Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 07:37 AM EST

PDB ID	:	7L06
EMDB ID	:	EMD-23095
Title	:	Cryo-EM structure of SARS-CoV-2 2P S ectodomain bound to two copies of domain-swapped antibody 2G12
Authors	:	Manne, K.; Henderson, R.; Acharya, P.
Deposited on	:	2020-12-11
Resolution	:	3.30 Å(reported)
Based on initial model	:	6VXX

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:

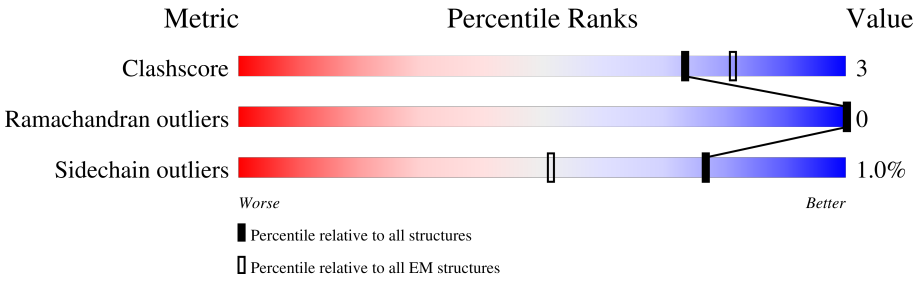
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	1121	5% 82% 5% 13%
1	B	1121	6% 83% • 13%
1	C	1121	6% 84% • 13%
2	D	226	17% 88% 7% • •
2	G	226	30% 88% 7% • •
2	H	226	10% 88% 7% • •
2	M	226	20% 89% 5% • •
3	E	213	24% 96% •

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Mol	Chain	Length	Quality of chain
3	F	213	41% 90% 8%
3	K	213	11% 95%
3	L	213	29% 91% 8%
4	I	2	100%
4	O	2	50% 50%
4	Q	2	100%
4	R	2	100%
4	S	2	50% 50%
4	T	2	50% 100%
4	V	2	100%
4	Y	2	50% 50%
5	J	5	40% 60%
5	W	5	60% 40%
6	N	8	12% 62% 25%
6	X	8	75% 25%
7	P	5	20% 40% 20% 40%
7	U	5	60% 20% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	V	1	X	-	-	-
5	MAN	W	4	-	-	X	-
5	MAN	W	5	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 72820 atoms, of which 35948 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	972	Total	C	H	N	O	S	0	0
			15038	4861	7434	1262	1448	33		
1	B	972	Total	C	H	N	O	S	0	0
			15038	4861	7434	1262	1448	33		
1	C	972	Total	C	H	N	O	S	0	0
			15018	4861	7414	1262	1448	33		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called 2G12 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		
2	G	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		
2	H	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		
2	M	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		

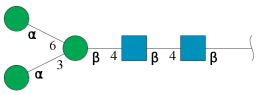
- Molecule 3 is a protein called 2G12 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	213	Total	C	H	N	O	S	0	0
			3228	1027	1593	274	329	5		
3	F	211	Total	C	H	N	O	S	0	0
			3198	1018	1580	272	323	5		
3	K	213	Total	C	H	N	O	S	0	0
			3228	1027	1593	274	329	5		
3	L	211	Total	C	H	N	O	S	0	0
			3198	1018	1580	272	323	5		

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

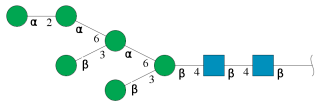
Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
4	O	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	Q	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	R	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	S	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	T	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	V	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
4	Y	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



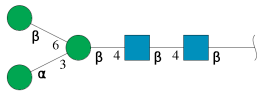
Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
5	W	5	Total	C	H	N	O	0	0
			118	34	57	2	25		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



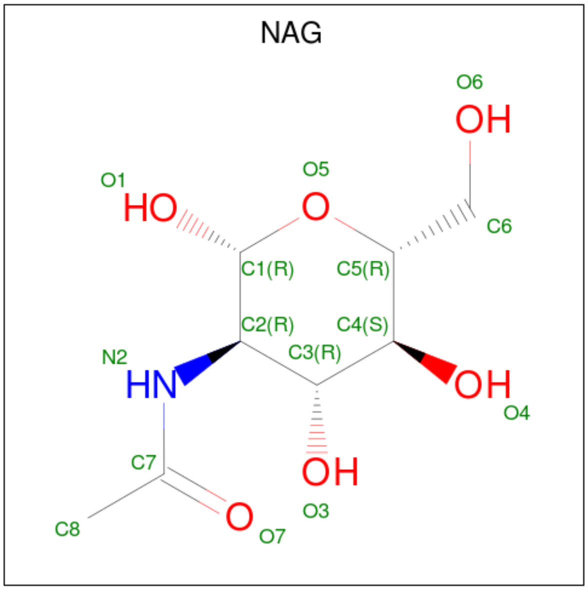
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	8	Total	C	H	N	O	0	0
			181	52	87	2	40		
6	X	8	Total	C	H	N	O	0	0
			181	52	87	2	40		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]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
7	P	5	Total	C	H	N	O	0	0
			74	34	13	2	25		
7	U	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	A	1	Total 216	C 64	H 104	N 8	O 40	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0

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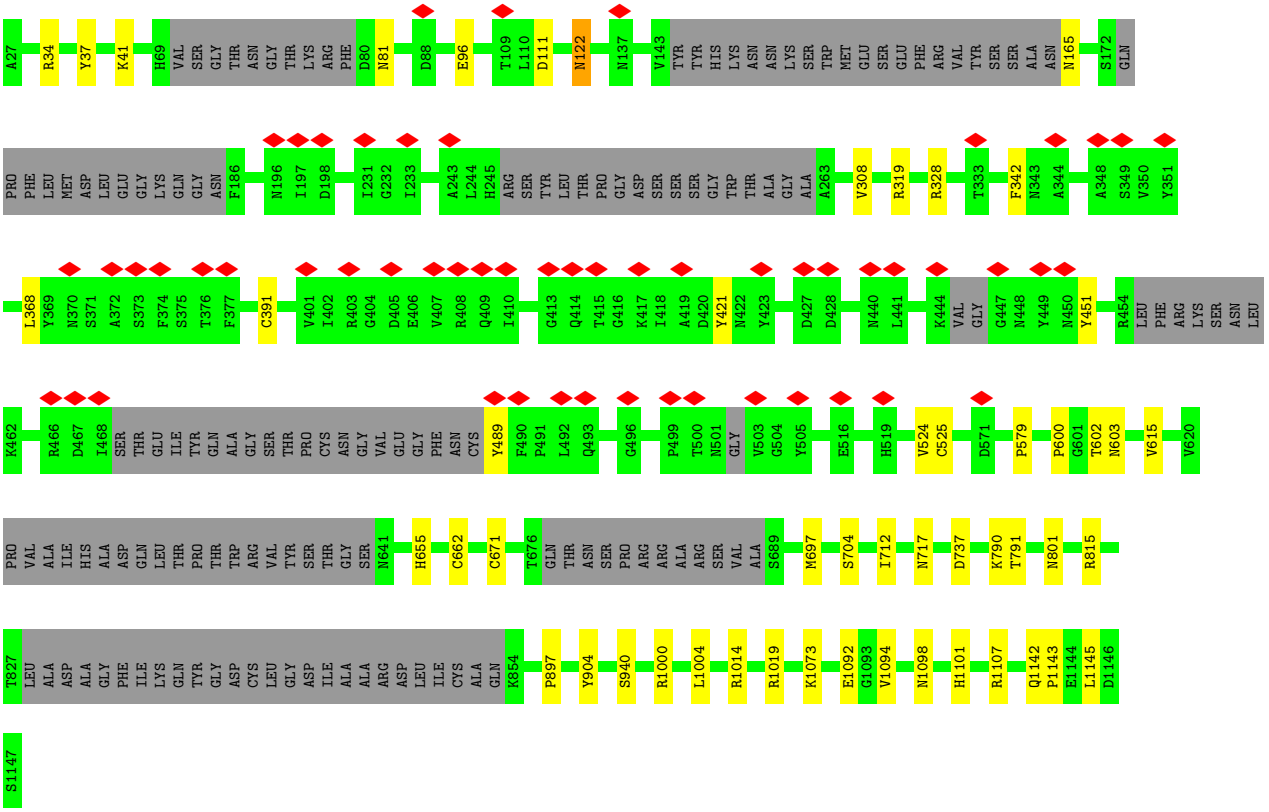
Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	B	1	Total 243	C 72	H 117	N 9	O 45	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0
8	C	1	Total 216	C 64	H 104	N 8	O 40	0

