Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:39 AM JST

PDB ID	:	8K45
EMDB ID	:	EMD-36877
Title	:	A potent and broad-spectrum neutralizing nanobody for SARS-CoV-2 viruses including all major Omicron strains
Authors	:	Lu, Y.; Gao, Y.; Yao, H.; Xu, W.; Yang, H.
Deposited on	:	2023-07-17
Resolution	:	3.66 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

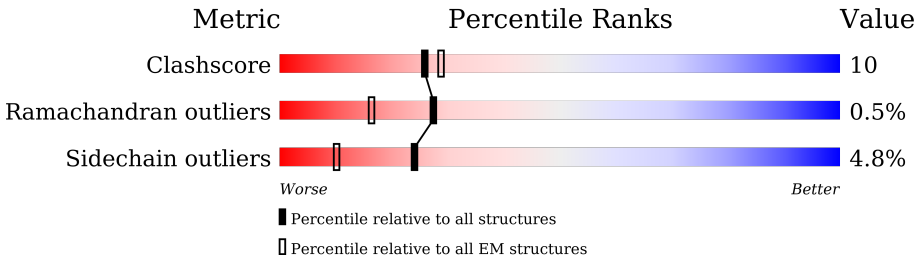
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.66 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%

Mol	Chain	Length	Quality of chain
1	A	1285	60% 19% • 19%
1	B	1285	59% 21% • 20%
1	C	1285	61% 17% • 21%
2	D	124	69% 31%
2	E	124	67% 31% •
3	K	2	100%
3	L	2	100%
3	M	2	50% 50%
3	R	2	100%

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Mol	Chain	Length	Quality of chain
3	S	2	100%
3	T	2	100%
3	U	2	100%
3	X	2	100%
3	Z	2	100%
3	a	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26877 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	1035	Total	C	N	O	S	0	0
			8111	5200	1347	1527	37		
1	B	1034	Total	C	N	O	S	0	0
			8117	5202	1351	1527	37		
1	C	1021	Total	C	N	O	S	0	0
			8003	5127	1330	1511	35		

There are 387 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	ASP	TYR	variant	UNP P0DTC2
A	210A	ILE	-	insertion	UNP P0DTC2
A	210B	VAL	-	insertion	UNP P0DTC2
A	210C	ARG	ASN	variant	UNP P0DTC2
A	210D	GLU	LEU	variant	UNP P0DTC2
A	210E	PRO	VAL	variant	UNP P0DTC2
A	210F	GLU	ARG	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	ASP	TYR	variant	UNP P0DTC2
B	210A	ILE	-	insertion	UNP P0DTC2
B	210B	VAL	-	insertion	UNP P0DTC2
B	210C	ARG	ASN	variant	UNP P0DTC2
B	210D	GLU	LEU	variant	UNP P0DTC2
B	210E	PRO	VAL	variant	UNP P0DTC2
B	210F	GLU	ARG	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	ASP	TYR	variant	UNP P0DTC2
C	210A	ILE	-	insertion	UNP P0DTC2
C	210B	VAL	-	insertion	UNP P0DTC2
C	210C	ARG	ASN	variant	UNP P0DTC2
C	210D	GLU	LEU	variant	UNP P0DTC2
C	210E	PRO	VAL	variant	UNP P0DTC2
C	210F	GLU	ARG	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2

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

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

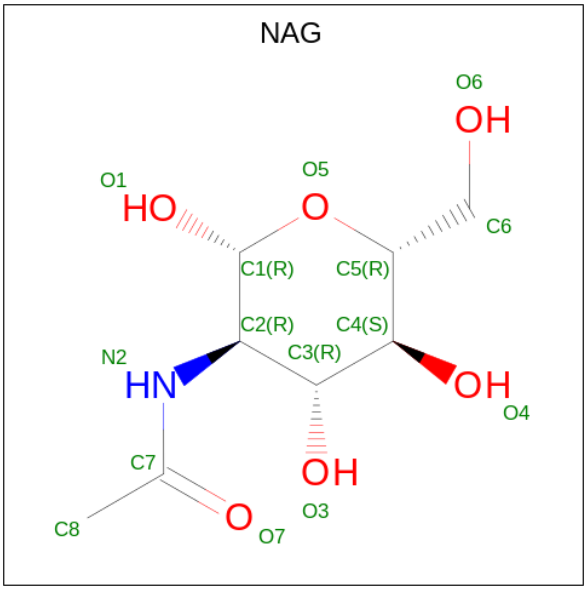
- Molecule 2 is a protein called Nb4 nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	124	Total	C	N	O	S	1	0
			987	623	168	191	5		
2	E	124	Total	C	N	O	S	1	0
			987	623	168	191	5		

- 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	K	2	Total C N O 28 16 2 10	0	0
3	L	2	Total C N O 28 16 2 10	0	0
3	M	2	Total C N O 28 16 2 10	0	0
3	R	2	Total C N O 28 16 2 10	0	0
3	S	2	Total C N O 28 16 2 10	0	0
3	T	2	Total C N O 28 16 2 10	0	0
3	U	2	Total C N O 28 16 2 10	0	0
3	X	2	Total C N O 28 16 2 10	0	0
3	Z	2	Total C N O 28 16 2 10	0	0
3	a	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

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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	A	1	Total	C	N	O	0
			14	8	1	5	
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	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	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	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	

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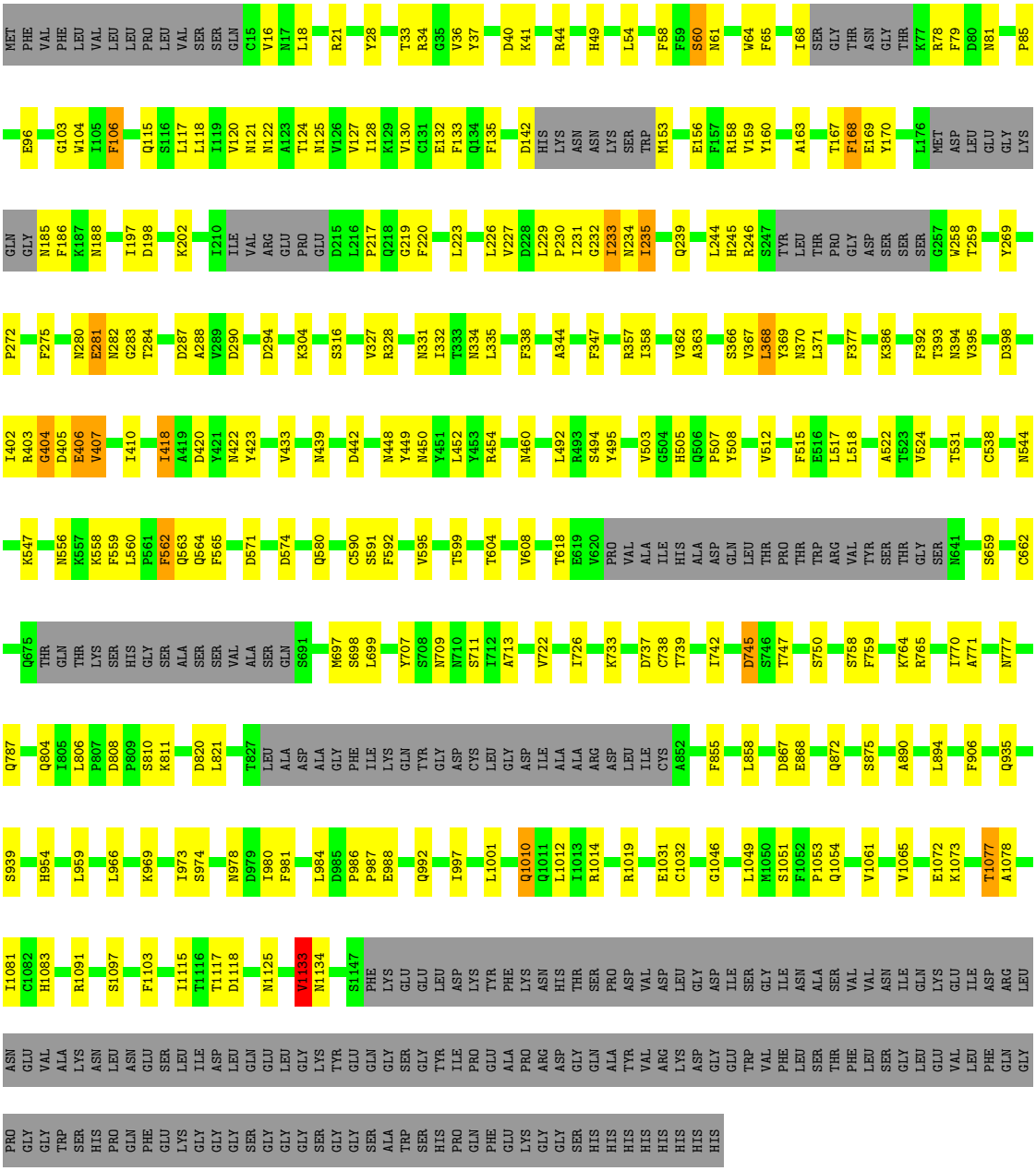
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

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. 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. 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.

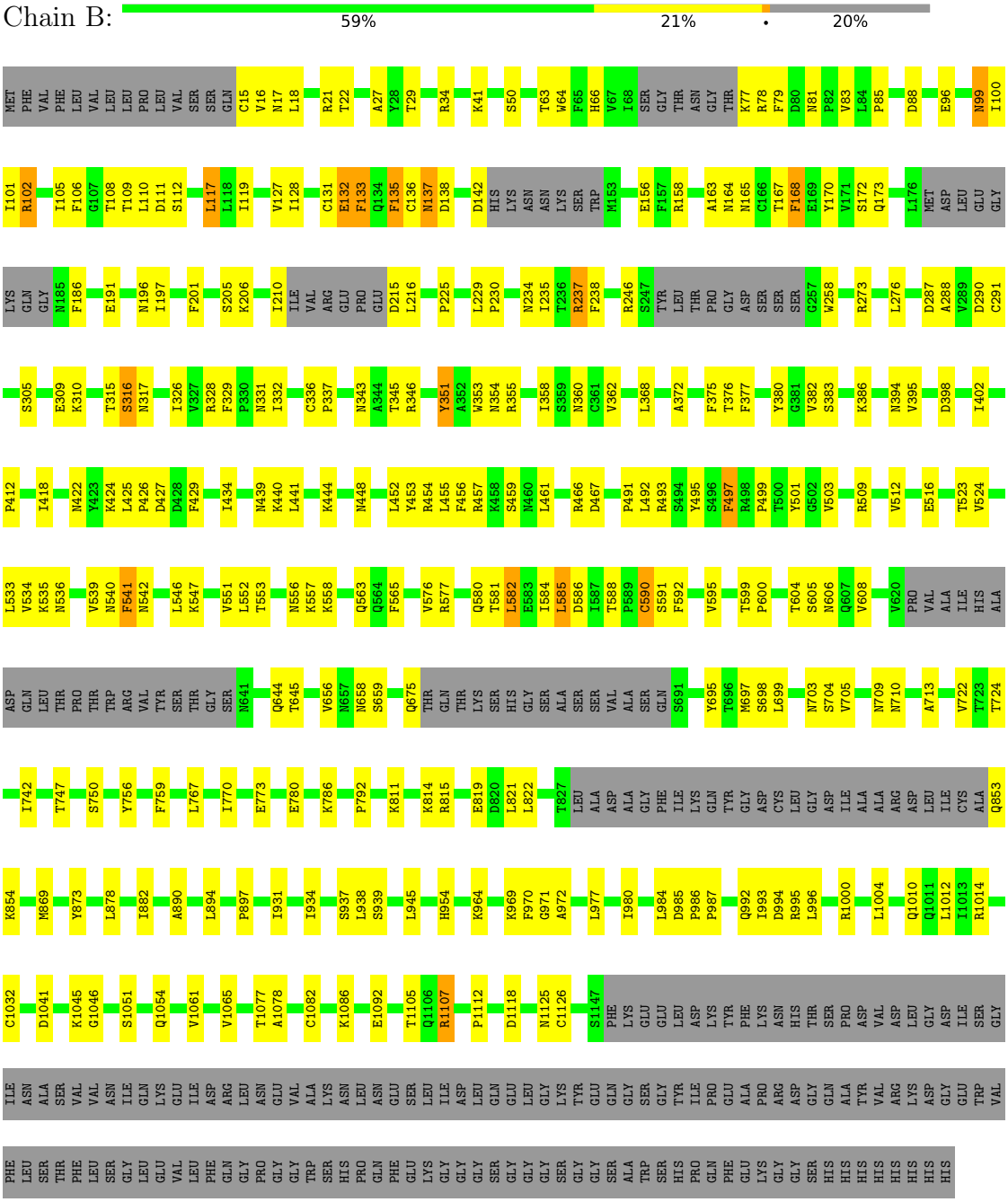
- Molecule 1: Spike glycoprotein

Chain A:



