Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 01:07 PM JST

PDB ID	:	7WG7
EMDB ID	:	EMD-32479
Title	:	Acidic Omicron Spike Trimer
Authors	:	Cui, Z.
Deposited on	:	2021-12-28
Resolution	:	4.00 Å(reported)

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

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

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

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

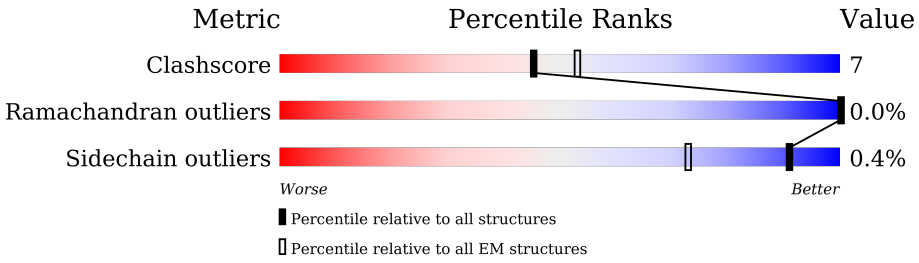
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.00 Å.

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



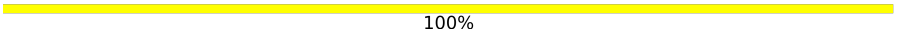
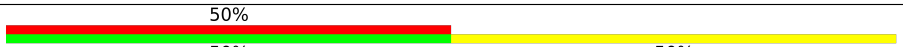
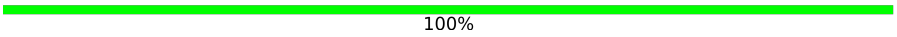
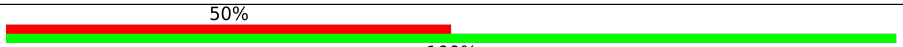
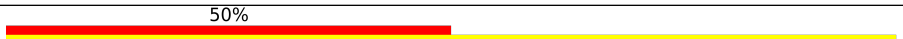
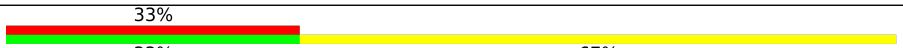
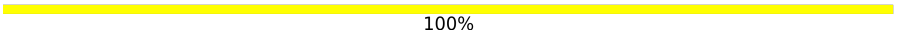
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1270	5% 71% 16% 14%
1	B	1270	8% 71% 15% 14%
1	C	1270	17% 70% 18% 12%
2	D	2	100% 50% 50%
2	E	2	50% 100%
2	F	2	100%
2	G	2	50% 100%
2	H	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
3	I	3	
3	J	3	
3	O	3	
3	U	3	
3	V	3	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27041 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	B	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
1	A	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
1	C	1117	Total	C	N	O	S	0	0
			8770	5611	1462	1657	40		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	208	ILE	-	insertion	UNP P0DTC2
B	209	VAL	-	insertion	UNP P0DTC2
B	210	ARG	ASN	conflict	UNP P0DTC2
B	211	GLU	LEU	conflict	UNP P0DTC2
B	212	PRO	VAL	conflict	UNP P0DTC2
B	213	GLU	ARG	conflict	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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	683	ALA	ARG	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
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	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	208	ILE	-	insertion	UNP P0DTC2
A	209	VAL	-	insertion	UNP P0DTC2
A	210	ARG	ASN	conflict	UNP P0DTC2
A	211	GLU	LEU	conflict	UNP P0DTC2
A	212	PRO	VAL	conflict	UNP P0DTC2
A	213	GLU	ARG	conflict	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	GLU	variant	UNP P0DTC2
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	683	ALA	ARG	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	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	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	208	ILE	-	insertion	UNP P0DTC2
C	209	VAL	-	insertion	UNP P0DTC2
C	210	ARG	ASN	conflict	UNP P0DTC2
C	211	GLU	LEU	conflict	UNP P0DTC2
C	212	PRO	VAL	conflict	UNP P0DTC2
C	213	GLU	ARG	conflict	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
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	683	ALA	ARG	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2

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

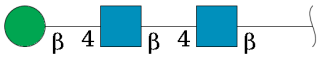
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

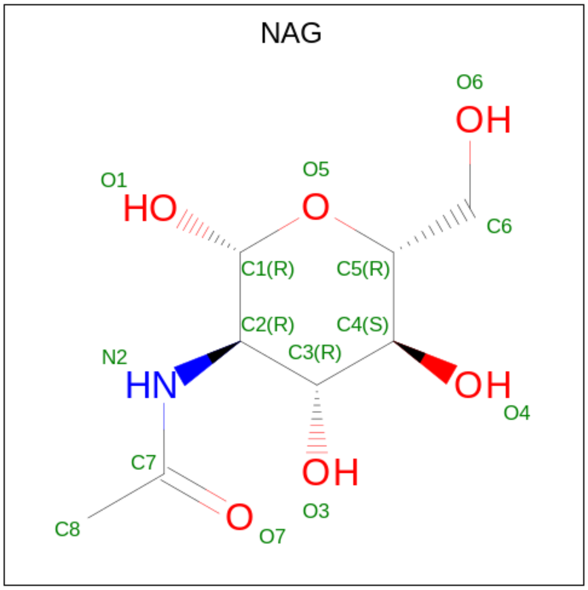
Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 140 80 10 50	0
4	A	1	Total C N O 140 80 10 50	0
4	A	1	Total C N O 140 80 10 50	0
4	A	1	Total C N O 140 80 10 50	0
4	A	1	Total C N O 140 80 10 50	0

Continued on next page...

Continued from previous page...

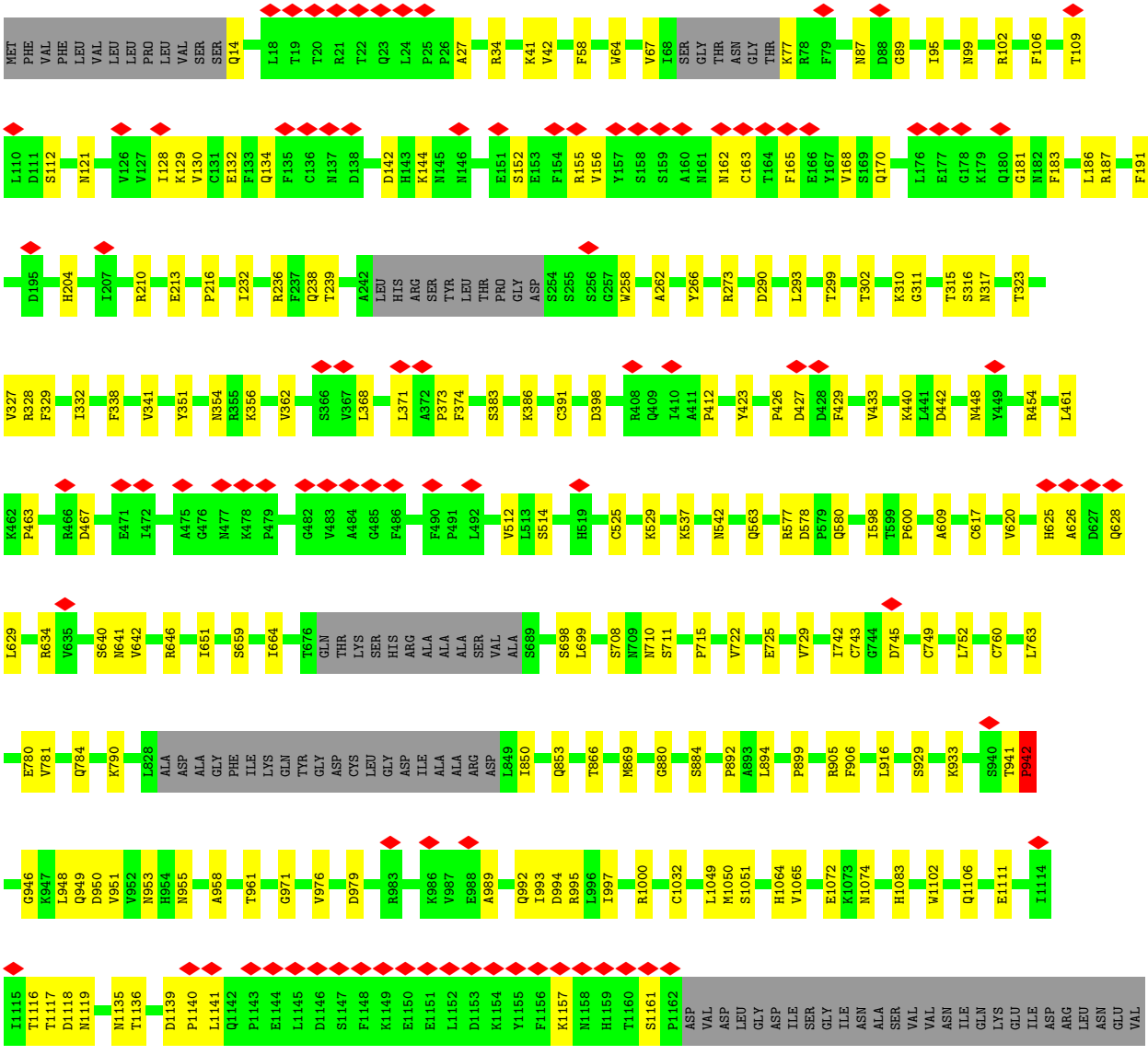
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 140	C 80	N 10	O 50	0
4	A	1	Total 140	C 80	N 10	O 50	0
4	A	1	Total 140	C 80	N 10	O 50	0
4	A	1	Total 140	C 80	N 10	O 50	0
4	A	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0

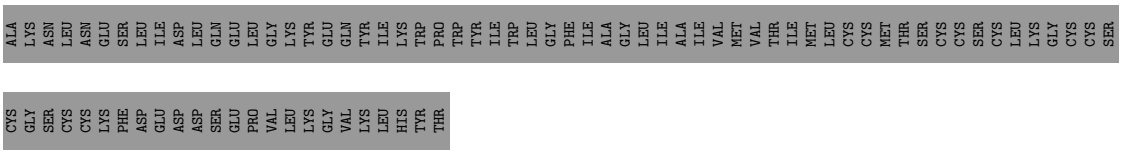
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

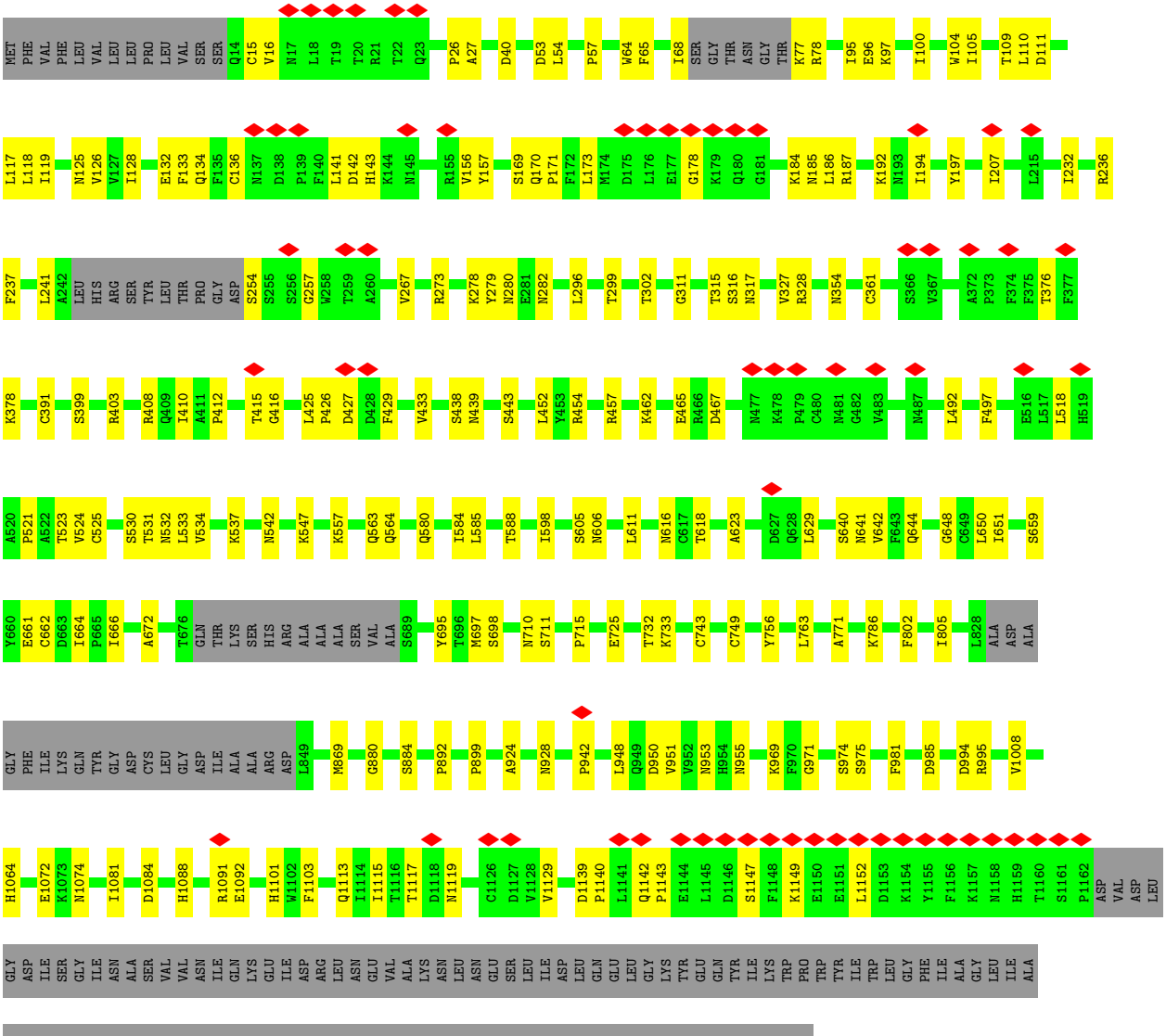
Chain B:





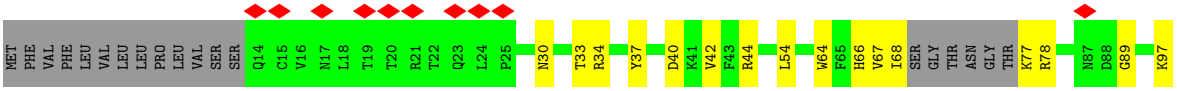
• Molecule 1: Spike glycoprotein

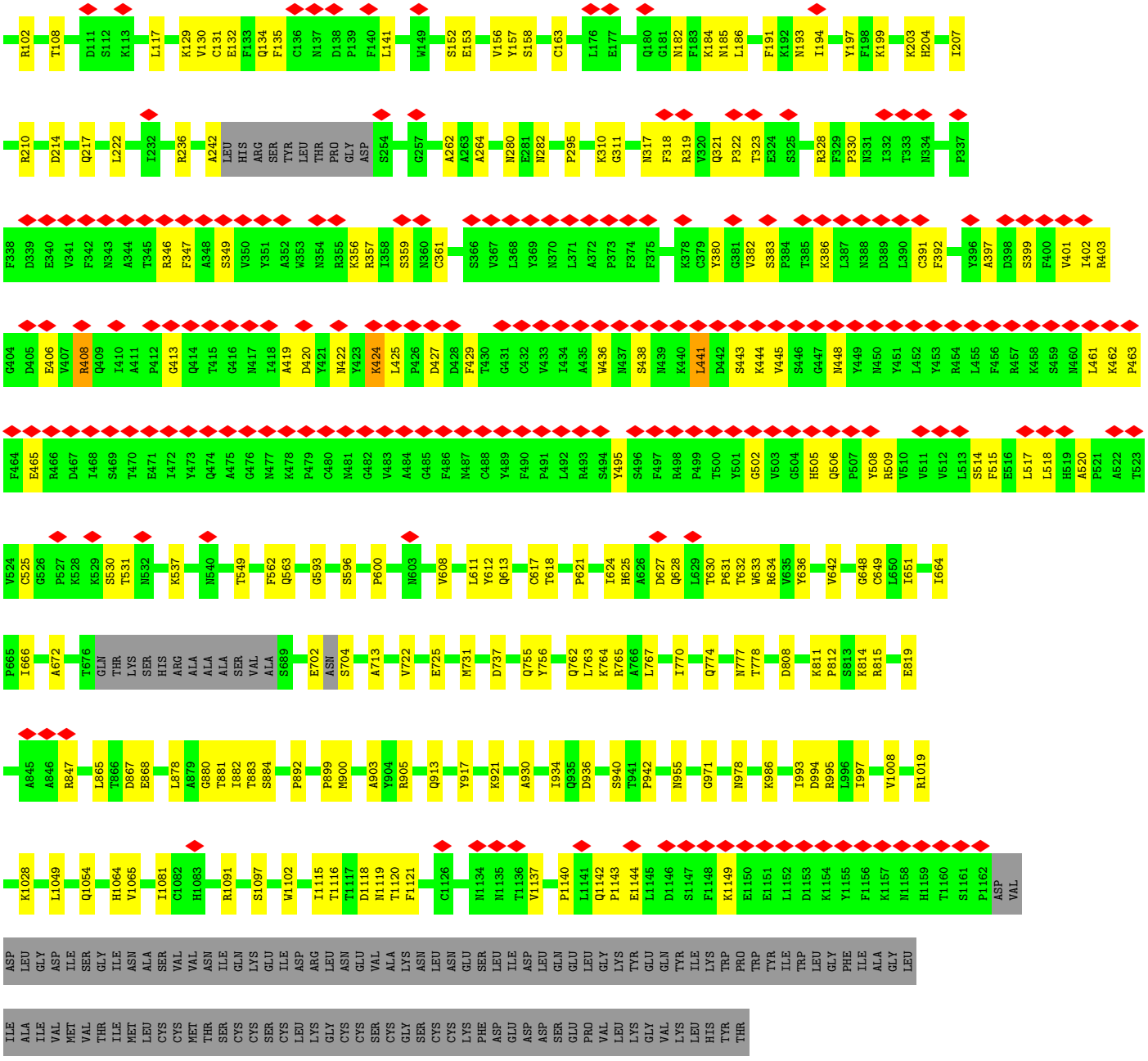
Chain A:



• Molecule 1: Spike glycoprotein

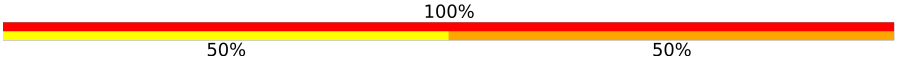
Chain C:





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

Chain D:

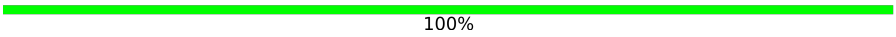


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

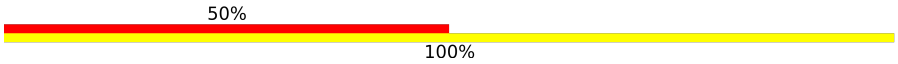
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain G:

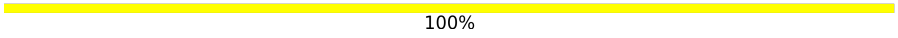


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain K:

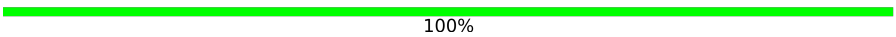


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

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

Chain M:



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

Chain N:

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

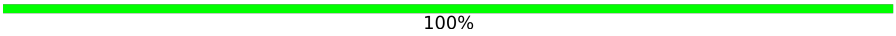
Chain P:

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

Chain Q:

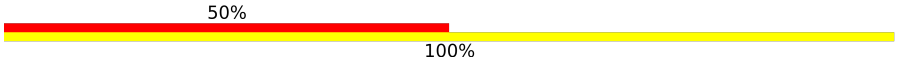
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



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

Chain S:



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

Chain T:

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

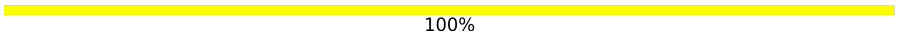
Chain I:

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

Chain J:

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

Chain O:



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

Chain U:

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

Chain V:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371808	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.28	0/8837	0.56	5/12019 (0.0%)
1	B	0.28	0/8837	0.56	3/12019 (0.0%)
1	C	0.29	0/8977	0.59	6/12207 (0.0%)
All	All	0.28	0/26651	0.57	14/36245 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	3
All	All	0	6

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	627	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	111	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	518	LEU	CA-CB-CG	6.45	130.13	115.30
1	B	942	PRO	N-CA-CB	6.39	110.97	103.30
1	C	892	PRO	N-CA-CB	6.10	110.62	103.30
1	A	518	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	892	PRO	N-CA-CB	6.03	110.53	103.30
1	B	892	PRO	N-CA-CB	5.80	110.26	103.30
1	C	517	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	942	PRO	N-CA-CB	5.75	110.19	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	942	PRO	N-CA-CB	5.72	110.16	103.30
1	A	899	PRO	N-CA-CB	5.66	110.10	103.30
1	B	899	PRO	N-CA-CB	5.51	109.92	103.30
1	C	899	PRO	N-CA-CB	5.44	109.82	103.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLU	Peptide
1	A	133	PHE	Peptide
1	B	1117	THR	Peptide
1	C	330	PRO	Peptide
1	C	359	SER	Peptide
1	C	441	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8632	0	8437	119	0
1	B	8632	0	8436	110	0
1	C	8770	0	8564	141	0
2	D	28	0	25	2	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	39	0	34	0	0
3	J	39	0	34	0	0
3	O	39	0	34	1	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
4	A	140	0	128	4	0
4	B	126	0	115	0	0
4	C	154	0	141	1	0
All	All	27041	0	26341	358	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 7.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TRP:HE1	1:C:438:SER:HG	1.23	0.81
1:A:96:GLU:O	1:A:185:ASN:HB2	1.82	0.80
1:A:254:SER:N	4:A:1301:NAG:HO6	1.82	0.77
1:B:790:LYS:HZ2	1:C:704:SER:HB2	1.55	0.71
1:A:134:GLN:HB2	1:A:157:TYR:HB2	1.73	0.71
1:B:433:VAL:HG12	1:B:512:VAL:HG12	1.73	0.69
1:A:403:ARG:HG2	1:A:497:PHE:HZ	1.56	0.68
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.57	0.68
1:C:625:HIS:HB3	1:C:628:GLN:HE21	1.60	0.67
1:C:356:LYS:HB3	1:C:397:ALA:HB3	1.77	0.66
1:B:628:GLN:H	1:B:634:ARG:HH12	1.44	0.66
1:C:495:TYR:OH	1:C:505:HIS:ND1	2.28	0.65
1:A:1117:THR:H	1:A:1140:PRO:HD2	1.61	0.65
1:A:327:VAL:HG12	1:A:542:ASN:HB3	1.77	0.64
1:C:441:LEU:O	1:C:448:ASN:ND2	2.29	0.64
1:C:444:LYS:H	1:C:506:GLN:H	1.45	0.64
1:A:126:VAL:HG23	1:A:171:PRO:HA	1.79	0.63
1:C:403:ARG:HB2	1:C:495:TYR:HB3	1.80	0.63
1:A:376:THR:HB	1:A:378:LYS:HD3	1.81	0.63
1:B:64:TRP:HD1	1:B:266:TYR:HE1	1.47	0.63
1:B:371:LEU:HG	1:B:373:PRO:HD2	1.81	0.62
1:A:141:LEU:HD21	1:A:156:VAL:HG22	1.80	0.62
1:C:882:ILE:HG23	1:C:883:THR:HG23	1.80	0.62
1:C:392:PHE:HB3	1:C:520:ALA:HB3	1.81	0.61
1:B:752:LEU:HD22	1:B:993:ILE:HD11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:HG3	1:A:465:GLU:HG3	1.83	0.61
1:C:131:CYS:SG	1:C:132:GLU:N	2.73	0.61
1:C:102:ARG:HB2	1:C:242:ALA:HB2	1.82	0.60
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.82	0.60
1:B:905:ARG:HH12	1:B:1050:MET:HB3	1.66	0.60
1:A:1143:PRO:HA	1:A:1147:SER:H	1.67	0.59
1:A:317:ASN:ND2	1:C:737:ASP:OD2	2.35	0.59
1:B:311:GLY:HA2	1:B:664:ILE:HD12	1.83	0.59
1:A:110:LEU:HD22	1:A:236:ARG:HH22	1.67	0.59
1:A:97:LYS:HB3	1:A:178:GLY:HA3	1.84	0.58
1:C:1116:THR:HB	1:C:1144:GLU:HB2	1.85	0.58
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.86	0.58
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.37	0.57
1:B:442:ASP:O	1:B:448:ASN:ND2	2.37	0.57
1:C:194:ILE:HG22	1:C:199:LYS:HZ1	1.69	0.57
1:B:238:GLN:NE2	1:B:239:THR:O	2.37	0.57
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.87	0.57
1:C:89:GLY:HA2	1:C:191:PHE:O	2.04	0.57
1:B:341:VAL:HG12	1:B:356:LYS:HD2	1.86	0.57
1:B:850:ILE:O	1:B:853:GLN:NE2	2.37	0.56
1:C:632:THR:O	1:C:634:ARG:NH1	2.38	0.56
1:B:745:ASP:HB2	1:C:549:THR:HB	1.88	0.56
2:H:1:NAG:H5	2:H:2:NAG:H82	1.88	0.56
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.87	0.56
1:A:611:LEU:HD12	1:A:650:LEU:HD12	1.87	0.56
1:A:521:PRO:HD3	1:A:564:GLN:HB2	1.87	0.56
1:A:77:LYS:HE2	1:A:257:GLY:HA2	1.87	0.56
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.40	0.55
1:C:420:ASP:HB2	1:C:461:LEU:HA	1.88	0.55
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.39	0.55
1:C:815:ARG:NH2	1:C:867:ASP:OD2	2.37	0.55
1:B:989:ALA:O	1:B:992:GLN:HB2	2.06	0.55
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.88	0.55
1:C:380:TYR:HB2	1:C:429:PHE:HB3	1.89	0.55
1:C:134:GLN:O	1:C:158:SER:N	2.40	0.54
1:C:317:ASN:ND2	1:C:593:GLY:O	2.40	0.54
1:C:328:ARG:NH1	1:C:530:SER:OG	2.40	0.54
1:C:462:LYS:NZ	1:C:465:GLU:OE1	2.41	0.54
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.41	0.54
1:B:629:LEU:O	1:B:634:ARG:NH2	2.41	0.54
1:A:623:ALA:HB1	1:A:629:LEU:HD11	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LYS:NZ	1:A:981:PHE:O	2.41	0.54
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.89	0.54
1:B:338:PHE:HA	1:B:341:VAL:HG22	1.89	0.54
1:A:640:SER:OG	1:A:641:ASN:N	2.41	0.54
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.25	0.54
1:B:77:LYS:N	1:B:258:TRP:O	2.41	0.54
1:C:502:GLY:O	1:C:506:GLN:NE2	2.41	0.54
1:B:42:VAL:O	1:C:563:GLN:NE2	2.40	0.53
1:C:328:ARG:NH1	1:C:531:THR:O	2.41	0.53
1:A:68:ILE:HD11	1:A:78:ARG:HH11	1.73	0.53
1:A:948:LEU:O	1:A:951:VAL:HB	2.07	0.53
1:B:299:THR:HA	1:B:302:THR:HG22	1.89	0.53
1:A:311:GLY:HA2	1:A:664:ILE:HD12	1.90	0.53
1:A:427:ASP:N	1:A:427:ASP:OD1	2.41	0.53
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.90	0.53
1:C:762:GLN:OE1	1:C:765:ARG:NH1	2.41	0.53
1:B:640:SER:OG	1:B:641:ASN:N	2.42	0.53
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.90	0.53
1:C:33:THR:OG1	1:C:34:ARG:NH1	2.42	0.53
1:B:642:VAL:HG22	1:B:651:ILE:HG22	1.91	0.53
1:C:68:ILE:O	1:C:77:LYS:N	2.42	0.53
1:B:327:VAL:HG12	1:B:542:ASN:HB3	1.90	0.53
1:A:1103:PHE:HB3	1:A:1113:GLN:H	1.74	0.53
1:C:318:PHE:HB2	1:C:630:THR:HG21	1.90	0.52
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.42	0.52
1:B:625:HIS:CD2	1:B:626:ALA:H	2.27	0.52
1:A:16:VAL:HA	4:A:1302:NAG:H82	1.91	0.52
1:A:733:LYS:HE3	1:A:771:ALA:HB1	1.91	0.52
1:C:182:ASN:HD21	1:C:207:ILE:HD12	1.74	0.52
1:A:659:SER:HB2	1:A:698:SER:HB3	1.91	0.52
1:A:563:GLN:NE2	1:C:42:VAL:O	2.42	0.52
1:C:1142:GLN:HG2	1:C:1143:PRO:HD3	1.91	0.52
1:B:354:ASN:O	1:B:398:ASP:HA	2.10	0.52
1:C:867:ASP:OD1	1:C:868:GLU:N	2.43	0.52
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.91	0.52
1:B:729:VAL:HG21	1:B:781:VAL:HG11	1.91	0.52
1:C:37:TYR:OH	1:C:54:LEU:O	2.27	0.52
1:C:702:GLU:O	1:C:704:SER:N	2.42	0.52
1:A:254:SER:N	4:A:1301:NAG:O6	2.42	0.52
1:A:530:SER:OG	1:A:531:THR:N	2.42	0.52
1:B:1118:ASP:N	1:B:1139:ASP:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:THR:O	1:C:236:ARG:NH1	2.42	0.51
1:C:311:GLY:HA2	1:C:664:ILE:HD12	1.92	0.51
1:A:971:GLY:O	1:A:995:ARG:NH1	2.43	0.51
1:B:711:SER:OG	1:B:1074:ASN:OD1	2.29	0.51
1:A:971:GLY:H	1:C:755:GLN:HE22	1.57	0.51
1:B:971:GLY:O	1:B:995:ARG:NH1	2.43	0.51
1:A:880:GLY:O	1:A:884:SER:OG	2.29	0.51
1:B:351:TYR:OH	1:B:454:ARG:O	2.28	0.51
1:C:67:VAL:HG22	1:C:78:ARG:HB3	1.91	0.51
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.92	0.51
1:A:644:GLN:NE2	1:A:648:GLY:O	2.43	0.51
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.93	0.51
1:B:95:ILE:HG22	1:B:186:LEU:HD13	1.93	0.51
1:B:210:ARG:HE	1:B:213:GLU:HB3	1.76	0.51
1:C:184:LYS:O	1:C:204:HIS:NE2	2.39	0.51
1:A:454:ARG:NH1	1:A:467:ASP:OD2	2.40	0.50
1:A:457:ARG:NH2	2:Q:1:NAG:O7	2.39	0.50
1:B:273:ARG:NH2	1:B:290:ASP:OD2	2.42	0.50
1:A:412:PRO:HD3	1:A:425:LEU:HD12	1.94	0.50
1:A:1091:ARG:NH2	1:A:1117:THR:O	2.44	0.50
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.93	0.50
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.93	0.50
1:B:894:LEU:HB3	1:C:713:ALA:HB3	1.93	0.50
1:C:413:GLY:H	1:C:419:ALA:HB3	1.76	0.50
1:A:26:PRO:HB3	1:A:65:PHE:HE1	1.77	0.50
1:C:210:ARG:NH1	1:C:217:GLN:O	2.44	0.50
1:C:425:LEU:HD23	1:C:429:PHE:HA	1.92	0.50
1:C:767:LEU:HA	1:C:770:ILE:HG22	1.94	0.50
1:A:54:LEU:HB2	1:A:192:LYS:HE3	1.94	0.49
1:A:53:ASP:OD1	1:A:54:LEU:N	2.45	0.49
1:A:1074:ASN:HB3	4:A:1310:NAG:HN2	1.77	0.49
1:B:14:GLN:HB3	1:B:156:VAL:HG12	1.94	0.49
1:B:144:LYS:HD2	1:B:152:SER:H	1.76	0.49
1:A:534:VAL:HG11	1:A:537:LYS:HE3	1.94	0.49
1:A:439:ASN:O	1:A:443:SER:OG	2.30	0.49
1:B:1106:GLN:NE2	1:B:1111:GLU:OE2	2.46	0.49
1:B:1116:THR:HG21	1:B:1140:PRO:HB3	1.95	0.49
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.95	0.49
1:A:328:ARG:HH12	1:A:533:LEU:HB2	1.78	0.49
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.46	0.49
1:A:105:ILE:HG12	1:A:118:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HA	1:A:302:THR:HG22	1.94	0.49
1:A:1129:VAL:HG23	1:C:917:TYR:HB3	1.94	0.49
1:A:117:LEU:HD22	1:A:232:ILE:HD11	1.93	0.48
1:C:321:GLN:NE2	1:C:322:PRO:O	2.46	0.48
1:B:1119:ASN:HD21	1:B:1141:LEU:HD13	1.78	0.48
1:C:280:ASN:HD21	1:C:282:ASN:HB2	1.79	0.48
1:C:812:PRO:O	1:C:814:LYS:NZ	2.46	0.48
1:A:1092:GLU:OE2	1:A:1119:ASN:ND2	2.46	0.48
1:B:34:ARG:NH2	1:B:216:PRO:O	2.46	0.48
1:A:354:ASN:OD1	1:A:399:SER:OG	2.24	0.48
1:A:547:LYS:O	1:C:978:ASN:ND2	2.47	0.48
1:C:135:PHE:HA	1:C:157:TYR:HA	1.96	0.48
2:D:1:NAG:H62	2:D:2:NAG:H83	1.95	0.48
1:B:976:VAL:HG13	1:B:979:ASP:HB2	1.96	0.48
1:B:58:PHE:HB2	1:B:293:LEU:HD11	1.96	0.48
1:B:1157:LYS:O	1:B:1161:SER:OG	2.30	0.48
1:C:880:GLY:O	1:C:884:SER:OG	2.27	0.48
1:B:106:PHE:HE2	1:B:232:ILE:HD11	1.79	0.47
1:B:760:CYS:HA	1:B:763:LEU:HB2	1.96	0.47
1:B:121:ASN:HA	1:B:155:ARG:HH22	1.79	0.47
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.94	0.47
1:A:173:LEU:O	1:A:187:ARG:NH1	2.48	0.47
1:A:974:SER:OG	1:A:975:SER:N	2.45	0.47
1:C:621:PRO:HA	1:C:624:ILE:HB	1.95	0.47
1:A:557:LYS:HG2	1:A:584:ILE:HG21	1.96	0.47
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.95	0.47
1:C:444:LYS:N	1:C:506:GLN:O	2.48	0.47
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.97	0.47
1:A:142:ASP:H	1:A:143:HIS:HA	1.78	0.47
1:C:214:ASP:OD1	1:C:214:ASP:N	2.44	0.47
1:C:403:ARG:HH22	1:C:448:ASN:HB3	1.79	0.47
1:C:993:ILE:O	1:C:997:ILE:HG12	2.14	0.47
1:C:295:PRO:HG2	1:C:608:VAL:HG21	1.96	0.47
1:C:617:CYS:HB2	1:C:649:CYS:HB3	1.66	0.47
1:B:89:GLY:HA3	1:B:191:PHE:O	2.15	0.47
1:B:128:ILE:HG13	1:B:168:VAL:HB	1.97	0.47
1:B:1032:CYS:SG	1:B:1051:SER:OG	2.67	0.47
1:A:184:LYS:HB3	1:A:207:ILE:HA	1.96	0.47
1:A:410:ILE:HG21	1:A:433:VAL:HG21	1.97	0.47
1:A:1101:HIS:ND1	3:O:2:NAG:O7	2.48	0.46
1:C:618:THR:HG23	4:C:1308:NAG:H83	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.96	0.46
1:A:711:SER:OG	1:A:1074:ASN:OD1	2.34	0.46
1:C:356:LYS:NZ	1:C:361:CYS:SG	2.75	0.46
1:B:112:SER:HB2	1:B:134:GLN:HA	1.98	0.46
1:B:948:LEU:O	1:B:951:VAL:HB	2.15	0.46
1:C:295:PRO:HD3	1:C:633:TRP:CD2	2.50	0.46
1:B:129:LYS:HB3	1:B:165:PHE:HB3	1.98	0.46
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.30	0.46
1:C:194:ILE:HG22	1:C:199:LYS:NZ	2.29	0.46
1:C:631:PRO:HB3	1:C:633:TRP:CE2	2.50	0.46
1:C:900:MET:SD	1:C:900:MET:N	2.86	0.46
1:C:1091:ARG:NH2	1:C:1118:ASP:O	2.48	0.46
1:C:509:ARG:HA	1:C:509:ARG:HD2	1.85	0.46
1:B:332:ILE:HG22	1:B:362:VAL:HG23	1.97	0.46
1:A:924:ALA:HB1	1:A:928:ASN:HD21	1.81	0.46
1:C:443:SER:N	1:C:508:TYR:O	2.32	0.46
1:C:1120:THR:OG1	1:C:1121:PHE:N	2.49	0.46
1:A:1117:THR:N	1:A:1140:PRO:HD2	2.30	0.46
1:B:121:ASN:ND2	1:B:170:GLN:O	2.49	0.46
1:B:132:GLU:N	1:B:163:CYS:SG	2.84	0.46
1:A:315:THR:OG1	1:A:316:SER:N	2.49	0.46
1:A:732:THR:OG1	1:A:955:ASN:OD1	2.34	0.46
1:A:1115:ILE:HG22	1:A:1139:ASP:HB3	1.98	0.46
1:A:950:ASP:HA	1:A:953:ASN:HB2	1.98	0.46
1:C:129:LYS:NZ	1:C:163:CYS:SG	2.84	0.46
1:B:129:LYS:HG3	1:B:130:VAL:H	1.81	0.45
1:A:533:LEU:HD11	1:A:585:LEU:HD11	1.97	0.45
1:A:662:CYS:HB2	1:A:697:MET:HG3	1.98	0.45
1:C:346:ARG:HA	1:C:509:ARG:HH22	1.81	0.45
1:C:819:GLU:OE2	1:C:1054:GLN:NE2	2.48	0.45
1:B:708:SER:OG	1:B:710:ASN:OD1	2.33	0.45
1:B:880:GLY:O	1:B:884:SER:OG	2.28	0.45
1:B:181:GLY:H	1:B:183:PHE:HE1	1.64	0.45
1:A:40:ASP:OD1	1:A:40:ASP:N	2.49	0.45
1:C:347:PHE:HD2	1:C:399:SER:HB2	1.81	0.45
1:C:357:ARG:NH1	1:C:422:ASN:OD1	2.50	0.45
1:A:280:ASN:HD21	1:A:282:ASN:HB2	1.81	0.45
1:A:452:LEU:HB3	1:A:492:LEU:HB3	1.99	0.45
1:A:605:SER:OG	1:A:606:ASN:N	2.48	0.45
1:A:1139:ASP:O	1:A:1143:PRO:HD2	2.17	0.45
1:C:68:ILE:HA	1:C:262:ALA:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:HIS:HB2	1:B:1136:THR:HA	1.99	0.45
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.77	0.45
1:C:777:ASN:HD21	1:C:1019:ARG:HD2	1.82	0.45
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.61	0.45
1:A:119:ILE:HG12	1:A:128:ILE:HD12	1.99	0.45
1:C:1115:ILE:HG22	1:C:1140:PRO:HB3	1.97	0.45
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.99	0.44
1:C:37:TYR:HA	1:C:222:LEU:H	1.83	0.44
1:C:596:SER:HB2	1:C:611:LEU:HB3	1.99	0.44
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.81	0.44
1:C:986:LYS:HA	1:C:986:LYS:HD2	1.75	0.44
1:B:780:GLU:O	1:B:784:GLN:NE2	2.48	0.44
1:C:323:THR:HG21	1:C:537:LYS:HE2	1.99	0.44
1:C:40:ASP:N	1:C:40:ASP:OD1	2.50	0.44
1:C:383:SER:HB3	1:C:386:LYS:HG2	2.00	0.44
1:C:514:SER:OG	1:C:515:PHE:N	2.50	0.44
1:B:629:LEU:H	1:B:634:ARG:HH22	1.66	0.44
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.98	0.44
1:C:97:LYS:O	1:C:185:ASN:ND2	2.43	0.44
1:C:319:ARG:NH1	1:C:628:GLN:O	2.50	0.44
1:C:402:ILE:HD11	1:C:505:HIS:HB3	2.00	0.44
1:C:406:GLU:OE1	1:C:408:ARG:NH1	2.50	0.44
1:C:413:GLY:HA2	1:C:424:LYS:HA	1.98	0.44
1:B:187:ARG:HD3	1:B:204:HIS:HD2	1.82	0.44
1:B:467:ASP:OD1	1:B:467:ASP:N	2.51	0.44
1:B:994:ASP:HA	1:B:997:ILE:HG22	2.00	0.44
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.81	0.44
1:B:89:GLY:CA	1:B:191:PHE:O	2.65	0.44
1:B:142:ASP:OD1	1:B:142:ASP:N	2.50	0.44
1:C:349:SER:HA	1:C:401:VAL:HB	2.00	0.44
1:C:930:ALA:O	1:C:934:ILE:HG12	2.18	0.44
1:B:429:PHE:HE1	1:B:514:SER:HB2	1.83	0.43
1:C:778:THR:HG22	1:C:865:LEU:HD12	2.00	0.43
1:C:633:TRP:HD1	1:C:636:TYR:HB2	1.82	0.43
1:A:710:ASN:OD1	1:A:710:ASN:N	2.51	0.43
1:C:971:GLY:O	1:C:995:ARG:NH1	2.51	0.43
1:B:383:SER:OG	1:A:985:ASP:N	2.52	0.43
1:B:1102:TRP:HD1	1:B:1135:ASN:HD22	1.67	0.43
1:A:95:ILE:HB	1:A:186:LEU:HD13	2.00	0.43
1:A:125:ASN:HA	1:A:171:PRO:HD3	2.01	0.43
1:A:438:SER:O	1:A:438:SER:OG	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:HG12	1:C:386:LYS:HG3	2.01	0.43
1:B:1074:ASN:HD22	2:G:2:NAG:H2	1.83	0.43
1:A:104:TRP:H	1:A:119:ILE:HB	1.84	0.43
1:C:731:MET:HG3	1:C:774:GLN:NE2	2.33	0.43
1:A:104:TRP:HB2	1:A:119:ILE:HD12	2.01	0.43
1:C:295:PRO:HD3	1:C:633:TRP:CE2	2.53	0.43
1:C:424:LYS:HE3	1:C:463:PRO:HG3	2.01	0.43
1:A:531:THR:OG1	1:A:532:ASN:N	2.50	0.43
1:C:443:SER:O	1:C:508:TYR:HB2	2.19	0.43
1:B:134:GLN:NE2	1:B:162:ASN:OD1	2.52	0.43
1:B:617:CYS:O	1:B:620:VAL:HG12	2.19	0.43
1:B:906:PHE:HD2	1:B:916:LEU:HB2	1.84	0.43
1:A:100:ILE:HG22	1:A:241:LEU:HB2	2.00	0.43
1:A:661:GLU:O	1:A:695:TYR:OH	2.36	0.43
1:C:1081:ILE:HG12	1:C:1137:VAL:HG11	2.00	0.43
1:A:1084:ASP:OD1	1:A:1084:ASP:N	2.49	0.42
1:B:563:GLN:O	1:B:577:ARG:NH1	2.51	0.42
1:A:1149:LYS:HB3	1:A:1152:LEU:HB2	2.01	0.42
1:B:323:THR:HG21	1:B:537:LYS:HE2	1.99	0.42
1:C:391:CYS:HB3	1:C:525:CYS:HB3	1.32	0.42
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.51	0.42
1:B:329:PHE:O	1:B:580:GLN:NE2	2.53	0.42
1:B:426:PRO:HD3	1:B:463:PRO:HB3	2.01	0.42
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.02	0.42
1:C:186:LEU:H	1:C:204:HIS:HD2	1.68	0.42
1:B:41:LYS:NZ	1:C:562:PHE:O	2.42	0.42
1:B:699:LEU:HD21	1:A:869:MET:HB2	2.02	0.42
1:A:642:VAL:HG22	1:A:651:ILE:HG23	2.02	0.42
1:A:1092:GLU:N	1:A:1119:ASN:OD1	2.42	0.42
1:C:403:ARG:NH1	1:C:403:ARG:HA	2.33	0.42
1:C:436:TRP:NE1	1:C:438:SER:OG	2.32	0.42
1:B:423:TYR:HA	1:B:461:LEU:HD11	2.02	0.42
1:B:625:HIS:CG	1:B:626:ALA:H	2.38	0.42
1:B:958:ALA:O	1:B:961:THR:OG1	2.32	0.42
1:A:169:SER:OG	1:A:170:GLN:N	2.52	0.42
1:B:315:THR:OG1	1:B:316:SER:N	2.52	0.42
1:B:950:ASP:HA	1:B:953:ASN:HB2	2.02	0.42
1:A:194:ILE:HG23	1:A:197:TYR:HB2	2.02	0.42
1:C:936:ASP:O	1:C:940:SER:OG	2.28	0.42
1:B:316:SER:OG	1:B:317:ASN:N	2.52	0.42
1:B:929:SER:OG	1:B:933:LYS:NZ	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:NZ	1:A:279:TYR:O	2.44	0.42
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.02	0.42
1:A:1139:ASP:O	1:A:1142:GLN:N	2.38	0.42
1:C:808:ASP:OD2	1:C:811:LYS:N	2.51	0.42
1:B:646:ARG:O	1:B:646:ARG:NH1	2.53	0.41
1:A:237:PHE:HZ	1:A:267:VAL:HG21	1.84	0.41
1:C:141:LEU:HD11	1:C:156:VAL:HG11	2.02	0.41
1:C:152:SER:OG	1:C:153:GLU:N	2.53	0.41
1:C:403:ARG:NH2	1:C:448:ASN:O	2.53	0.41
1:B:710:ASN:OD1	1:B:710:ASN:N	2.52	0.41
1:A:109:THR:OG1	1:A:110:LEU:N	2.53	0.41
1:A:415:THR:OG1	1:A:416:GLY:N	2.52	0.41
1:C:633:TRP:CD1	1:C:636:TYR:HB2	2.55	0.41
1:B:368:LEU:HB3	1:B:374:PHE:HE2	1.86	0.41
1:C:117:LEU:HD23	1:C:130:VAL:HB	2.01	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.56	0.41
1:A:786:LYS:HA	1:A:786:LYS:HD3	1.87	0.41
1:C:612:TYR:O	1:C:648:GLY:HA3	2.21	0.41
1:B:866:THR:H	1:B:869:MET:HE3	1.86	0.41
1:C:193:ASN:HA	1:C:197:TYR:O	2.20	0.41
1:C:427:ASP:OD1	1:C:427:ASP:N	2.54	0.41
1:B:99:ASN:O	1:B:102:ARG:NH2	2.43	0.41
1:B:659:SER:HB2	1:B:698:SER:HB3	2.02	0.41
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.96	0.41
1:A:588:THR:OG1	1:C:847:ARG:NH1	2.54	0.41
1:C:764:LYS:HB2	1:C:764:LYS:HE3	1.77	0.41
2:D:1:NAG:H62	2:D:2:NAG:H2	2.01	0.41
1:B:109:THR:O	1:B:236:ARG:NH2	2.53	0.41
1:C:30:ASN:OD1	1:C:30:ASN:N	2.54	0.41
1:C:66:HIS:O	1:C:78:ARG:NH2	2.54	0.41
1:C:102:ARG:HA	1:C:102:ARG:HD3	1.80	0.41
1:C:921:LYS:HE3	1:C:921:LYS:HB3	1.92	0.41
1:B:946:GLY:HA2	1:B:949:GLN:HB2	2.03	0.41
1:C:878:LEU:HA	1:C:881:THR:HG22	2.03	0.41
1:C:357:ARG:HA	1:C:357:ARG:HD2	1.87	0.40
1:C:444:LYS:HG2	1:C:445:VAL:H	1.86	0.40
1:B:67:VAL:O	1:B:262:ALA:HA	2.22	0.40
1:B:412:PRO:HB2	1:B:427:ASP:HA	2.02	0.40
1:B:941:THR:OG1	1:B:942:PRO:N	2.55	0.40
1:A:361:CYS:H	1:A:524:VAL:HG22	1.86	0.40
1:A:616:ASN:OD1	1:A:618:THR:OG1	2.31	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LYS:HG2	1:C:664:ILE:HD11	2.04	0.40
1:B:1049:LEU:HD23	1:B:1049:LEU:HA	1.87	0.40
1:A:15:CYS:HB2	1:A:136:CYS:HB3	1.99	0.40
1:A:969:LYS:HB2	1:C:755:GLN:NE2	2.36	0.40
1:A:1081:ILE:HG23	1:A:1088:HIS: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	1088/1270 (86%)	1016 (93%)	72 (7%)	0	100	100
1	B	1088/1270 (86%)	997 (92%)	90 (8%)	1 (0%)	51	84
1	C	1107/1270 (87%)	1013 (92%)	94 (8%)	0	100	100
All	All	3283/3810 (86%)	3026 (92%)	256 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	942	PRO