3 Residue-property plots (i)

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

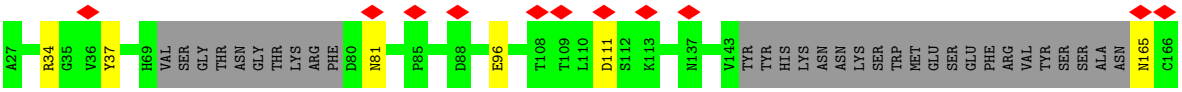
• Molecule 1: Spike glycoprotein

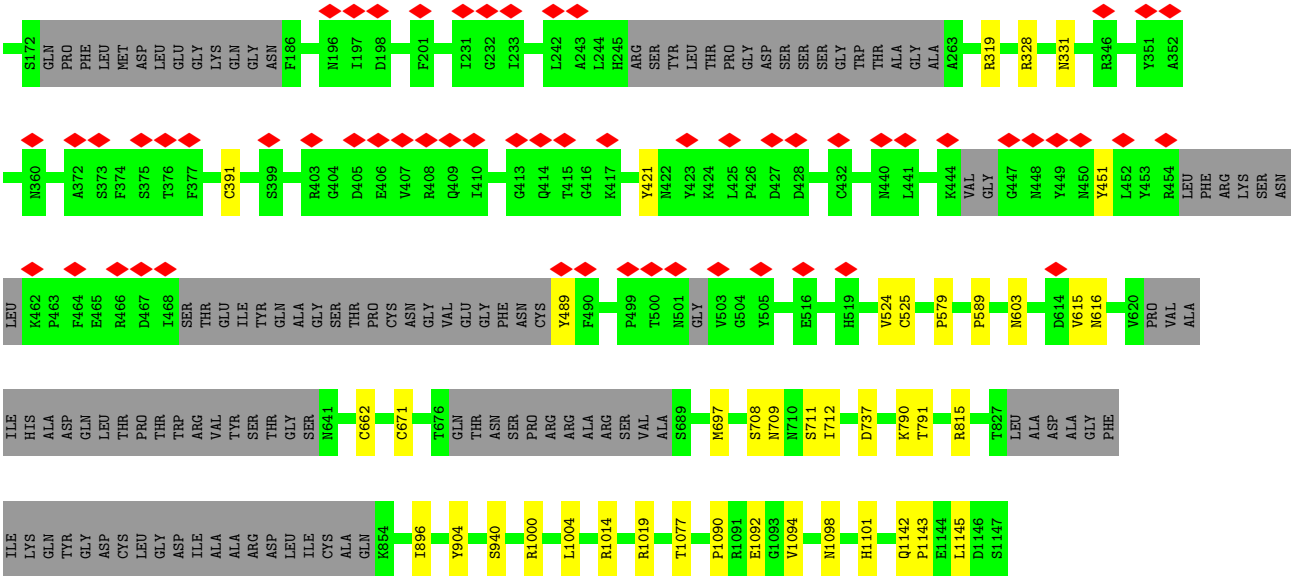
Chain A:



• Molecule 1: Spike glycoprotein

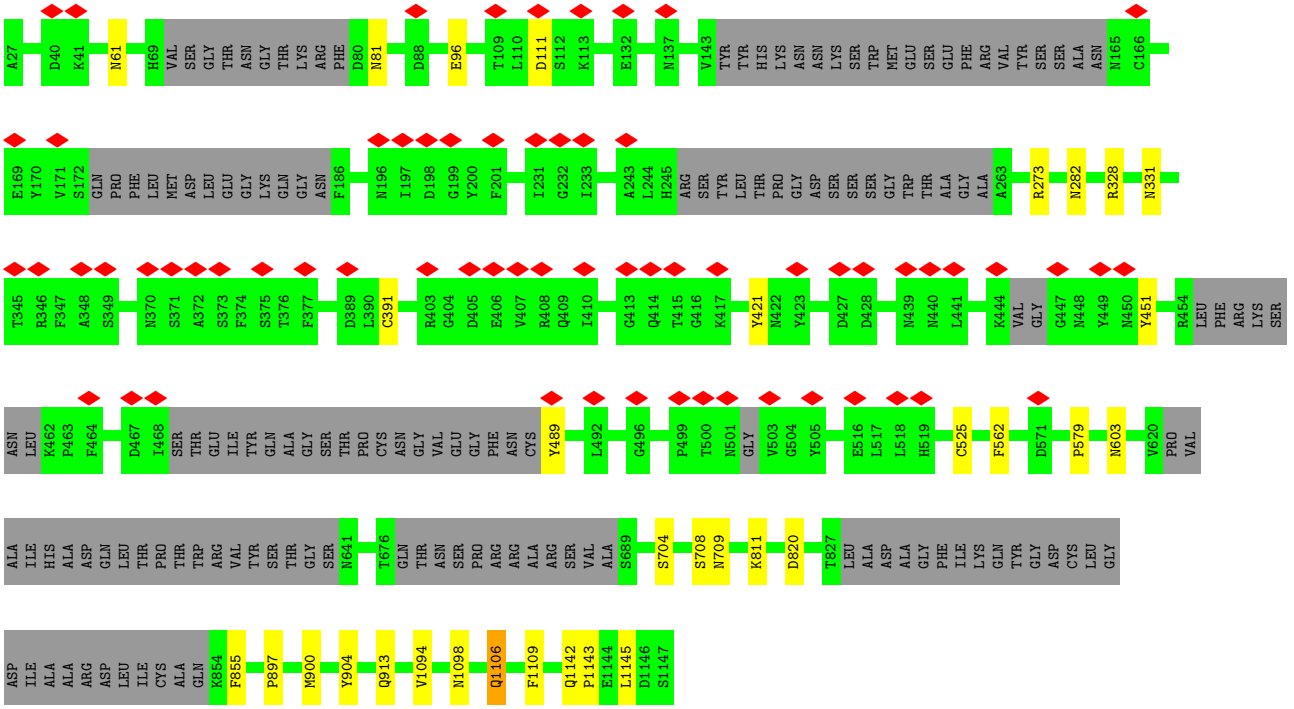
Chain B:





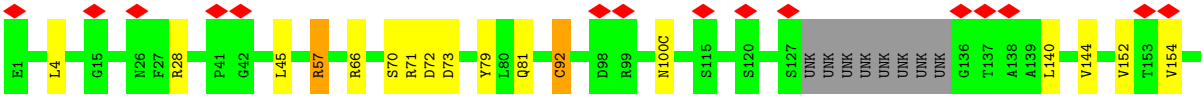
• Molecule 1: Spike glycoprotein

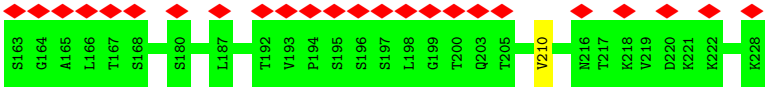
Chain C:



• Molecule 2: 2G12 heavy chain

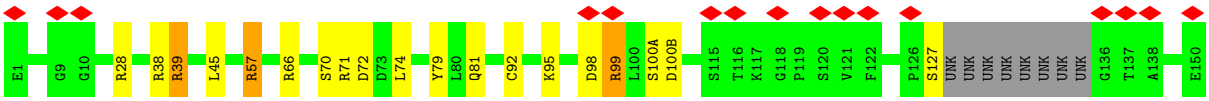
Chain D:

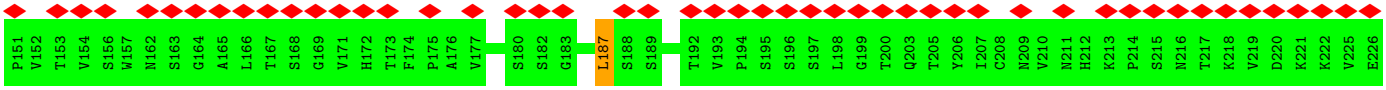




• Molecule 2: 2G12 heavy chain

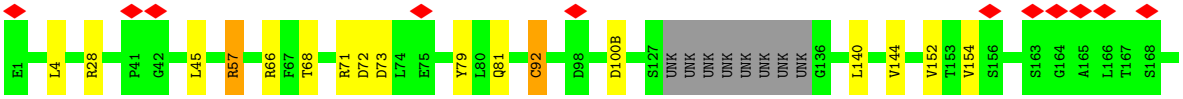
Chain G:

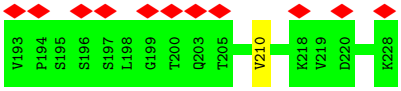




• Molecule 2: 2G12 heavy chain

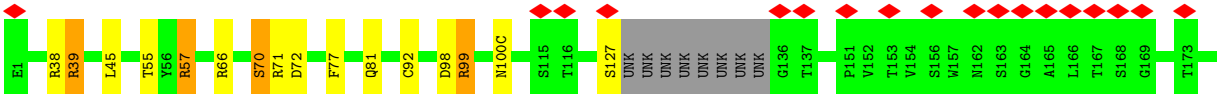
Chain H:

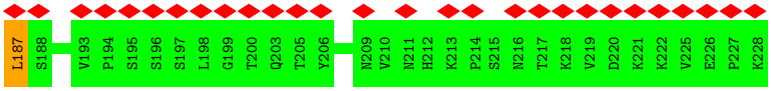




• Molecule 2: 2G12 heavy chain

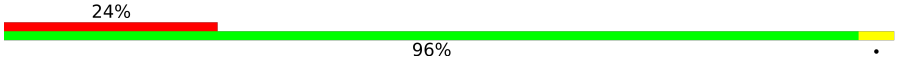
Chain M:

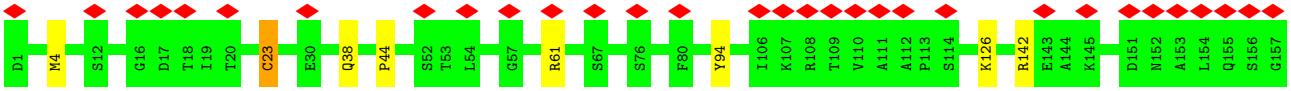


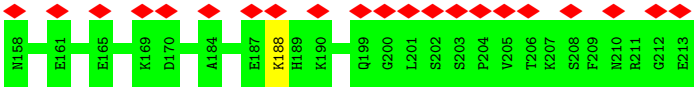


• Molecule 3: 2G12 light chain

Chain E:

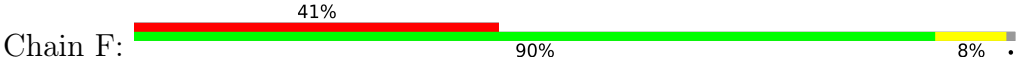


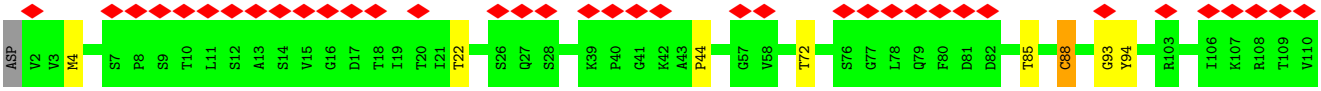


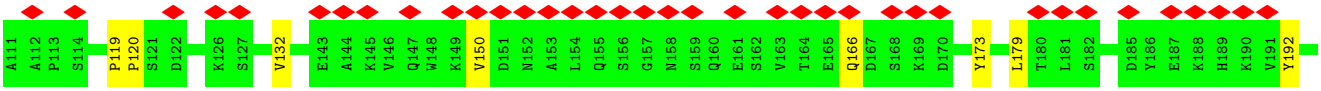


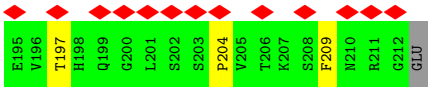
• Molecule 3: 2G12 light chain

Chain F:



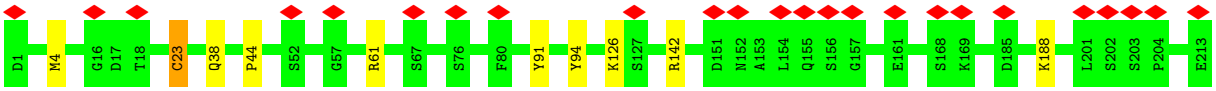






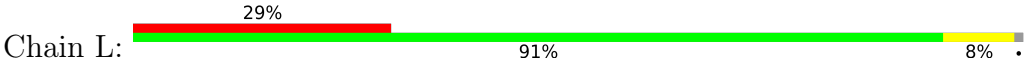
• Molecule 3: 2G12 light chain

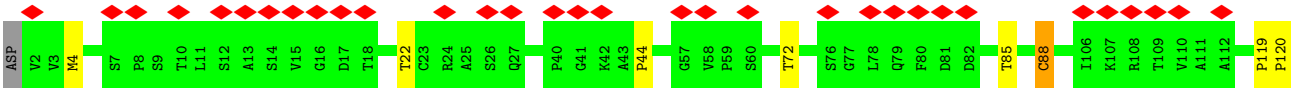
Chain K:

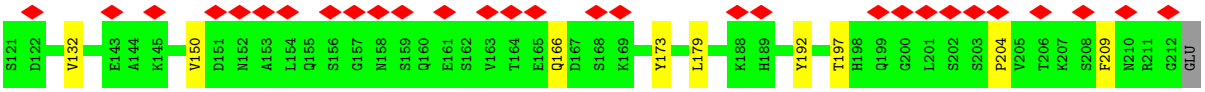


• Molecule 3: 2G12 light chain

Chain L:

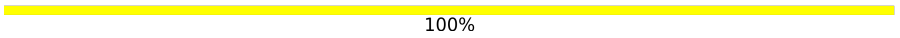






• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

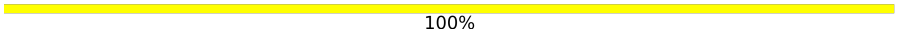


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

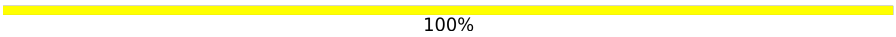
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:



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

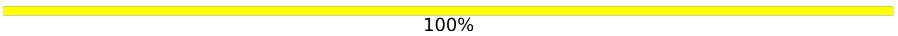
Chain S:

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

Chain T:

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

Chain V:

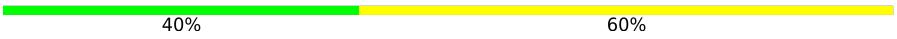


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

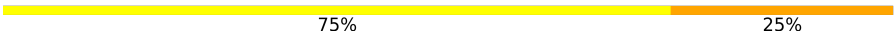
Chain W:

• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

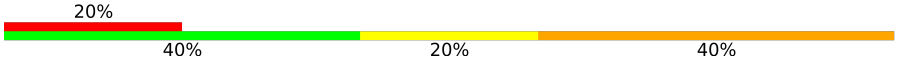
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

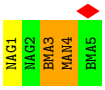
Chain X:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:





• Molecule 7: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109774	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 ($e^-/Å^2$)	66.43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.636	Depositor
Minimum map value	-0.689	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.204	Depositor
Map size (Å)	338.56, 338.56, 338.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, 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	0.72	5/7772 (0.1%)	0.87	10/10572 (0.1%)
1	B	0.72	5/7772 (0.1%)	0.87	10/10572 (0.1%)
1	C	0.83	5/7772 (0.1%)	0.69	4/10572 (0.0%)
2	D	0.65	0/1675	1.02	4/2281 (0.2%)
2	G	0.58	0/1675	0.97	6/2281 (0.3%)
2	H	0.65	0/1675	1.02	4/2281 (0.2%)
2	M	0.58	0/1675	0.97	7/2281 (0.3%)
3	E	0.60	0/1671	0.89	2/2269 (0.1%)
3	F	0.57	0/1654	0.77	0/2246
3	K	0.60	0/1671	0.90	2/2269 (0.1%)
3	L	0.57	0/1654	0.77	0/2246
All	All	0.71	15/36666 (0.0%)	0.85	49/49870 (0.1%)

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	1
1	B	0	1
3	E	0	1
3	K	0	1
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	489	TYR	CG-CD1	5.65	1.46	1.39
1	A	489	TYR	CG-CD1	5.61	1.46	1.39
1	A	489	TYR	CG-CD2	5.61	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	489	TYR	CG-CD2	5.61	1.46	1.39
1	B	489	TYR	CG-CD2	5.58	1.46	1.39
1	C	489	TYR	CG-CD1	5.43	1.46	1.39
1	B	489	TYR	CE1-CZ	5.28	1.45	1.38
1	A	489	TYR	CE1-CZ	5.25	1.45	1.38
1	C	489	TYR	CE1-CZ	5.24	1.45	1.38
1	C	489	TYR	CE2-CZ	5.21	1.45	1.38
1	B	96	GLU	CD-OE2	-5.11	1.20	1.25
1	A	96	GLU	CD-OE2	-5.07	1.20	1.25
1	B	489	TYR	CE2-CZ	5.06	1.45	1.38
1	C	96	GLU	CD-OE2	-5.03	1.20	1.25
1	A	489	TYR	CE2-CZ	5.02	1.45	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	99	ARG	NE-CZ-NH2	8.66	124.63	120.30
2	M	99	ARG	NE-CZ-NH2	8.64	124.62	120.30
2	M	71	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	G	71	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	B	1019	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	1019	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	319	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	815	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	708	SER	C-N-CA	7.24	139.80	121.70
1	B	319	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	1014	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	904	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	A	34	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	1014	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	34	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	815	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	G	66	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	451	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	B	451	TYR	CB-CG-CD2	-6.89	116.86	121.00
3	K	142	ARG	NE-CZ-NH1	6.89	123.74	120.30
2	D	71	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	M	66	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	C	451	TYR	CB-CG-CD2	-6.80	116.92	121.00
3	E	142	ARG	NE-CZ-NH1	6.76	123.68	120.30
2	H	71	ARG	NE-CZ-NH1	6.71	123.65	120.30
2	M	39	ARG	NE-CZ-NH1	6.67	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	38	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	M	57	ARG	NE-CZ-NH1	6.63	123.62	120.30
2	G	39	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	G	38	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	G	57	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	H	66	ARG	NE-CZ-NH1	6.53	123.56	120.30
3	K	61	ARG	NE-CZ-NH1	6.49	123.54	120.30
3	E	61	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	D	66	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	600	PRO	N-CA-C	-6.32	95.67	112.10
1	B	1000	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	1000	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	421	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	421	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	B	421	TYR	CB-CG-CD1	-5.30	117.82	121.00
2	H	57	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	D	57	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	737	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	737	ASP	CB-CG-OD2	-5.08	113.73	118.30
2	D	28	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	C	273	ARG	NE-CZ-NH2	-5.07	117.76	120.30
2	H	28	ARG	NE-CZ-NH2	5.07	122.83	120.30
2	M	71	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	TYR	Sidechain
1	B	37	TYR	Sidechain
3	E	94	TYR	Sidechain
3	K	94	TYR	Sidechain

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	7604	7434	7420	55	0
1	B	7604	7434	7419	53	0
1	C	7604	7414	7419	38	0
2	D	1637	1610	1609	29	0
2	G	1637	1610	1608	56	0
2	H	1637	1610	1609	19	0
2	M	1637	1610	1609	25	0
3	E	1635	1593	1593	13	0
3	F	1618	1580	1580	17	0
3	K	1635	1593	1593	9	0
3	L	1618	1580	1580	13	0
4	I	28	26	25	0	0
4	O	28	25	25	5	0
4	Q	28	25	25	0	0
4	R	28	25	25	0	0
4	S	28	25	25	3	0
4	T	28	25	25	0	0
4	V	28	26	25	0	0
4	Y	28	25	25	6	0
5	J	61	57	52	4	0
5	W	61	57	52	12	0
6	N	94	87	79	5	0
6	X	94	87	79	6	0
7	P	61	13	52	3	0
7	U	61	52	52	4	0
8	A	112	104	104	10	0
8	B	126	117	117	13	0
8	C	112	104	104	10	0
All	All	36872	35948	35930	239	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 3.