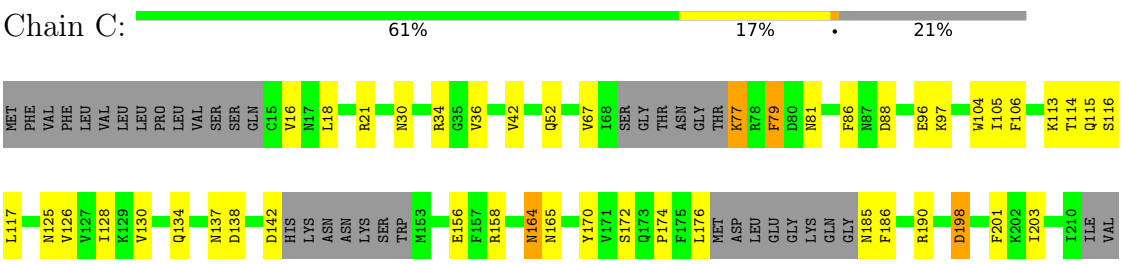
• Molecule 1: Spike glycoprotein

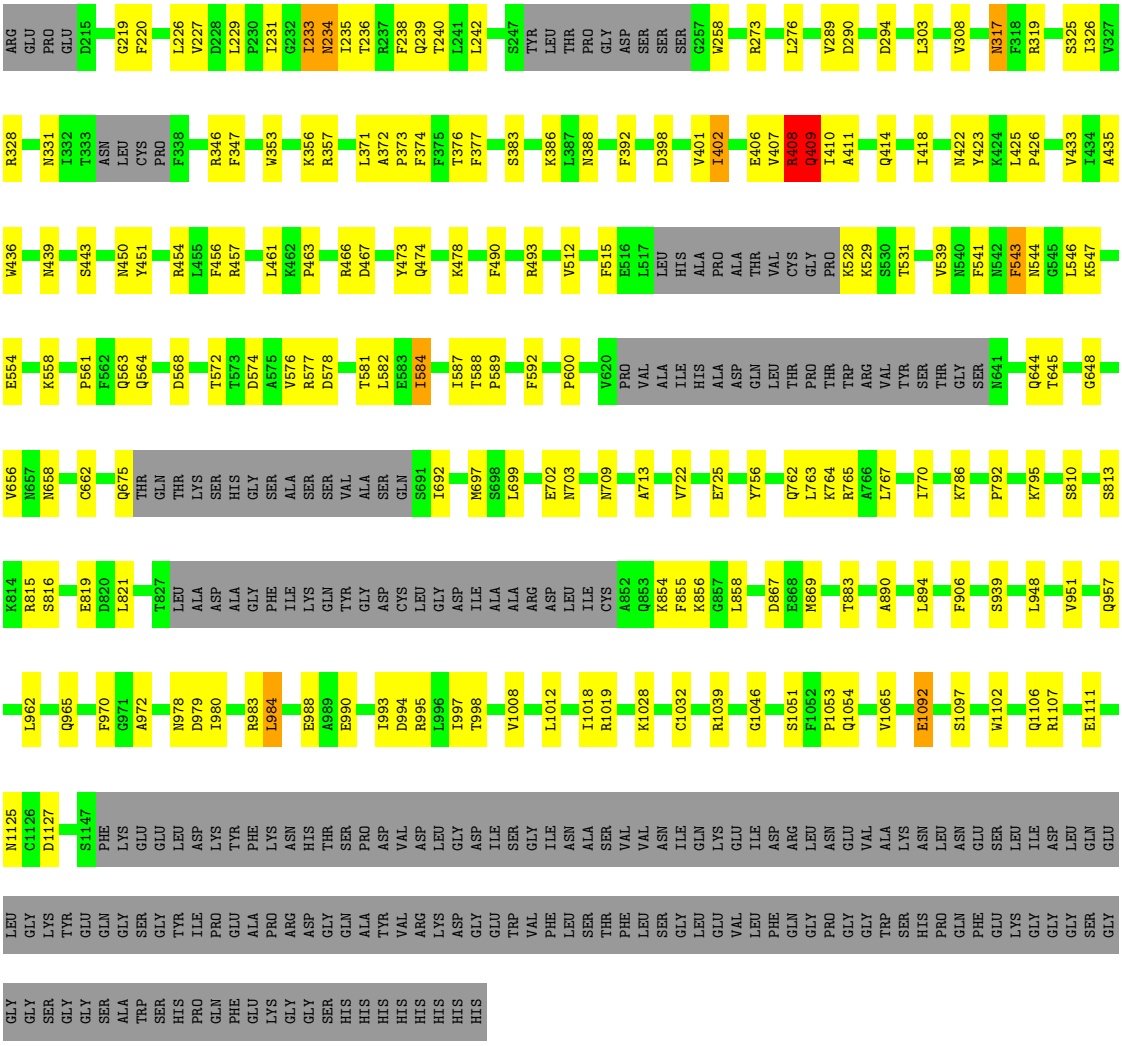
Chain B:



• Molecule 1: Spike glycoprotein

Chain C:



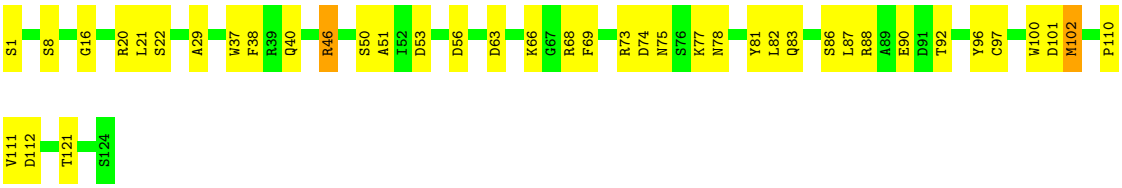


• Molecule 2: Nb4 nanobody

Chain D:

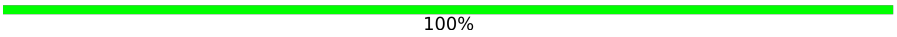
• Molecule 2: Nb4 nanobody

Chain E:



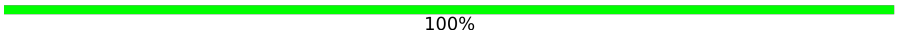
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:

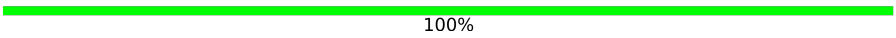


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

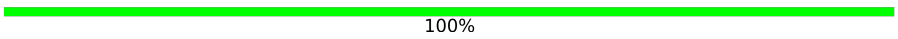
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



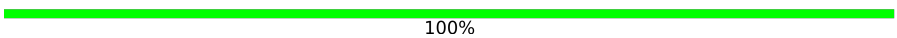
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



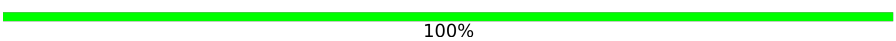
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

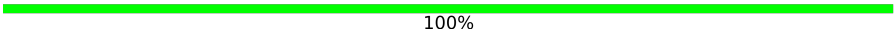


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

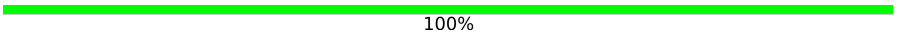
Chain U:



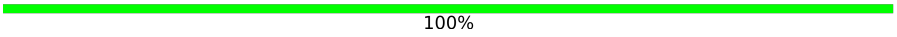
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

• 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: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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	0.34	0/8303	0.51	0/11297
1	B	0.31	0/8309	0.50	0/11303
1	C	0.30	0/8187	0.49	0/11133
2	D	0.26	0/1016	0.56	0/1382
2	E	0.27	0/1016	0.54	0/1382
All	All	0.31	0/26831	0.51	0/36497

There are no bond length outliers.

There are no bond angle outliers.

