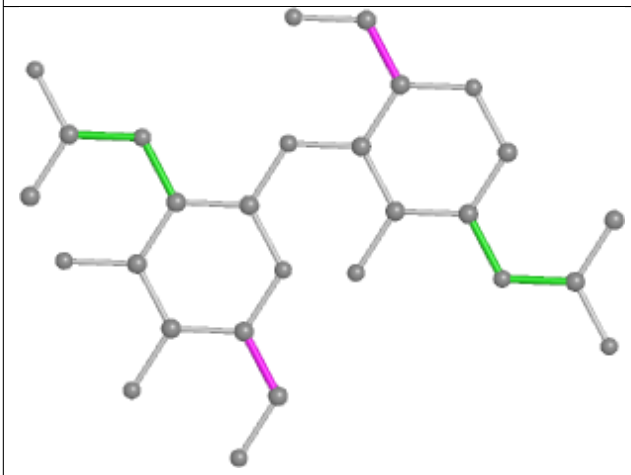
Oligosaccharide Chain b



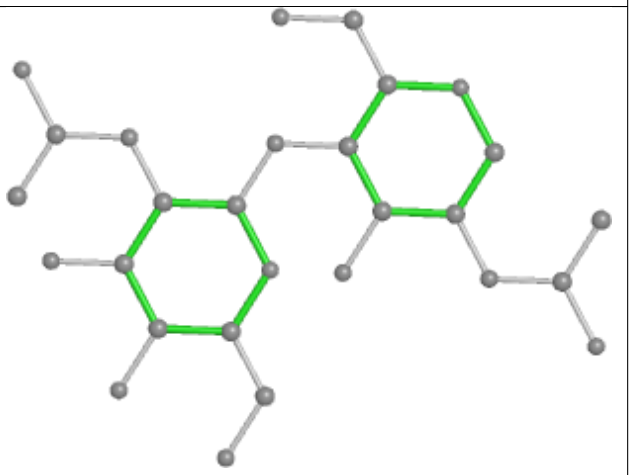
Bond lengths



Bond angles

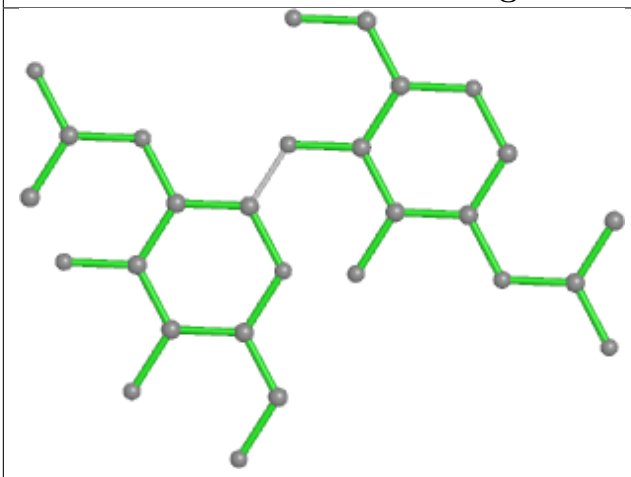


Torsions

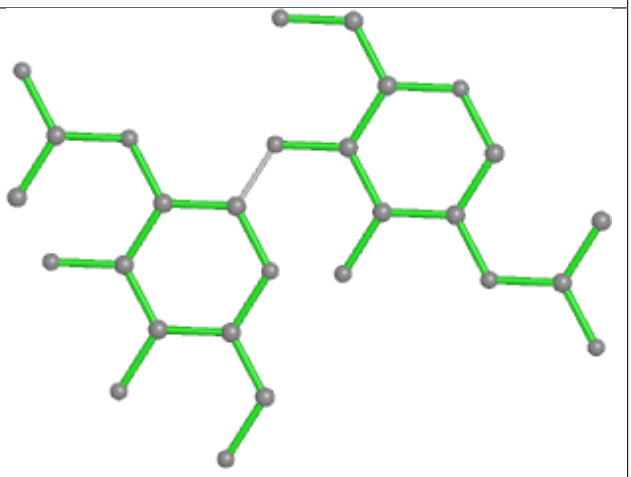


Rings

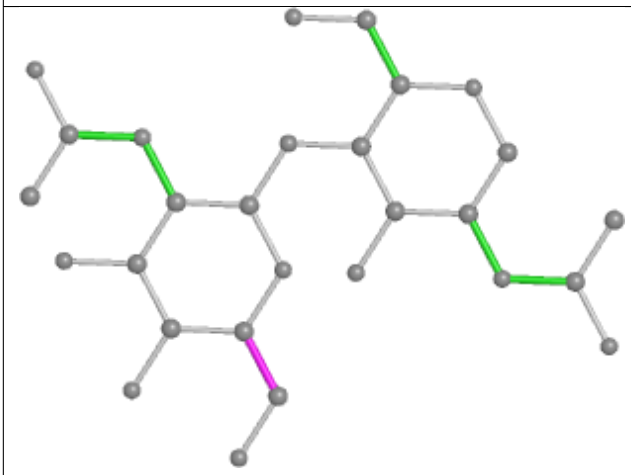
Oligosaccharide Chain c



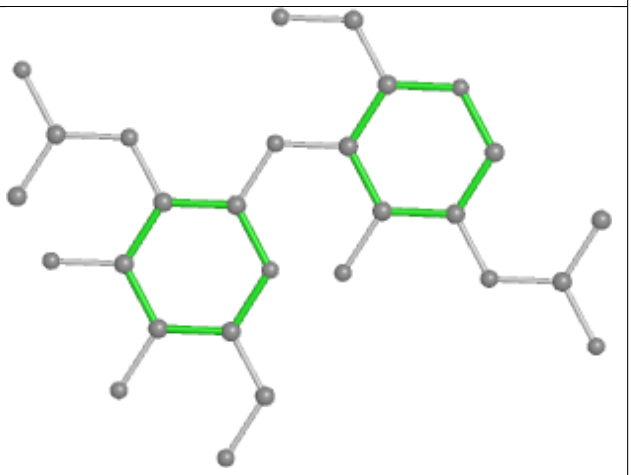
Bond lengths



Bond angles

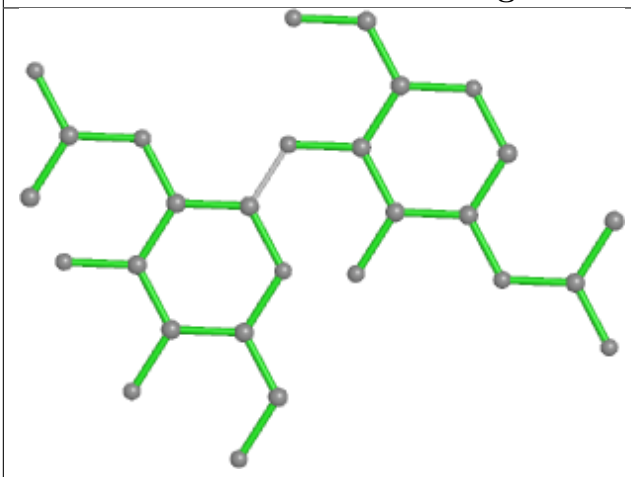


Torsions

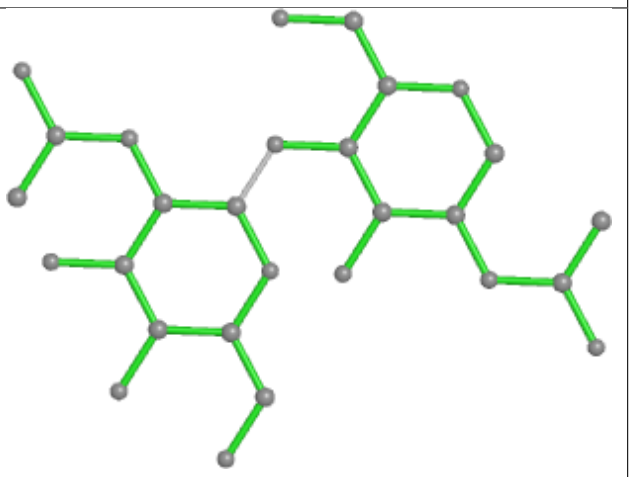


Rings

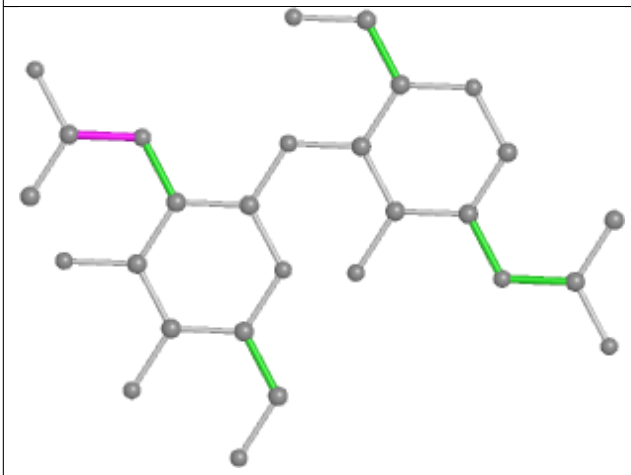
Oligosaccharide Chain d



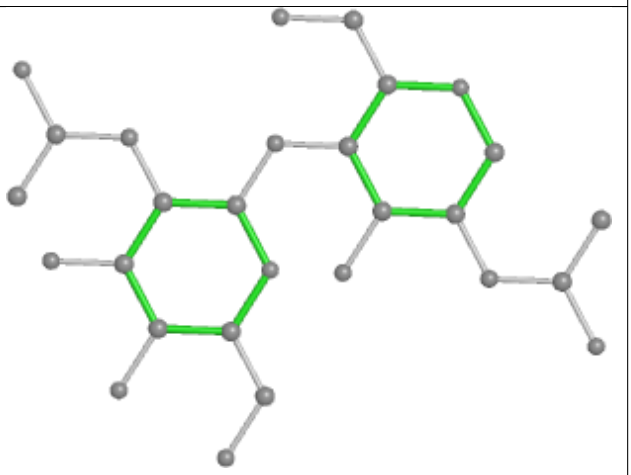
Bond lengths



Bond angles

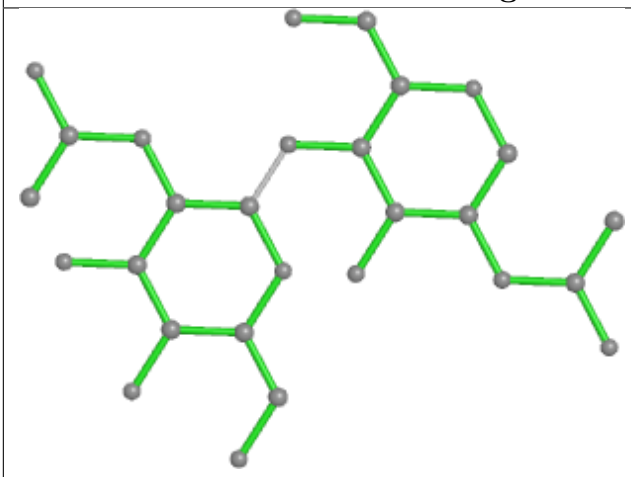


Torsions

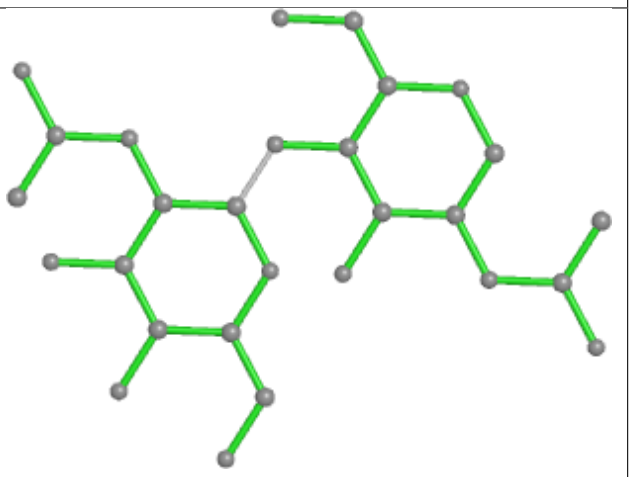


Rings

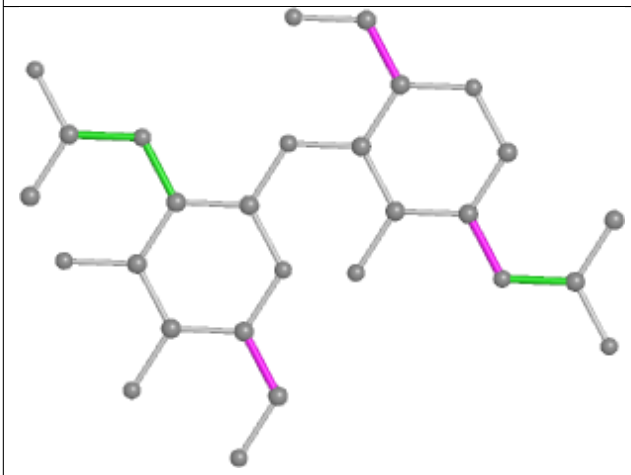
Oligosaccharide Chain e



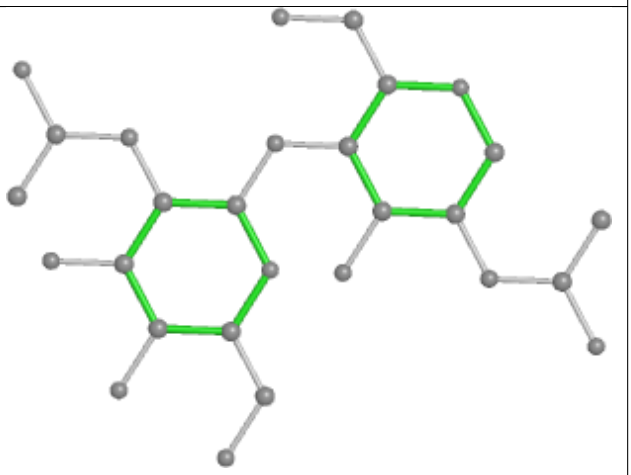
Bond lengths



Bond angles

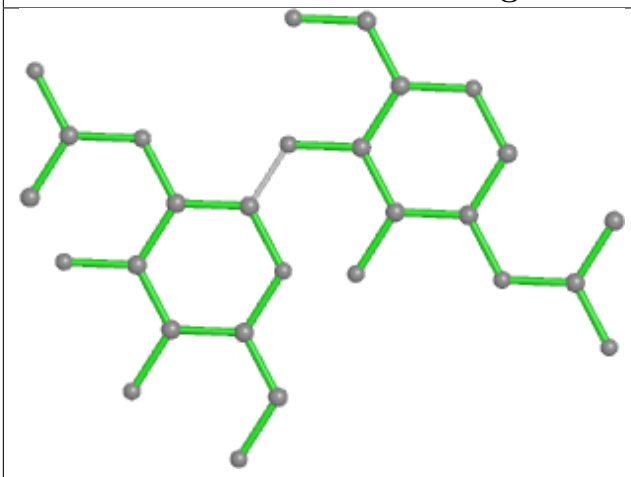


Torsions