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	964/1113 (87%)	963 (100%)	1 (0%)	93 97
1	B	964/1113 (87%)	960 (100%)	4 (0%)	91 94
1	C	976/1113 (88%)	968 (99%)	8 (1%)	81 89
All	All	2904/3339 (87%)	2891 (100%)	13 (0%)	91 94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	B	440	LYS
1	B	529	LYS
1	B	955	ASN
1	A	408	ARG
1	C	44	ARG
1	C	203	LYS
1	C	408	ARG
1	C	424	LYS
1	C	613	GLN
1	C	955	ASN
1	C	1119	ASN
1	C	1149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	238	GLN
1	B	1119	ASN
1	C	628	GLN
1	C	755	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)

43 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	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	1.56	2 (14%)	17,19,21	1.09	1 (5%)
2	NAG	D	2	2	14,14,15	0.47	0	17,19,21	0.44	0
2	NAG	E	1	2,1	14,14,15	1.17	1 (7%)	17,19,21	1.78	1 (5%)
2	NAG	E	2	2	14,14,15	0.95	1 (7%)	17,19,21	1.18	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	G	1	2	14,14,15	0.33	0	17,19,21	0.90	1 (5%)
2	NAG	G	2	2	14,14,15	0.36	0	17,19,21	0.41	0
2	NAG	H	1	2,1	14,14,15	0.63	0	17,19,21	0.71	0
2	NAG	H	2	2	14,14,15	0.65	0	17,19,21	1.96	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	I	2	3	14,14,15	1.23	1 (7%)	17,19,21	1.56	1 (5%)
3	BMA	I	3	3	11,11,12	0.74	0	15,15,17	0.76	0
3	NAG	J	1	3,1	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	J	2	3	14,14,15	1.38	1 (7%)	17,19,21	1.40	1 (5%)
3	BMA	J	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.35	3 (20%)
2	NAG	K	1	2,1	14,14,15	0.62	1 (7%)	17,19,21	0.58	0
2	NAG	K	2	2	14,14,15	0.40	0	17,19,21	0.61	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	L	2	2	14,14,15	1.09	1 (7%)	17,19,21	1.14	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	M	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	N	1	2,1	14,14,15	0.32	0	17,19,21	0.77	1 (5%)
2	NAG	N	2	2	14,14,15	0.36	0	17,19,21	0.41	0
3	NAG	O	1	3	14,14,15	0.44	0	17,19,21	0.74	1 (5%)
3	NAG	O	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	O	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.60	3 (20%)
2	NAG	P	1	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	P	2	2	14,14,15	0.30	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	Q	1	2,1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	Q	2	2	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	R	1	2,1	14,14,15	0.35	0	17,19,21	0.35	0
2	NAG	R	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	S	1	2,1	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
2	NAG	S	2	2	14,14,15	1.34	1 (7%)	17,19,21	1.71	2 (11%)
2	NAG	T	1	2,1	14,14,15	0.28	0	17,19,21	0.57	0
2	NAG	T	2	2	14,14,15	0.29	0	17,19,21	0.42	0
3	NAG	U	1	3	14,14,15	0.67	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	U	2	3	14,14,15	0.38	0	17,19,21	0.36	0
3	BMA	U	3	3	11,11,12	0.63	0	15,15,17	0.85	0
3	NAG	V	1	3,1	14,14,15	0.27	0	17,19,21	0.76	1 (5%)
3	NAG	V	2	3	14,14,15	0.26	0	17,19,21	0.69	0
3	BMA	V	3	3	11,11,12	0.75	0	15,15,17	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	5/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
2	NAG	P	1	2	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	4/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	1/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C1	5.05	1.51	1.43
3	J	2	NAG	O5-C1	4.84	1.51	1.43
2	S	2	NAG	O5-C1	4.80	1.51	1.43
3	I	2	NAG	O5-C1	4.46	1.50	1.43
2	E	1	NAG	O5-C1	4.27	1.50	1.43
2	L	2	NAG	O5-C1	3.63	1.49	1.43
2	E	2	NAG	O5-C1	3.19	1.48	1.43
2	D	1	NAG	C1-C2	2.61	1.56	1.52
3	O	3	BMA	C1-C2	2.41	1.57	1.52
3	O	3	BMA	C2-C3	2.31	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	C1-C2	2.09	1.55	1.52
3	U	1	NAG	O5-C1	2.03	1.47	1.43
3	J	3	BMA	C1-C2	2.01	1.56	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-O5-C5	6.92	121.57	112.19
2	H	2	NAG	C2-N2-C7	6.89	132.71	122.90
3	I	2	NAG	C1-O5-C5	6.21	120.61	112.19
2	S	2	NAG	C1-O5-C5	6.17	120.55	112.19
3	J	2	NAG	C1-O5-C5	5.57	119.73	112.19
2	E	2	NAG	C1-O5-C5	4.64	118.48	112.19
2	L	2	NAG	C1-O5-C5	4.50	118.29	112.19
3	O	3	BMA	C1-O5-C5	4.43	118.19	112.19
2	D	1	NAG	C1-O5-C5	4.02	117.63	112.19
3	U	1	NAG	C1-O5-C5	3.51	116.95	112.19
2	H	2	NAG	C1-C2-N2	3.09	115.78	110.49
3	O	1	NAG	C1-O5-C5	2.80	115.98	112.19
3	J	3	BMA	C1-O5-C5	2.72	115.87	112.19
2	S	2	NAG	C2-N2-C7	2.50	126.46	122.90
2	G	1	NAG	C2-N2-C7	2.48	126.44	122.90
2	S	1	NAG	C2-N2-C7	2.47	126.42	122.90
2	N	1	NAG	C1-O5-C5	2.40	115.44	112.19
3	O	3	BMA	O5-C1-C2	2.24	114.23	110.77
3	J	3	BMA	C2-C3-C4	2.19	114.68	110.89
3	O	3	BMA	C1-C2-C3	2.14	112.29	109.67
2	K	2	NAG	C1-O5-C5	2.12	115.07	112.19
3	V	1	NAG	C1-O5-C5	2.04	114.95	112.19
3	J	3	BMA	O5-C1-C2	2.00	113.86	110.77

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	R	2	NAG	C8-C7-N2-C2
2	R	2	NAG	O7-C7-N2-C2
2	S	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	S	1	NAG	C3-C2-N2-C7
3	U	3	BMA	O5-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	S	2	NAG	C3-C2-N2-C7
2	S	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6

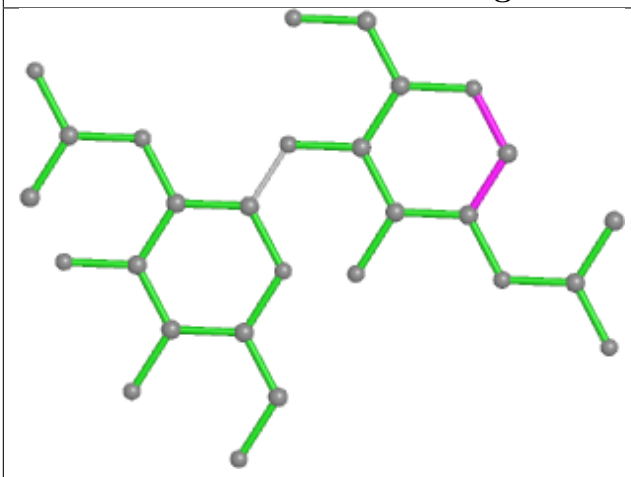
There are no ring outliers.