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	8111	0	7929	169	0
1	B	8117	0	7940	181	0
1	C	8003	0	7826	162	0
2	D	987	0	906	22	0
2	E	987	0	906	28	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	X	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
4	A	112	0	104	3	0
4	B	154	0	143	0	0
4	C	126	0	117	2	0
All	All	26877	0	26121	530	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (530) 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:111:ASP:OD1	1:B:112:SER:N	1.99	0.96
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.38	0.87
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.66	0.78
1:C:546:LEU:HD21	1:C:576:VAL:HG11	1.67	0.77
1:C:164:ASN:OD1	1:C:164:ASN:N	2.17	0.77
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.69	0.73
2:E:21:LEU:HB2	2:E:82:LEU:HD21	1.70	0.73
1:B:402:ILE:HD11	1:B:418:ILE:HG21	1.72	0.72
1:A:130:VAL:HB	1:A:167:THR:HB	1.73	0.70
1:B:329:PHE:O	1:B:580:GLN:NE2	2.25	0.70
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.24	0.70
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.56	0.70
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.74	0.70
1:B:133:PHE:HB3	1:B:163:ALA:HA	1.73	0.70
1:B:454:ARG:HH12	1:B:457:ARG:HB2	1.56	0.69
1:B:34:ARG:NH2	1:B:191:GLU:OE2	2.26	0.69
1:A:503:VAL:HG11	2:E:73:ARG:HE	1.58	0.69
1:B:309:GLU:N	1:B:309:GLU:OE1	2.24	0.69
1:B:328:ARG:NH2	1:B:580:GLN:OE1	2.26	0.69
1:C:528:LYS:HG3	1:C:529:LYS:HG3	1.75	0.68
2:E:40:GLN:HB2	2:E:46:ARG:HG3	1.75	0.68
1:B:360:ASN:N	1:B:523:THR:OG1	2.25	0.68
1:A:393:THR:HA	1:A:522:ALA:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TRP:HB2	1:A:106:PHE:CE1	2.29	0.67
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.77	0.67
1:B:108:THR:C	1:B:110:LEU:H	1.96	0.67
1:B:452:LEU:HD13	1:B:492:LEU:HB3	1.75	0.67
1:A:106:PHE:HB3	1:A:235:ILE:HD12	1.76	0.67
1:C:402:ILE:HG13	1:C:407:VAL:HG22	1.75	0.66
1:A:81:ASN:O	1:A:239:GLN:NE2	2.28	0.66
1:A:281:GLU:OE2	1:A:282:ASN:OD1	2.14	0.66
1:A:358:ILE:HG13	1:A:395:VAL:HG23	1.75	0.66
1:C:346:ARG:NH1	1:C:347:PHE:O	2.28	0.66
1:B:377:PHE:HB2	1:B:434:ILE:HD13	1.77	0.65
1:A:21:ARG:HB2	1:A:79:PHE:HB2	1.78	0.65
1:A:386:LYS:NZ	1:B:984:LEU:O	2.30	0.65
1:B:398:ASP:HB2	1:B:512:VAL:HG12	1.78	0.65
1:C:984:LEU:HD21	1:C:988:GLU:HG2	1.79	0.65
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.31	0.64
1:A:777:ASN:HD21	1:A:1019:ARG:HA	1.63	0.64
2:E:73:ARG:HH12	2:E:78:ASN:HA	1.62	0.64
1:B:66:HIS:HB3	1:B:78:ARG:HH12	1.63	0.64
1:C:563:GLN:O	1:C:564:GLN:NE2	2.31	0.64
1:C:113:LYS:HG3	1:C:114:THR:HG23	1.80	0.64
1:C:656:VAL:HG12	1:C:658:ASN:H	1.63	0.64
1:A:978:ASN:HB3	1:C:547:LYS:HD3	1.79	0.64
1:C:970:PHE:O	1:C:995:ARG:NH1	2.30	0.63
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.31	0.63
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.32	0.63
1:C:474:GLN:NE2	1:C:478:LYS:O	2.32	0.62
1:C:821:LEU:HD11	1:C:939:SER:HB3	1.81	0.62
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.33	0.62
1:B:656:VAL:HG12	1:B:658:ASN:H	1.64	0.62
1:B:556:ASN:HB2	1:B:584:ILE:HG21	1.80	0.62
1:A:418:ILE:HA	1:A:422:ASN:ND2	2.13	0.62
1:A:974:SER:HB3	1:A:980:ILE:HD11	1.81	0.62
1:A:739:THR:HA	1:A:742:ILE:HG22	1.80	0.61
1:A:821:LEU:HD11	1:A:939:SER:HB2	1.82	0.61
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.29	0.61
1:A:245:HIS:HB2	1:A:259:THR:HB	1.80	0.61
1:B:96:GLU:OE2	1:B:101:ILE:N	2.33	0.61
1:B:644:GLN:NE2	1:B:645:THR:O	2.33	0.61
1:B:412:PRO:HB3	1:B:427:ASP:HA	1.81	0.61
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:NH2	1:B:398:ASP:OD2	2.33	0.61
1:C:558:LYS:HE2	1:C:561:PRO:HB3	1.83	0.61
2:E:20:ARG:HH22	2:E:81:TYR:HB3	1.65	0.61
1:B:724:THR:HG22	1:B:934:ILE:HD11	1.82	0.61
1:A:868:GLU:OE2	1:A:872:GLN:NE2	2.34	0.60
1:A:737:ASP:OD1	1:C:317:ASN:ND2	2.35	0.60
1:A:858:LEU:HD13	1:A:959:LEU:HD22	1.83	0.60
1:C:231:ILE:HG13	1:C:233:ILE:HG12	1.84	0.59
1:B:172:SER:OG	1:B:173:GLN:N	2.34	0.59
1:C:383:SER:H	1:C:386:LYS:HE3	1.67	0.59
1:C:1092:GLU:O	1:C:1107:ARG:NE	2.35	0.59
1:B:331:ASN:HB2	1:B:580:GLN:HG3	1.84	0.59
1:B:980:ILE:HD11	1:B:992:GLN:HB3	1.82	0.59
2:D:62:ALA:HB3	2:D:65:VAL:HG22	1.84	0.59
1:A:167:THR:HG22	1:A:168:PHE:H	1.67	0.59
1:C:115:GLN:NE2	1:C:165:ASN:O	2.36	0.59
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.84	0.59
1:B:128:ILE:HG21	1:B:229:LEU:HD11	1.83	0.59
1:B:156:GLU:OE2	1:B:158:ARG:NH1	2.36	0.59
1:A:294:ASP:OD1	1:A:294:ASP:N	2.36	0.58
1:C:644:GLN:NE2	1:C:645:THR:O	2.37	0.58
1:A:335:LEU:HD23	1:A:362:VAL:HG13	1.84	0.58
1:C:816:SER:N	1:C:819:GLU:OE1	2.34	0.58
1:A:128:ILE:HD13	1:A:170:TYR:HB3	1.86	0.58
1:B:786:LYS:HE3	1:B:786:LYS:HA	1.86	0.58
2:D:63:ASP:HA	2:D:66:LYS:HG3	1.85	0.58
1:A:34:ARG:NH1	1:A:217:PRO:O	2.36	0.58
2:E:20:ARG:HH21	2:E:22:SER:HB3	1.68	0.58
1:A:128:ILE:HG21	1:A:229:LEU:HD21	1.85	0.57
1:A:699:LEU:HD21	1:B:869:MET:HB3	1.85	0.57
1:B:345:THR:O	1:B:509:ARG:NH2	2.31	0.57
1:B:547:LYS:HB2	1:C:978:ASN:ND2	2.19	0.57
1:B:811:LYS:O	1:B:814:LYS:NZ	2.37	0.57
2:E:20:ARG:NH1	2:E:83:GLN:OE1	2.36	0.57
1:A:115:GLN:HA	1:A:132:GLU:HG2	1.86	0.57
2:D:31:THR:OG1	2:D:32:PHE:N	2.36	0.57
1:A:33:THR:OG1	1:A:219:GLY:O	2.22	0.57
2:E:92:THR:HG23	2:E:121:THR:HA	1.87	0.57
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.86	0.57
1:A:197:ILE:HG13	1:A:198:ASP:H	1.70	0.57
1:B:108:THR:O	1:B:110:LEU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:O	1:B:127:VAL:HG12	2.05	0.57
1:C:328:ARG:NH1	1:C:581:THR:OG1	2.34	0.57
2:D:92:THR:HG23	2:D:121:THR:HA	1.87	0.57
1:C:142:ASP:HB2	1:C:156:GLU:HB3	1.87	0.56
1:C:786:LYS:HE3	1:C:786:LYS:HA	1.88	0.56
1:A:40:ASP:O	1:C:563:GLN:NE2	2.38	0.56
1:B:316:SER:OG	1:B:317:ASN:N	2.38	0.56
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.39	0.56
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.86	0.56
1:C:407:VAL:O	1:C:409:GLN:N	2.39	0.56
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.87	0.56
1:A:1032:CYS:O	1:A:1051:SER:OG	2.24	0.55
1:A:54:LEU:HA	1:A:272:PRO:HA	1.89	0.55
1:A:709:ASN:OD1	1:A:709:ASN:N	2.37	0.55
1:C:294:ASP:OD1	1:C:294:ASP:N	2.39	0.55
1:A:230:PRO:O	1:A:231:ILE:HD13	2.07	0.55
1:A:442:ASP:O	1:A:448:ASN:ND2	2.38	0.55
1:C:326:ILE:HG22	1:C:328:ARG:HD2	1.88	0.54
1:B:108:THR:C	1:B:110:LEU:N	2.61	0.54
1:B:439:ASN:HD21	1:B:499:PRO:HA	1.71	0.54
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.38	0.54
2:D:92:THR:HA	2:D:120:VAL:O	2.08	0.54
1:A:403:ARG:O	1:A:404:GLY:C	2.46	0.54
1:C:105:ILE:HB	1:C:239:GLN:HB2	1.88	0.54
1:C:858:LEU:HD11	1:C:962:LEU:HD22	1.90	0.54
1:A:1046:GLY:HA2	1:B:890:ALA:HB1	1.90	0.54
1:B:461:LEU:HD21	1:B:467:ASP:HB2	1.90	0.54
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.90	0.54
1:A:524:VAL:HG12	1:A:524:VAL:O	2.08	0.54
1:B:88:ASP:OD1	1:B:88:ASP:N	2.39	0.54
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.90	0.54
1:B:41:LYS:HE2	1:B:225:PRO:HD2	1.89	0.54
1:B:106:PHE:HA	1:B:238:PHE:HB2	1.90	0.54
1:B:954:HIS:O	1:B:1014:ARG:NH1	2.41	0.54
1:A:226:LEU:HD23	1:A:227:VAL:HB	1.90	0.53
1:A:439:ASN:OD1	1:A:507:PRO:HD2	2.08	0.53
1:B:456:PHE:HD2	1:B:491:PRO:HA	1.73	0.53
1:A:787:GLN:OE1	1:C:703:ASN:ND2	2.37	0.53
1:B:1041:ASP:OD2	1:B:1045:LYS:NZ	2.39	0.53
1:A:890:ALA:HB1	1:C:1046:GLY:HA2	1.91	0.53
1:B:215:ASP:OD1	1:B:216:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:TYR:HB3	1:A:223:LEU:HB2	1.90	0.53
1:A:197:ILE:H	1:A:202:LYS:HZ1	1.57	0.52
1:B:105:ILE:HD11	1:B:135:PHE:CD2	2.44	0.52
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.91	0.52
1:C:371:LEU:HD13	1:C:374:PHE:CE2	2.44	0.52
2:D:21:LEU:HD12	2:D:82:LEU:HD23	1.91	0.52
1:B:290:ASP:OD1	1:B:291:CYS:N	2.42	0.52
1:C:1125:ASN:OD1	1:C:1125:ASN:N	2.40	0.52
1:A:21:ARG:NE	1:A:79:PHE:O	2.43	0.52
1:A:452:LEU:HD13	1:A:492:LEU:HD13	1.91	0.52
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.92	0.52
2:E:20:ARG:NH2	2:E:21:LEU:O	2.42	0.52
1:C:176:LEU:HD21	1:C:190:ARG:HE	1.74	0.52
1:A:395:VAL:HG22	1:A:524:VAL:HG21	1.92	0.52
1:C:106:PHE:HB3	1:C:235:ILE:HD12	1.92	0.52
1:A:231:ILE:HG22	1:A:232:GLY:H	1.73	0.52
1:C:490:PHE:HB3	1:C:493:ARG:HH21	1.74	0.51
1:A:366:SER:HA	1:A:369:TYR:HD2	1.76	0.51
1:B:815:ARG:HB3	1:B:819:GLU:HG3	1.92	0.51
1:C:18:LEU:O	1:C:21:ARG:NH1	2.43	0.51
2:D:34:HIS:NE2	2:D:103:ASP:O	2.39	0.51
1:A:118:LEU:HD21	1:A:135:PHE:HE1	1.75	0.51
1:B:547:LYS:HB2	1:C:978:ASN:HD22	1.76	0.51
1:B:563:GLN:NE2	1:C:42:VAL:O	2.43	0.51
2:D:14:GLN:NE2	2:D:124:SER:O	2.42	0.51
2:D:70:THR:OG1	2:D:83:GLN:HB2	2.10	0.51
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.93	0.51
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.91	0.51
2:D:69:PHE:HE1	2:D:84:MET:HG3	1.76	0.51
1:A:395:VAL:HG12	1:A:515:PHE:HD1	1.75	0.51
1:B:605:SER:OG	1:B:606:ASN:N	2.44	0.51
1:A:867:ASP:OD1	1:A:868:GLU:N	2.44	0.51
1:B:21:ARG:HH21	1:B:138:ASP:HB3	1.76	0.51
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.35	0.51
1:C:117:LEU:HD22	1:C:130:VAL:HG22	1.93	0.50
2:E:101:ASP:N	2:E:112:ASP:OD2	2.42	0.50
1:A:327:VAL:H	1:A:531:THR:HG22	1.74	0.50
1:A:556:ASN:O	1:A:558:LYS:NZ	2.39	0.50
2:D:69:PHE:CE1	2:D:84:MET:HG3	2.45	0.50
2:E:53:ASP:OD1	2:E:56:ASP:N	2.43	0.50
1:B:201:PHE:HB3	1:B:229:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ARG:HA	1:B:346:ARG:NE	2.26	0.50
1:B:1054:GLN:HB2	1:B:1061:VAL:HG12	1.92	0.50
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.94	0.50
1:C:792:PRO:O	1:C:795:LYS:NZ	2.42	0.50
1:B:546:LEU:HD12	1:B:546:LEU:H	1.76	0.50
1:B:977:LEU:HG	1:B:993:ILE:HD11	1.93	0.50
1:B:383:SER:HB2	1:B:386:LYS:HG2	1.93	0.50
1:B:1125:ASN:OD1	1:B:1125:ASN:N	2.44	0.50
1:A:168:PHE:CE1	1:A:170:TYR:HB2	2.47	0.50
1:A:367:VAL:HG23	1:A:368:LEU:HD23	1.93	0.50
1:A:420:ASP:OD1	1:A:460:ASN:ND2	2.45	0.50
1:A:563:GLN:HG2	1:B:41:LYS:O	2.10	0.50
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.94	0.50
1:B:142:ASP:OD2	1:B:246:ARG:NH2	2.44	0.50
1:C:137:ASN:ND2	1:C:138:ASP:OD2	2.44	0.50
1:C:346:ARG:HH21	1:C:450:ASN:HB3	1.76	0.50
1:A:765:ARG:CZ	1:C:957:GLN:HE22	2.24	0.50
1:B:699:LEU:HD21	1:C:869:MET:HB3	1.94	0.50
1:C:115:GLN:HE21	1:C:165:ASN:HB2	1.76	0.50
1:C:406:GLU:O	1:C:418:ILE:HG13	2.11	0.50
1:A:121:ASN:ND2	1:A:122:ASN:O	2.44	0.50
1:C:156:GLU:HG3	1:C:158:ARG:HH11	1.77	0.50
1:C:454:ARG:NH2	1:C:467:ASP:O	2.45	0.50
1:B:454:ARG:NH2	1:B:456:PHE:O	2.45	0.49
1:C:97:LYS:NZ	1:C:185:ASN:O	2.44	0.49
1:A:406:GLU:O	1:A:407:VAL:C	2.49	0.49
1:B:551:VAL:HG12	1:B:588:THR:OG1	2.12	0.49
1:B:970:PHE:HB2	1:B:996:LEU:HD23	1.94	0.49
2:D:34:HIS:ND1	2:D:105:LEU:HB2	2.27	0.49
1:C:113:LYS:O	1:C:113:LYS:NZ	2.42	0.49
1:A:733:LYS:HE2	1:A:771:ALA:HB1	1.94	0.49
1:B:703:ASN:OD1	1:B:704:SER:N	2.46	0.49
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.45	0.49
1:B:351:TYR:HB2	1:B:454:ARG:HG3	1.94	0.49
1:C:990:GLU:HA	1:C:993:ILE:HG12	1.94	0.49
1:A:125:ASN:OD1	1:A:125:ASN:N	2.46	0.49
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.30	0.49
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.95	0.49
1:C:328:ARG:NH2	1:C:531:THR:H	2.10	0.49
1:C:422:ASN:ND2	1:C:454:ARG:O	2.45	0.49
1:B:22:THR:OG1	1:B:77:LYS:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:TRP:HB3	1:C:106:PHE:HE1	1.77	0.49
1:C:356:LYS:NZ	1:C:357:ARG:O	2.33	0.49
1:C:644:GLN:NE2	1:C:648:GLY:O	2.46	0.48
2:E:100:TRP:HE1	2:E:111:VAL:HA	1.78	0.48
1:A:41:LYS:HA	1:C:563:GLN:HG2	1.94	0.48
1:A:44:ARG:HH11	1:A:49:HIS:CG	2.32	0.48
1:A:197:ILE:HG22	1:A:202:LYS:HZ1	1.79	0.48
1:A:280:ASN:HD21	1:A:284:THR:HB	1.77	0.48
1:B:112:SER:O	1:B:132:GLU:HG3	2.12	0.48
1:C:34:ARG:NH1	1:C:219:GLY:O	2.46	0.48
1:C:461:LEU:HD21	1:C:467:ASP:HB2	1.95	0.48
2:E:16:GLY:N	2:E:87:LEU:O	2.40	0.48
1:A:1103:PHE:HZ	3:M:1:NAG:H62	1.79	0.48
1:B:96:GLU:OE2	1:B:100:ILE:N	2.46	0.48
1:B:457:ARG:NH1	1:B:459:SER:OG	2.45	0.48
2:E:63:ASP:HA	2:E:66:LYS:HD3	1.94	0.48
1:A:118:LEU:HD11	1:A:135:PHE:HZ	1.78	0.48
1:B:85:PRO:HA	1:B:237:ARG:HB3	1.95	0.48
1:A:197:ILE:HG22	1:A:202:LYS:NZ	2.29	0.48
1:A:560:LEU:HB2	1:A:563:GLN:HG3	1.94	0.48
1:C:539:VAL:HG12	1:C:541:PHE:H	1.78	0.48
1:A:1081:ILE:HD13	1:A:1133:VAL:HG23	1.94	0.48
1:B:659:SER:HB3	1:B:698:SER:HB3	1.95	0.48
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.47	0.48
1:C:319:ARG:HG2	1:C:592:PHE:HB2	1.95	0.48
2:D:65:VAL:HA	2:D:68:ARG:NH1	2.29	0.48
2:E:1:SER:HB2	2:E:29:ALA:HA	1.95	0.48
1:A:973:ILE:HG22	1:A:992:GLN:HE21	1.79	0.48
1:A:60:SER:OG	1:A:61:ASN:N	2.47	0.47
1:A:124:THR:OG1	1:A:125:ASN:OD1	2.19	0.47
1:B:1046:GLY:HA2	1:C:890:ALA:HB1	1.96	0.47
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.48	0.47
2:E:73:ARG:HH22	2:E:78:ASN:HA	1.80	0.47
1:B:1010:GLN:HE22	1:B:1014:ARG:NE	2.13	0.47
1:A:246:ARG:HA	1:A:258:TRP:HA	1.94	0.47