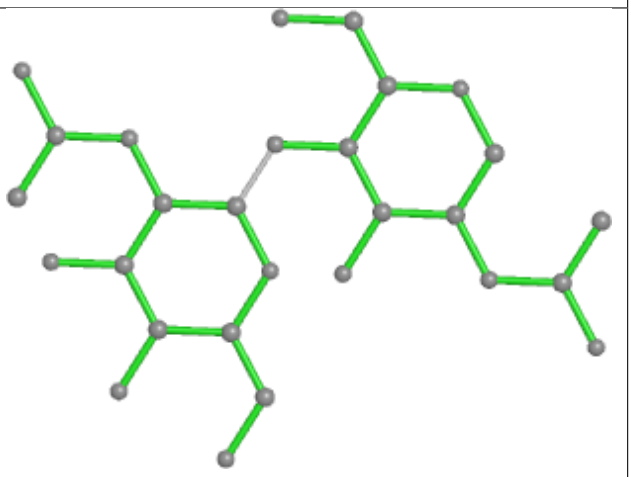


Rings

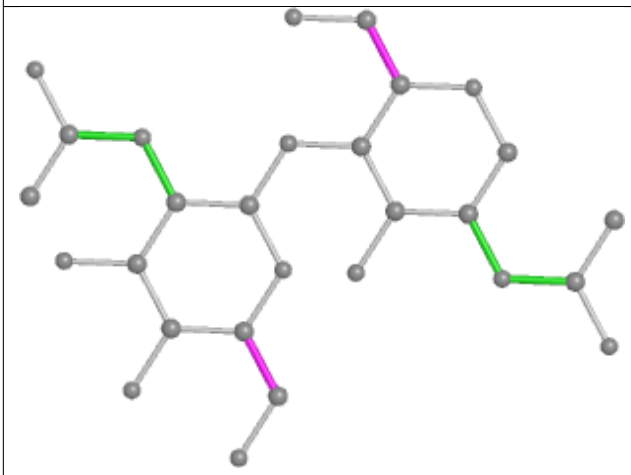
Oligosaccharide Chain f



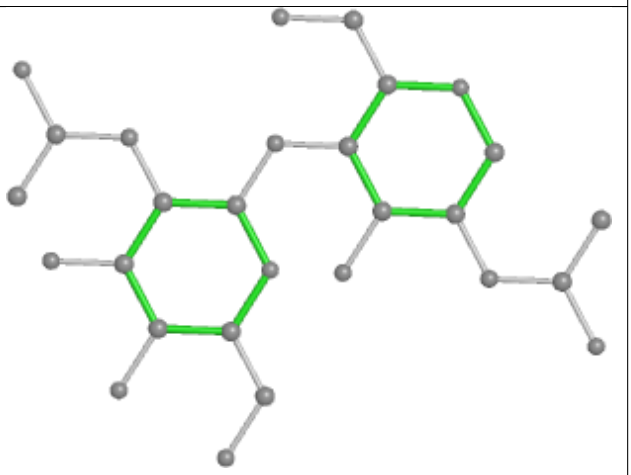
Bond lengths



Bond angles

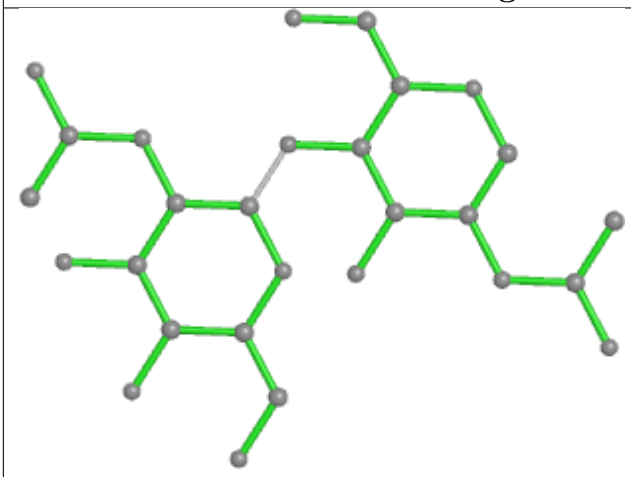


Torsions

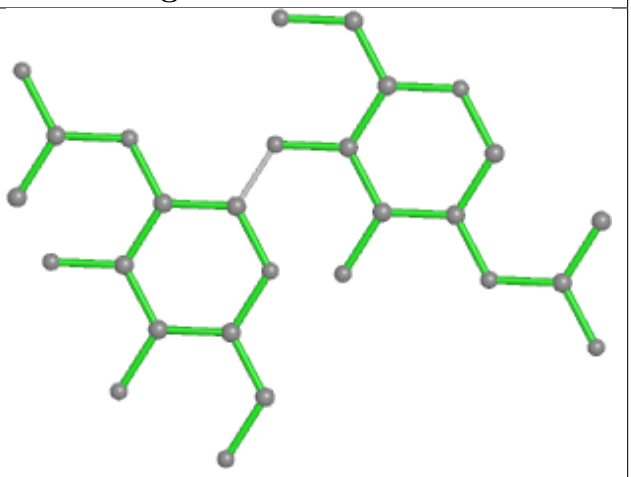


Rings

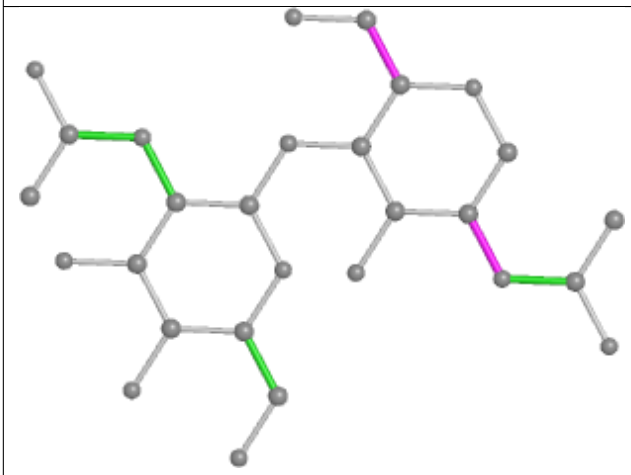
Oligosaccharide Chain g



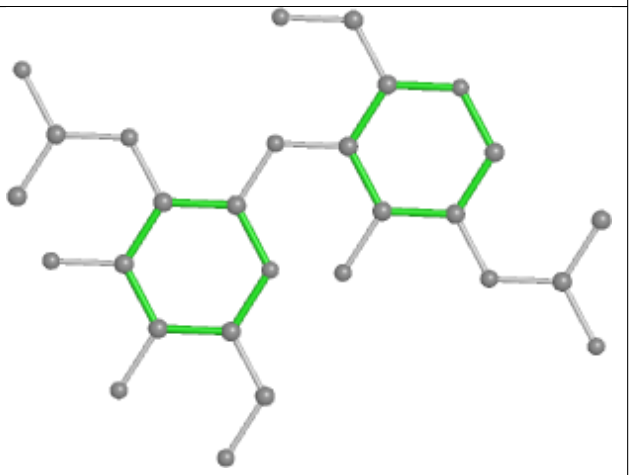
Bond lengths



Bond angles

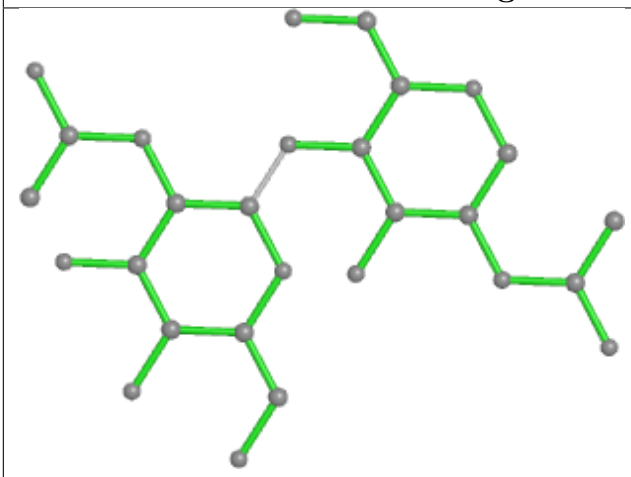


Torsions

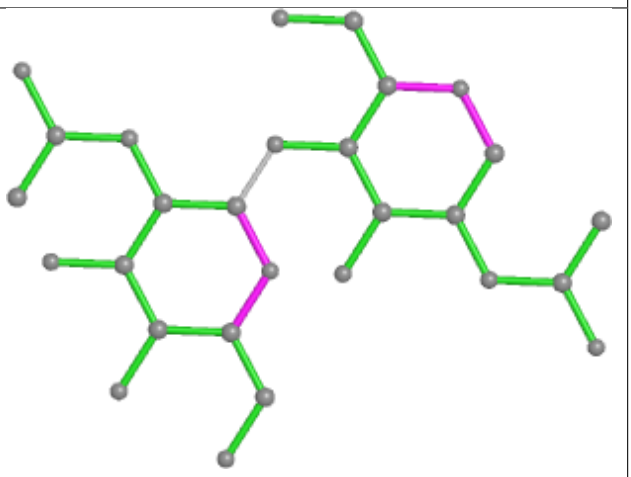


Rings

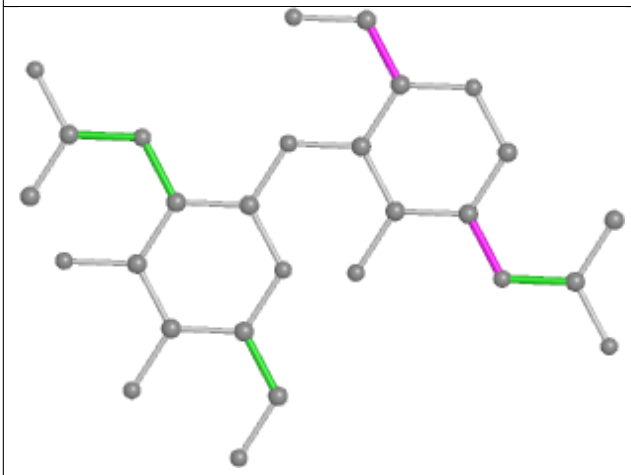
Oligosaccharide Chain h



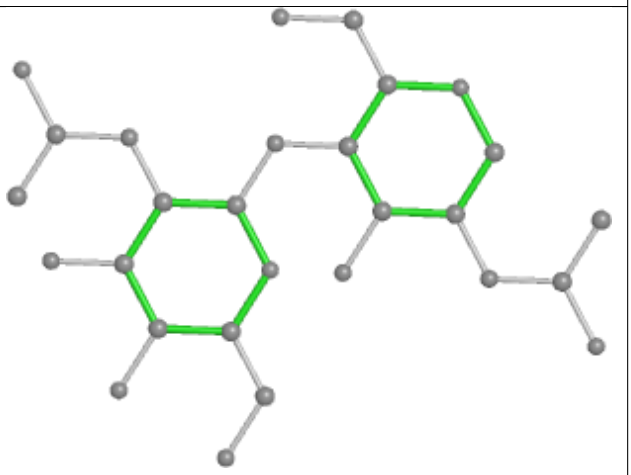
Bond lengths



Bond angles

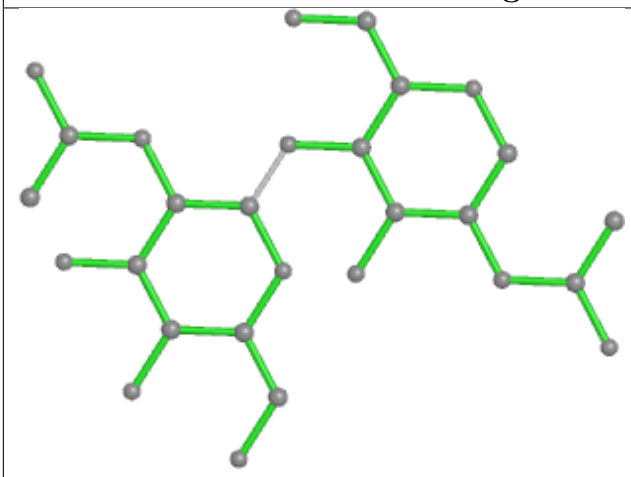


Torsions

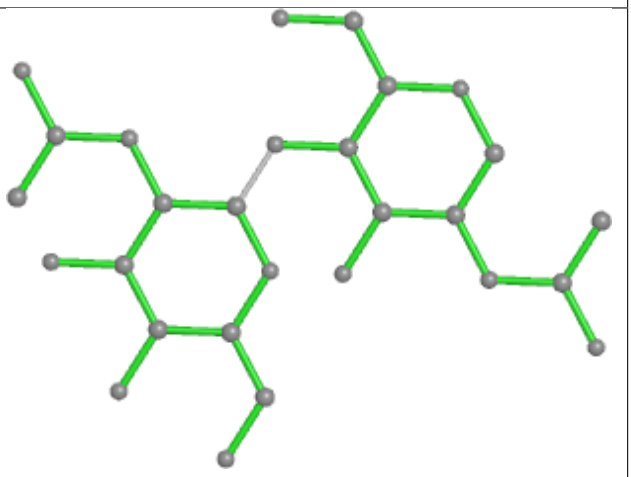


Rings

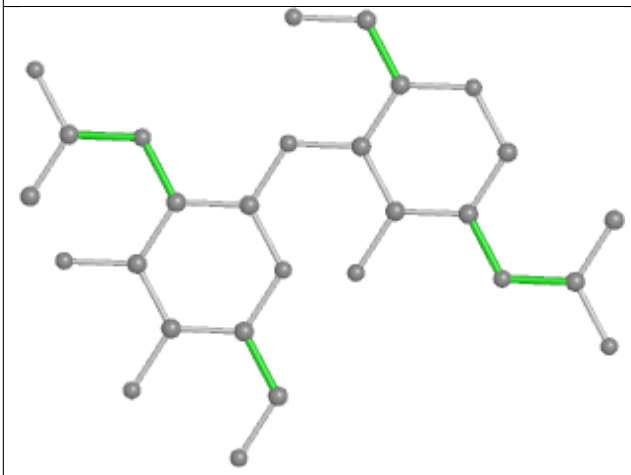
Oligosaccharide Chain i



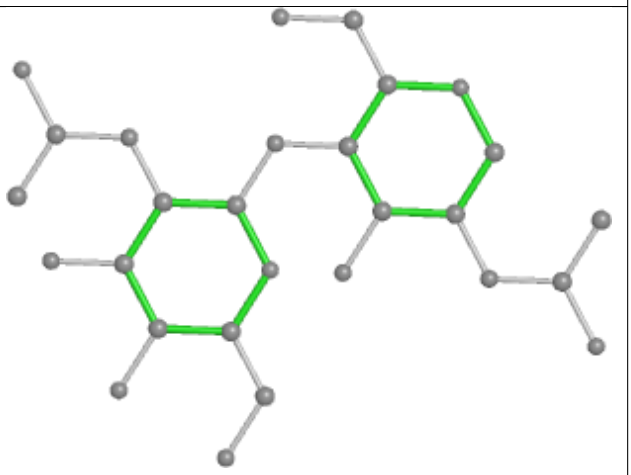
Bond lengths



Bond angles