All (239) 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:1098:ASN:HD21	4:S:1:NAG:C1	0.98	1.62
1:A:603:ASN:HD21	8:A:1304:NAG:C1	0.98	1.56
1:C:61:ASN:HD21	8:C:1203:NAG:C1	0.97	1.56
1:C:282:ASN:HD21	8:C:1204:NAG:C1	0.91	1.55
1:B:709:ASN:HD21	8:B:1309:NAG:C1	0.89	1.54
1:C:331:ASN:ND2	8:C:1205:NAG:C1	1.68	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1098:ASN:ND2	4:Y:1:NAG:C1	1.69	1.52
1:B:616:ASN:HD21	8:B:1308:NAG:C1	0.90	1.52
1:A:1098:ASN:ND2	4:O:1:NAG:C1	1.68	1.52
1:A:717:ASN:ND2	6:N:1:NAG:C1	1.71	1.49
1:C:709:ASN:ND2	7:U:1:NAG:C1	1.71	1.49
1:A:801:ASN:ND2	5:J:1:NAG:C1	1.71	1.48
1:B:616:ASN:ND2	8:B:1308:NAG:C1	1.74	1.46
1:B:709:ASN:ND2	8:B:1309:NAG:C1	1.75	1.45
1:A:603:ASN:ND2	8:A:1304:NAG:C1	1.73	1.43
1:C:61:ASN:ND2	8:C:1203:NAG:C1	1.83	1.42
1:C:282:ASN:ND2	8:C:1204:NAG:C1	1.75	1.39
1:C:1098:ASN:ND2	4:S:1:NAG:C1	1.83	1.37
2:D:72:ASP:OD1	2:G:57:ARG:NH2	1.66	1.28
1:B:331:ASN:OD1	8:B:1302:NAG:C1	1.83	1.27
2:H:45:LEU:HD11	3:L:44:PRO:CG	1.70	1.19
1:A:704:SER:HB3	1:B:790:LYS:HE3	1.23	1.17
2:G:28:ARG:NH1	5:W:5:MAN:H5	1.68	1.08
2:H:45:LEU:HD11	3:L:44:PRO:HG2	1.06	1.06
2:H:57:ARG:NH1	2:M:72:ASP:OD2	1.89	1.04
2:H:45:LEU:CD1	3:L:44:PRO:HG2	1.88	1.02
2:H:72:ASP:OD2	2:M:57:ARG:NH1	1.93	1.00
2:D:45:LEU:HD11	3:F:44:PRO:HG2	1.43	0.99
2:D:57:ARG:NH1	2:G:72:ASP:OD2	1.96	0.99
3:E:38:GLN:HE22	2:G:39:ARG:HD2	1.27	0.96
2:D:79:TYR:OH	2:G:81:GLN:NE2	1.99	0.94
3:E:44:PRO:HG2	2:G:45:LEU:HD11	1.50	0.93
1:B:1098:ASN:CG	4:Y:1:NAG:C1	2.38	0.91
1:A:717:ASN:CG	6:N:1:NAG:C1	2.39	0.89
2:G:100(B):ASP:OD2	6:X:5:MAN:O6	1.91	0.89
1:A:801:ASN:CG	5:J:1:NAG:C1	2.45	0.85
2:D:45:LEU:HD11	3:F:44:PRO:CG	2.08	0.83
2:G:28:ARG:HD3	5:W:5:MAN:H62	1.59	0.83
1:A:940:SER:CB	2:M:99:ARG:HD2	2.10	0.82
1:A:1094:VAL:CG2	1:B:904:TYR:OH	2.27	0.82
1:A:1098:ASN:CG	4:O:1:NAG:C1	2.48	0.82
1:B:940:SER:CB	2:G:99:ARG:HD2	2.09	0.82
2:D:79:TYR:HE1	2:G:81:GLN:HG3	1.45	0.80
2:H:72:ASP:OD1	2:M:57:ARG:NH2	2.14	0.80
2:G:74:LEU:HD13	5:W:4:MAN:O4	1.82	0.79
2:G:28:ARG:NH1	5:W:5:MAN:C5	2.47	0.77
2:D:81:GLN:NE2	2:G:79:TYR:OH	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:ASN:ND2	4:O:1:NAG:C2	2.49	0.76
2:D:57:ARG:NH2	2:G:72:ASP:OD1	2.18	0.76
2:D:79:TYR:CE1	2:G:81:GLN:HG3	2.20	0.76
1:B:616:ASN:CG	8:B:1308:NAG:C1	2.54	0.76
1:A:603:ASN:CG	8:A:1304:NAG:C1	2.54	0.75
2:D:79:TYR:HE1	2:G:81:GLN:CG	2.00	0.73
1:A:704:SER:HB3	1:B:790:LYS:CE	2.12	0.72
2:D:72:ASP:CG	2:G:57:ARG:HH22	1.92	0.72
2:D:72:ASP:OD1	2:G:57:ARG:CZ	2.33	0.72
2:H:57:ARG:NH2	2:M:72:ASP:OD1	2.19	0.71
2:G:95:LYS:HE3	6:X:6:MAN:O4	1.90	0.70
1:A:1094:VAL:HG22	1:B:904:TYR:OH	1.91	0.70
2:M:55:THR:HG21	6:N:3:BMA:H62	1.72	0.70
3:E:38:GLN:NE2	2:G:39:ARG:HD2	2.03	0.70
1:A:940:SER:OG	2:M:99:ARG:NH2	2.25	0.69
2:D:100(C):ASN:HB2	3:F:93:GLY:HA2	1.72	0.69
3:F:94:TYR:HE1	7:P:4:MAN:HO6	1.41	0.69
1:B:940:SER:OG	2:G:99:ARG:NH2	2.26	0.69
1:B:1101:HIS:ND1	4:Y:1:NAG:H5	2.08	0.69
2:D:100(C):ASN:CG	3:F:93:GLY:HA2	2.13	0.69
2:G:74:LEU:HD13	5:W:4:MAN:H5	1.75	0.68
1:C:331:ASN:ND2	8:C:1205:NAG:C2	2.55	0.68
2:H:72:ASP:CG	2:M:57:ARG:HH12	1.95	0.68
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.76	0.67
2:D:79:TYR:CZ	2:G:81:GLN:NE2	2.61	0.67
3:E:38:GLN:CD	2:G:39:ARG:CZ	2.63	0.67
2:M:187:LEU:C	2:M:187:LEU:HD12	2.15	0.67
1:A:790:LYS:HE3	1:C:704:SER:HB3	1.76	0.67
2:D:57:ARG:HH12	2:G:72:ASP:CG	1.98	0.67
2:D:100(C):ASN:CB	3:F:93:GLY:HA2	2.24	0.67
2:H:45:LEU:HD11	3:L:44:PRO:HG3	1.69	0.67
1:A:1094:VAL:HG21	1:B:904:TYR:OH	1.94	0.67
2:G:28:ARG:HH12	5:W:5:MAN:H5	1.59	0.66
2:G:187:LEU:HD12	2:G:187:LEU:C	2.15	0.66
1:A:1145:LEU:HD21	1:B:1145:LEU:HD12	1.78	0.65
3:E:38:GLN:CD	2:G:39:ARG:NH1	2.50	0.65
1:C:391:CYS:CB	1:C:525:CYS:HA	2.27	0.65
1:C:709:ASN:CG	7:U:1:NAG:C1	2.62	0.65
3:E:44:PRO:CG	2:G:45:LEU:HD11	2.24	0.65
3:E:188:LYS:HE2	3:E:188:LYS:HA	1.79	0.64
1:B:391:CYS:HB2	1:B:524:VAL:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:188:LYS:HE2	3:K:188:LYS:HA	1.79	0.64
1:A:391:CYS:HB2	1:A:524:VAL:O	1.97	0.63
1:B:1098:ASN:OD1	4:Y:1:NAG:C1	2.47	0.63
1:A:391:CYS:CB	1:A:525:CYS:HA	2.29	0.63
1:A:940:SER:HB2	2:M:99:ARG:HD2	1.80	0.62
1:B:391:CYS:CB	1:B:525:CYS:HA	2.29	0.62
2:G:74:LEU:HD13	5:W:4:MAN:C5	2.29	0.62
1:B:603:ASN:OD1	8:B:1304:NAG:C1	2.48	0.61
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.82	0.61
1:B:589:PRO:HD2	1:C:855:PHE:CD1	2.36	0.61
1:B:1145:LEU:HD21	1:C:1145:LEU:HD12	1.83	0.61
1:A:41:LYS:HG2	1:C:562:PHE:HD1	1.66	0.61
1:A:579:PRO:O	8:A:1302:NAG:H82	2.00	0.61
2:D:79:TYR:CE1	2:G:81:GLN:CG	2.80	0.61
2:D:81:GLN:NE2	2:G:79:TYR:CZ	2.68	0.61
1:A:717:ASN:OD1	6:N:1:NAG:C1	2.50	0.60
2:D:45:LEU:CD1	3:F:44:PRO:HG2	2.27	0.60
3:E:38:GLN:OE1	2:G:39:ARG:CZ	2.50	0.59
1:A:342:PHE:HB2	8:A:1303:NAG:H82	1.84	0.59
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.82	0.59
1:C:579:PRO:O	8:C:1205:NAG:H82	2.02	0.59
1:A:717:ASN:ND2	6:N:1:NAG:C2	2.61	0.59
2:D:70:SER:HG	2:G:79:TYR:HE2	1.50	0.59
1:B:1098:ASN:ND2	4:Y:1:NAG:C2	2.63	0.58
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	2.39	0.58
1:A:655:HIS:ND1	8:A:1306:NAG:H62	2.20	0.57
3:K:44:PRO:CG	2:M:45:LEU:HD11	2.34	0.57
1:C:282:ASN:CG	8:C:1204:NAG:C1	2.68	0.57
2:H:100(B):ASP:OD1	7:U:3:BMA:O3	2.23	0.57
1:B:589:PRO:HG2	1:C:855:PHE:HB3	1.87	0.57
2:H:57:ARG:HH22	2:M:72:ASP:CG	2.07	0.56
1:A:704:SER:CB	1:B:790:LYS:HE3	2.16	0.56
1:A:122:ASN:HD22	1:A:122:ASN:H	1.51	0.56
1:A:801:ASN:ND2	5:J:1:NAG:O5	2.34	0.56
1:B:709:ASN:CG	8:B:1309:NAG:C1	2.69	0.56
2:G:28:ARG:NH1	5:W:5:MAN:O4	2.38	0.56
2:D:81:GLN:HG2	2:G:79:TYR:HE1	1.71	0.56
1:B:712:ILE:HD13	1:B:1094:VAL:HG11	1.90	0.54
3:K:44:PRO:HG2	2:M:45:LEU:HD11	1.90	0.54
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	1.90	0.53
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.43	0.53
1:C:61:ASN:CG	8:C:1203:NAG:C1	2.70	0.53
2:G:74:LEU:CD1	5:W:4:MAN:O4	2.53	0.53
3:F:94:TYR:HE1	7:P:4:MAN:O6	1.92	0.53