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.79	0.47
1:B:336:CYS:N	1:B:362:VAL:O	2.45	0.47
1:B:821:LEU:HD11	1:B:939:SER:HB3	1.96	0.47
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.95	0.47
1:A:142:ASP:HB2	1:A:156:GLU:HB2	1.96	0.47
1:A:244:LEU:HB3	1:A:258:TRP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:GLN:OE1	1:C:765:ARG:NH2	2.47	0.47
1:C:856:LYS:HA	1:C:856:LYS:HD3	1.61	0.47
2:E:20:ARG:O	2:E:21:LEU:HD23	2.15	0.47
2:E:21:LEU:HD12	2:E:82:LEU:HD11	1.95	0.47
1:B:709:ASN:OD1	1:B:710:ASN:N	2.48	0.47
1:A:68:ILE:HG22	1:A:78:ARG:H	1.80	0.47
1:A:759:PHE:HD2	1:A:1001:LEU:HD21	1.79	0.47
1:B:394:ASN:HB3	1:B:516:GLU:HB3	1.96	0.47
1:B:931:ILE:O	1:B:934:ILE:HG22	2.15	0.47
2:E:77:LYS:HA	2:E:77:LYS:HE2	1.96	0.47
1:A:393:THR:HG23	1:A:517:LEU:HA	1.97	0.46
1:A:433:VAL:HG22	1:A:512:VAL:HG22	1.97	0.46
1:B:17:ASN:HB3	1:B:137:ASN:HD21	1.80	0.46
1:B:383:SER:HB2	1:B:386:LYS:HE3	1.96	0.46
1:B:541:PHE:CE2	1:B:552:LEU:HD11	2.50	0.46
1:C:236:THR:HG21	4:C:1302:NAG:H62	1.97	0.46
1:C:407:VAL:O	1:C:408:ARG:C	2.53	0.46
1:C:983:ARG:HH22	1:C:984:LEU:HB2	1.79	0.46
1:B:551:VAL:O	1:B:552:LEU:HD13	2.14	0.46
1:B:580:GLN:C	1:B:582:LEU:H	2.19	0.46
1:C:353:TRP:O	1:C:466:ARG:NH2	2.32	0.46
2:E:101:ASP:N	2:E:102:MET:HE3	2.31	0.46
1:A:16:VAL:HG23	1:A:158:ARG:HH21	1.81	0.46
1:B:444:LYS:HE2	1:B:448:ASN:HA	1.98	0.46
1:C:303:LEU:HD23	1:C:308:VAL:HG12	1.98	0.46
1:C:426:PRO:HD3	1:C:463:PRO:HB3	1.98	0.46
1:C:422:ASN:OD1	1:C:454:ARG:N	2.41	0.46
1:B:354:ASN:O	1:B:398:ASP:HA	2.16	0.46
1:B:394:ASN:ND2	1:B:516:GLU:OE2	2.48	0.46
1:C:376:THR:HB	1:C:435:ALA:HB3	1.98	0.46
1:C:392:PHE:CG	1:C:515:PHE:HB3	2.51	0.46
1:C:972:ALA:HA	1:C:995:ARG:HH22	1.80	0.46
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.81	0.46
1:C:128:ILE:HG21	1:C:229:LEU:HD21	1.97	0.46
1:B:440:LYS:HA	1:B:440:LYS:HD3	1.85	0.46
1:B:986:PRO:N	1:B:987:PRO:HD2	2.31	0.46
1:C:983:ARG:HH12	1:C:984:LEU:HB2	1.80	0.46
1:A:338:PHE:HE2	1:A:363:ALA:HB1	1.81	0.46
1:B:168:PHE:CZ	1:B:230:PRO:HD2	2.51	0.46
1:C:67:VAL:HG21	1:C:242:LEU:HD21	1.98	0.46
1:C:582:LEU:HD12	1:C:582:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.97	0.45
1:B:453:TYR:CE1	1:B:493:ARG:HB3	2.51	0.45
1:C:558:LYS:NZ	1:C:561:PRO:HG3	2.31	0.45
1:C:303:LEU:HD12	1:C:303:LEU:HA	1.80	0.45
2:E:37:TRP:CH2	2:E:97:CYS:HB3	2.52	0.45
1:A:156:GLU:OE2	1:A:246:ARG:NH2	2.49	0.45
1:A:197:ILE:N	1:A:202:LYS:HZ1	2.14	0.45
1:A:745:ASP:OD1	1:A:745:ASP:N	2.48	0.45
1:A:747:THR:O	1:A:750:SER:OG	2.33	0.45
1:B:1092:GLU:O	1:B:1107:ARG:NH1	2.49	0.45
1:C:373:PRO:O	1:C:436:TRP:HB2	2.17	0.45
1:C:18:LEU:HG	1:C:21:ARG:HH11	1.80	0.45
1:C:81:ASN:OD1	1:C:239:GLN:NE2	2.50	0.45
1:A:562:PHE:HD2	1:B:41:LYS:HE3	1.82	0.45
1:A:64:TRP:HD1	1:A:65:PHE:N	2.15	0.45
1:A:118:LEU:HD11	1:A:135:PHE:CZ	2.52	0.45
1:A:404:GLY:O	1:A:405:ASP:C	2.54	0.45
1:B:99:ASN:O	1:B:102:ARG:NH1	2.50	0.45
1:B:353:TRP:O	1:B:466:ARG:NH2	2.42	0.45
1:A:96:GLU:O	1:A:188:ASN:HB2	2.17	0.45
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.35	0.45
1:B:1032:CYS:O	1:B:1051:SER:OG	2.26	0.45
1:A:758:SER:H	1:C:965:GLN:HE21	1.65	0.45
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.83	0.45
1:A:1049:LEU:HD23	1:A:1049:LEU:HA	1.84	0.45
1:C:948:LEU:O	1:C:951:VAL:HG12	2.16	0.45
1:B:117:LEU:HD22	1:B:119:ILE:HD11	1.98	0.45
1:C:326:ILE:HG23	1:C:531:THR:HG21	1.99	0.45
1:B:382:VAL:HG13	1:B:386:LYS:HZ2	1.82	0.45
1:B:878:LEU:HD23	1:B:878:LEU:HA	1.82	0.45
1:C:201:PHE:CD2	1:C:203:ILE:HD11	2.52	0.45
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.99	0.45
1:C:568:ASP:OD1	1:C:572:THR:N	2.34	0.45
1:B:328:ARG:HH11	1:B:533:LEU:HD13	1.83	0.44
1:C:756:TYR:OH	1:C:998:THR:HG22	2.17	0.44
1:A:153:MET:HA	1:A:245:HIS:HA	1.99	0.44
1:B:273:ARG:HE	1:B:273:ARG:HB3	1.67	0.44
1:B:577:ARG:HD3	1:B:582:LEU:HD12	1.99	0.44
1:C:401:VAL:HB	1:C:451:TYR:CE1	2.52	0.44
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.52	0.44
1:A:969:LYS:NZ	1:A:973:ILE:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:N	1:B:81:ASN:OD1	2.50	0.44
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.82	0.44
1:B:599:THR:HB	1:B:608:VAL:HG12	2.00	0.44
1:B:853:GLN:HB3	1:B:854:LYS:H	1.60	0.44
1:C:18:LEU:HD21	1:C:79:PHE:HB2	2.00	0.44
1:C:993:ILE:O	1:C:997:ILE:HG12	2.17	0.44
1:A:449:TYR:HD1	1:A:494:SER:HG	1.64	0.44
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.52	0.44
1:C:77:LYS:HE2	1:C:77:LYS:HB2	1.71	0.44
1:A:64:TRP:HD1	1:A:65:PHE:H	1.65	0.44
1:A:855:PHE:HZ	1:C:589:PRO:HA	1.83	0.44
1:B:586:ASP:OD1	1:B:586:ASP:N	2.47	0.44
1:C:86:PHE:HA	1:C:238:PHE:HE1	1.82	0.44
1:A:564:GLN:HG3	1:A:565:PHE:CD1	2.53	0.44
1:A:1031:GLU:OE2	1:C:1039:ARG:NH1	2.51	0.44
1:C:16:VAL:HG23	1:C:158:ARG:HD3	2.00	0.44
2:E:88:ARG:HB2	2:E:90:GLU:OE1	2.18	0.44
1:B:985:ASP:HB3	1:B:987:PRO:HD2	1.99	0.44
1:A:133:PHE:HB3	1:A:160:TYR:HB2	2.00	0.44
1:C:544:ASN:HD21	1:C:577:ARG:HB3	1.83	0.44
1:A:185:ASN:OD1	1:A:186:PHE:N	2.50	0.43
1:A:659:SER:HB3	1:A:698:SER:HB3	2.00	0.43
1:B:495:TYR:HB2	1:B:497:PHE:CZ	2.52	0.43
1:B:1105:THR:HG22	1:B:1112:PRO:HA	2.00	0.43
1:C:980:ILE:HD12	1:C:980:ILE:HA	1.87	0.43
2:D:84:MET:SD	2:D:87:LEU:HD11	2.58	0.43
1:A:68:ILE:HA	1:A:68:ILE:HD12	1.86	0.43
1:A:984:LEU:HD23	1:A:988:GLU:HG2	2.00	0.43
1:A:1091:ARG:HH11	1:A:1091:ARG:HB2	1.84	0.43
1:B:383:SER:H	1:B:386:LYS:HE3	1.82	0.43
1:B:1012:LEU:HD23	1:B:1012:LEU:HA	1.81	0.43
1:B:576:VAL:O	1:B:585:LEU:HD23	2.17	0.43
1:B:780:GLU:OE2	1:B:780:GLU:HA	2.18	0.43
1:C:106:PHE:O	1:C:116:SER:HB3	2.17	0.43
1:B:315:THR:HG22	1:B:595:VAL:O	2.19	0.43
1:B:854:LYS:HA	1:B:854:LYS:HD2	1.85	0.43
1:C:978:ASN:OD1	1:C:979:ASP:N	2.51	0.43
2:D:38:PHE:HB3	2:D:46:ARG:HG2	2.00	0.43
1:A:316:SER:O	1:A:595:VAL:HG12	2.19	0.43
1:C:96:GLU:OE1	1:C:190:ARG:HD3	2.19	0.43
2:D:10:GLY:HA2	2:D:120:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:TYR:CG	4:A:1301:NAG:H61	2.54	0.43
1:A:287:ASP:OD1	1:A:288:ALA:N	2.51	0.43
1:A:986:PRO:N	1:A:987:PRO:HD2	2.34	0.43
1:A:1125:ASN:N	1:A:1125:ASN:OD1	2.49	0.43
1:B:168:PHE:HZ	1:B:230:PRO:HD2	1.83	0.43
1:B:747:THR:O	1:B:750:SER:OG	2.26	0.43
1:A:699:LEU:HD12	1:B:873:TYR:CZ	2.53	0.43
1:C:203:ILE:HB	1:C:227:VAL:HG12	2.01	0.43
1:C:770:ILE:HD13	1:C:770:ILE:HA	1.81	0.43
1:B:590:CYS:SG	1:B:591:SER:N	2.91	0.43
1:B:969:LYS:HE2	1:B:969:LYS:HB2	1.85	0.43
1:A:168:PHE:HD1	1:A:169:GLU:N	2.17	0.43
1:A:454:ARG:HA	1:A:492:LEU:HA	2.01	0.43
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.92	0.43
1:B:287:ASP:OD1	1:B:288:ALA:N	2.52	0.43
1:C:125:ASN:HB2	1:C:172:SER:O	2.19	0.43
1:C:574:ASP:N	1:C:574:ASP:OD1	2.51	0.43
1:A:231:ILE:HG22	1:A:232:GLY:N	2.34	0.42
1:B:310:LYS:HE3	1:B:310:LYS:HB3	1.72	0.42
1:A:562:PHE:CE2	1:B:41:LYS:HG3	2.54	0.42
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.02	0.42
1:C:81:ASN:ND2	1:C:240:THR:O	2.52	0.42
1:C:231:ILE:CG1	1:C:233:ILE:HG12	2.49	0.42
2:D:39:ARG:HB2	2:D:49:VAL:HG21	2.01	0.42
1:B:535:LYS:HA	1:B:552:LEU:HD23	2.01	0.42
1:C:276:LEU:HB3	1:C:289:VAL:HG22	2.01	0.42
1:C:983:ARG:NH2	1:C:984:LEU:HB2	2.34	0.42
2:E:74:ASP:OD1	2:E:75:ASN:N	2.53	0.42
1:A:404:GLY:HA2	1:A:508:TYR:CD1	2.54	0.42
1:A:738:CYS:HB3	1:A:739:THR:HG23	2.01	0.42
1:B:326:ILE:HG21	1:B:534:VAL:HG22	2.00	0.42
1:B:542:ASN:HB2	1:B:547:LYS:NZ	2.35	0.42
1:B:557:LYS:HD3	1:B:558:LYS:HG2	2.02	0.42
2:E:68:ARG:HG2	2:E:69:PHE:CE1	2.54	0.42
1:A:558:LYS:HA	1:A:558:LYS:HD3	1.71	0.42
1:A:742:ILE:HD12	1:A:742:ILE:HA	1.87	0.42
1:B:50:SER:HB2	1:B:276:LEU:HD12	2.01	0.42
1:B:358:ILE:HD12	1:B:395:VAL:HG13	2.02	0.42
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.87	0.42
1:C:983:ARG:NH1	1:C:984:LEU:HB2	2.35	0.42
1:B:972:ALA:N	1:B:995:ARG:HH12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ALA:N	1:C:373:PRO:HD2	2.35	0.42
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.80	0.42
1:B:552:LEU:HG	1:B:585:LEU:HD12	2.02	0.42
1:B:1004:LEU:HD12	1:B:1004:LEU:HA	1.76	0.42
1:A:331:ASN:HB3	4:A:1302:NAG:O5	2.19	0.42
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.82	0.42
1:B:425:LEU:HA	1:B:425:LEU:HD23	1.87	0.42
1:B:713:ALA:HB3	1:C:894:LEU:HB3	2.02	0.42
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.79	0.42
1:C:234:ASN:HB3	4:C:1302:NAG:H82	2.02	0.42
1:C:234:ASN:OD1	1:C:234:ASN:N	2.53	0.42
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.72	0.42
1:A:44:ARG:HD2	1:A:49:HIS:CD2	2.55	0.41
1:C:328:ARG:HH21	1:C:531:THR:H	1.67	0.41
1:C:456:PHE:HB3	1:C:473:TYR:CG	2.55	0.41
1:C:763:LEU:HD12	1:C:1008:VAL:HG21	2.02	0.41
1:A:707:TYR:HE1	1:B:897:PRO:HA	1.85	0.41
1:A:954:HIS:HB3	1:A:1014:ARG:NH1	2.35	0.41
1:B:110:LEU:HG	1:B:135:PHE:CZ	2.55	0.41
1:B:380:TYR:CZ	1:B:412:PRO:HD2	2.55	0.41
1:C:226:LEU:HD23	1:C:227:VAL:HB	2.02	0.41
1:C:439:ASN:O	1:C:443:SER:HB2	2.21	0.41
1:A:16:VAL:HG23	1:A:158:ARG:NH2	2.35	0.41
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.53	0.41
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.55	0.41
1:B:376:THR:HG21	2:D:32:PHE:CD1	2.55	0.41
1:C:994:ASP:O	1:C:998:THR:HG23	2.20	0.41
2:D:109:ILE:HG13	2:D:110:PRO:CD	2.50	0.41
1:A:282:ASN:O	1:A:283:GLY:C	2.58	0.41
1:A:997:ILE:HD13	1:A:997:ILE:HA	1.84	0.41
1:A:1010:GLN:HE21	1:A:1010:GLN:HB3	1.69	0.41
1:B:439:ASN:HB3	1:B:440:LYS:NZ	2.36	0.41
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.87	0.41
1:C:541:PHE:HB2	1:C:543:PHE:CE1	2.56	0.41
2:D:40:GLN:O	2:D:93:ALA:HB1	2.20	0.41
2:E:16:GLY:HA2	2:E:86:SER:HA	2.02	0.41
1:A:103:GLY:HA3	1:A:120:VAL:HA	2.01	0.41
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.87	0.41
1:B:83:VAL:HG11	1:B:237:ARG:HH21	1.85	0.41
1:B:372:ALA:HB3	1:B:375:PHE:HD2	1.85	0.41
1:B:455:LEU:N	1:B:491:PRO:O	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:HG23	1:B:524:VAL:HG23	2.03	0.41
1:C:433:VAL:HG12	1:C:512:VAL:HG22	2.02	0.41
1:C:1018:ILE:HD13	1:C:1018:ILE:HA	1.89	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.55	0.41
2:E:20:ARG:HH22	2:E:81:TYR:CB	2.32	0.41
1:A:159:VAL:HG13	1:A:160:TYR:HD1	1.86	0.41
1:B:882:ILE:HA	1:B:882:ILE:HD13	1.81	0.41
1:B:971:GLY:C	1:B:995:ARG:HH12	2.23	0.41
1:A:599:THR:HB	1:A:608:VAL:HG12	2.02	0.41
1:A:1133:VAL:HB	1:A:1134:ASN:H	1.70	0.41
1:B:196:ASN:O	1:B:197:ILE:HD13	2.20	0.41
1:B:503:VAL:HG11	2:D:73:ARG:NH1	2.36	0.41
1:B:539:VAL:HG12	1:B:540:ASN:N	2.36	0.41
1:C:408:ARG:HE	1:C:408:ARG:HB2	1.79	0.41
1:B:15:CYS:SG	1:B:16:VAL:N	2.94	0.41
1:B:563:GLN:O	1:B:577:ARG:NH1	2.54	0.41
1:C:21:ARG:HB3	1:C:79:PHE:HD2	1.83	0.41
1:C:582:LEU:O	1:C:584:ILE:N	2.54	0.41
1:C:699:LEU:H	1:C:699:LEU:HD22	1.85	0.41
1:C:1032:CYS:O	1:C:1051:SER:OG	2.36	0.41
1:C:1106:GLN:NE2	1:C:1111:GLU:OE2	2.53	0.41
1:A:133:PHE:HD1	1:A:163:ALA:HA	1.86	0.41
1:A:808:ASP:HB3	1:A:811:LYS:HG2	2.02	0.41
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.02	0.41
1:B:822:LEU:HD21	1:B:938:LEU:HD13	2.03	0.41
1:C:433:VAL:HG12	1:C:512:VAL:HG13	2.03	0.41
2:E:100:TRP:NE1	2:E:110:PRO:O	2.53	0.41
1:A:18:LEU:HD22	1:A:258:TRP:CZ2	2.55	0.41
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.73	0.41
1:A:562:PHE:HE2	1:B:41:LYS:HG3	1.85	0.41
1:A:707:TYR:HD2	1:B:792:PRO:HG3	1.85	0.41
1:B:210:ILE:HD13	1:B:210:ILE:HA	1.85	0.41
1:B:229:LEU:HA	1:B:230:PRO:HD3	1.91	0.41
1:B:418:ILE:HG23	1:B:422:ASN:HB2	2.03	0.41
1:A:40:ASP:OD2	1:A:44:ARG:NH2	2.53	0.40
1:A:759:PHE:CD2	1:A:1001:LEU:HD21	2.55	0.40
1:C:170:TYR:CZ	1:C:172:SER:HB2	2.56	0.40
1:C:198:ASP:O	1:C:198:ASP:CG	2.59	0.40
1:C:407:VAL:O	1:C:410:ILE:HG12	2.20	0.40
1:B:96:GLU:HG3	1:B:101:ILE:HD12	2.03	0.40
1:B:99:ASN:HB3	1:B:102:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:O	1:A:269:TYR:OH	2.33	0.40
1:A:544:ASN:OD1	1:A:544:ASN:N	2.55	0.40
1:B:553:THR:O	1:B:585:LEU:HA	2.21	0.40
1:C:644:GLN:HE21	1:C:645:THR:N	2.20	0.40
1:C:709:ASN:N	1:C:709:ASN:OD1	2.52	0.40
1:C:764:LYS:HE3	1:C:764:LYS:HB2	1.87	0.40
1:C:813:SER:OG	1:C:815:ARG:NH1	2.54	0.40
2:D:109:ILE:HG13	2:D:110:PRO:N	2.37	0.40
2:E:50:SER:OG	2:E:51:ALA:N	2.54	0.40
1:B:205:SER:OG	1:B:206:LYS:N	2.54	0.40
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.33	0.40
1:A:61:ASN:HB2	4:A:1301:NAG:H2	2.03	0.40
1:A:764:LYS:HB3	1:A:764:LYS:HE3	1.90	0.40
1:B:705:VAL:HG21	1:C:883:THR:OG1	2.21	0.40
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.90	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	1017/1285 (79%)	925 (91%)	86 (8%)	6 (1%)	22	54
1	B	1016/1285 (79%)	938 (92%)	74 (7%)	4 (0%)	30	62
1	C	999/1285 (78%)	927 (93%)	65 (6%)	7 (1%)	19	51
2	D	123/124 (99%)	120 (98%)	3 (2%)	0	100	100
2	E	123/124 (99%)	119 (97%)	4 (3%)	0	100	100
All	All	3278/4103 (80%)	3029 (92%)	232 (7%)	17 (0%)	27	57