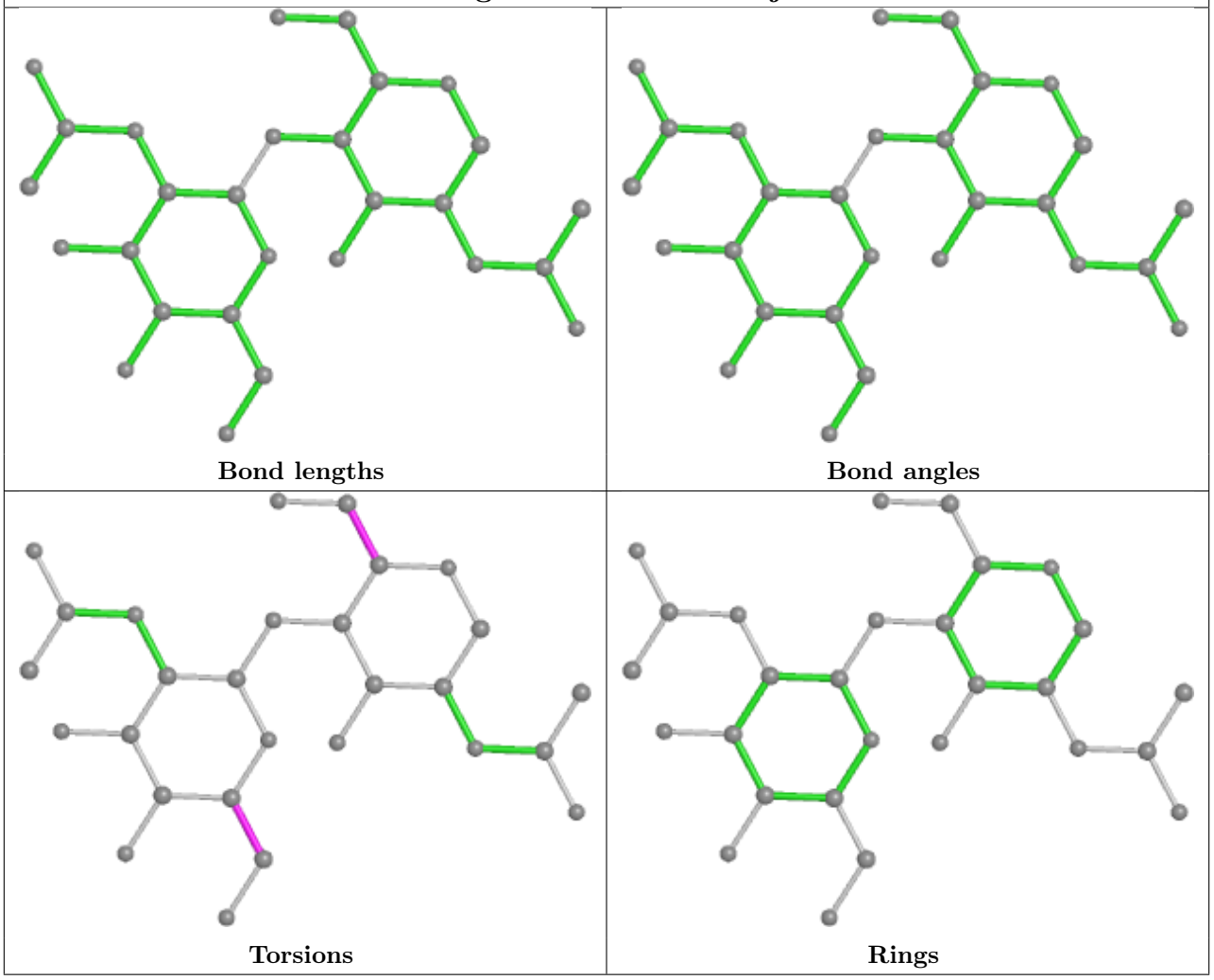


Torsions



Rings

Oligosaccharide Chain j



5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	2001	1	14,14,15	0.42	0	17,19,21	0.49	0
4	NAG	B	2003	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	A	2004	1	14,14,15	0.36	0	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	2001	1	14,14,15	0.23	0	17,19,21	0.34	0
4	NAG	A	2001	1	14,14,15	0.31	0	17,19,21	0.33	0
4	NAG	A	2003	1	14,14,15	0.30	0	17,19,21	0.43	0
4	NAG	B	2002	1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	C	2005	1	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	C	2002	1	14,14,15	0.22	0	17,19,21	0.70	1 (5%)
4	NAG	C	2003	1	14,14,15	0.23	0	17,19,21	0.37	0
4	NAG	A	2002	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	2004	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	B	2004	1	14,14,15	0.28	0	17,19,21	0.45	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	C	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2004	NAG	C2-N2-C7	4.31	129.04	122.90