1:C:1106:GLN:HG3	1:C:1109:PHE:O	2.09	0.53
3:F:166:GLN:HG3	3:F:173:TYR:CZ	2.43	0.52
3:E:38:GLN:HE22	2:G:39:ARG:CD	2.13	0.52
1:A:1145:LEU:HD21	1:B:1145:LEU:CD1	2.40	0.51
2:D:57:ARG:HH22	2:G:72:ASP:CG	2.14	0.51
1:A:1101:HIS:ND1	4:O:1:NAG:H3	2.26	0.51
1:B:603:ASN:CG	8:B:1304:NAG:C1	2.79	0.51
3:F:132:VAL:CG2	3:F:179:LEU:HB3	2.41	0.50
2:G:100(A):SER:O	6:X:6:MAN:H3	2.11	0.50
3:L:132:VAL:CG2	3:L:179:LEU:HB3	2.41	0.50
2:G:187:LEU:HD12	2:G:187:LEU:O	2.12	0.50
2:D:81:GLN:CG	2:G:79:TYR:HE1	2.25	0.50
2:G:74:LEU:HD22	5:W:4:MAN:H5	1.93	0.50
1:A:1107:ARG:HG2	1:B:904:TYR:CZ	2.46	0.50
2:D:81:GLN:HG3	2:G:79:TYR:OH	2.11	0.50
3:E:38:GLN:NE2	2:G:39:ARG:NH1	2.60	0.50
2:G:100(B):ASP:CG	6:X:5:MAN:O6	2.49	0.49
2:H:4:LEU:HD23	2:H:92:CYS:SG	2.52	0.49
2:H:68:THR:HG21	2:M:77:PHE:CE2	2.47	0.49
2:D:4:LEU:HD23	2:D:92:CYS:SG	2.52	0.49
1:A:391:CYS:HB3	1:A:525:CYS:HA	1.94	0.49
1:B:331:ASN:CG	8:B:1302:NAG:C1	2.74	0.49
1:B:391:CYS:HB3	1:B:525:CYS:HA	1.94	0.49
1:A:1107:ARG:HG2	1:B:904:TYR:OH	2.13	0.48
1:C:61:ASN:ND2	8:C:1203:NAG:C2	2.72	0.48
2:M:187:LEU:HD12	2:M:187:LEU:O	2.12	0.48
1:A:904:TYR:OH	1:C:1094:VAL:HG11	2.13	0.48
1:B:940:SER:HB2	2:G:99:ARG:HD2	1.91	0.48
2:D:154:VAL:HG22	2:D:210:VAL:HG22	1.96	0.47
2:H:154:VAL:HG22	2:H:210:VAL:HG22	1.96	0.47
3:F:4:MET:CE	3:F:88:CYS:SG	3.03	0.47
3:K:38:GLN:HE22	2:M:39:ARG:HD2	1.79	0.47
3:E:38:GLN:NE2	2:G:39:ARG:CD	2.75	0.47
3:L:4:MET:CE	3:L:88:CYS:SG	3.03	0.47
1:A:801:ASN:OD1	5:J:1:NAG:C1	2.62	0.47
2:D:81:GLN:CG	2:G:79:TYR:CE1	2.98	0.46
3:E:4:MET:HB3	3:E:23:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:4:MET:HB3	3:K:23:CYS:SG	2.55	0.46
2:H:72:ASP:OD2	2:M:70:SER:HA	2.15	0.46
1:A:1098:ASN:OD1	4:O:1:NAG:C1	2.64	0.46
2:H:144:VAL:HG11	2:H:152:VAL:HG11	1.98	0.46
3:L:4:MET:HE3	3:L:88:CYS:SG	2.56	0.46
2:H:81:GLN:NE2	2:M:77:PHE:CG	2.79	0.46
2:D:144:VAL:HG11	2:D:152:VAL:HG11	1.98	0.45
1:A:81:ASN:OD1	1:A:81:ASN:N	2.49	0.45
2:G:187:LEU:C	2:G:187:LEU:CD1	2.84	0.45
1:C:81:ASN:OD1	1:C:81:ASN:N	2.49	0.45
1:B:81:ASN:OD1	1:B:81:ASN:N	2.49	0.45
3:F:197:THR:HG22	3:F:204:PRO:HB3	1.99	0.45
1:A:897:PRO:CG	1:C:709:ASN:O	2.65	0.45
2:G:95:LYS:HE3	6:X:6:MAN:C4	2.47	0.45
3:K:44:PRO:HG3	2:M:45:LEU:HD11	1.99	0.45
3:K:91:TYR:CD2	2:M:100(C):ASN:ND2	2.85	0.45
3:F:22:THR:HG22	3:F:72:THR:HG22	1.99	0.45
1:B:589:PRO:HG2	1:C:855:PHE:CB	2.46	0.45
3:F:4:MET:HE3	3:F:88:CYS:SG	2.56	0.45
3:L:197:THR:HG22	3:L:204:PRO:HB3	1.99	0.44
7:P:3:BMA:H3	7:P:4:MAN:H2	1.51	0.44
1:C:709:ASN:OD1	1:C:709:ASN:N	2.50	0.44
1:A:712:ILE:HD11	1:B:896:ILE:HD12	2.00	0.44
1:A:1107:ARG:CD	1:B:904:TYR:CE2	3.01	0.44
1:C:111:ASP:N	1:C:111:ASP:OD1	2.48	0.44
2:M:187:LEU:C	2:M:187:LEU:CD1	2.84	0.44
3:F:120:PRO:HD3	3:F:132:VAL:HG12	2.00	0.44
1:B:671:CYS:SG	1:B:697:MET:HB3	2.58	0.43
3:E:126:LYS:HA	3:E:126:LYS:CE	2.48	0.43
3:L:22:THR:HG22	3:L:72:THR:HG22	1.99	0.43
3:K:126:LYS:HA	3:K:126:LYS:CE	2.48	0.43
3:L:120:PRO:HD3	3:L:132:VAL:HG12	2.00	0.43
1:A:111:ASP:N	1:A:111:ASP:OD1	2.48	0.43
2:M:92:CYS:O	2:M:92:CYS:SG	2.77	0.43
1:A:671:CYS:SG	1:A:697:MET:HB3	2.58	0.43
1:B:711:SER:O	1:C:897:PRO:HD3	2.18	0.43
2:G:74:LEU:HD13	5:W:4:MAN:C4	2.48	0.43
2:H:72:ASP:CG	2:M:57:ARG:HH22	2.13	0.43
1:B:1145:LEU:HD21	1:C:1145:LEU:CD1	2.47	0.43
1:A:790:LYS:CE	1:C:704:SER:HB3	2.48	0.42
1:B:940:SER:OG	2:G:99:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:CYS:O	2:G:92:CYS:SG	2.77	0.42
1:A:368:LEU:HD21	8:A:1303:NAG:H83	2.00	0.42
1:B:616:ASN:OD1	8:B:1308:NAG:C1	2.67	0.42
1:B:1090:PRO:O	1:C:913:GLN:NE2	2.52	0.42
1:C:709:ASN:ND2	7:U:1:NAG:C2	2.70	0.42
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.34	0.42
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.34	0.42
3:F:150:VAL:HG22	3:F:192:TYR:CD2	2.55	0.42
2:G:28:ARG:NH1	5:W:5:MAN:C4	2.82	0.42
1:A:603:ASN:ND2	8:A:1304:NAG:C2	2.73	0.42
8:B:1309:NAG:H3	8:B:1309:NAG:H82	2.01	0.42
1:A:368:LEU:CD2	8:A:1303:NAG:H83	2.50	0.42
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.35	0.42
3:L:119:PRO:HB3	3:L:209:PHE:CE1	2.55	0.42
3:F:119:PRO:HB3	3:F:209:PHE:CE1	2.55	0.41
1:C:1098:ASN:CG	4:S:1:NAG:C1	2.74	0.41
3:L:150:VAL:HG22	3:L:192:TYR:CD2	2.55	0.41
2:G:100(B):ASP:CG	6:X:5:MAN:HO6	2.08	0.41
3:K:38:GLN:NE2	2:M:39:ARG:HD2	2.35	0.41
1:A:1073:LYS:HA	8:A:1305:NAG:H81	2.03	0.41
2:H:79:TYR:OH	2:M:81:GLN:NE2	2.39	0.41
1:B:579:PRO:O	8:B:1302:NAG:H82	2.21	0.41
1:A:308:VAL:HB	1:A:602:THR:HG23	2.03	0.40
1:B:1101:HIS:ND1	4:Y:1:NAG:H3	2.36	0.40
1:B:111:ASP:N	1:B:111:ASP:OD1	2.48	0.40
1:B:712:ILE:HG22	1:B:1077:THR:HB	2.03	0.40
1:B:1094:VAL:HG13	1:C:900:MET:CE	2.51	0.40
1:C:391:CYS:HB3	1:C:525:CYS:HA	2.01	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	948/1121 (85%)	905 (96%)	43 (4%)	0	100	100
1	B	948/1121 (85%)	906 (96%)	42 (4%)	0	100	100
1	C	948/1121 (85%)	924 (98%)	24 (2%)	0	100	100
2	D	214/226 (95%)	204 (95%)	10 (5%)	0	100	100
2	G	214/226 (95%)	206 (96%)	8 (4%)	0	100	100
2	H	214/226 (95%)	203 (95%)	11 (5%)	0	100	100
2	M	214/226 (95%)	206 (96%)	8 (4%)	0	100	100
3	E	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
3	F	209/213 (98%)	203 (97%)	6 (3%)	0	100	100
3	K	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
3	L	209/213 (98%)	203 (97%)	6 (3%)	0	100	100
All	All	4540/5119 (89%)	4368 (96%)	172 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	852/972 (88%)	844 (99%)	8 (1%)	78	87
1	B	852/972 (88%)	845 (99%)	7 (1%)	81	89
1	C	852/972 (88%)	848 (100%)	4 (0%)	88	93
2	D	184/184 (100%)	181 (98%)	3 (2%)	62	79
2	G	184/184 (100%)	180 (98%)	4 (2%)	52	74
2	H	184/184 (100%)	181 (98%)	3 (2%)	62	79
2	M	184/184 (100%)	180 (98%)	4 (2%)	52	74
3	E	184/184 (100%)	183 (100%)	1 (0%)	88	93
3	F	182/184 (99%)	180 (99%)	2 (1%)	73	85
3	K	184/184 (100%)	183 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	182/184 (99%)	180 (99%)	2 (1%)	73 85
All	All	4024/4388 (92%)	3985 (99%)	39 (1%)	77 86