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	THR
1	C	408	ARG
1	C	584	ILE
1	C	587	ILE
1	A	404	GLY
1	B	332	ILE
1	C	588	THR
1	A	410	ILE
1	B	536	ASN
1	C	233	ILE
1	B	164	ASN
1	C	409	GLN
1	C	234	ASN
1	A	233	ILE
1	A	1133	VAL
1	A	127	VAL
1	A	407	VAL

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	906/1115 (81%)	855 (94%)	51 (6%)	17	44
1	B	908/1115 (81%)	860 (95%)	48 (5%)	19	45
1	C	893/1115 (80%)	863 (97%)	30 (3%)	32	55
2	D	102/101 (101%)	96 (94%)	6 (6%)	16	42
2	E	102/101 (101%)	97 (95%)	5 (5%)	21	46
All	All	2911/3547 (82%)	2771 (95%)	140 (5%)	24	47

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	60	SER
1	A	106	PHE

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Mol	Chain	Res	Type
1	A	168	PHE
1	A	233	ILE
1	A	234	ASN
1	A	235	ILE
1	A	275	PHE
1	A	281	GLU
1	A	290	ASP
1	A	304	LYS
1	A	332	ILE
1	A	334	ASN
1	A	357	ARG
1	A	368	LEU
1	A	370	ASN
1	A	371	LEU
1	A	377	PHE
1	A	392	PHE
1	A	394	ASN
1	A	402	ILE
1	A	406	GLU
1	A	418	ILE
1	A	450	ASN
1	A	495	TYR
1	A	505	HIS
1	A	518	LEU
1	A	547	LYS
1	A	559	PHE
1	A	562	PHE
1	A	571	ASP
1	A	574	ASP
1	A	591	SER
1	A	592	PHE
1	A	604	THR
1	A	618	THR
1	A	711	SER
1	A	745	ASP
1	A	810	SER
1	A	875	SER
1	A	981	PHE
1	A	1010	GLN
1	A	1072	GLU
1	A	1073	LYS
1	A	1077	THR

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Mol	Chain	Res	Type
1	A	1083	HIS
1	A	1097	SER
1	A	1115	ILE
1	A	1117	THR
1	A	1118	ASP
1	A	1133	VAL
1	B	18	LEU
1	B	29	THR
1	B	63	THR
1	B	79	PHE
1	B	99	ASN
1	B	102	ARG
1	B	117	LEU
1	B	132	GLU
1	B	133	PHE
1	B	135	PHE
1	B	136	CYS
1	B	137	ASN
1	B	165	ASN
1	B	167	THR
1	B	168	PHE
1	B	186	PHE
1	B	234	ASN
1	B	235	ILE
1	B	237	ARG
1	B	258	TRP
1	B	305	SER
1	B	316	SER
1	B	337	PRO
1	B	343	ASN
1	B	351	TYR
1	B	368	LEU
1	B	424	LYS
1	B	441	LEU
1	B	497	PHE
1	B	501	TYR
1	B	541	PHE
1	B	565	PHE
1	B	581	THR
1	B	582	LEU
1	B	585	LEU
1	B	590	CYS

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Mol	Chain	Res	Type
1	B	592	PHE
1	B	604	THR
1	B	675	GLN
1	B	695	TYR
1	B	697	MET
1	B	759	PHE
1	B	773	GLU
1	B	937	SER
1	B	964	LYS
1	B	1086	LYS
1	B	1107	ARG
1	B	1118	ASP
1	C	30	ASN
1	C	52	GLN
1	C	77	LYS
1	C	79	PHE
1	C	88	ASP
1	C	134	GLN
1	C	164	ASN
1	C	186	PHE
1	C	198	ASP
1	C	258	TRP
1	C	317	ASN
1	C	325	SER
1	C	331	ASN
1	C	377	PHE
1	C	388	ASN
1	C	402	ILE
1	C	408	ARG
1	C	409	GLN
1	C	543	PHE
1	C	554	GLU
1	C	675	GLN
1	C	702	GLU
1	C	810	SER
1	C	854	LYS
1	C	855	PHE
1	C	867	ASP
1	C	906	PHE
1	C	984	LEU
1	C	1019	ARG
1	C	1092	GLU

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Mol	Chain	Res	Type
2	D	8	SER
2	D	48	PHE
2	D	88	ARG
2	D	100	TRP
2	D	102	MET
2	D	106	GLN
2	E	8	SER
2	E	38	PHE
2	E	46	ARG
2	E	96	TYR
2	E	102	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	965	GLN
1	A	1010	GLN
1	C	317	ASN
1	C	644	GLN
1	C	804	GLN
1	C	935	GLN
2	D	83	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

20 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	K	1	3,1	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	L	1	3,1	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	L	2	3	14,14,15	0.19	0	17,19,21	0.39	0
3	NAG	M	1	3,1	14,14,15	0.18	0	17,19,21	0.47	0
3	NAG	M	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	R	1	3,1	14,14,15	0.40	0	17,19,21	0.66	0
3	NAG	R	2	3	14,14,15	0.40	0	17,19,21	0.70	0
3	NAG	S	1	3,1	14,14,15	0.30	0	17,19,21	0.39	0
3	NAG	S	2	3	14,14,15	0.17	0	17,19,21	0.42	0
3	NAG	T	1	3,1	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	T	2	3	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	U	1	3,1	14,14,15	0.30	0	17,19,21	0.40	0
3	NAG	U	2	3	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	X	1	3,1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	X	2	3	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	Z	1	3,1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	Z	2	3	14,14,15	0.23	0	17,19,21	0.38	0
3	NAG	a	1	3,1	14,14,15	0.18	0	17,19,21	0.44	0
3	NAG	a	2	3	14,14,15	0.24	0	17,19,21	0.39	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	K	1	3,1	-	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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6

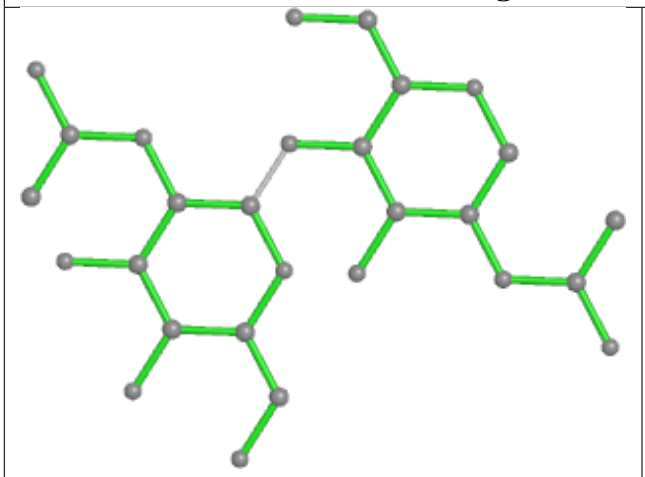
There are no ring outliers.