4	C	2002	NAG	C1-O5-C5	2.50	115.57	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2002	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	A	2002	NAG	O5-C5-C6-O6
4	A	2002	NAG	C4-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	B	2001	NAG	C4-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	C	2003	NAG	C4-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	B	2004	NAG	C4-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	A	2001	NAG	C8-C7-N2-C2
4	A	2001	NAG	O7-C7-N2-C2
4	A	2004	NAG	C8-C7-N2-C2
4	A	2004	NAG	O7-C7-N2-C2
4	B	2003	NAG	C8-C7-N2-C2
4	B	2003	NAG	O7-C7-N2-C2
4	C	2001	NAG	C8-C7-N2-C2
4	C	2001	NAG	O7-C7-N2-C2
4	C	2003	NAG	C8-C7-N2-C2
4	C	2003	NAG	O7-C7-N2-C2
4	C	2004	NAG	C8-C7-N2-C2
4	C	2004	NAG	O7-C7-N2-C2
4	C	2002	NAG	O5-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6
4	A	2004	NAG	O5-C5-C6-O6
4	C	2002	NAG	C4-C5-C6-O6
4	A	2004	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2001	NAG	2	0
4	A	2004	NAG	1	0
4	A	2001	NAG	2	0
4	B	2002	NAG	1	0
4	C	2004	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

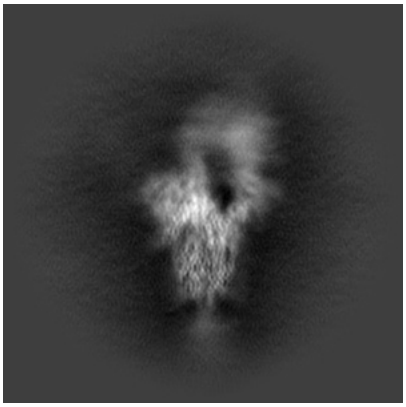
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31790. These allow visual inspection of the internal detail of the map and identification of artifacts.

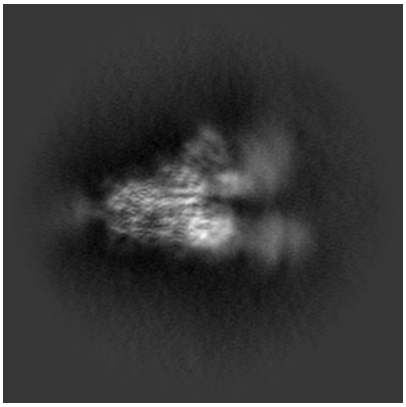
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

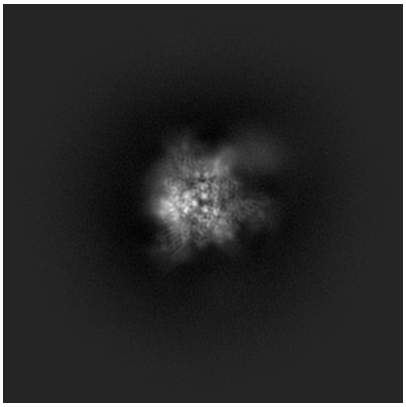
6.1.1 Primary map



X



Y



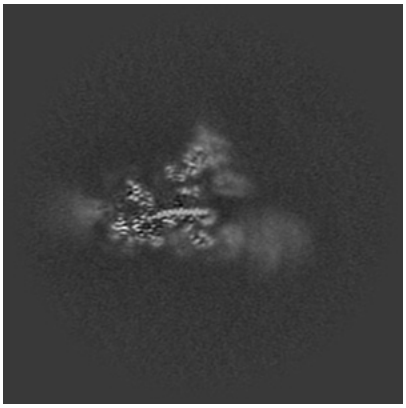
Z

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

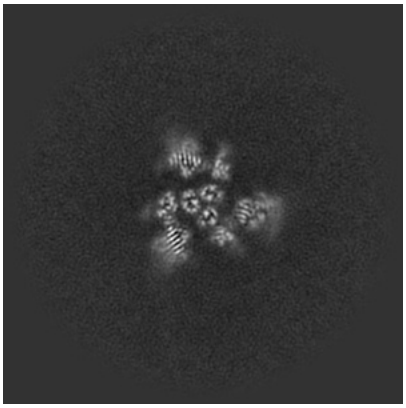
6.2 Central slices

6.2.1 Primary map

X Index: 192



Y Index: 192

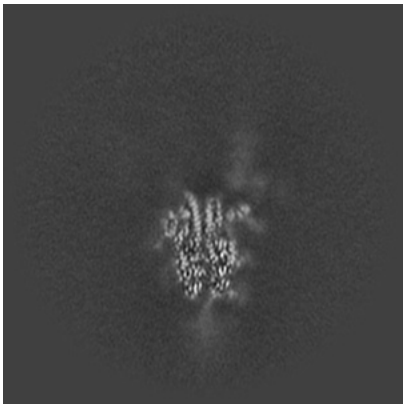


Z Index: 192

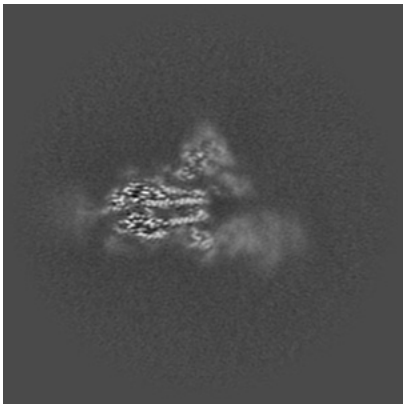
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