7 monomers are involved in 6 short contacts:

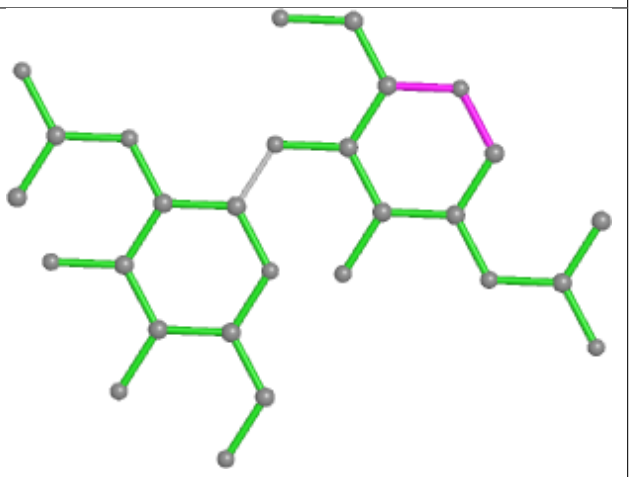
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
3	O	2	NAG	1	0
2	D	2	NAG	2	0
2	H	1	NAG	1	0
2	Q	1	NAG	1	0
2	G	2	NAG	1	0
2	H	2	NAG	1	0