1 monomer is involved in 1 short contact:

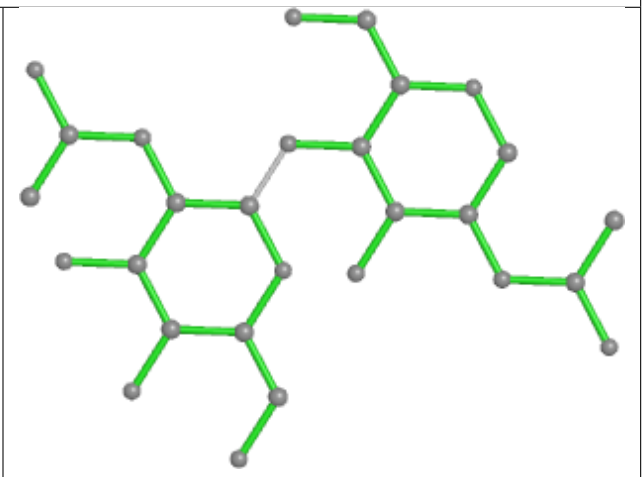
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0

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

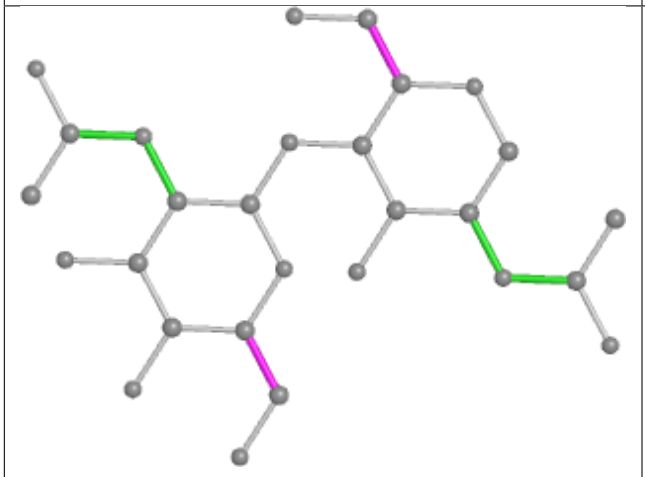
Oligosaccharide Chain K



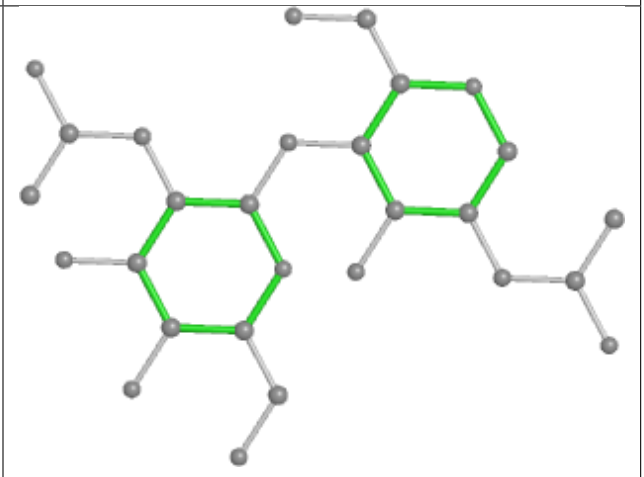
Bond lengths



Bond angles

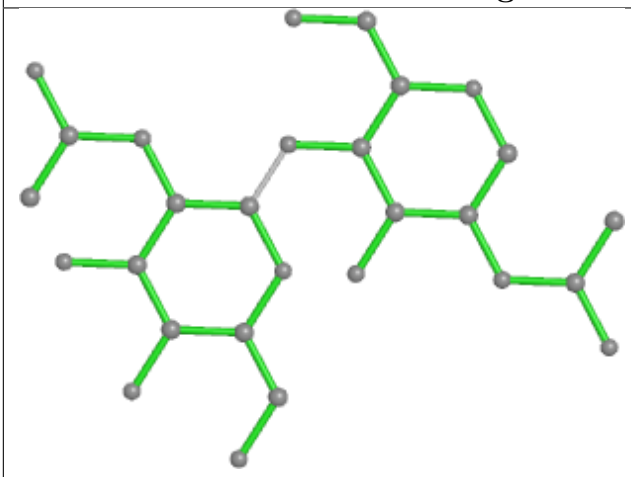


Torsions

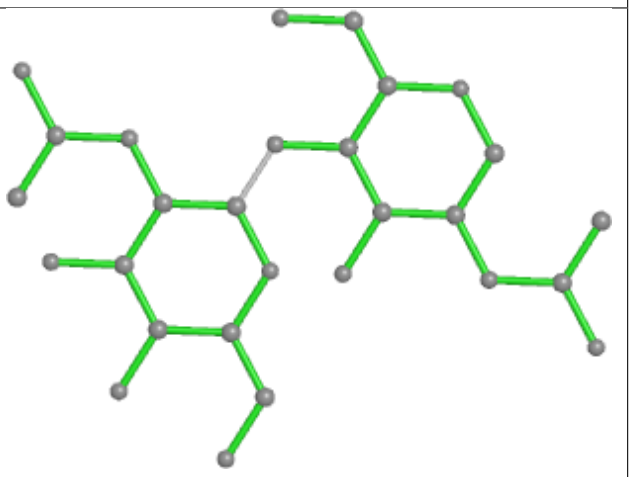


Rings

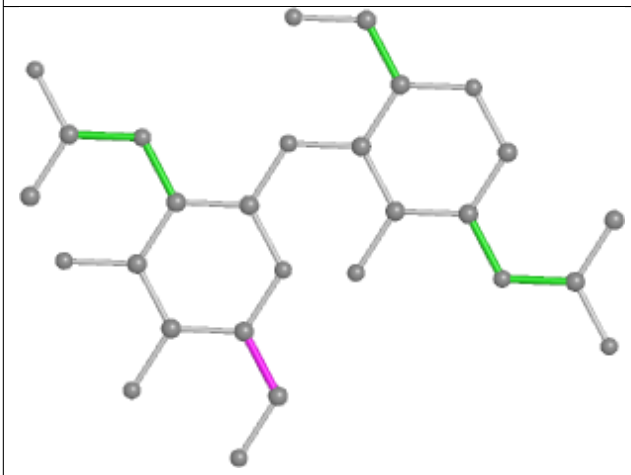
Oligosaccharide Chain L



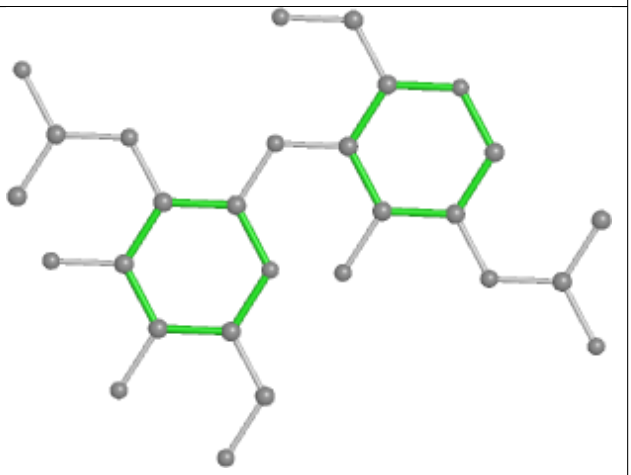
Bond lengths



Bond angles

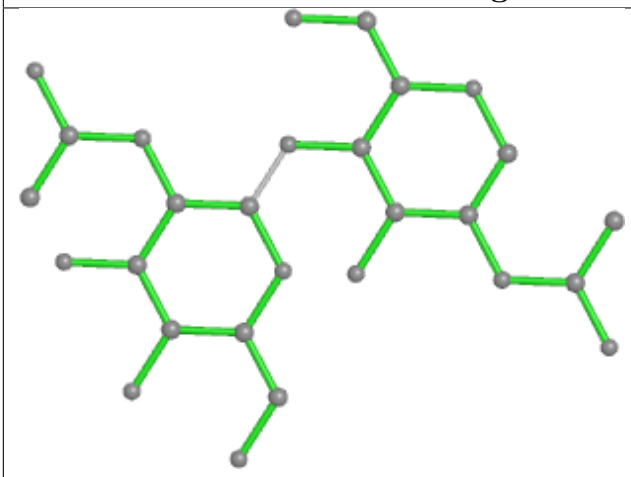


Torsions

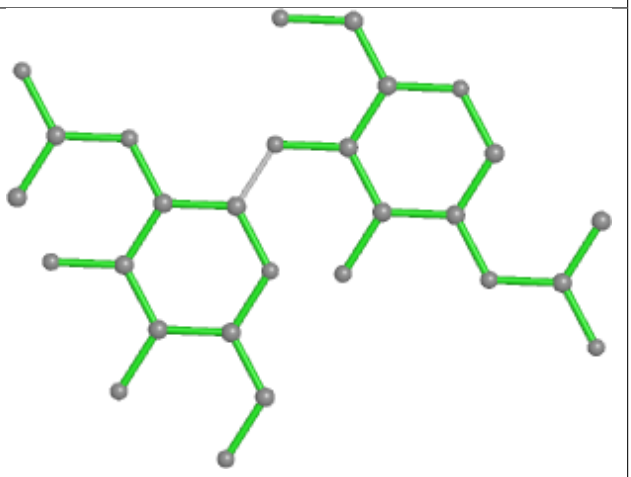


Rings

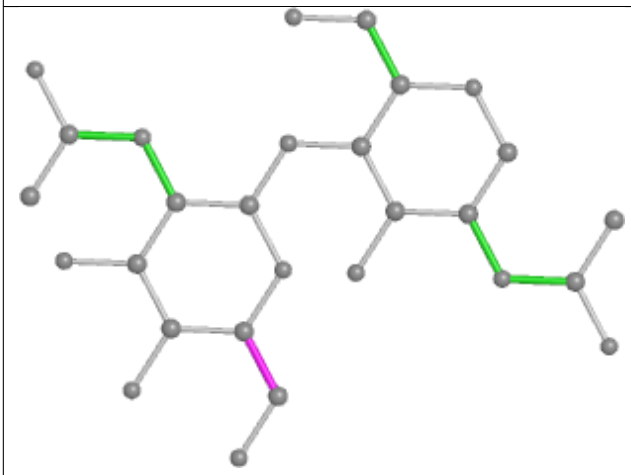
Oligosaccharide Chain M



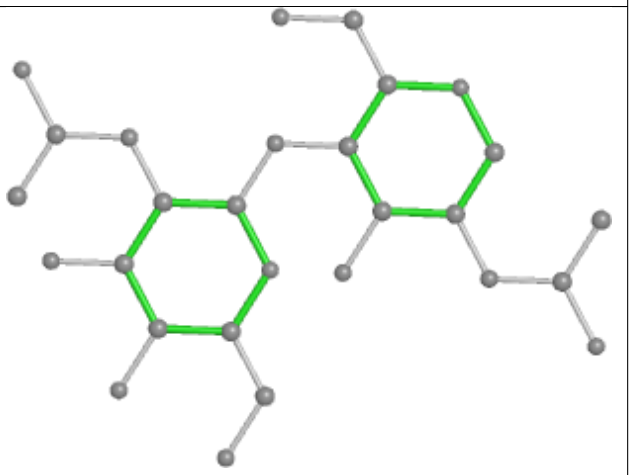
Bond lengths



Bond angles

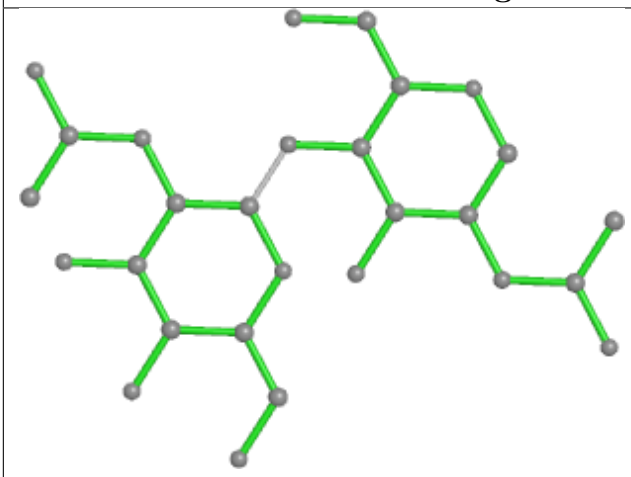


Torsions

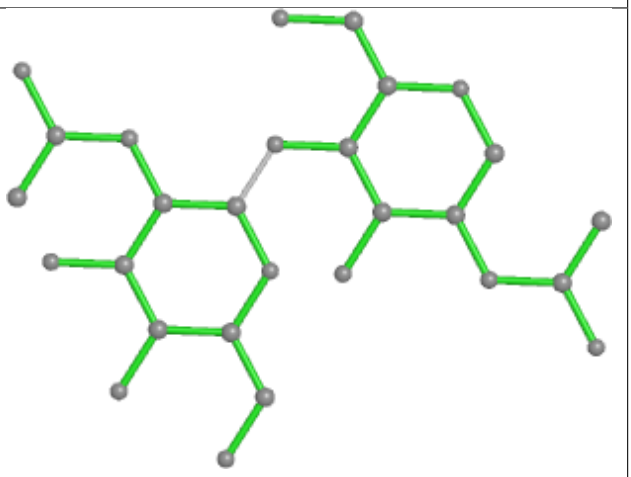


Rings

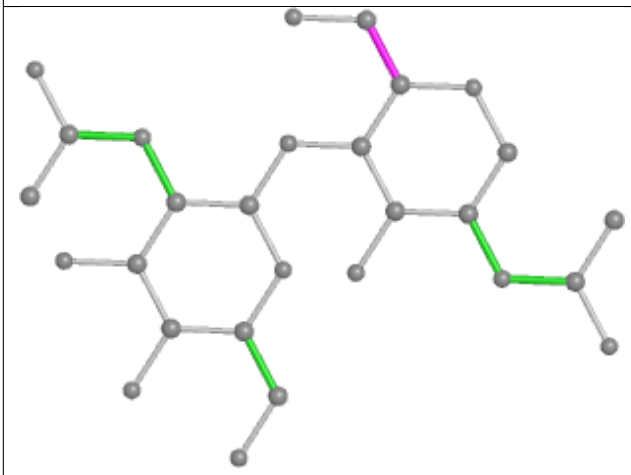
Oligosaccharide Chain R



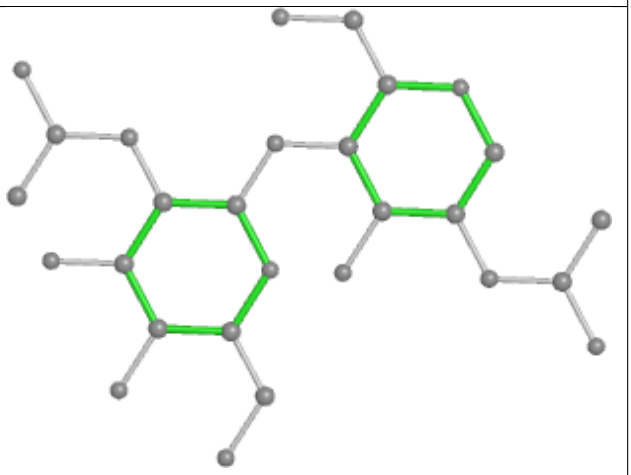
Bond lengths



Bond angles

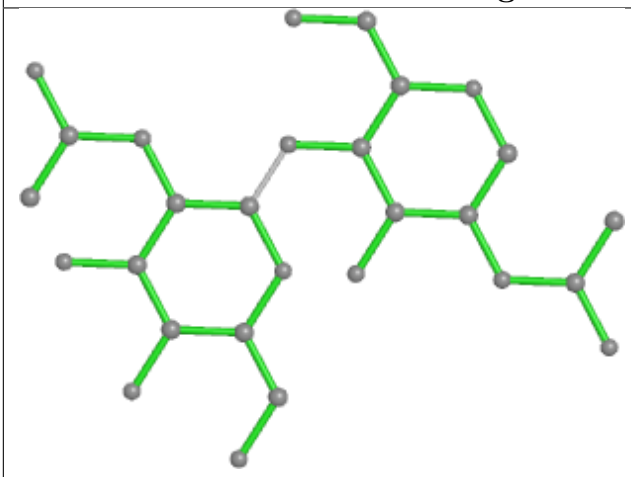


Torsions

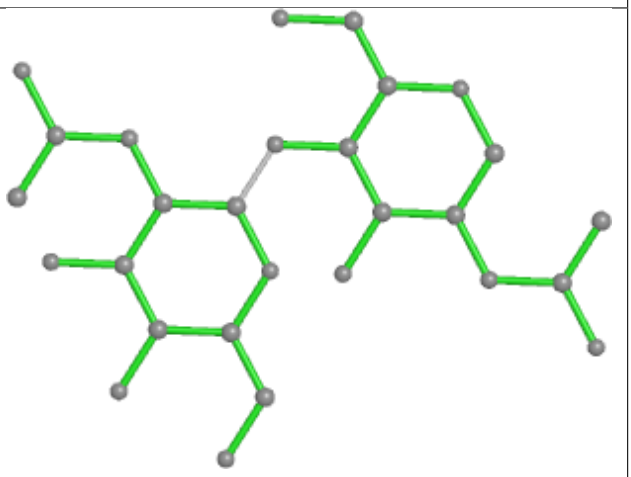


Rings

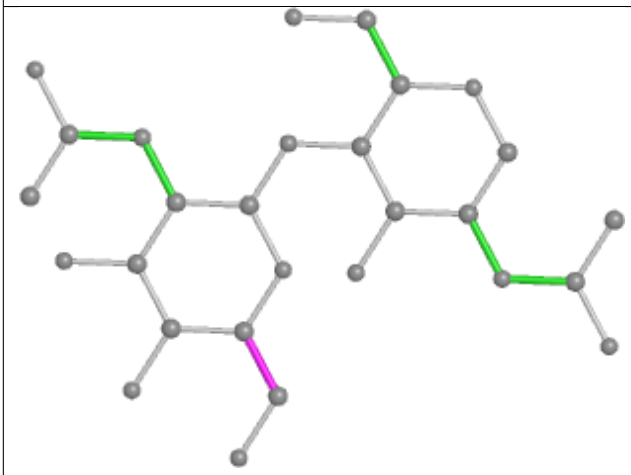
Oligosaccharide Chain S



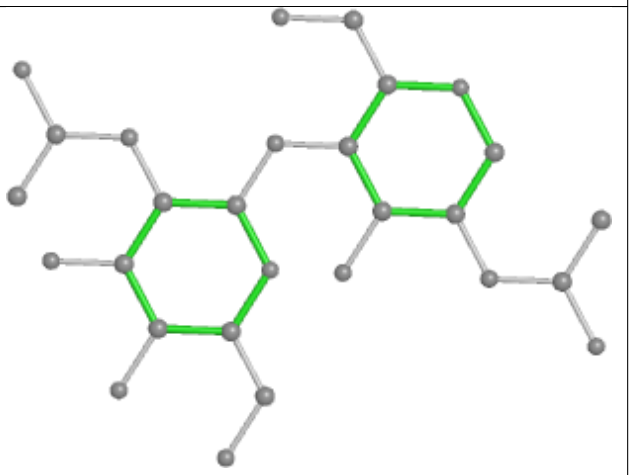
Bond lengths



Bond angles

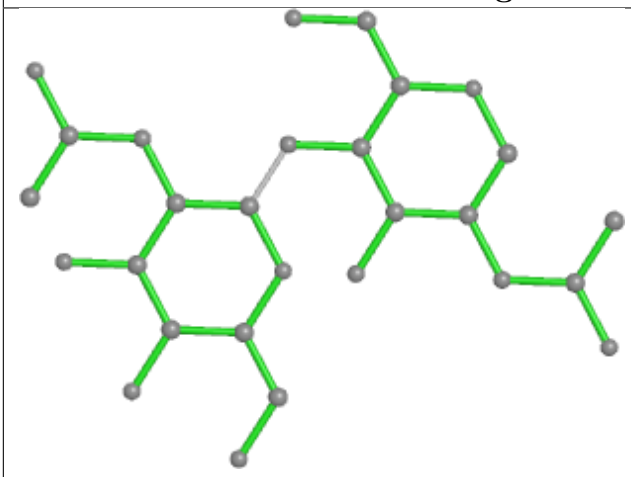


Torsions

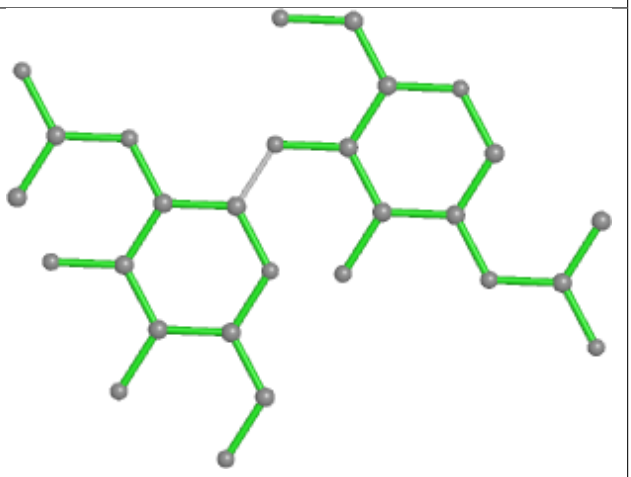


Rings

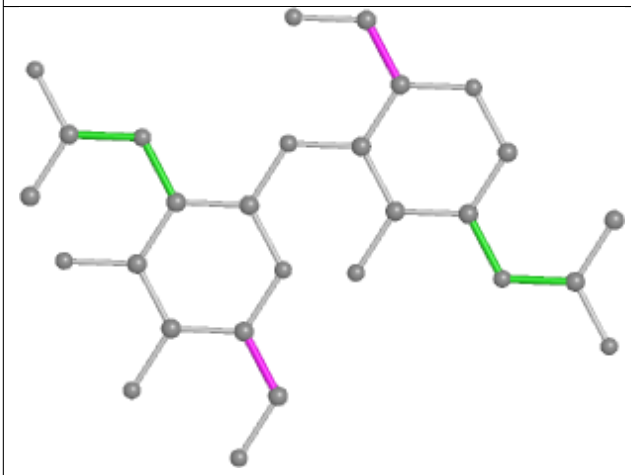
Oligosaccharide Chain T



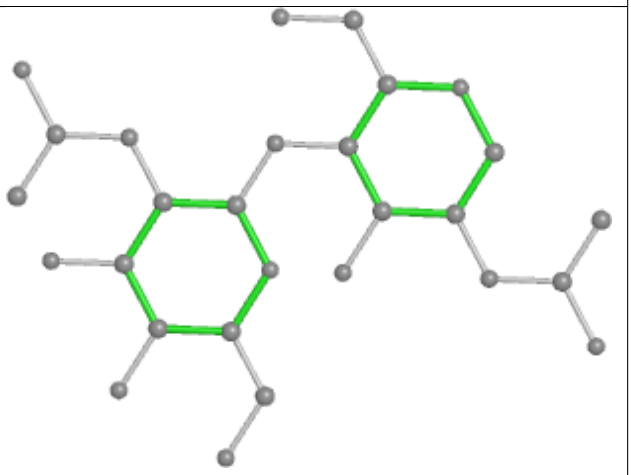
Bond lengths



Bond angles

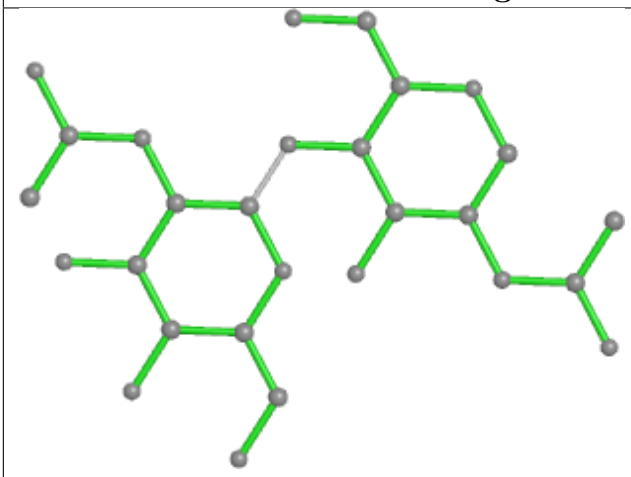


Torsions

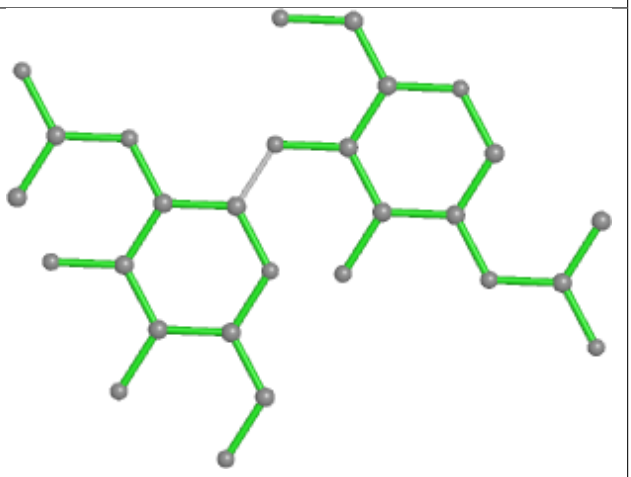


Rings

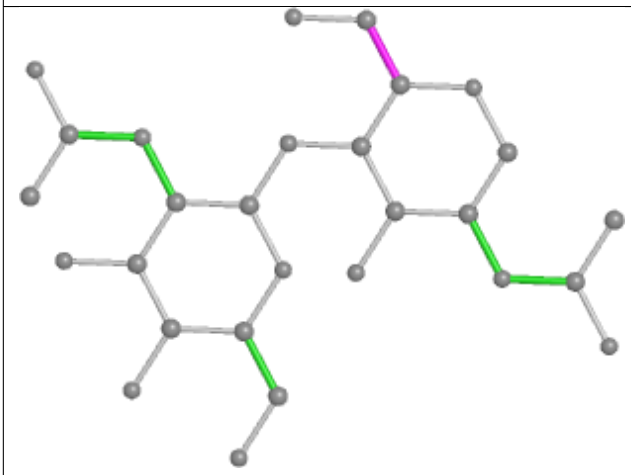
Oligosaccharide Chain U



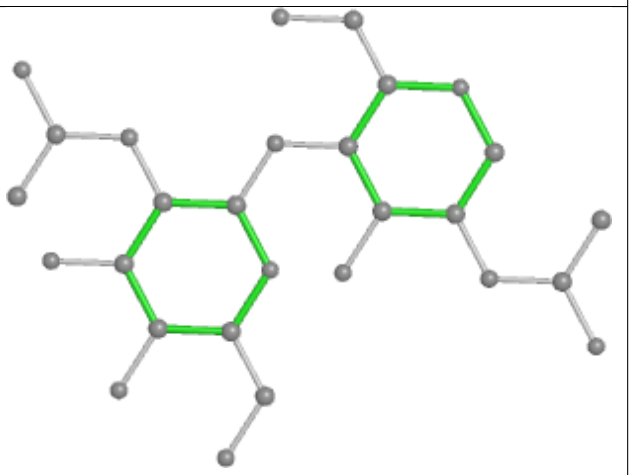
Bond lengths



Bond angles

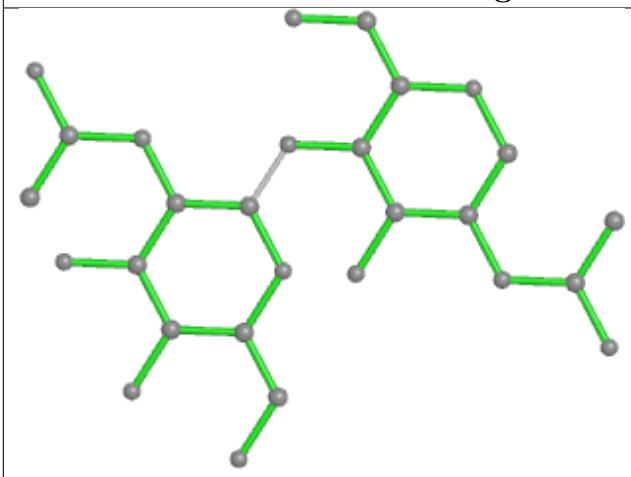


Torsions

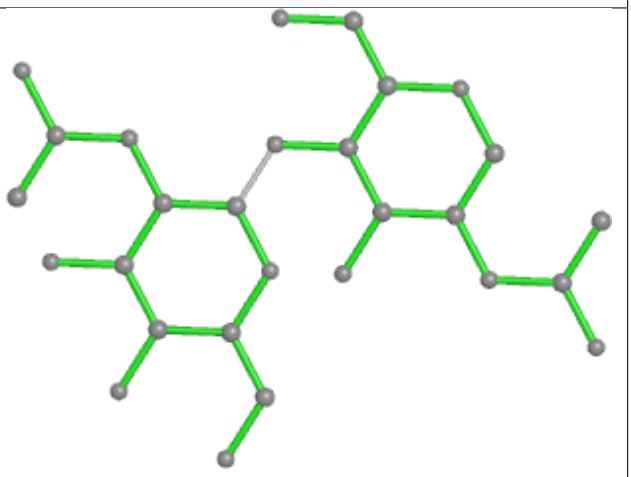


Rings

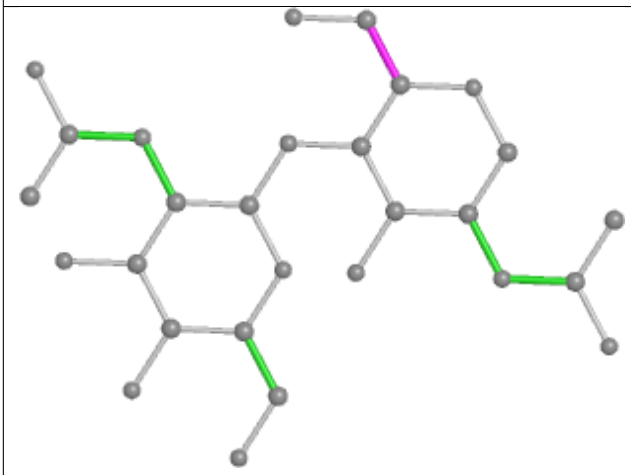
Oligosaccharide Chain X



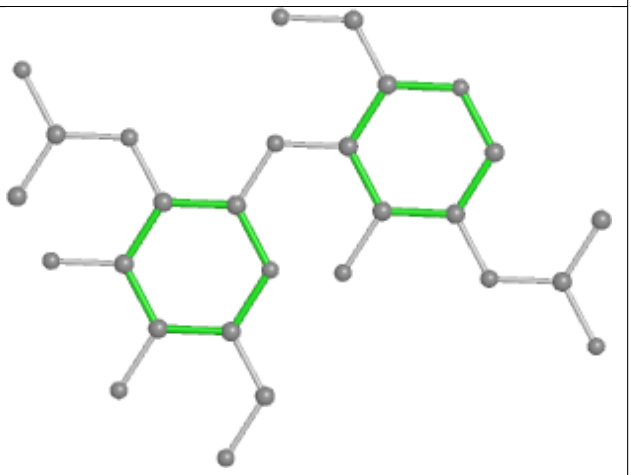
Bond lengths



Bond angles