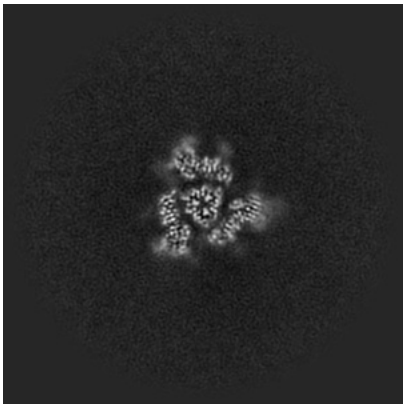
6.3.1 Primary map



X Index: 195



Y Index: 185



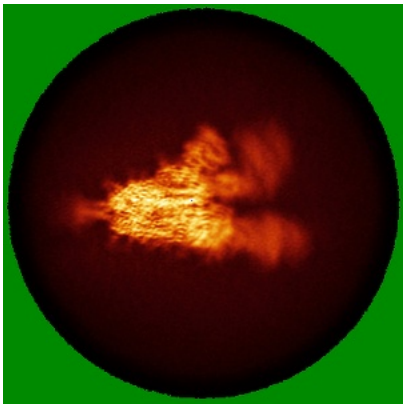
Z Index: 186

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

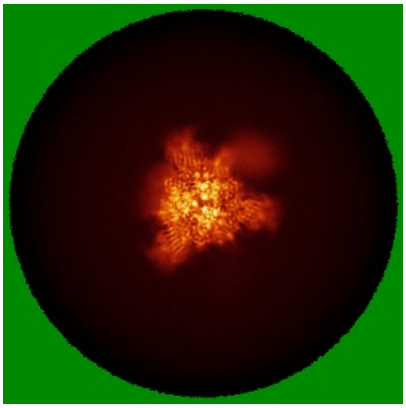
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

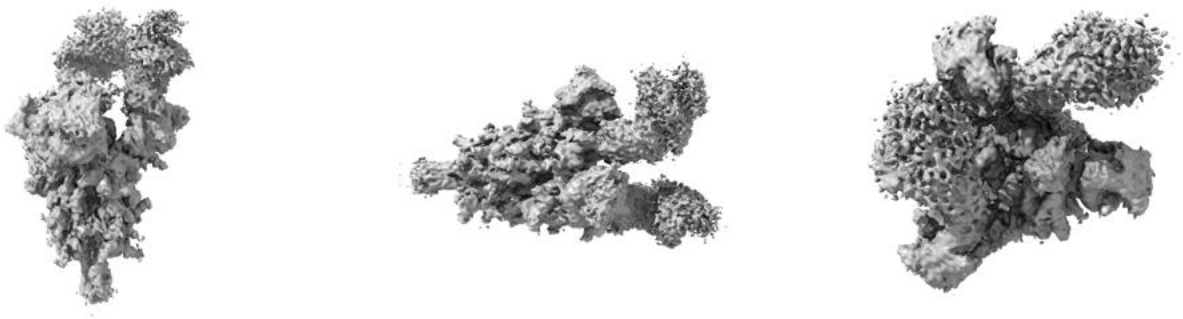


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

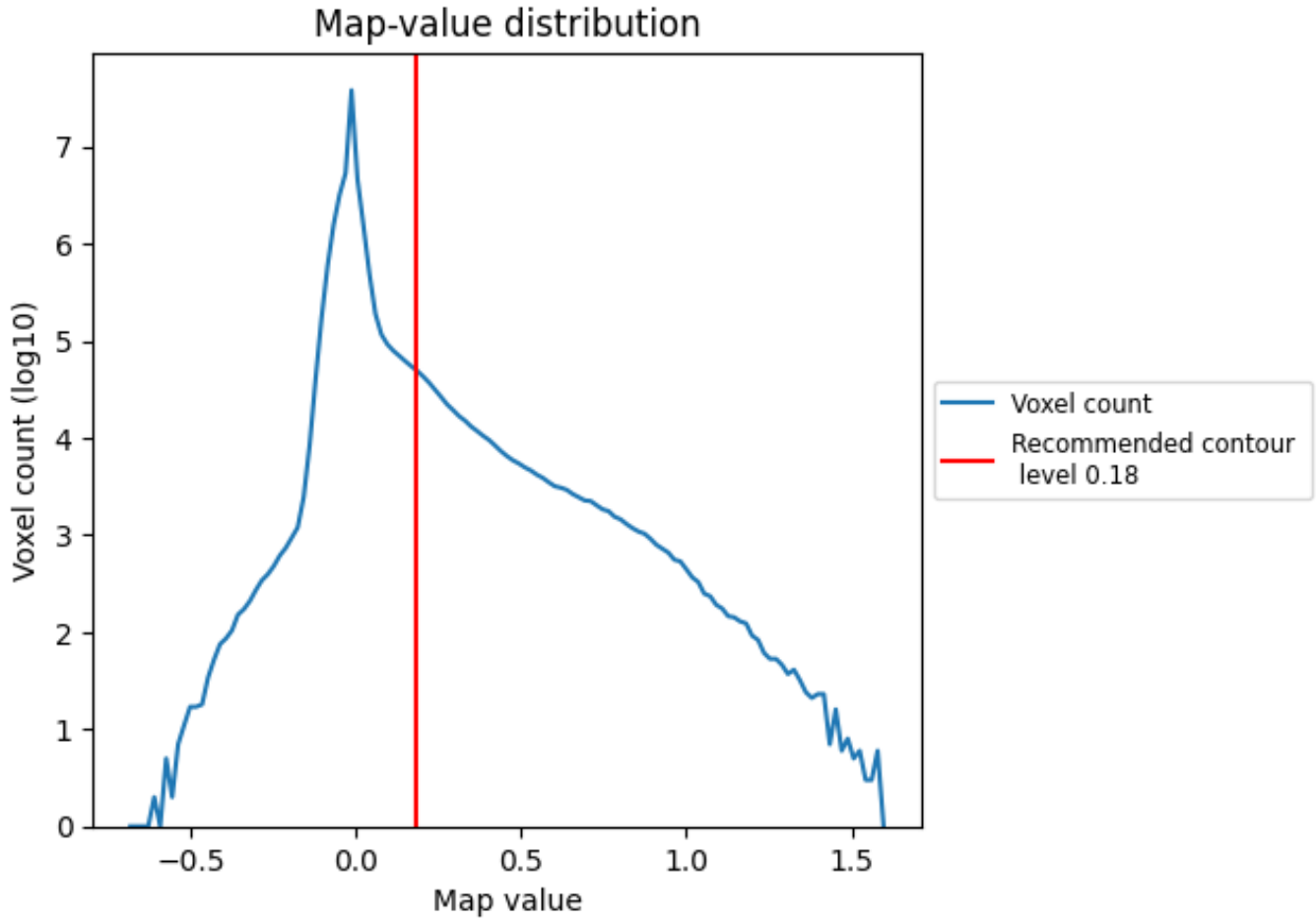
6.6 Mask visualisation (i)