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

Mol	Chain	Res	Type
1	A	122	ASN
1	A	165	ASN
1	A	328	ARG
1	A	615	VAL
1	A	662	CYS
1	A	791	THR
1	A	1004	LEU
1	A	1092	GLU
1	B	165	ASN
1	B	328	ARG
1	B	615	VAL
1	B	662	CYS
1	B	791	THR
1	B	1004	LEU
1	B	1092	GLU
1	C	328	ARG
1	C	603	ASN
1	C	708	SER
1	C	1106	GLN
2	D	73	ASP
2	D	92	CYS
2	D	140	LEU
3	E	23	CYS
3	F	85	THR
3	F	88	CYS
2	G	70	SER
2	G	98	ASP
2	G	127	SER
2	G	187	LEU
2	H	73	ASP
2	H	92	CYS
2	H	140	LEU
3	K	23	CYS
3	L	85	THR
3	L	88	CYS
2	M	70	SER

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Mol	Chain	Res	Type
2	M	98	ASP
2	M	127	SER
2	M	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	234	ASN
1	A	603	ASN
1	B	234	ASN
1	B	616	ASN
1	B	709	ASN
1	C	61	ASN
1	C	282	ASN
1	C	1005	GLN
1	C	1098	ASN
2	D	81	GLN
3	E	38	GLN
2	G	81	GLN
3	K	38	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)

52 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	I	1	4	14,14,15	1.46	2 (14%)	17,19,21	0.71	0
4	NAG	I	2	4	14,14,15	1.44	2 (14%)	17,19,21	0.63	0
5	NAG	J	1	5	14,14,15	0.98	0	17,19,21	0.73	0
5	NAG	J	2	5	14,14,15	0.96	0	17,19,21	0.82	0
5	BMA	J	3	5	11,11,12	1.04	0	15,15,17	0.93	0
5	MAN	J	4	5	11,11,12	1.12	1 (9%)	15,15,17	1.51	2 (13%)
5	MAN	J	5	5	11,11,12	1.31	2 (18%)	15,15,17	0.73	0
6	NAG	N	1	6	14,14,15	1.06	1 (7%)	17,19,21	0.77	0
6	NAG	N	2	6	14,14,15	1.01	0	17,19,21	1.02	0
6	BMA	N	3	6	11,11,12	1.21	1 (9%)	15,15,17	1.22	1 (6%)
6	MAN	N	4	6	11,11,12	1.35	2 (18%)	15,15,17	1.31	3 (20%)
6	MAN	N	5	6	11,11,12	1.17	2 (18%)	15,15,17	0.92	1 (6%)
6	MAN	N	6	6	11,11,12	1.23	2 (18%)	15,15,17	1.15	1 (6%)
6	BMA	N	7	6	11,11,12	1.03	1 (9%)	15,15,17	0.88	0
6	BMA	N	8	6	11,11,12	1.28	2 (18%)	15,15,17	1.03	1 (6%)
4	NAG	O	1	4	14,14,15	0.27	0	17,19,21	0.96	0
4	NAG	O	2	4	14,14,15	0.24	0	17,19,21	0.62	0
7	NAG	P	1	7	14,14,15	0.44	0	17,19,21	2.78	7 (41%)
7	NAG	P	2	7	14,14,15	0.47	0	17,19,21	0.97	0
7	BMA	P	3	7	11,11,12	0.41	0	15,15,17	0.92	1 (6%)
7	MAN	P	4	7	11,11,12	0.24	0	15,15,17	0.96	2 (13%)
7	BMA	P	5	7	11,11,12	0.22	0	15,15,17	0.59	0
4	NAG	Q	1	4,1	14,14,15	1.38	2 (14%)	17,19,21	0.70	0
4	NAG	Q	2	4	14,14,15	1.39	2 (14%)	17,19,21	0.61	0
4	NAG	R	1	4,1	14,14,15	1.41	1 (7%)	17,19,21	0.72	0
4	NAG	R	2	4	14,14,15	1.42	2 (14%)	17,19,21	0.60	0
4	NAG	S	1	4	14,14,15	1.50	2 (14%)	17,19,21	0.81	0
4	NAG	S	2	4	14,14,15	1.30	2 (14%)	17,19,21	0.62	0
4	NAG	T	1	4,1	14,14,15	1.46	2 (14%)	17,19,21	0.70	0
4	NAG	T	2	4	14,14,15	1.45	2 (14%)	17,19,21	0.63	0
7	NAG	U	1	7	14,14,15	0.31	0	17,19,21	0.59	0
7	NAG	U	2	7	14,14,15	0.31	0	17,19,21	0.68	0
7	BMA	U	3	7	11,11,12	0.32	0	15,15,17	1.01	2 (13%)
7	MAN	U	4	7	11,11,12	0.23	0	15,15,17	0.97	0
7	BMA	U	5	7	11,11,12	0.24	0	15,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	V	1	4,1	14,14,15	1.45	2 (14%)	17,19,21	0.70	0
4	NAG	V	2	4	14,14,15	1.43	2 (14%)	17,19,21	0.64	0
5	NAG	W	1	5	14,14,15	0.98	0	17,19,21	0.73	0
5	NAG	W	2	5	14,14,15	0.97	0	17,19,21	0.82	0
5	BMA	W	3	5	11,11,12	1.04	0	15,15,17	0.92	0
5	MAN	W	4	5	11,11,12	1.13	1 (9%)	15,15,17	1.52	2 (13%)
5	MAN	W	5	5	11,11,12	1.31	2 (18%)	15,15,17	0.73	0
6	NAG	X	1	6,1	14,14,15	1.05	1 (7%)	17,19,21	0.77	0
6	NAG	X	2	6	14,14,15	1.02	0	17,19,21	1.03	1 (5%)
6	BMA	X	3	6	11,11,12	1.20	1 (9%)	15,15,17	1.24	1 (6%)
6	MAN	X	4	6	11,11,12	1.35	2 (18%)	15,15,17	1.32	3 (20%)
6	MAN	X	5	6	11,11,12	1.19	2 (18%)	15,15,17	0.91	1 (6%)
6	MAN	X	6	6	11,11,12	1.23	2 (18%)	15,15,17	1.14	1 (6%)
6	BMA	X	7	6	11,11,12	1.03	1 (9%)	15,15,17	0.89	0
6	BMA	X	8	6	11,11,12	1.28	2 (18%)	15,15,17	1.04	1 (6%)
4	NAG	Y	1	4	14,14,15	0.26	0	17,19,21	0.96	0
4	NAG	Y	2	4	14,14,15	0.26	0	17,19,21	0.62	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	I	1	4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
6	MAN	N	6	6	-	0/2/19/22	0/1/1/1
6	BMA	N	7	6	-	0/2/19/22	0/1/1/1
6	BMA	N	8	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	1	4	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
7	NAG	P	1	7	-	4/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	2/2/19/22	0/1/1/1
7	MAN	P	4	7	-	1/2/19/22	0/1/1/1
7	BMA	P	5	7	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
7	NAG	U	1	7	-	4/6/23/26	0/1/1/1
7	NAG	U	2	7	-	4/6/23/26	0/1/1/1
7	BMA	U	3	7	-	2/2/19/22	0/1/1/1
7	MAN	U	4	7	-	1/2/19/22	0/1/1/1
7	BMA	U	5	7	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	1/1/6/7	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
5	NAG	W	1	5	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
5	MAN	W	4	5	-	2/2/19/22	0/1/1/1
5	MAN	W	5	5	-	0/2/19/22	0/1/1/1
6	NAG	X	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1
6	BMA	X	3	6	-	0/2/19/22	0/1/1/1
6	MAN	X	4	6	-	0/2/19/22	0/1/1/1
6	MAN	X	5	6	-	0/2/19/22	0/1/1/1
6	MAN	X	6	6	-	0/2/19/22	0/1/1/1
6	BMA	X	7	6	-	0/2/19/22	0/1/1/1
6	BMA	X	8	6	-	0/2/19/22	0/1/1/1
4	NAG	Y	1	4	-	4/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	3/6/23/26	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	C1-C2	3.79	1.58	1.52
4	R	1	NAG	C1-C2	3.75	1.57	1.52
4	T	1	NAG	C1-C2	3.75	1.57	1.52
4	I	1	NAG	C1-C2	3.74	1.57	1.52
4	V	1	NAG	C1-C2	3.71	1.57	1.52
4	T	2	NAG	C1-C2	3.71	1.57	1.52
4	Q	1	NAG	C1-C2	3.69	1.57	1.52
4	Q	2	NAG	C1-C2	3.65	1.57	1.52
4	I	2	NAG	C1-C2	3.61	1.57	1.52
4	R	2	NAG	C1-C2	3.59	1.57	1.52
4	V	2	NAG	C1-C2	3.58	1.57	1.52
4	S	2	NAG	C1-C2	2.87	1.56	1.52
6	N	8	BMA	O5-C5	2.85	1.49	1.43
6	X	8	BMA	O5-C5	2.82	1.49	1.43
6	X	6	MAN	O5-C5	2.76	1.49	1.43
6	N	6	MAN	O5-C5	2.75	1.49	1.43
5	J	5	MAN	O5-C5	2.66	1.48	1.43
6	X	4	MAN	O3-C3	2.64	1.49	1.43
6	N	4	MAN	O3-C3	2.63	1.49	1.43
5	W	5	MAN	O5-C5	2.59	1.48	1.43
6	N	6	MAN	O5-C1	2.57	1.47	1.43
6	X	6	MAN	O5-C1	2.54	1.47	1.43
6	N	3	BMA	O3-C3	2.51	1.48	1.43
6	X	3	BMA	O3-C3	2.51	1.48	1.43
4	S	1	NAG	O5-C5	2.50	1.48	1.43
5	W	4	MAN	O5-C5	2.47	1.48	1.43
5	J	4	MAN	O5-C5	2.46	1.48	1.43
4	V	2	NAG	O5-C5	2.44	1.48	1.43
4	I	2	NAG	O5-C5	2.42	1.48	1.43
4	S	2	NAG	O5-C5	2.41	1.48	1.43
4	R	2	NAG	O5-C5	2.40	1.48	1.43
4	T	2	NAG	O5-C5	2.36	1.48	1.43
6	X	5	MAN	O5-C1	2.32	1.47	1.43
6	X	7	BMA	O5-C5	2.30	1.48	1.43
6	N	8	BMA	O5-C1	2.29	1.47	1.43
6	X	8	BMA	O5-C1	2.29	1.47	1.43
6	N	7	BMA	O5-C5	2.29	1.48	1.43
4	Q	2	NAG	O5-C5	2.28	1.48	1.43
6	N	5	MAN	O5-C5	2.23	1.48	1.43
5	W	5	MAN	O5-C1	2.23	1.47	1.43
6	N	5	MAN	O5-C1	2.23	1.47	1.43
4	V	1	NAG	O5-C5	2.20	1.47	1.43
6	X	5	MAN	O5-C5	2.20	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	4	MAN	O5-C5	2.19	1.47	1.43
4	I	1	NAG	O5-C5	2.17	1.47	1.43
6	X	4	MAN	O5-C5	2.16	1.47	1.43
4	T	1	NAG	O5-C5	2.16	1.47	1.43
5	J	5	MAN	O5-C1	2.14	1.47	1.43
6	N	1	NAG	O5-C5	2.09	1.47	1.43
6	X	1	NAG	O5-C5	2.07	1.47	1.43
4	Q	1	NAG	O5-C5	2.05	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	1	NAG	C1-O5-C5	5.16	119.19	112.19
7	P	1	NAG	O3-C3-C2	4.77	119.33	109.47
5	W	4	MAN	C1-O5-C5	4.64	118.48	112.19
5	J	4	MAN	C1-O5-C5	4.61	118.43	112.19
6	X	3	BMA	C1-O5-C5	4.38	118.12	112.19
6	N	3	BMA	C1-O5-C5	4.30	118.01	112.19
7	P	1	NAG	O3-C3-C4	4.29	120.26	110.35
7	P	1	NAG	C4-C3-C2	3.93	116.78	111.02
7	P	1	NAG	C2-N2-C7	3.69	128.15	122.90
7	P	1	NAG	C8-C7-N2	3.34	121.76	116.10
6	N	6	MAN	C1-O5-C5	3.33	116.70	112.19
6	X	6	MAN	C1-O5-C5	3.30	116.66	112.19
7	P	1	NAG	O5-C5-C6	-3.25	102.11	107.20
6	X	4	MAN	C1-C2-C3	3.22	113.63	109.67
6	N	4	MAN	C1-C2-C3	3.21	113.61	109.67
6	N	8	BMA	C1-O5-C5	2.83	116.02	112.19
6	X	8	BMA	C1-O5-C5	2.82	116.02	112.19
5	W	4	MAN	O3-C3-C2	-2.82	104.59	109.99
5	J	4	MAN	O3-C3-C2	-2.80	104.64	109.99
6	N	5	MAN	C1-O5-C5	2.64	115.77	112.19
6	X	5	MAN	C1-O5-C5	2.62	115.74	112.19
7	U	3	BMA	O5-C5-C6	2.33	110.86	107.20
7	U	3	BMA	C2-C3-C4	-2.15	107.17	110.89
6	X	4	MAN	O3-C3-C2	2.12	114.05	109.99
7	P	3	BMA	C1-C2-C3	-2.12	107.06	109.67
7	P	4	MAN	C1-O5-C5	2.10	115.04	112.19
6	N	4	MAN	O3-C3-C2	2.09	114.00	109.99
7	P	4	MAN	O5-C5-C6	2.04	110.40	107.20
6	X	4	MAN	C1-O5-C5	2.04	114.95	112.19
6	X	2	NAG	C3-C4-C5	2.03	113.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	4	MAN	C1-O5-C5	2.02	114.94	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	V	1	NAG	C1