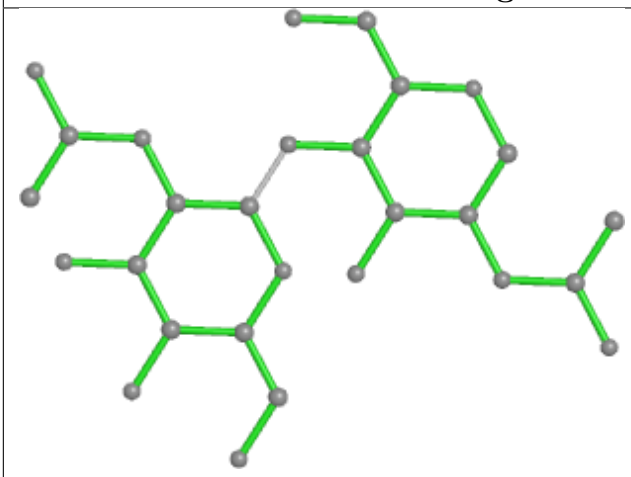


Torsions

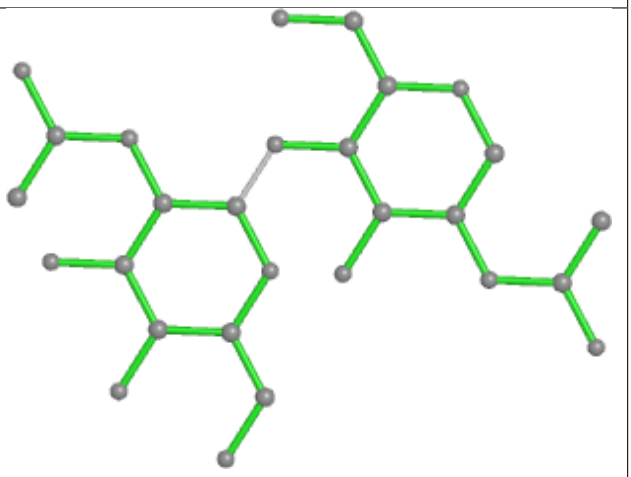


Rings

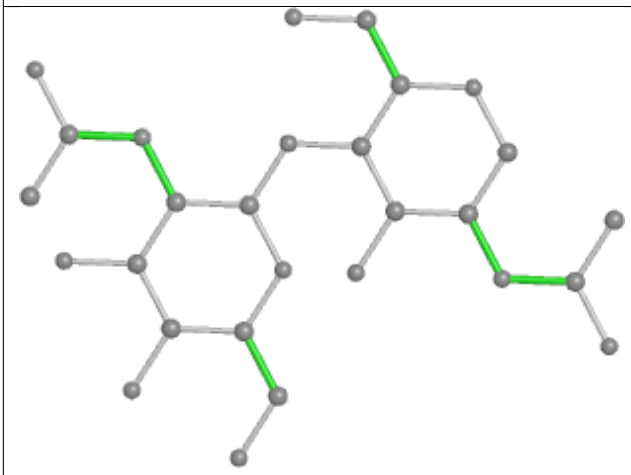
Oligosaccharide Chain Z



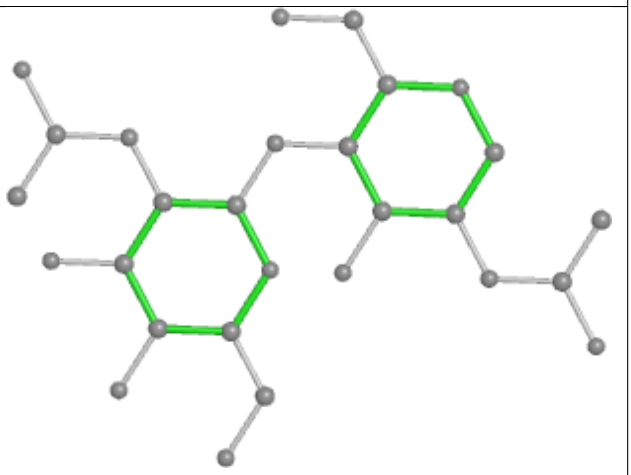
Bond lengths



Bond angles

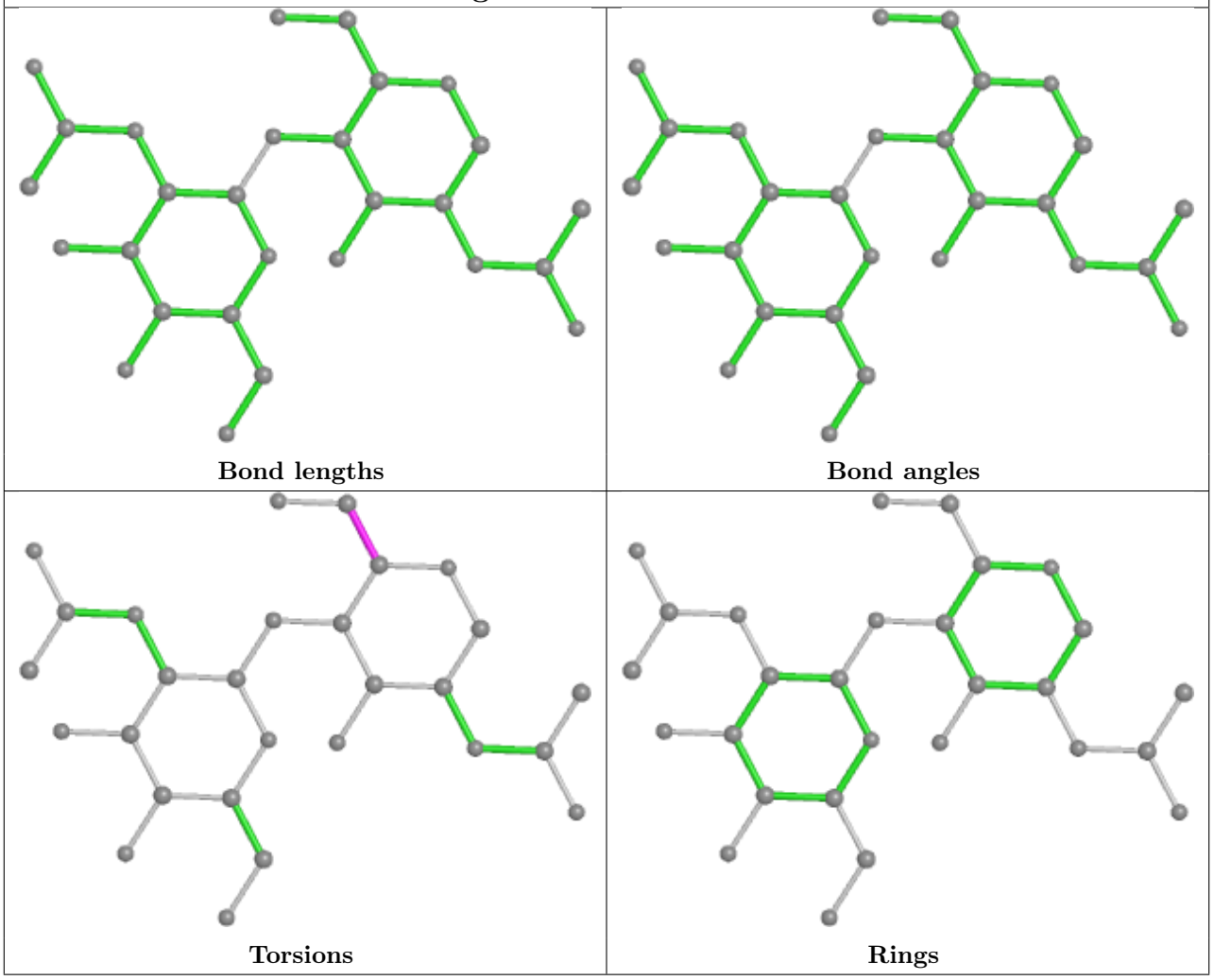


Torsions



Rings

Oligosaccharide Chain a



5.6 Ligand geometry (i)

28 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	1301	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	B	1302	1	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	A	1303	1	14,14,15	0.41	0	17,19,21	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1307	-	14,14,15	0.18	0	17,19,21	0.43	0
4	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	0.51	0
4	NAG	C	1304	-	14,14,15	0.19	0	17,19,21	0.41	0
4	NAG	B	1305	1	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
4	NAG	B	1306	1	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
4	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.31	0
4	NAG	C	1309	1	14,14,15	0.42	0	17,19,21	0.48	0
4	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	B	1310	-	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	B	1303	1	14,14,15	0.41	0	17,19,21	1.78	2 (11%)
4	NAG	A	1301	1	14,14,15	0.32	0	17,19,21	0.31	0
4	NAG	A	1304	1	14,14,15	0.40	0	17,19,21	0.50	0
4	NAG	C	1305	1	14,14,15	0.18	0	17,19,21	0.49	0
4	NAG	A	1307	1	14,14,15	0.40	0	17,19,21	0.92	2 (11%)
4	NAG	C	1308	-	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	C	1303	-	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	B	1308	1	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	B	1311	-	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	B	1301	1	14,14,15	0.43	0	17,19,21	1.61	1 (5%)
4	NAG	C	1306	-	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1305	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	A	1306	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1302	1	14,14,15	0.42	0	17,19,21	0.64	0