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

7 Map analysis

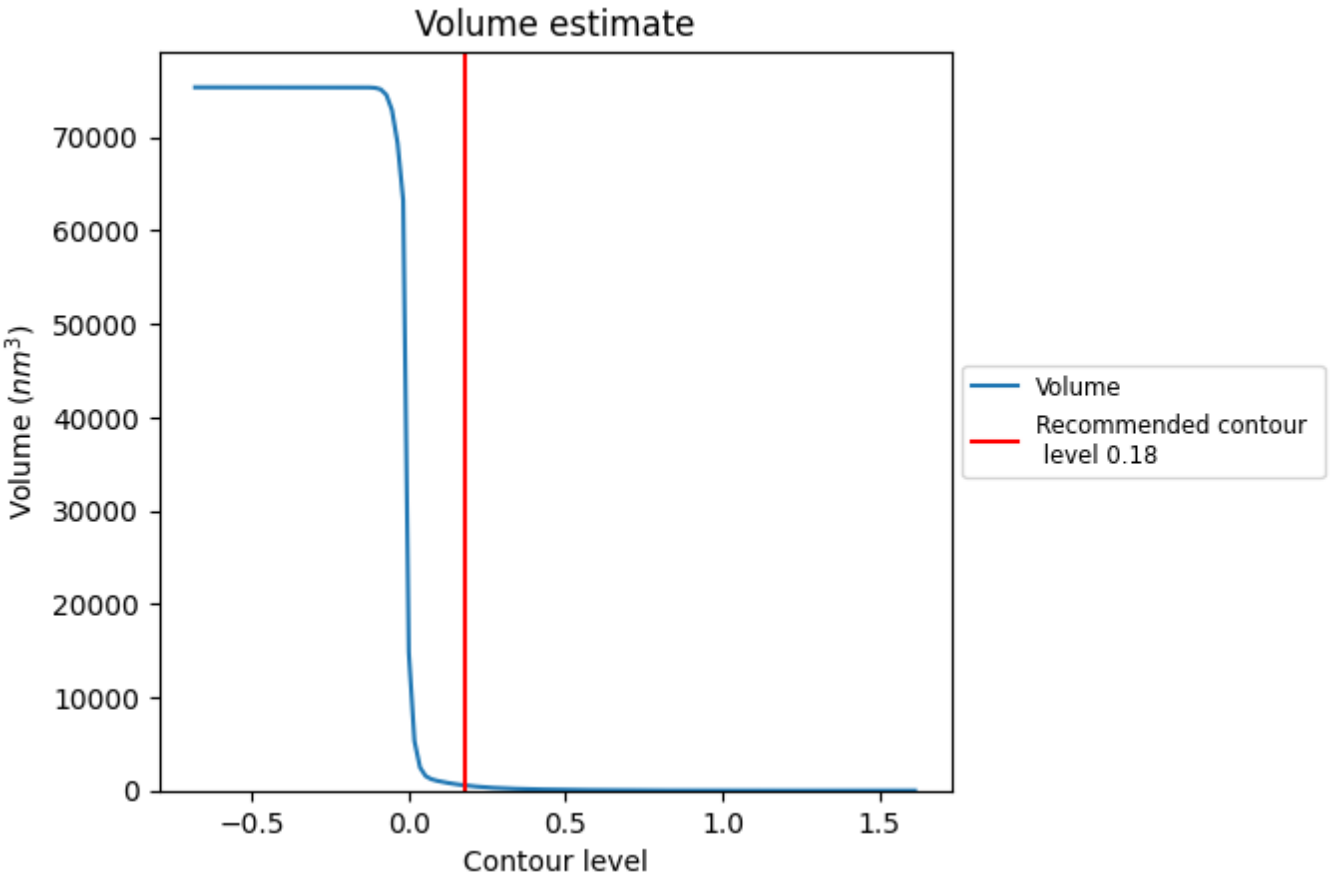
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

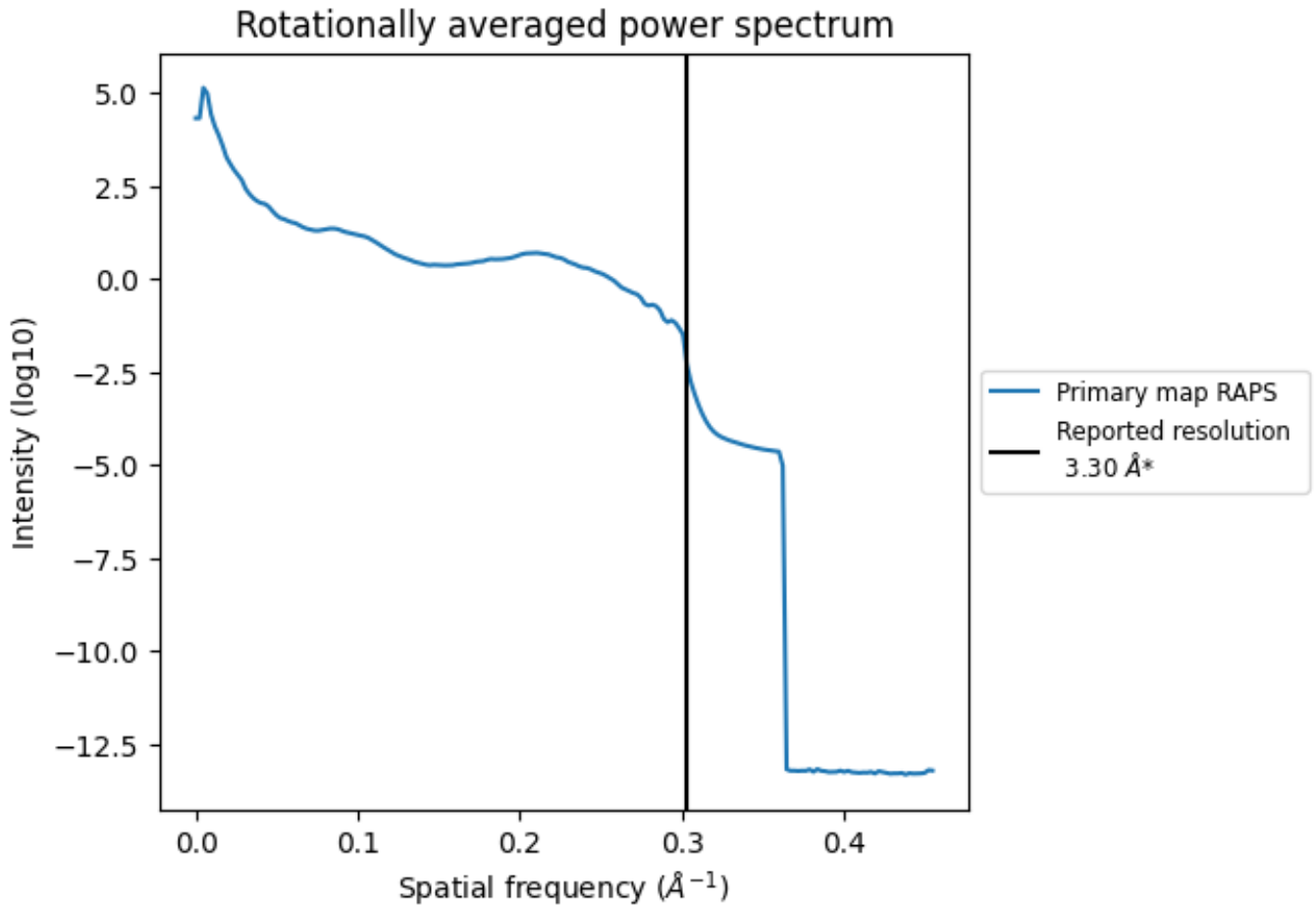
7.2 Volume estimate



The volume at the recommended contour level is 554 nm^3; this corresponds to an approximate mass of 501 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 0.303 $Å^{-1}$

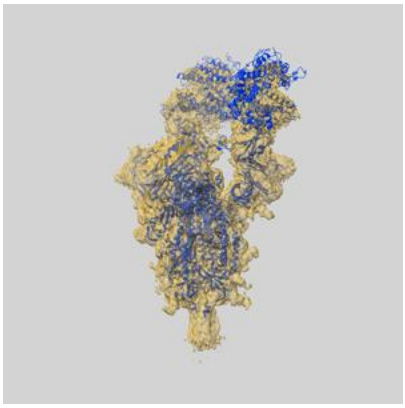
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

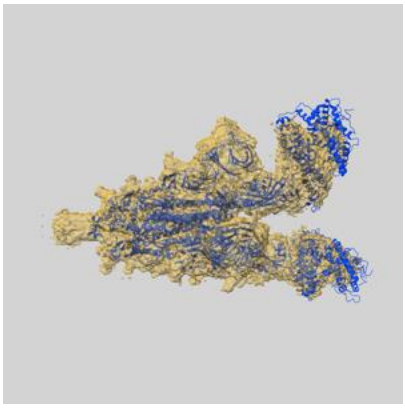
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31790 and PDB model 7V85. Per-residue inclusion information can be found in section 3 on page 15.