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

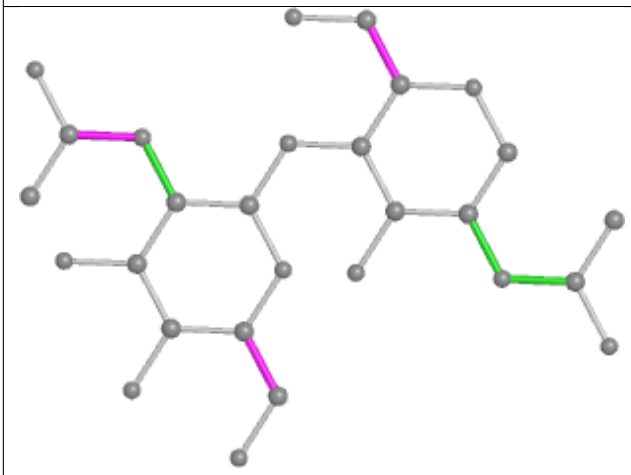
Oligosaccharide Chain D



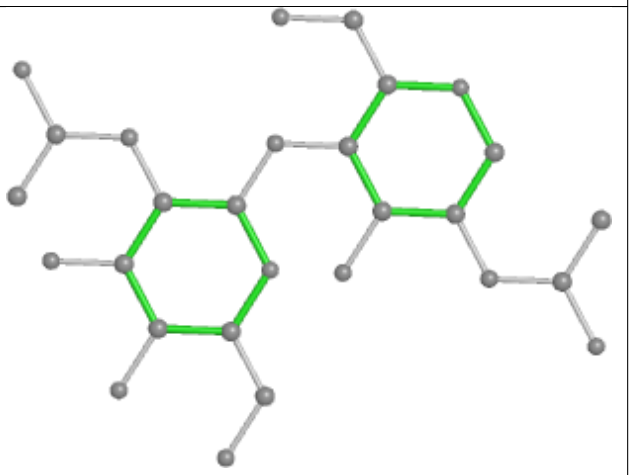
Bond lengths



Bond angles

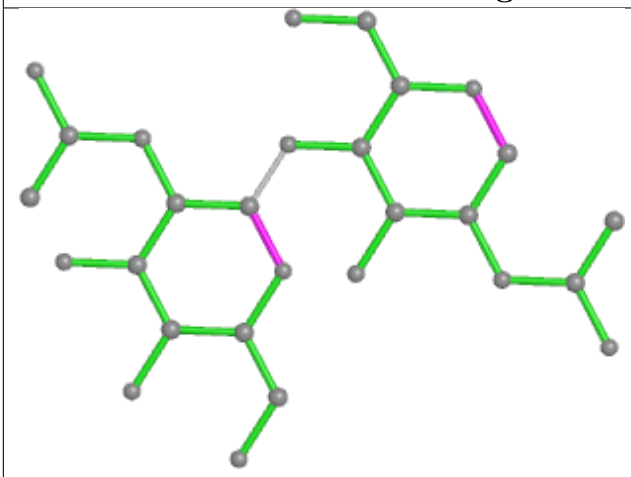


Torsions

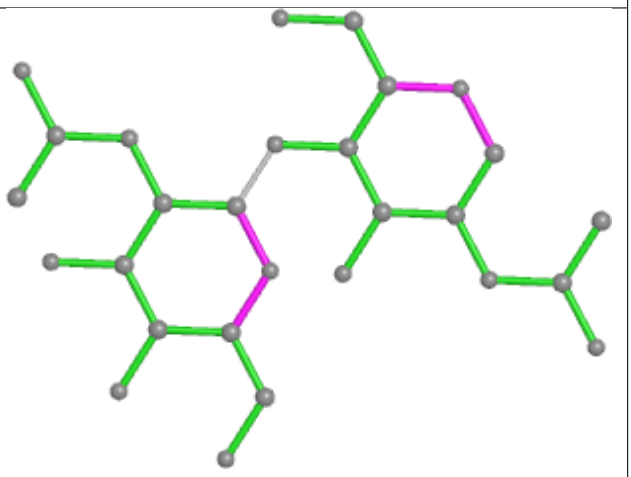


Rings

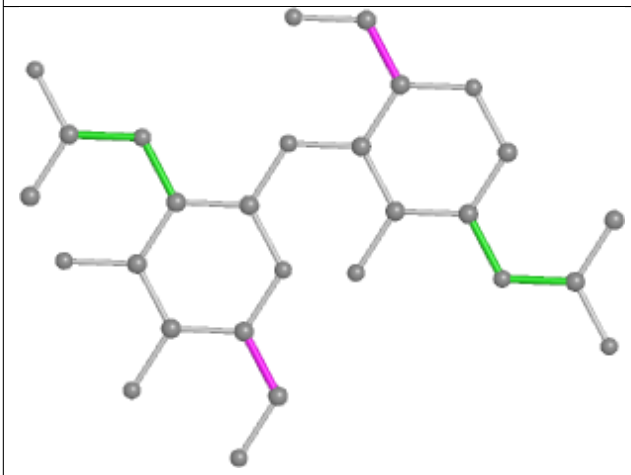
Oligosaccharide Chain E



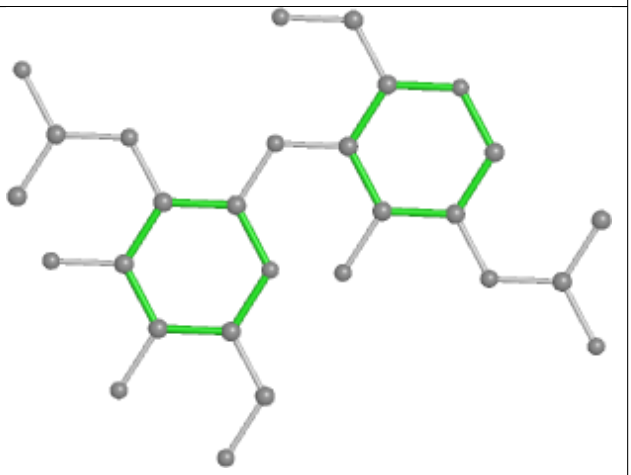
Bond lengths



Bond angles

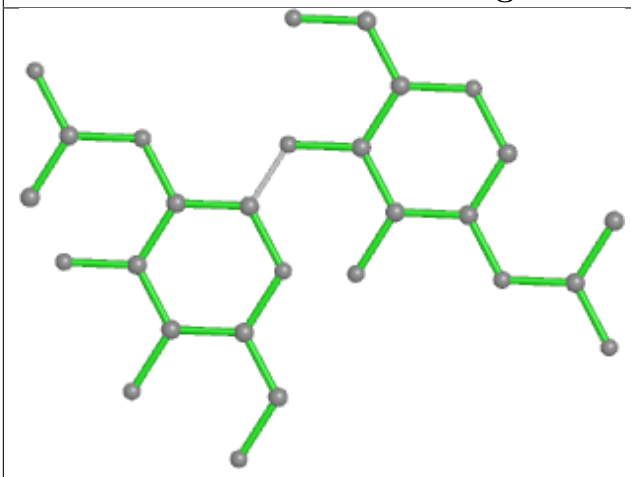


Torsions

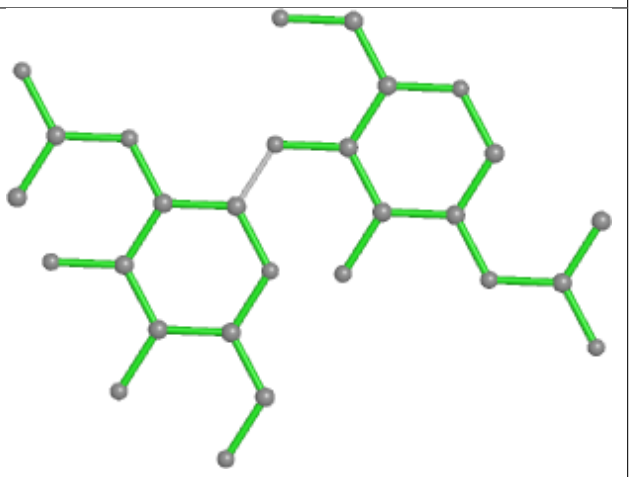


Rings

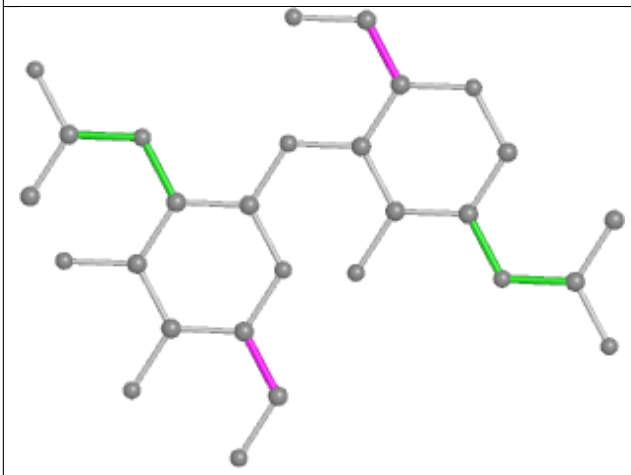
Oligosaccharide Chain F



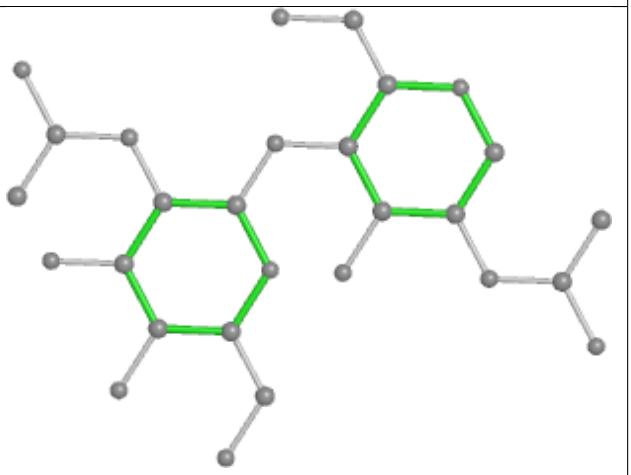
Bond lengths



Bond angles

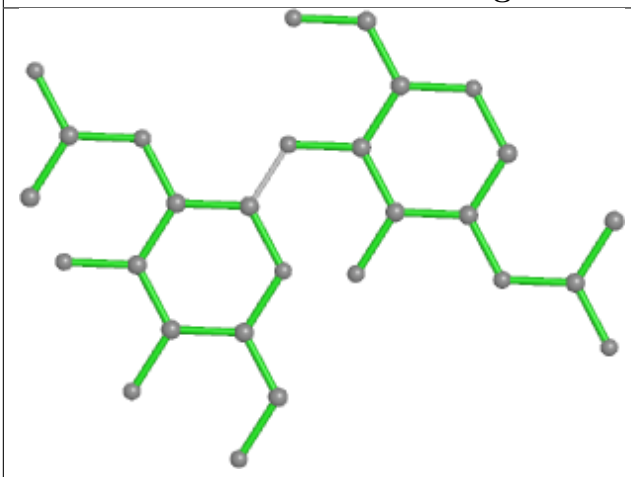


Torsions

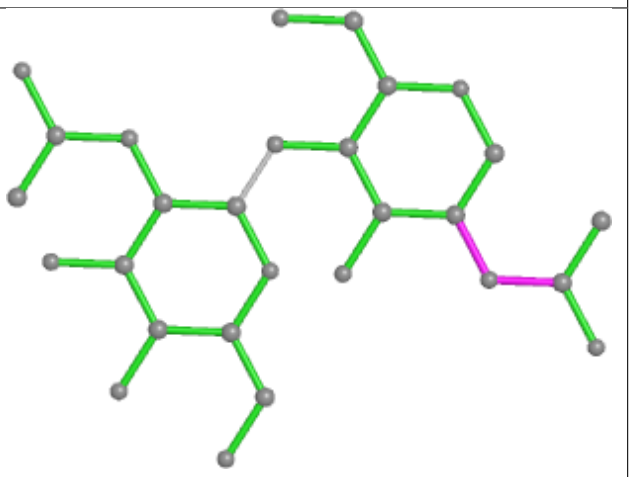


Rings

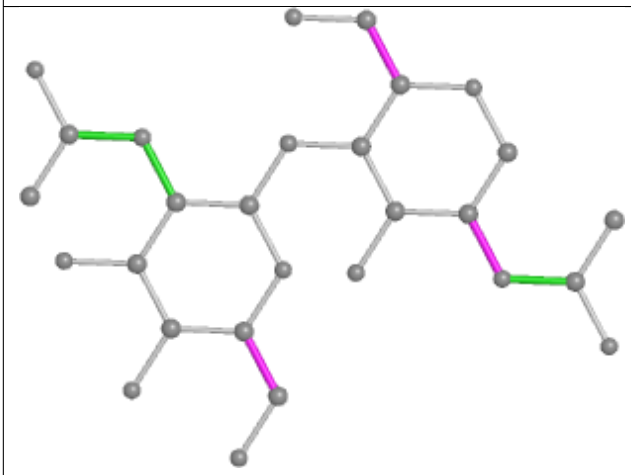
Oligosaccharide Chain G



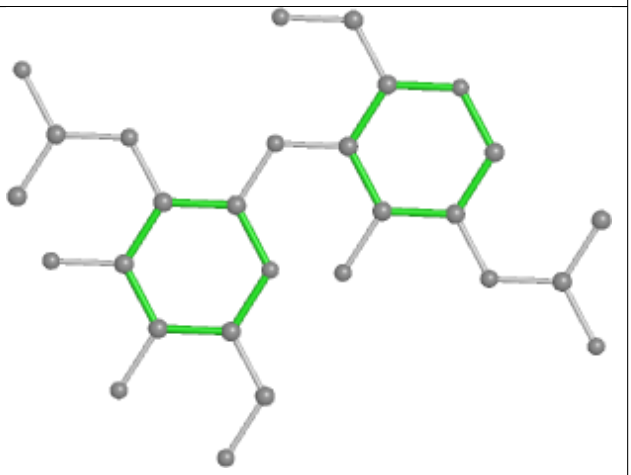
Bond lengths



Bond angles

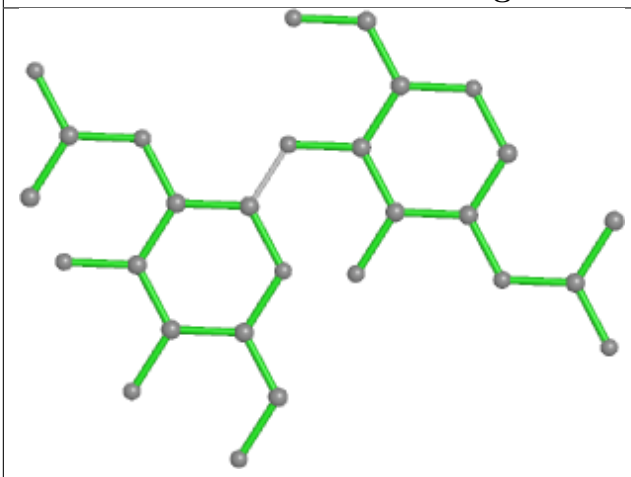


Torsions

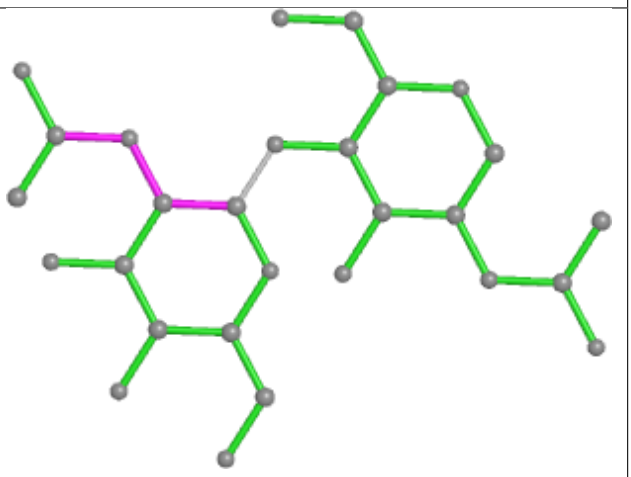


Rings

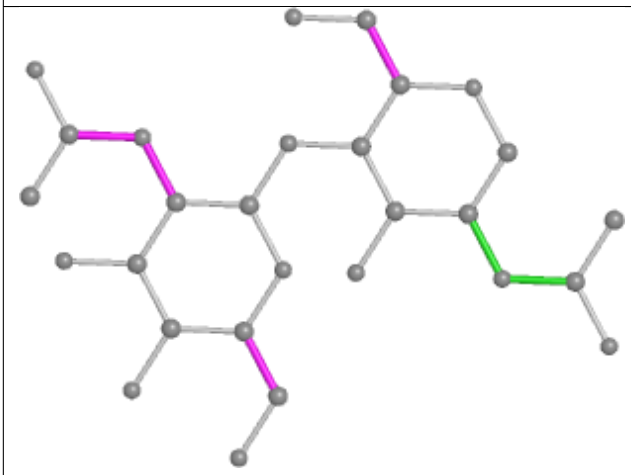
Oligosaccharide Chain H



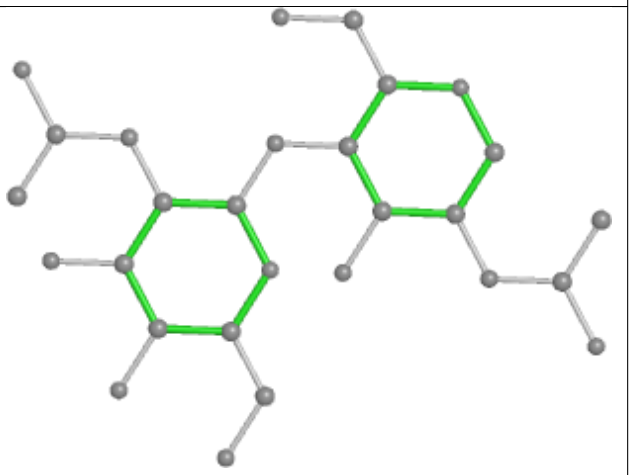
Bond lengths



Bond angles

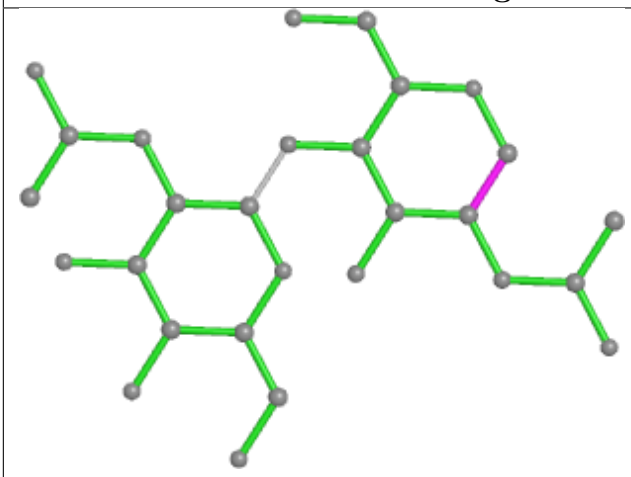


Torsions

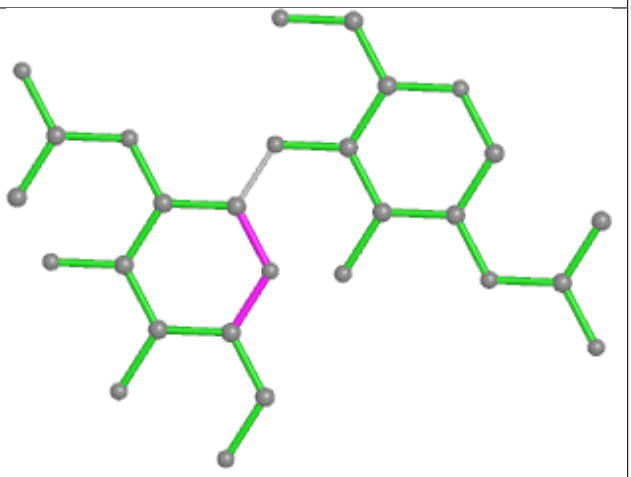


Rings

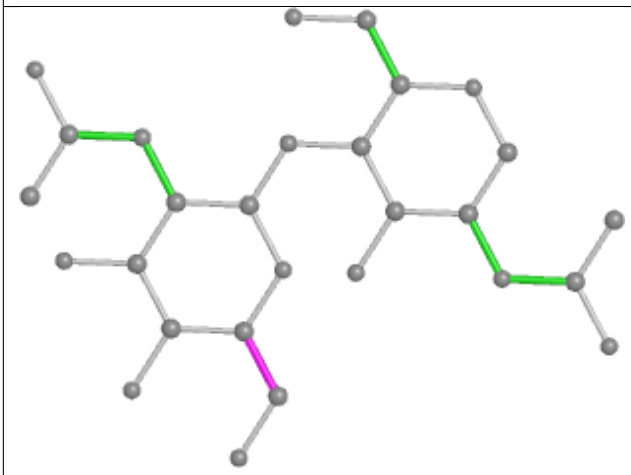
Oligosaccharide Chain K



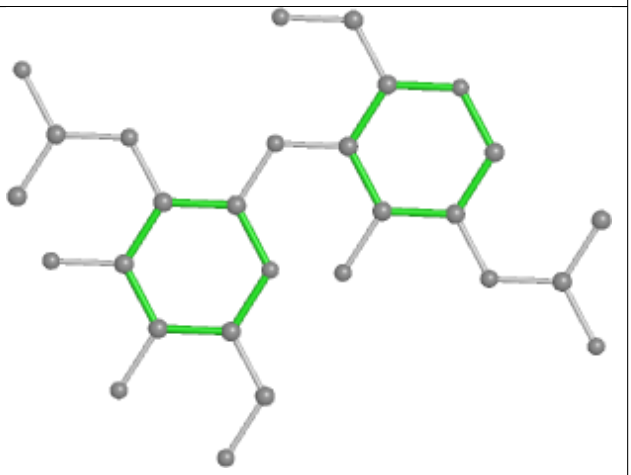
Bond lengths



Bond angles

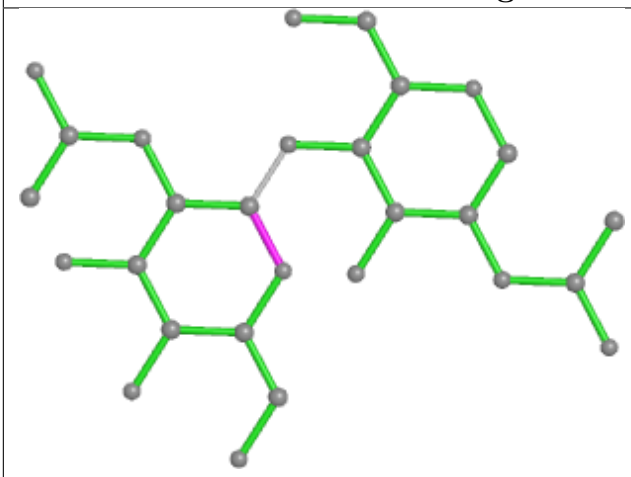


Torsions

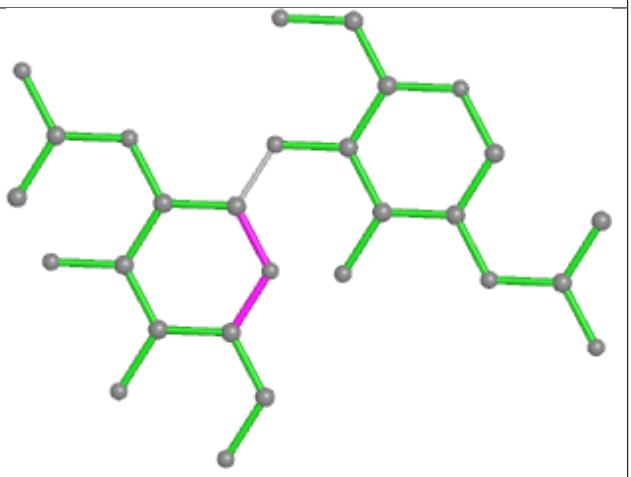


Rings

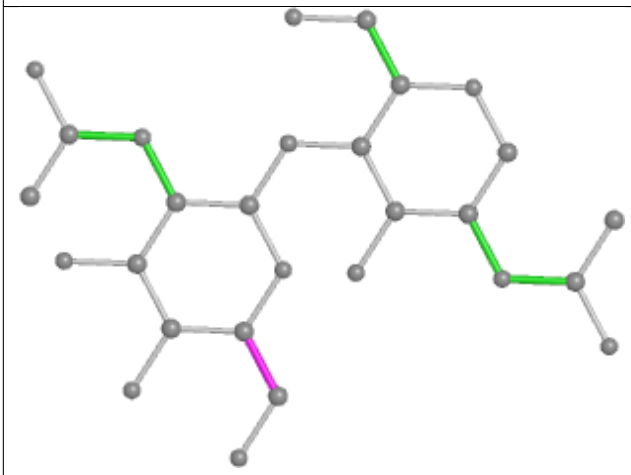
Oligosaccharide Chain L



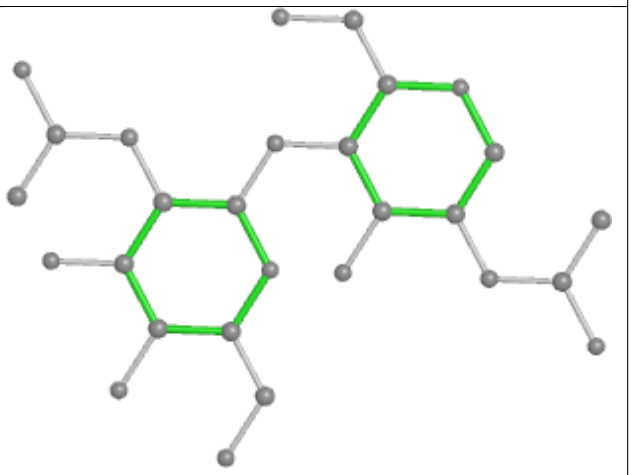
Bond lengths



Bond angles

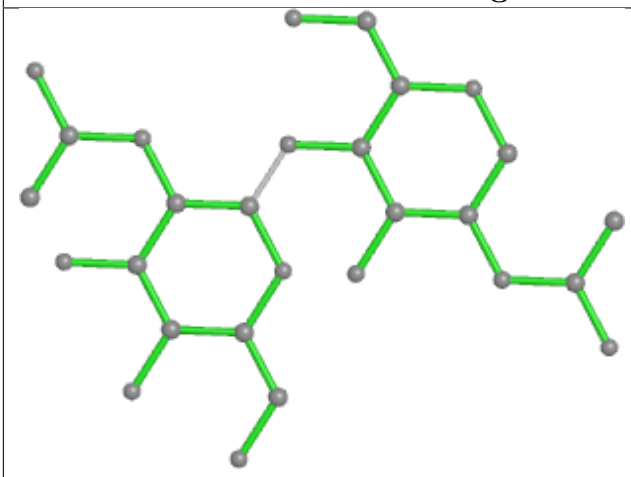


Torsions

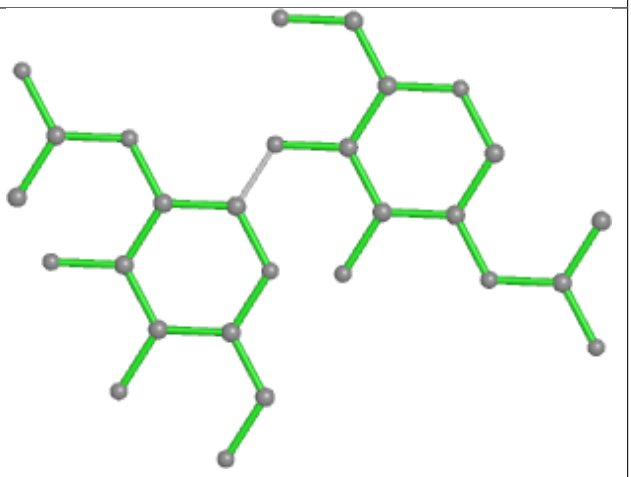


Rings

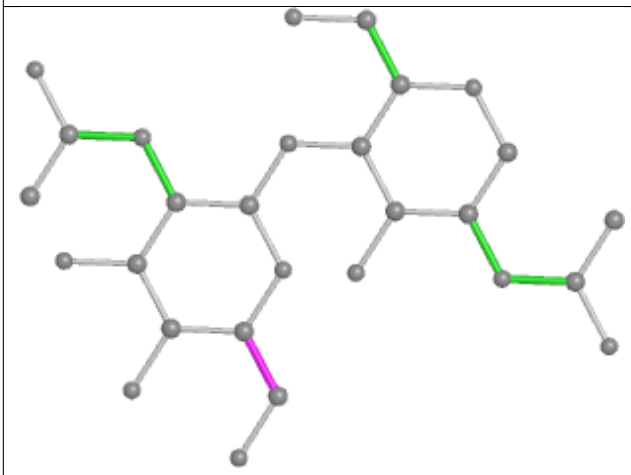
Oligosaccharide Chain M



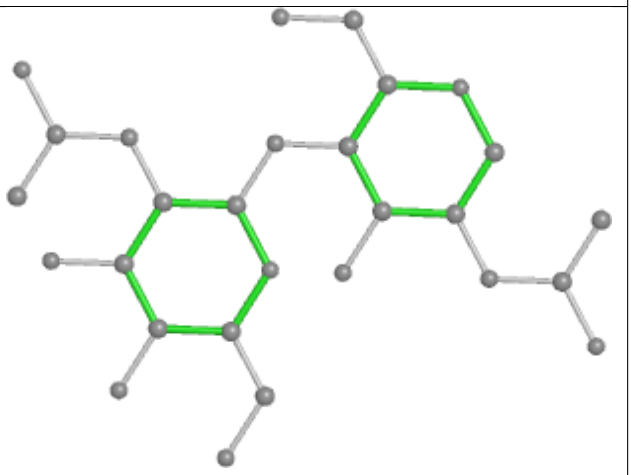
Bond lengths



Bond angles

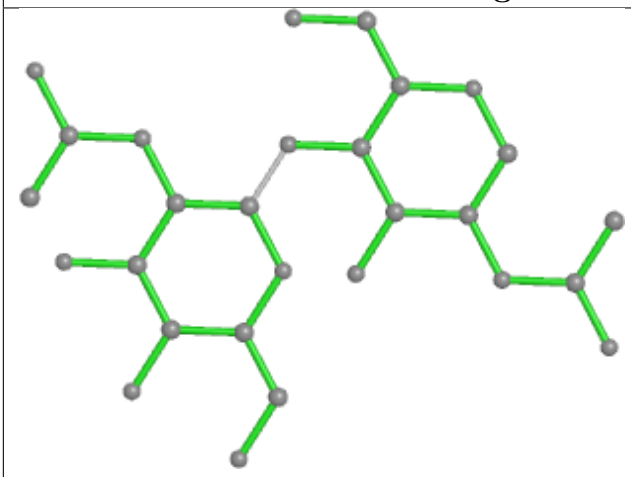


Torsions

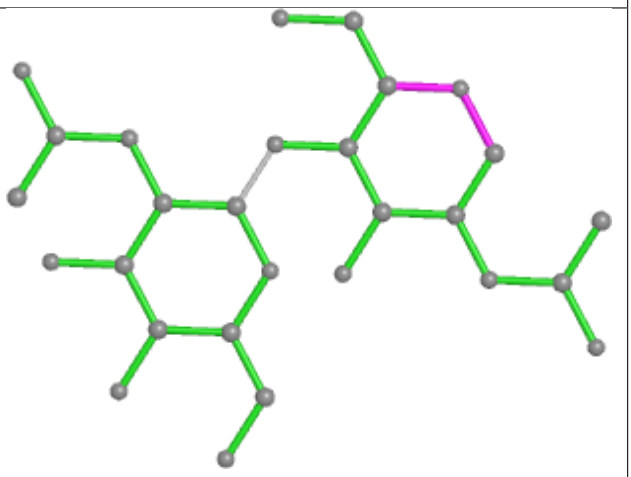


Rings

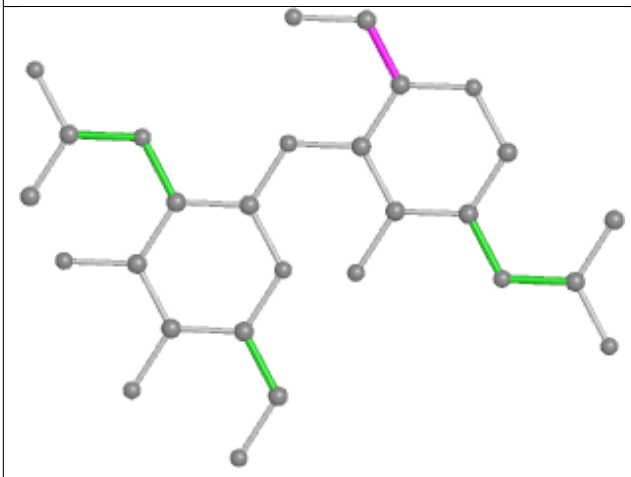
Oligosaccharide Chain N



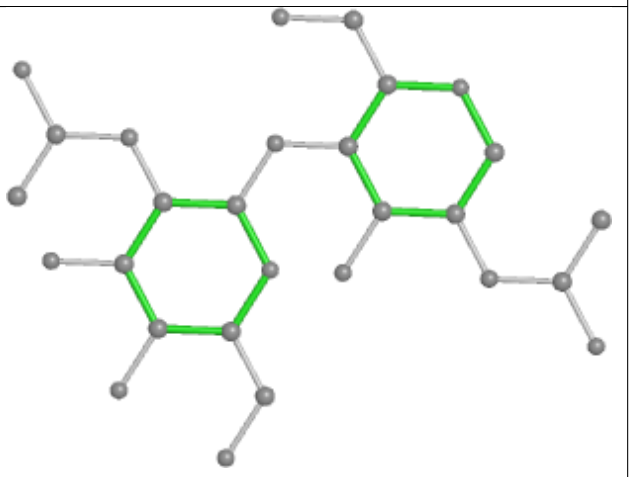
Bond lengths



Bond angles

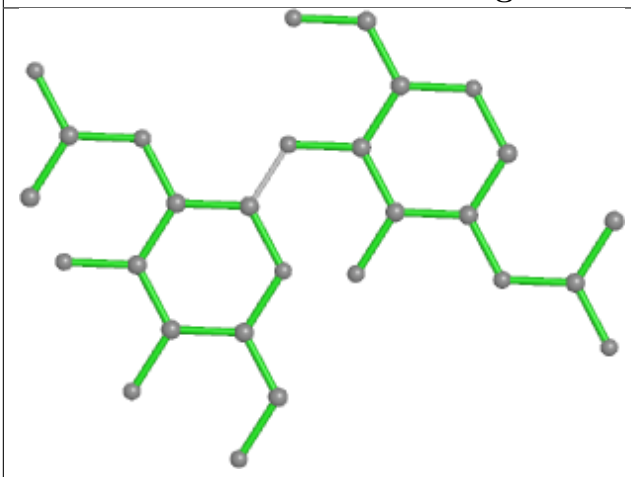


Torsions

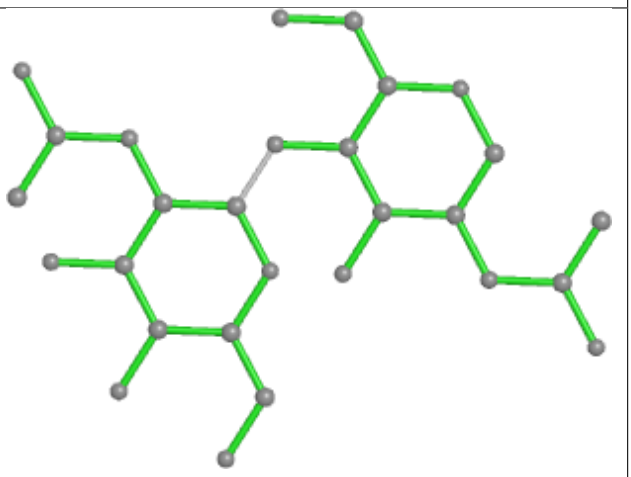


Rings

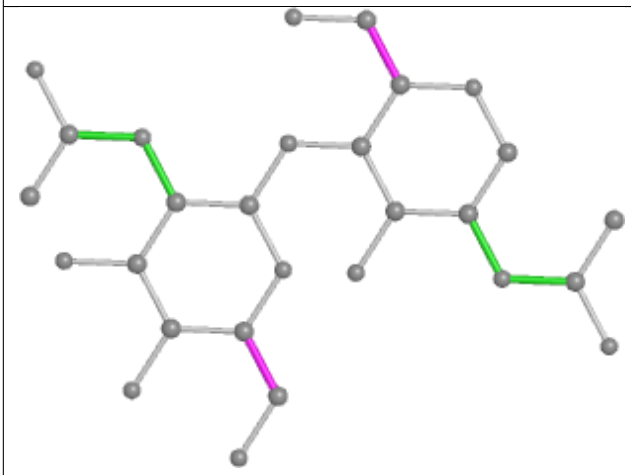
Oligosaccharide Chain P



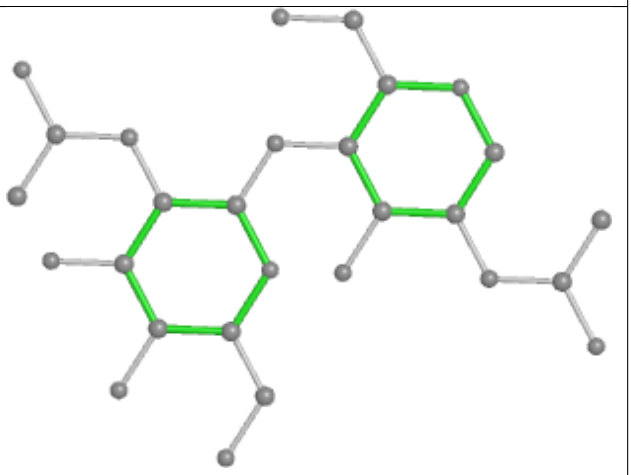
Bond lengths



Bond angles

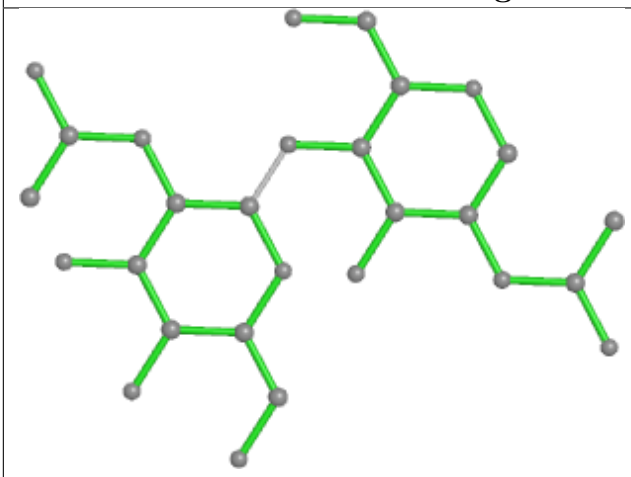


Torsions