4	NAG	A	1308	1	14,14,15	0.39	0	17,19,21	0.49	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	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1307	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	6/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1308	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1311	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	6/6/23/26	0/1/1/1
4	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1303	NAG	O5-C1-C2	6.82	122.05	111.29
4	B	1301	NAG	O5-C1-C2	5.61	120.15	111.29
4	A	1307	NAG	O5-C1-C2	2.66	115.49	111.29
4	B	1305	NAG	C1-O5-C5	2.66	115.80	112.19
4	A	1303	NAG	C1-O5-C5	2.49	115.57	112.19
4	B	1306	NAG	O5-C1-C2	2.48	115.20	111.29
4	A	1307	NAG	C1-O5-C5	2.40	115.44	112.19
4	B	1303	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1303	NAG	C3-C2-N2-C7
4	A	1303	NAG	O7-C7-N2-C2
4	A	1307	NAG	C3-C2-N2-C7
4	A	1307	NAG	C8-C7-N2-C2
4	A	1307	NAG	O7-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	C	1309	NAG	C8-C7-N2-C2
4	C	1309	NAG	O7-C7-N2-C2
4	A	1303	NAG	C8-C7-N2-C2
4	B	1301	NAG	C8-C7-N2-C2
4	B	1301	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	C	1305	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1304	NAG	C8-C7-N2-C2
4	C	1303	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	A	1304	NAG	O7-C7-N2-C2
4	A	1308	NAG	C8-C7-N2-C2
4	A	1308	NAG	O7-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	A	1305	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	O7-C7-N2-C2
4	A	1308	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	B	1301	NAG	C1-C2-N2-C7
4	C	1302	NAG	C4-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	B	1301	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	B	1305	NAG	C1-C2-N2-C7
4	B	1301	NAG	O5-C5-C6-O6
4	C	1302	NAG	C8-C7-N2-C2
4	A	1307	NAG	C1-C2-N2-C7
4	A	1302	NAG	C8-C7-N2-C2
4	A	1308	NAG	C4-C5-C6-O6
4	A	1303	NAG	C1-C2-N2-C7
4	C	1309	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	C	1302	NAG	O7-C7-N2-C2
4	B	1305	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	A	1302	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	1	0
4	A	1301	NAG	2	0
4	C	1302	NAG	2	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.