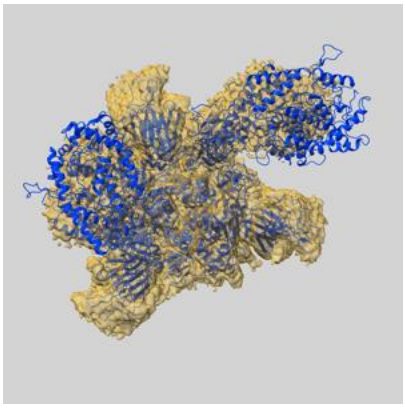
9.1 Map-model overlay



X



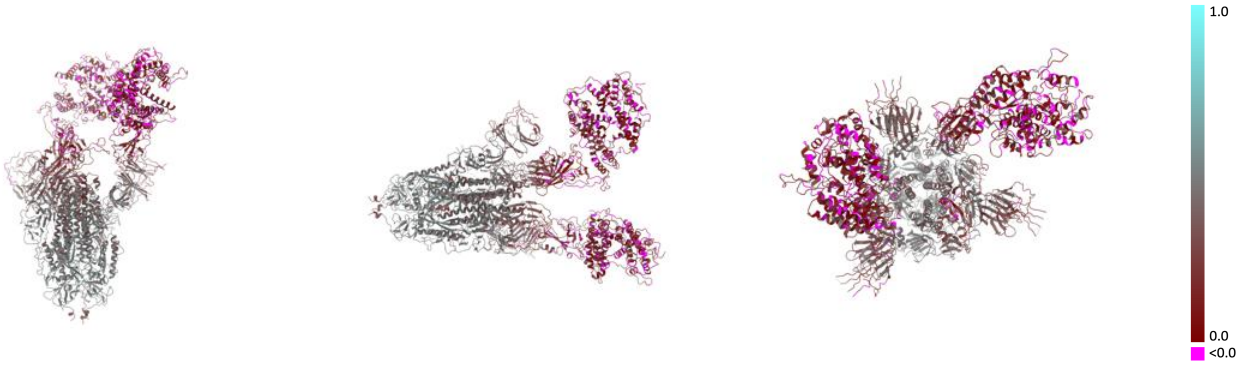
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

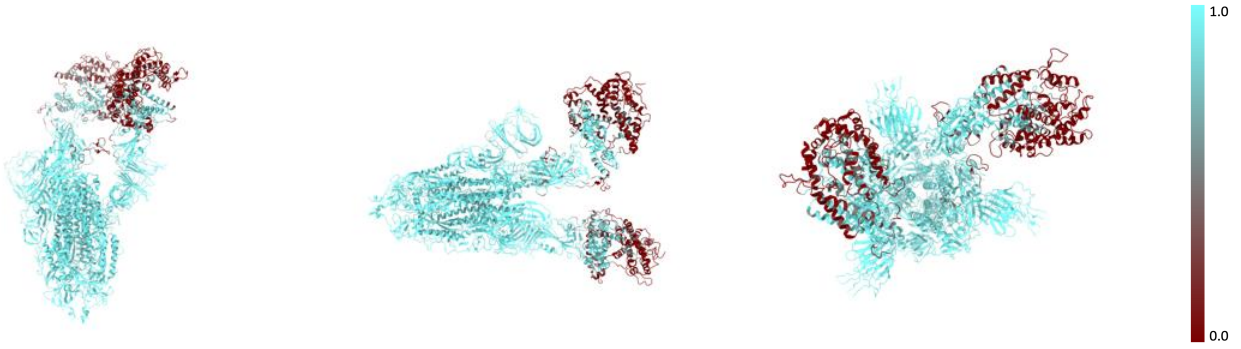
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

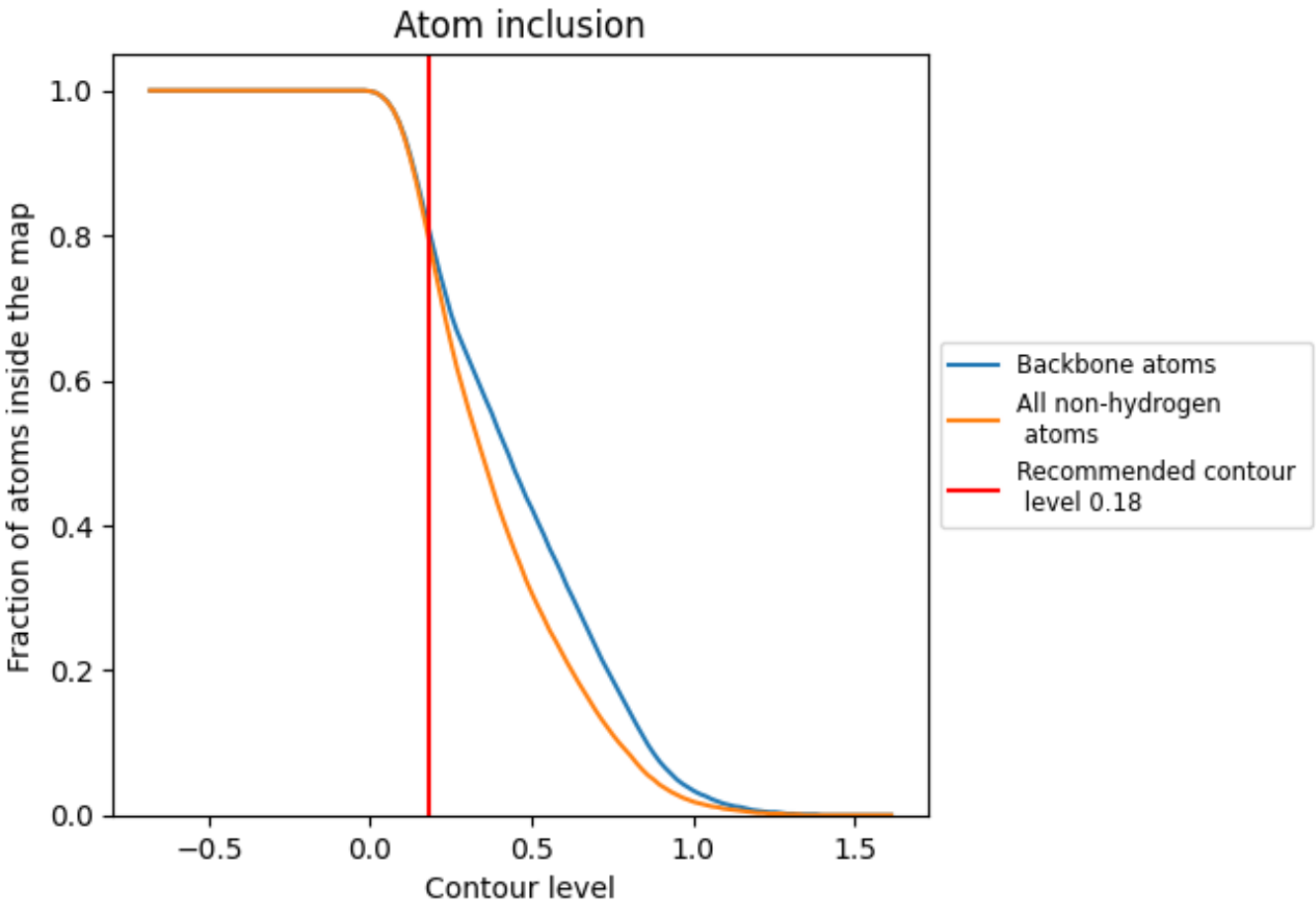
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.3030
A	0.9610	0.3670
B	0.9750	0.3730
C	0.9490	0.3890
D	0.8570	0.3360
E	0.7140	0.3090
F	0.3250	0.1070
G	0.8930	0.3110
H	0.4330	0.1170
I	1.0000	0.3870
J	0.9290	0.3060
K	0.9640	0.4400
L	1.0000	0.5030
M	1.0000	0.4410
N	0.7860	0.3410
O	0.9640	0.4470
P	0.9640	0.4730
Q	0.9290	0.4150
R	0.4290	0.2540
S	0.8930	0.2350
T	0.9640	0.3540
U	1.0000	0.4270
V	0.8570	0.4000
W	1.0000	0.4800
X	1.0000	0.4500
Y	0.7860	0.2960
Z	1.0000	0.4220
a	0.9640	0.4460
b	0.9290	0.2990
c	0.8930	0.4010
d	0.9290	0.3420
e	0.8210	0.3730
f	1.0000	0.4730
g	0.9640	0.4310
h	0.8570	0.3840

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Chain	Atom inclusion	Q-score
i	0.9640	0.4460
j	1.0000	0.4720