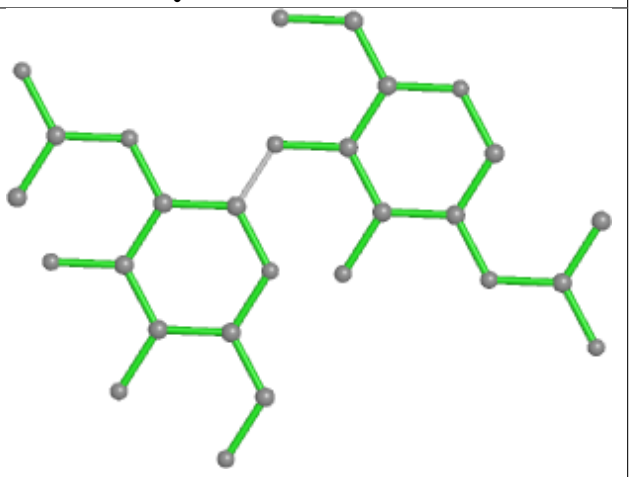


Rings

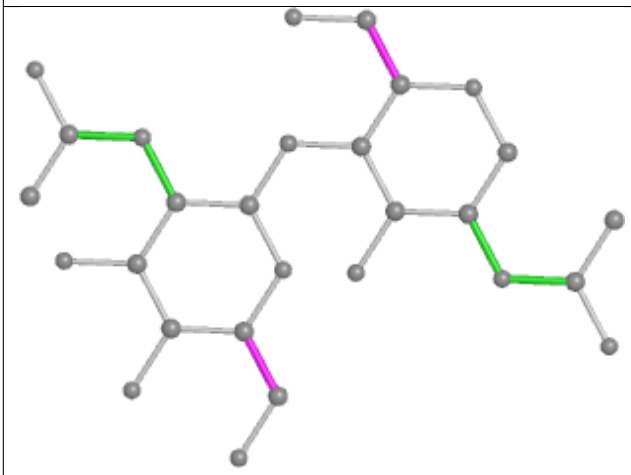
Oligosaccharide Chain Q



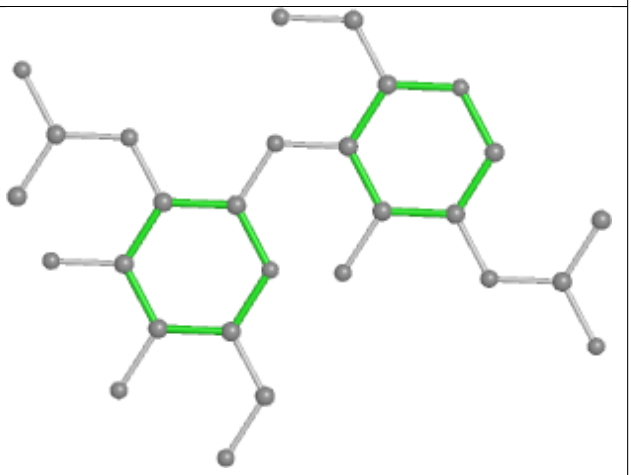
Bond lengths



Bond angles

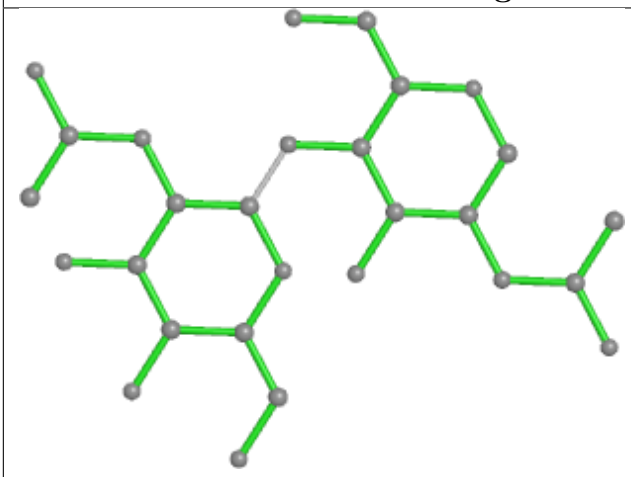


Torsions

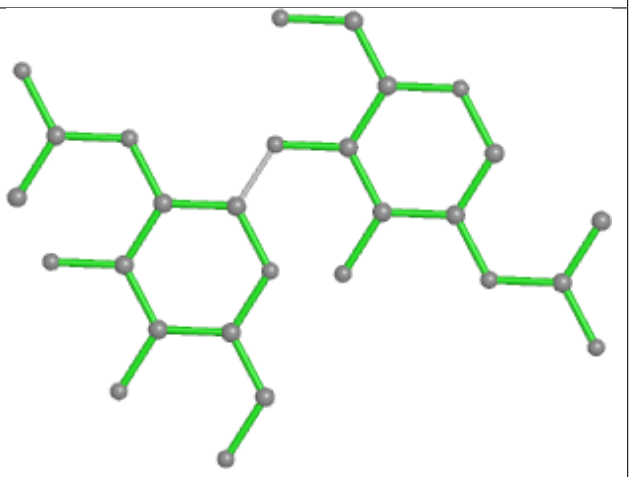


Rings

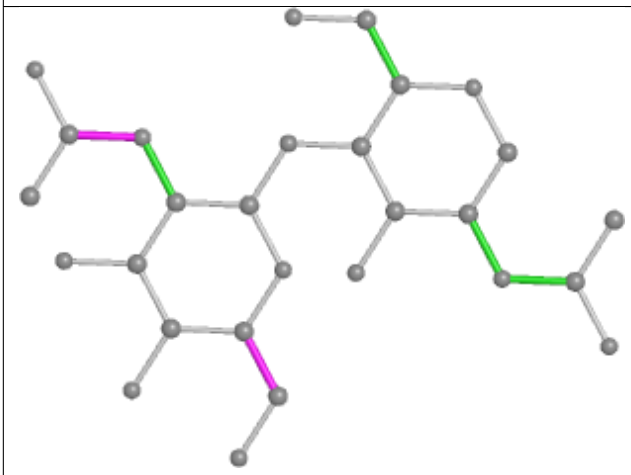
Oligosaccharide Chain R



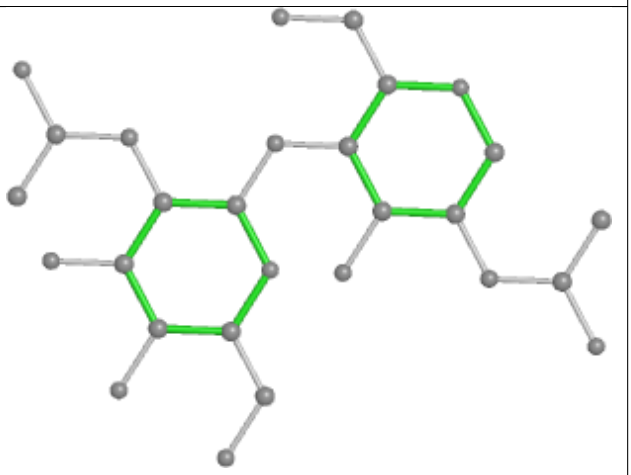
Bond lengths



Bond angles

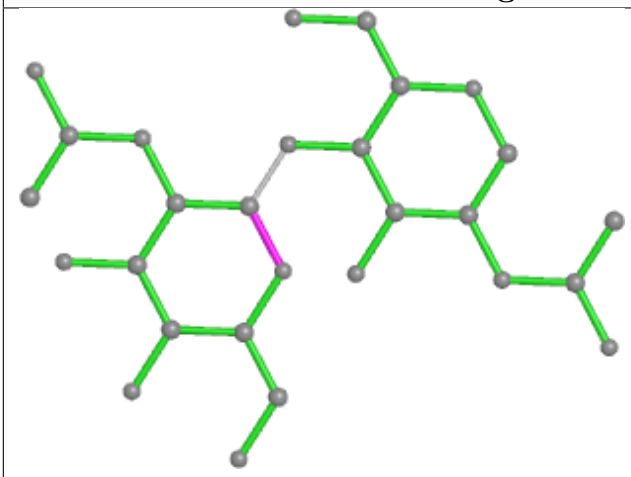


Torsions

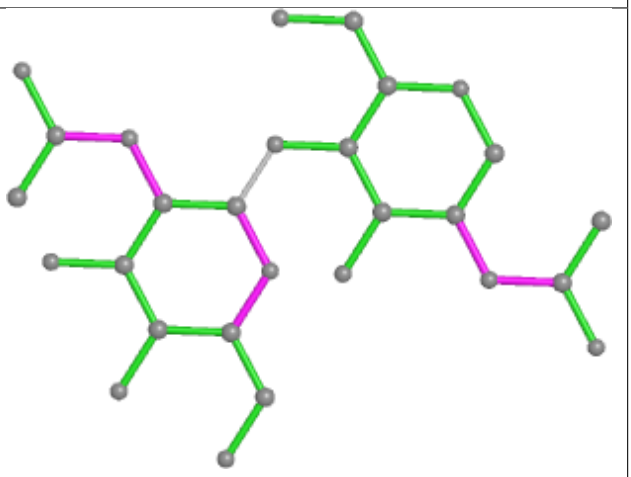


Rings

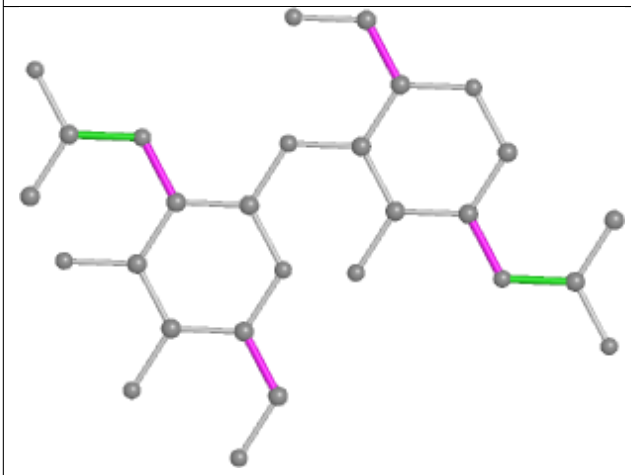
Oligosaccharide Chain S



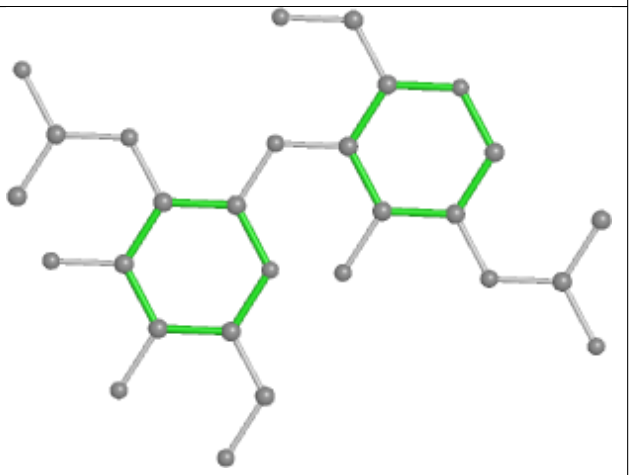
Bond lengths



Bond angles

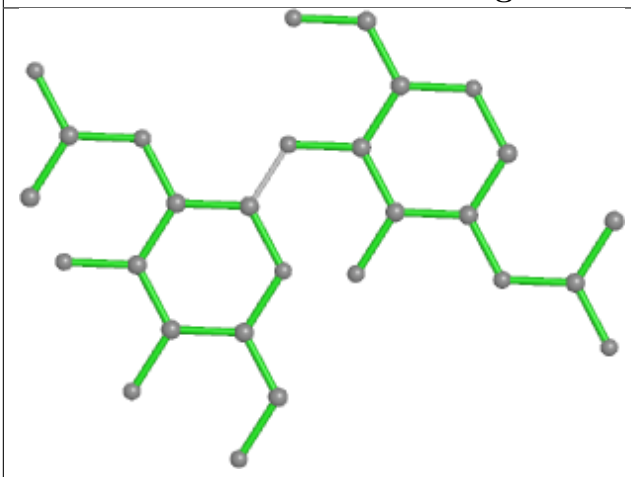


Torsions

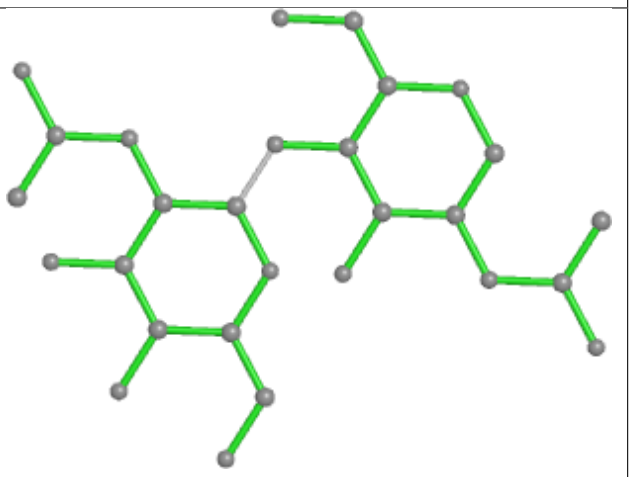


Rings

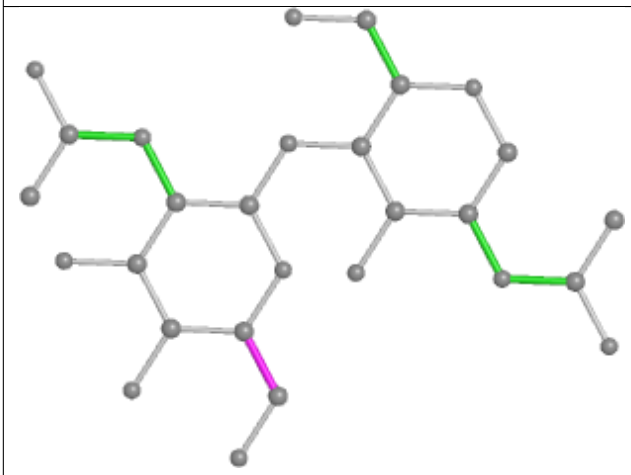
Oligosaccharide Chain T



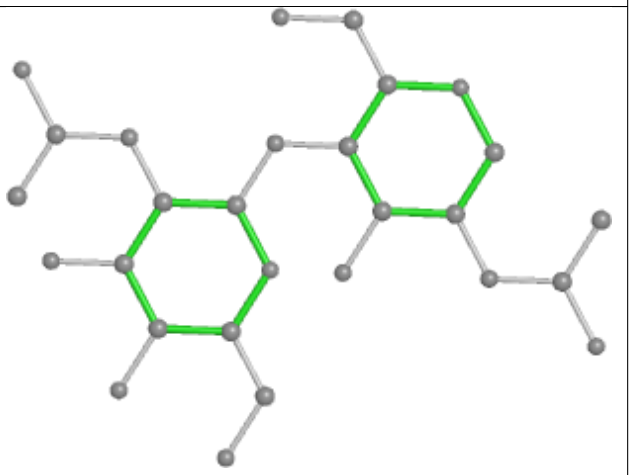
Bond lengths



Bond angles

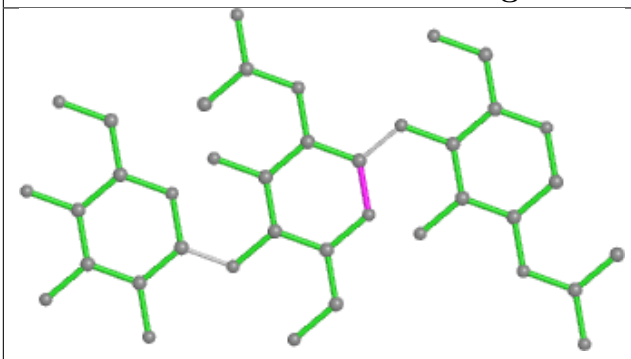


Torsions

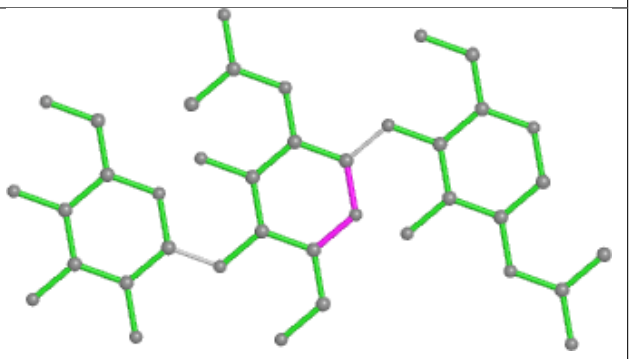


Rings

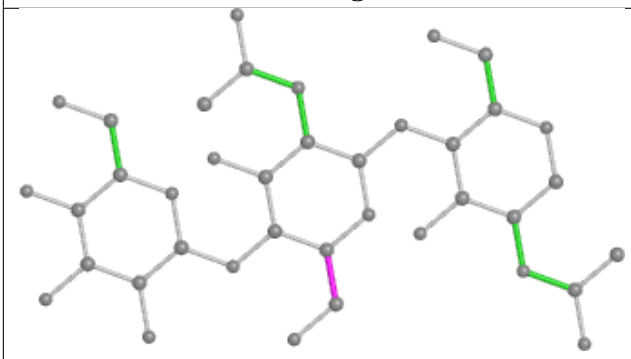
Oligosaccharide Chain I



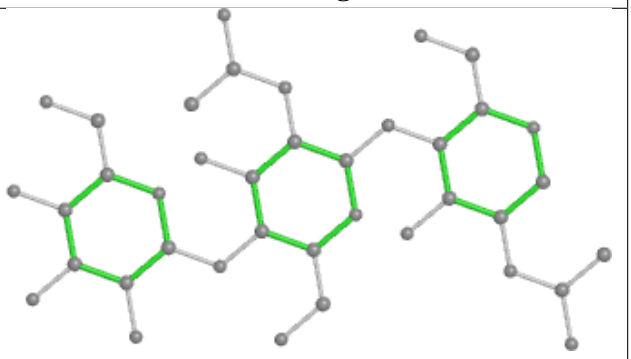
Bond lengths



Bond angles

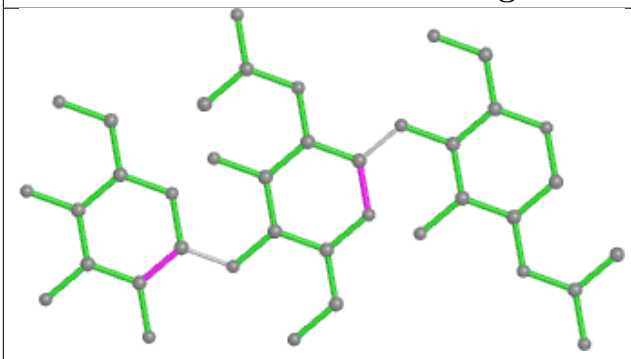


Torsions

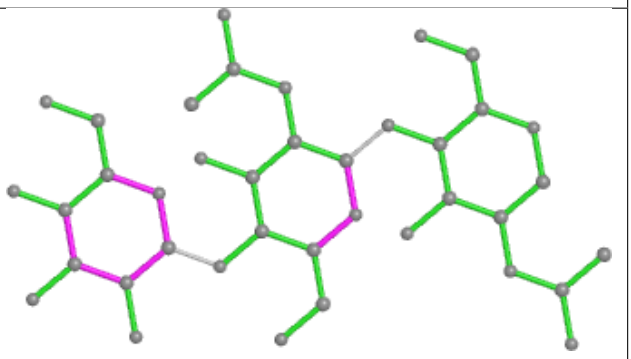


Rings

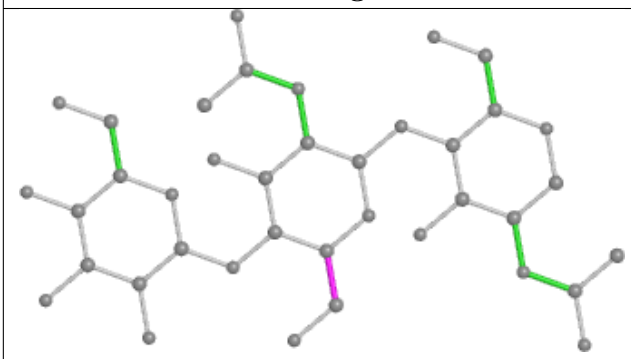
Oligosaccharide Chain J



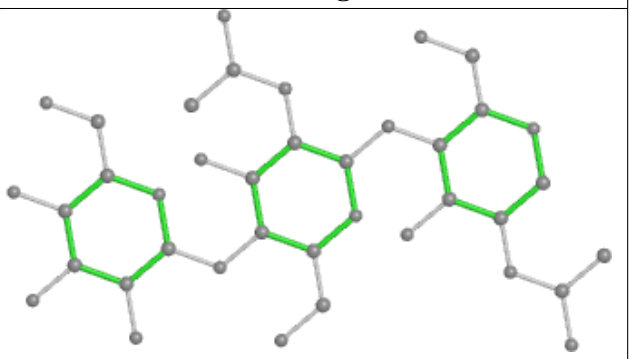
Bond lengths



Bond angles

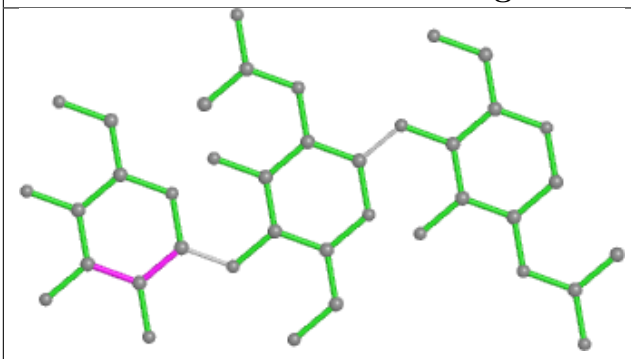


Torsions

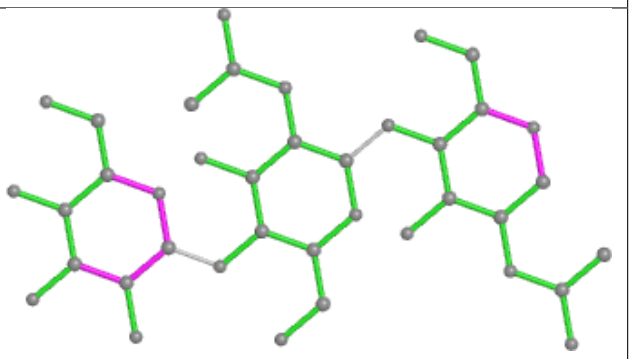


Rings

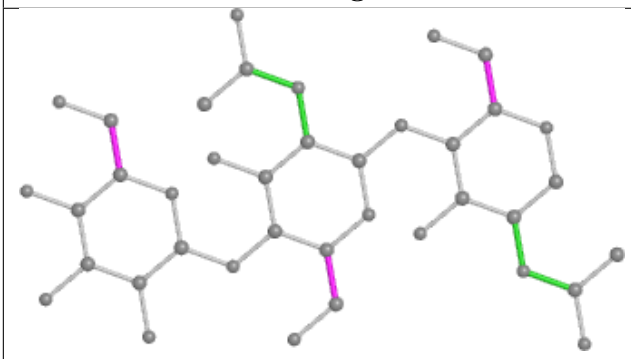
Oligosaccharide Chain O



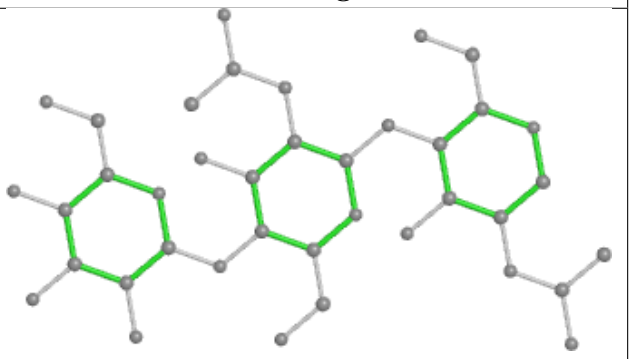
Bond lengths



Bond angles

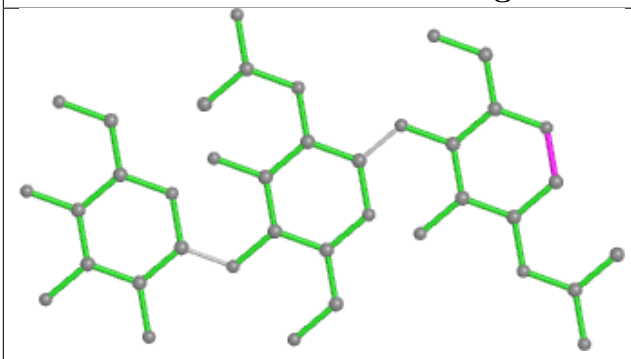


Torsions

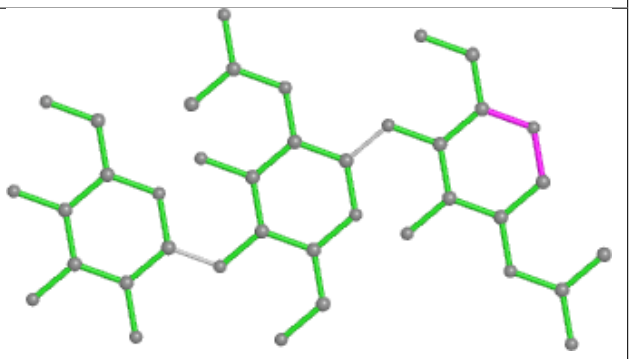


Rings

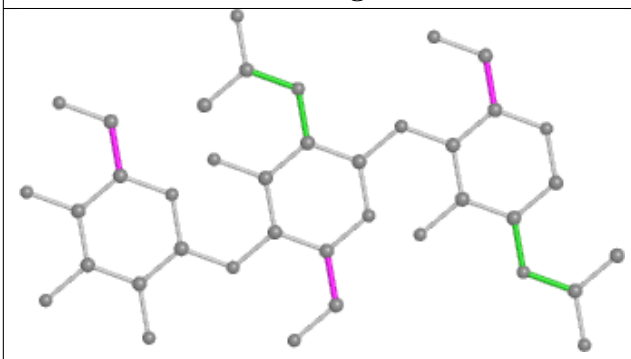
Oligosaccharide Chain U



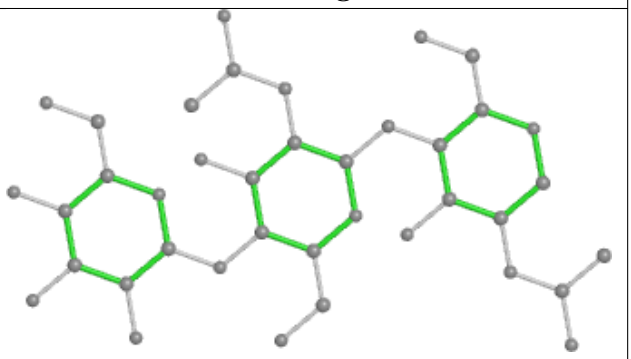
Bond lengths



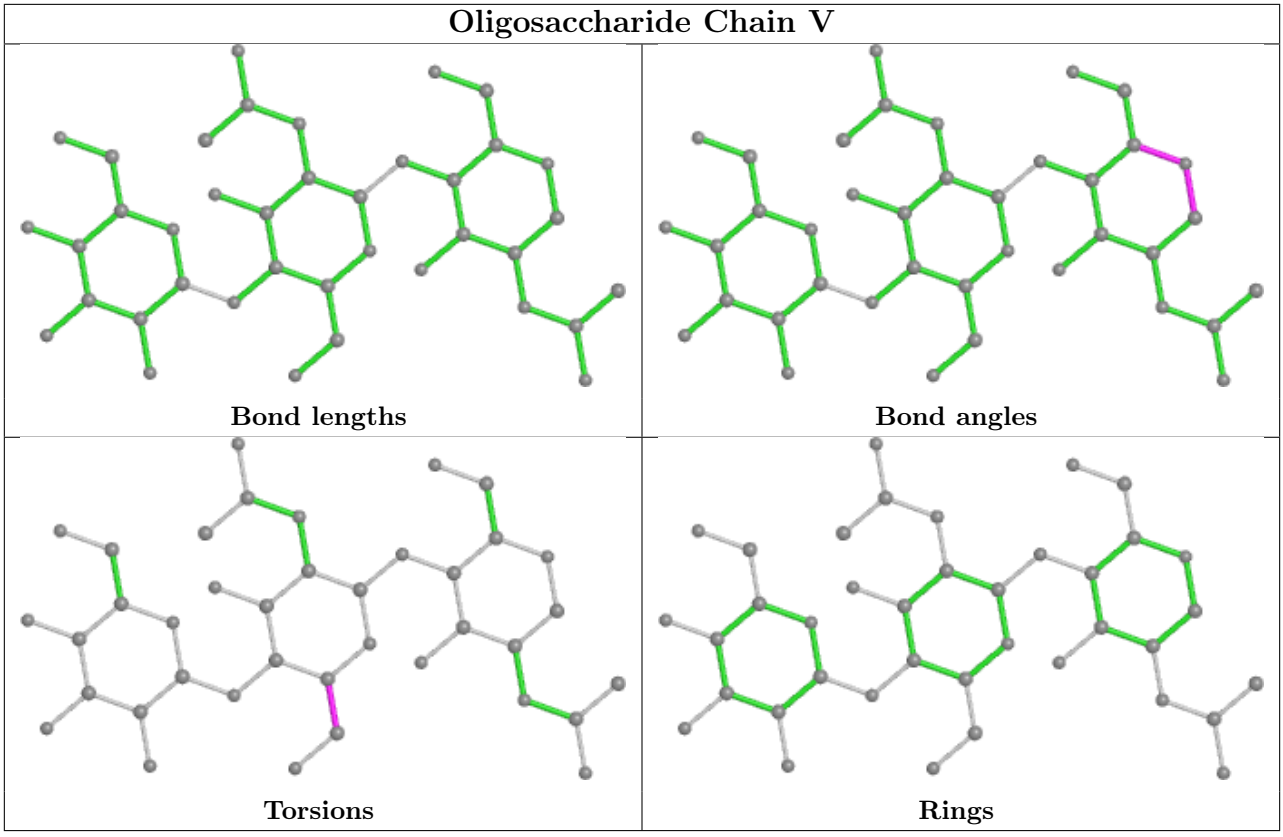
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	A	1310	-	14,14,15	0.53	0	17,19,21	0.46	0
4	NAG	C	1309	1	14,14,15	1.11	1 (7%)	17,19,21	1.46	1 (5%)
4	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	A	1302	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	B	1307	1	14,14,15	0.54	0	17,19,21	0.44	0
4	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	C	1303	1	14,14,15	0.28	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	0.94	2 (11%)