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
7	U	1	NAG	O7-C7-N2-C2
7	U	2	NAG	C8-C7-N2-C2
7	U	2	NAG	O7-C7-N2-C2
7	U	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C1-C2-N2-C7
4	O	2	NAG	C1-C2-N2-C7
4	Y	1	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
7	U	3	BMA	O5-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	U	3	BMA	C4-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
7	P	3	BMA	C4-C5-C6-O6
7	U	4	MAN	O5-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6
5	J	4	MAN	C4-C5-C6-O6
5	W	4	MAN	C4-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
5	J	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	W	4	MAN	O5-C5-C6-O6
4	O	1	NAG	C3-C2-N2-C7
4	Y	1	NAG	C3-C2-N2-C7
7	U	2	NAG	C4-C5-C6-O6
7	P	4	MAN	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6

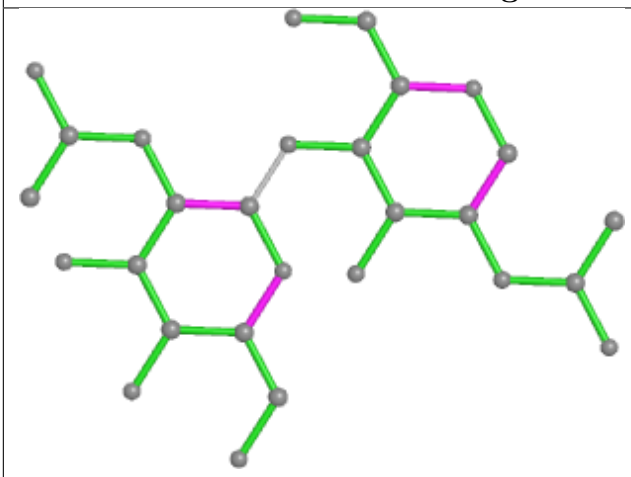
There are no ring outliers.

14 monomers are involved in 48 short contacts:

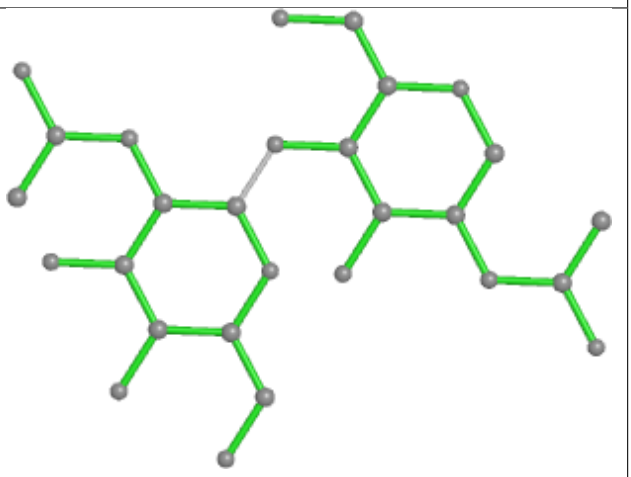
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	3	BMA	1	0
7	P	4	MAN	3	0
7	U	3	BMA	1	0
4	S	1	NAG	3	0
5	W	5	MAN	6	0
4	O	1	NAG	5	0
5	J	1	NAG	4	0
6	X	5	MAN	3	0
5	W	4	MAN	6	0
6	N	3	BMA	1	0
6	X	6	MAN	3	0
7	U	1	NAG	3	0
4	Y	1	NAG	6	0
6	N	1	NAG	4	0