4	NAG	C	1310	-	14,14,15	0.93	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	B	1302	-	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	C	1307	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	C	1308	1	14,14,15	0.53	0	17,19,21	0.53	0
4	NAG	A	1305	1	14,14,15	0.34	0	17,19,21	0.51	0
4	NAG	C	1305	1	14,14,15	1.09	1 (7%)	17,19,21	1.17	1 (5%)
4	NAG	B	1301	1	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	B	1303	1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	C	1302	1	14,14,15	1.18	1 (7%)	17,19,21	1.47	1 (5%)
4	NAG	B	1306	1	14,14,15	0.48	0	17,19,21	0.45	0
4	NAG	A	1304	1	14,14,15	0.40	0	17,19,21	0.30	0
4	NAG	A	1308	1	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	A	1309	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	C	1304	-	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	C	1306	1	14,14,15	0.64	0	17,19,21	0.82	1 (5%)
4	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.60	1 (5%)
4	NAG	C	1311	1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	B	1308	1	14,14,15	0.25	0	17,19,21	0.38	0

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	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)
4	C	1302	NAG	O5-C1	4.30	1.50	1.43
4	C	1309	NAG	O5-C1	4.00	1.50	1.43
4	C	1305	NAG	O5-C1	3.51	1.49	1.43
4	C	1310	NAG	O5-C1	2.78	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1302	NAG	C1-O5-C5	5.83	120.10	112.19
4	C	1309	NAG	C1-O5-C5	5.78	120.03	112.19
4	C	1305	NAG	C1-O5-C5	4.63	118.46	112.19
4	C	1310	NAG	C1-O5-C5	4.07	117.70	112.19
4	C	1306	NAG	C2-N2-C7	2.40	126.33	122.90
4	B	1304	NAG	C1-O5-C5	2.40	115.44	112.19
4	B	1304	NAG	C2-N2-C7	2.38	126.29	122.90
4	C	1301	NAG	C1-O5-C5	2.13	115.08	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1310	NAG	1	0
4	A	1302	NAG	1	0
4	C	1308	NAG	1	0
4	A	1301	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.

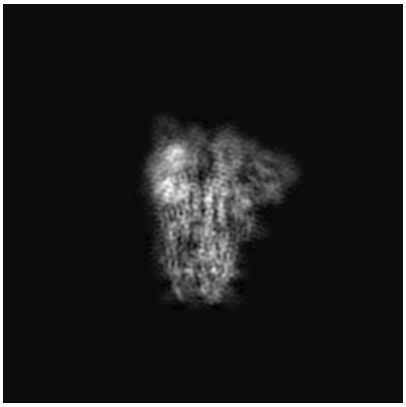
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32479. These allow visual inspection of the internal detail of the map and identification of artifacts.

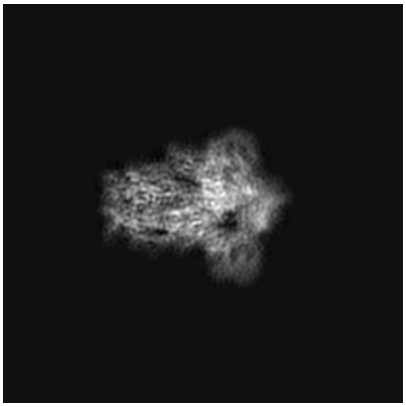
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

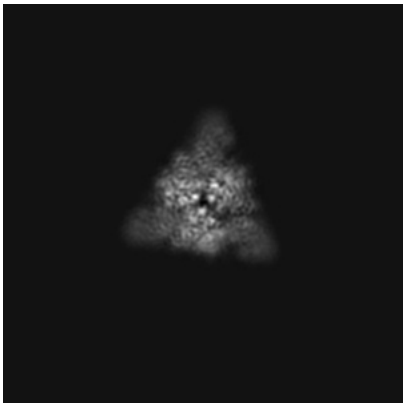
6.1.1 Primary map



X



Y



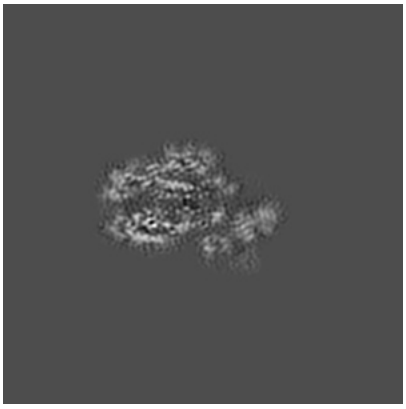
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 160



Y Index: 160

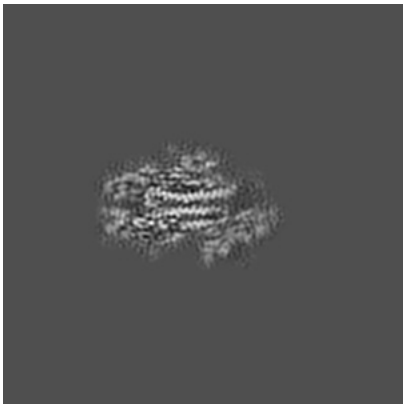
Z Index: 160

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

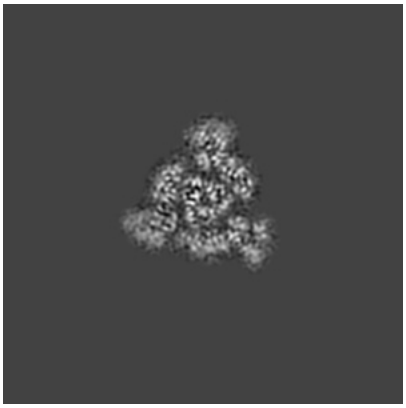
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 166



Y Index: 164

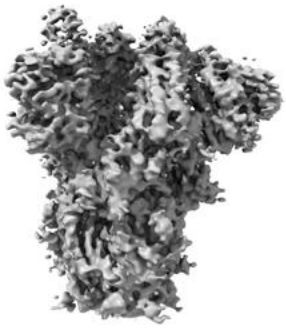


Z Index: 171

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

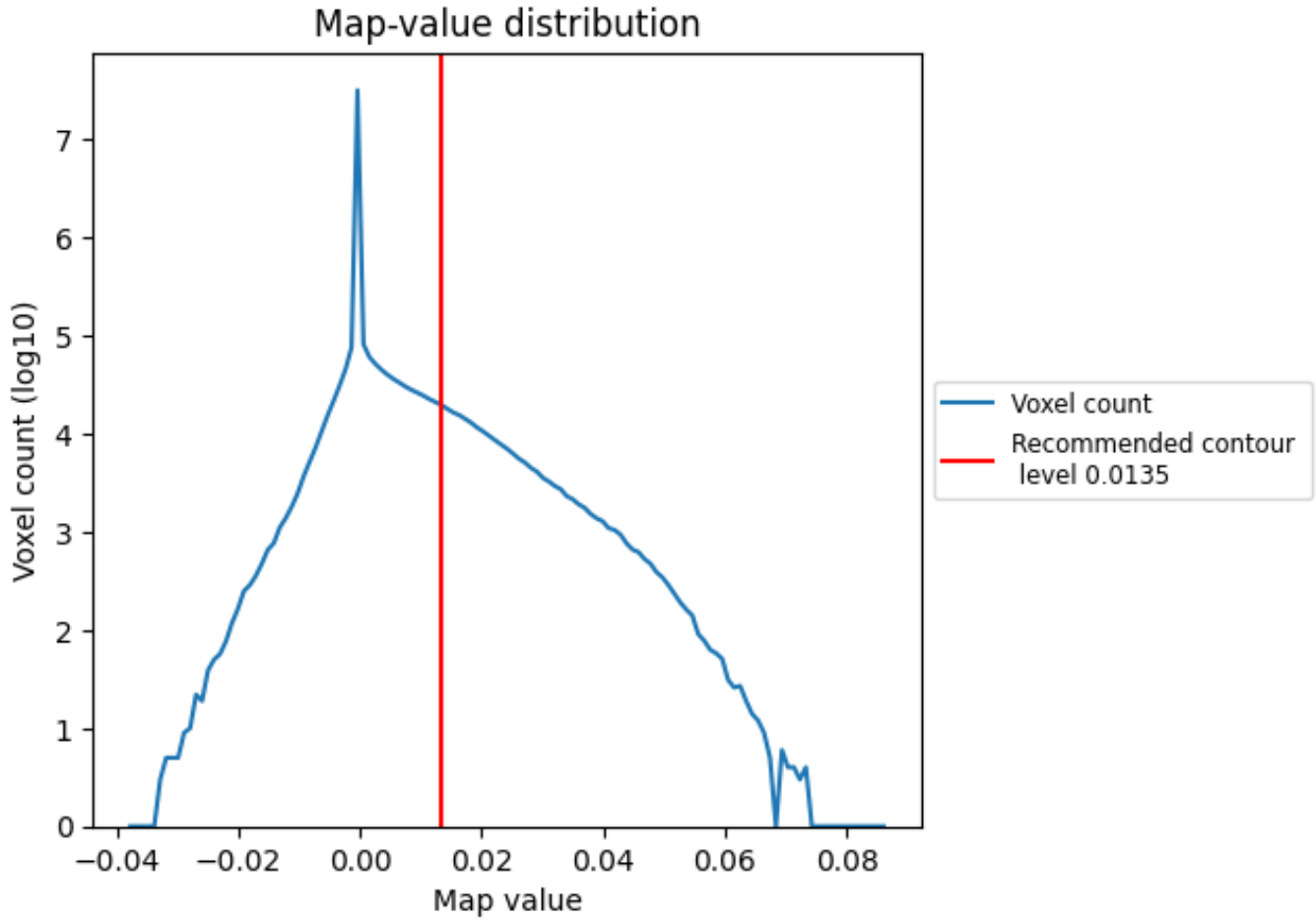
6.5 Mask visualisation (i)

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

7 Map analysis

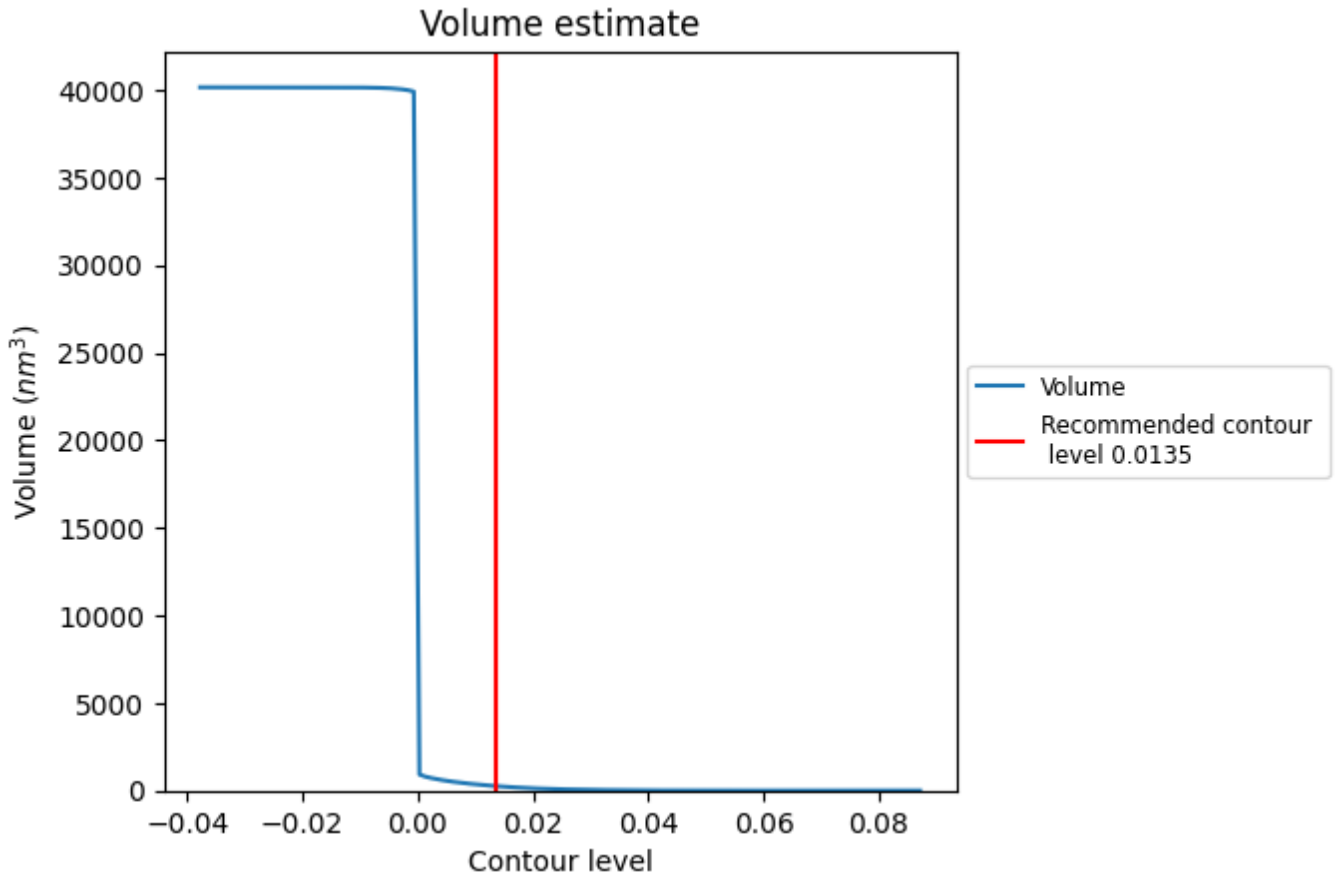
This section contains the results of statistical analysis of the map.

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.

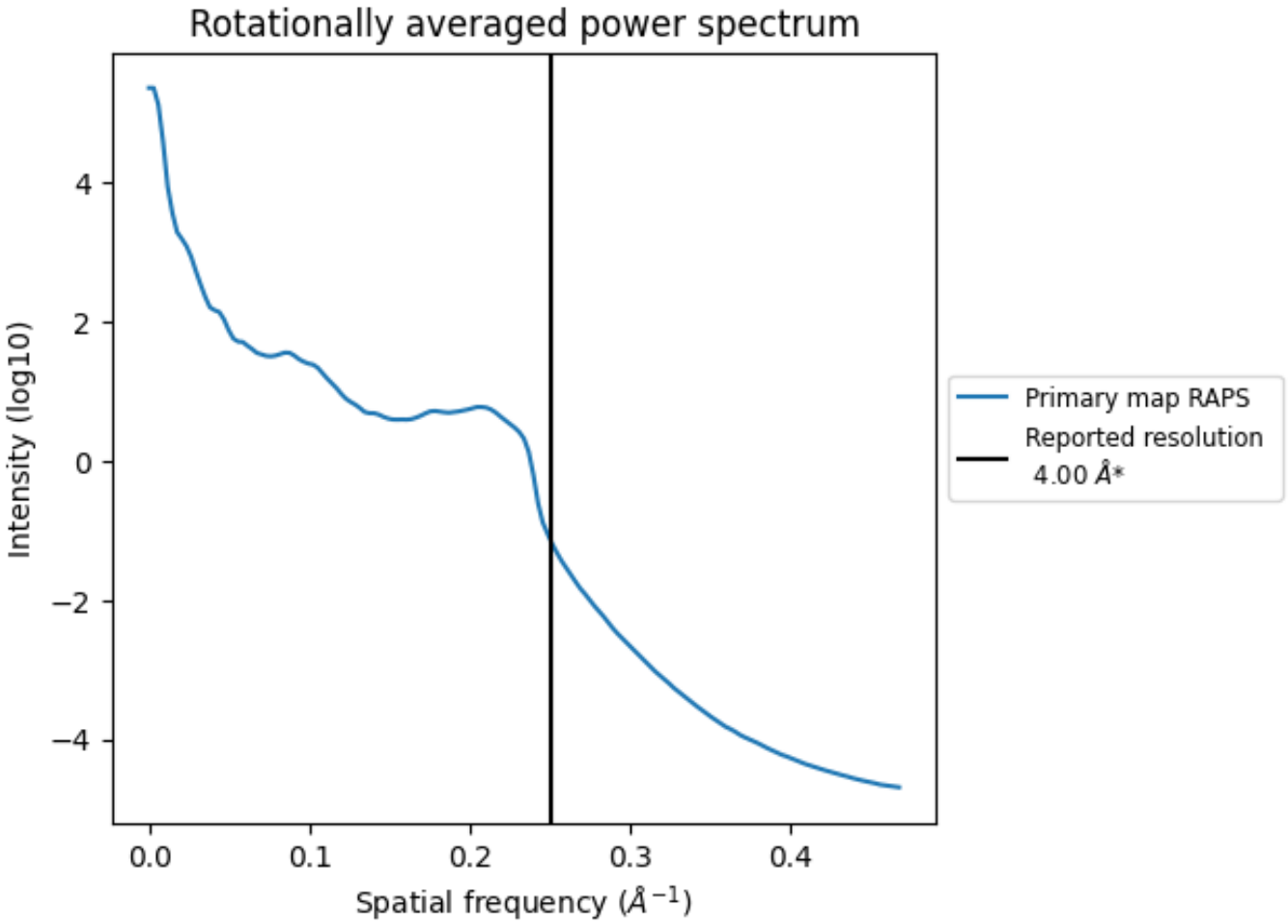
7.2 Volume estimate



The volume at the recommended contour level is 256 nm^3; this corresponds to an approximate mass of 231 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 0.250 Å^{-1}

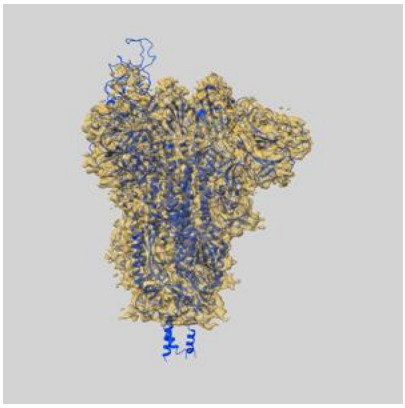
8 Fourier-Shell correlation (i)

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

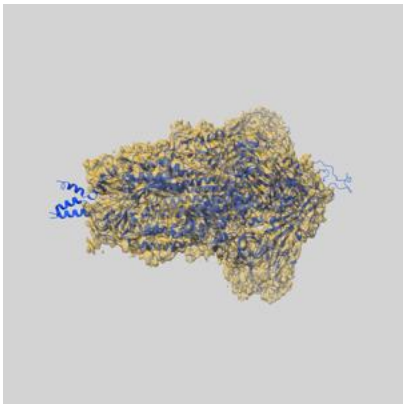
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32479 and PDB model 7WG7. Per-residue inclusion information can be found in section 3 on page 11.

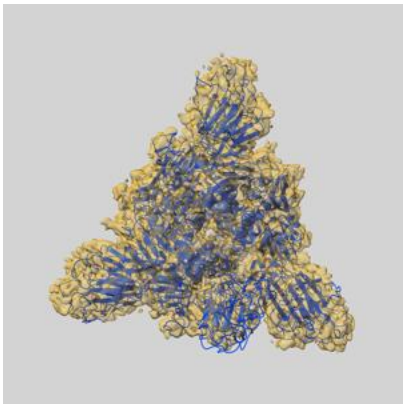
9.1 Map-model overlay



X



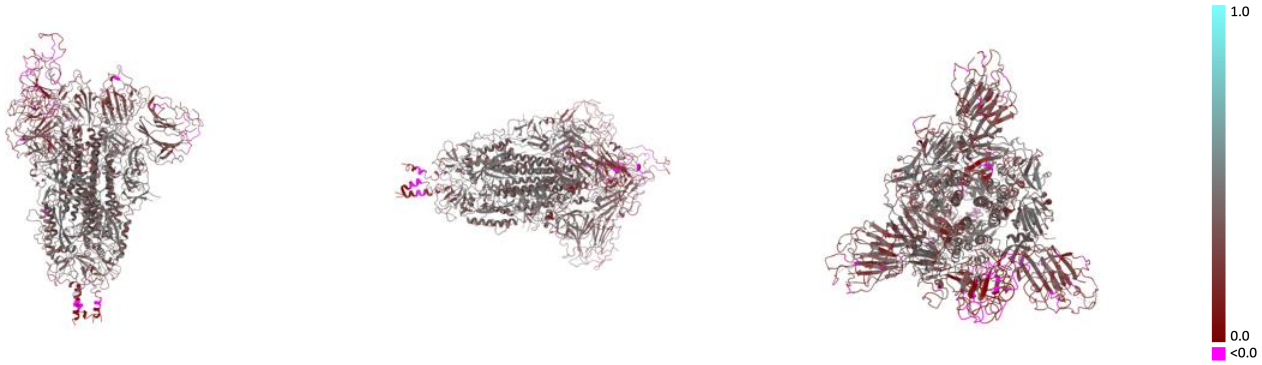
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135 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.

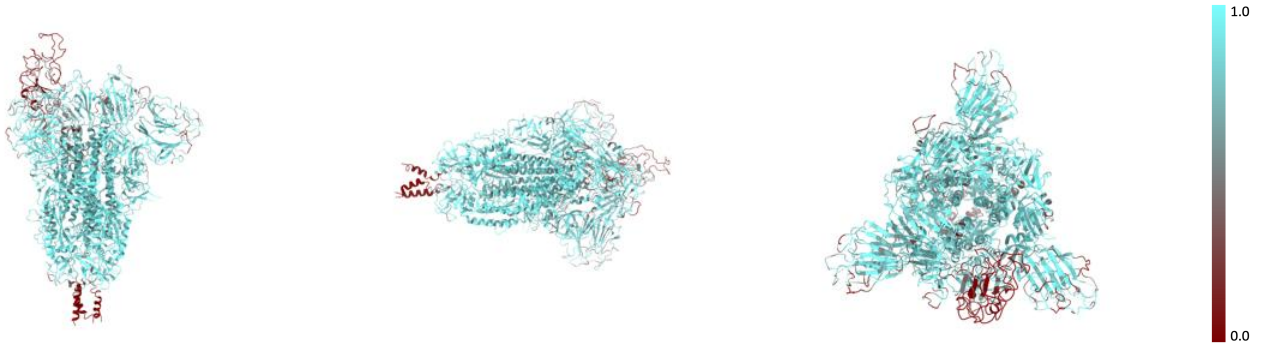
9.2 Q-score mapped to coordinate model (i)



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.

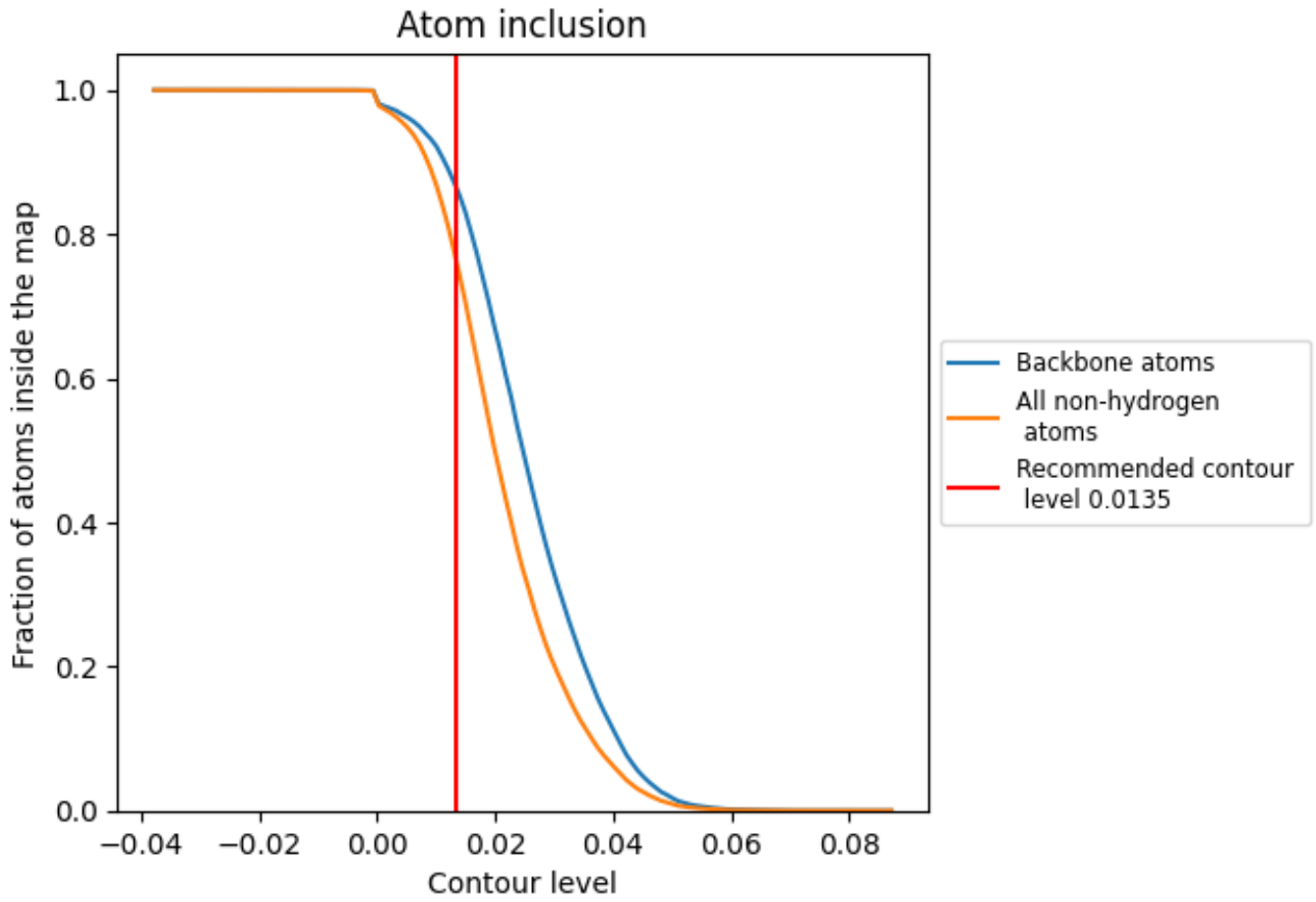
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0135).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7597	0.3380
A	0.8110	0.3580
B	0.7867	0.3440
C	0.6950	0.3120
D	0.0714	0.3190
E	0.2143	0.2010
F	0.8214	0.4670
G	0.5000	0.3100
H	0.8571	0.3330
I	0.5897	0.2400
J	0.4359	0.2370
K	0.6071	0.3750
L	0.3929	0.1630
M	0.8571	0.4690
N	0.8929	0.4560
O	0.7179	0.3930
P	0.6071	0.3930
Q	0.3929	0.3660
R	0.5714	0.3970
S	0.3929	0.3750
T	0.8214	0.4460
U	0.6410	0.3440
V	0.5385	0.2530