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

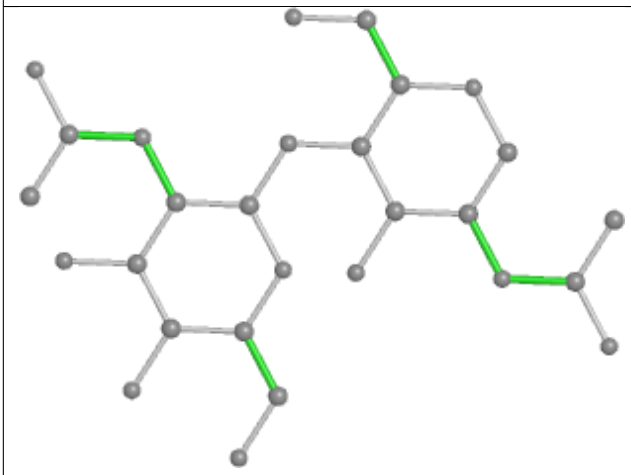
Oligosaccharide Chain I



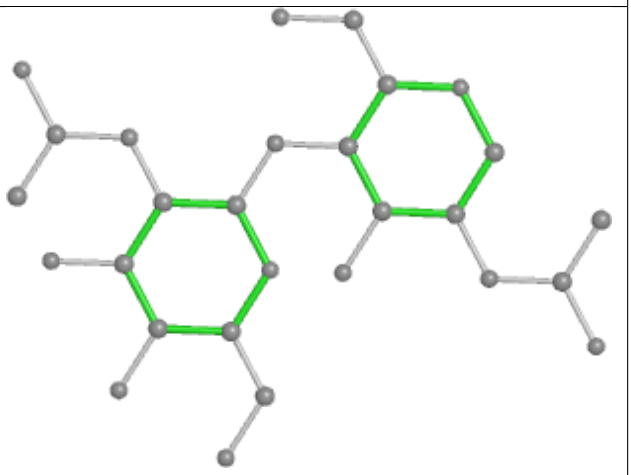
Bond lengths



Bond angles

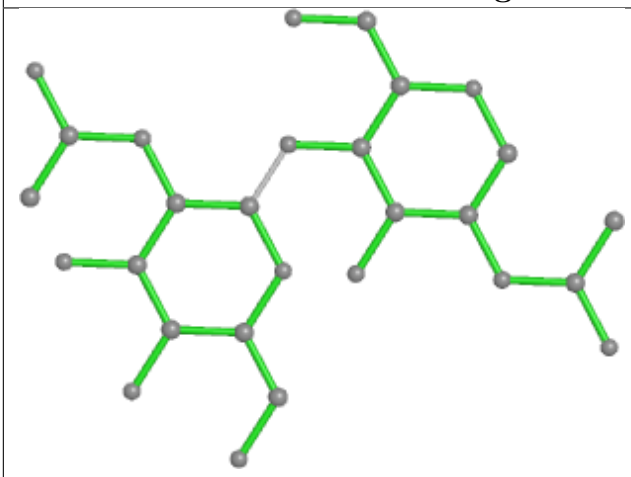


Torsions

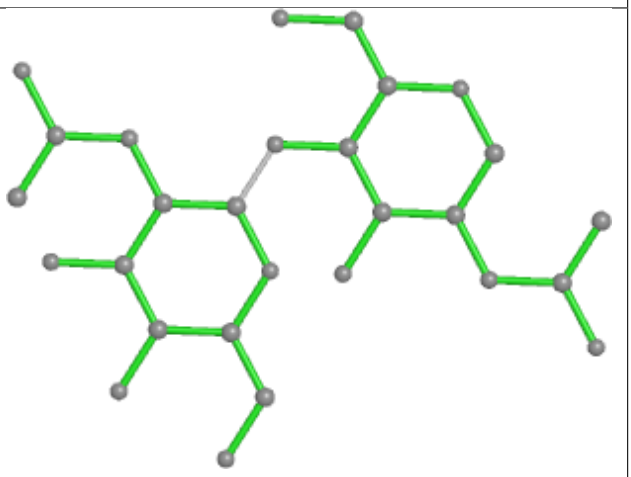


Rings

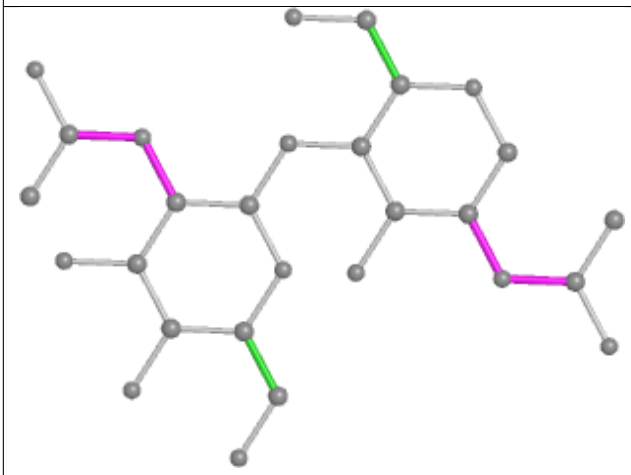
Oligosaccharide Chain O



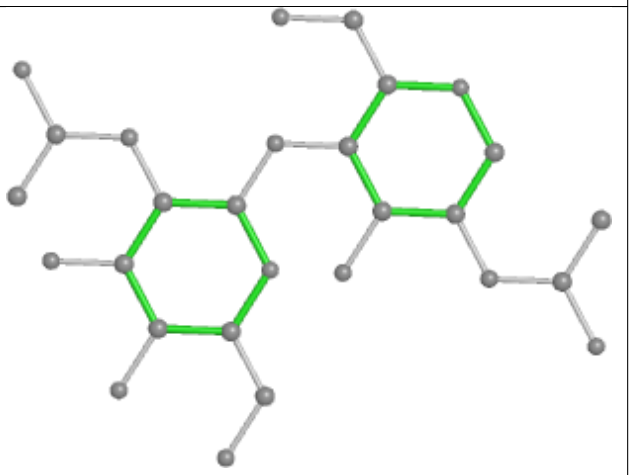
Bond lengths



Bond angles

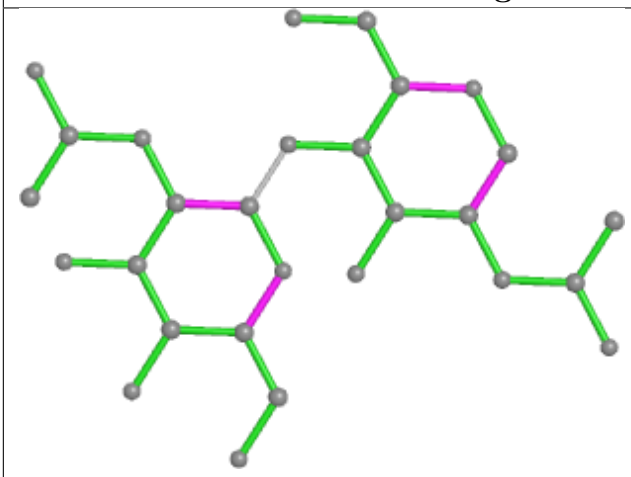


Torsions

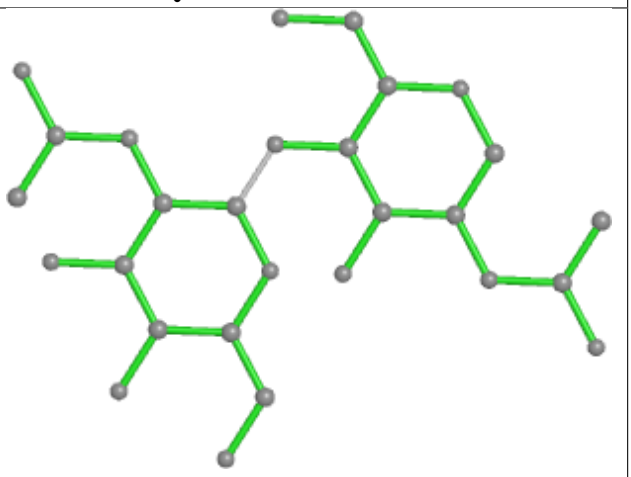


Rings

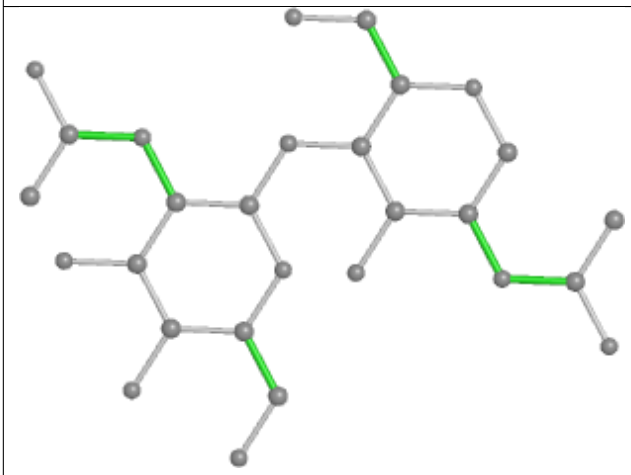
Oligosaccharide Chain Q



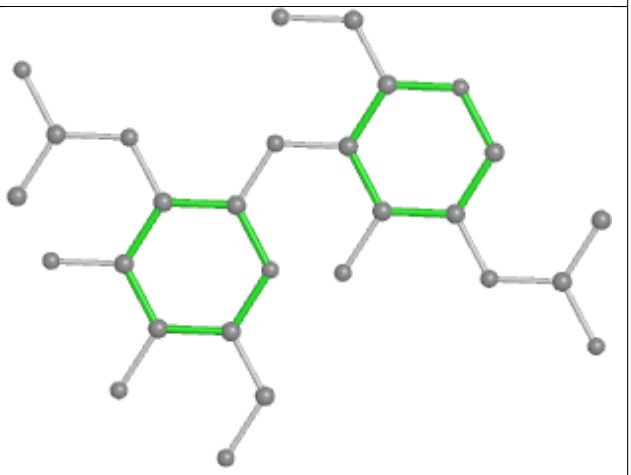
Bond lengths



Bond angles

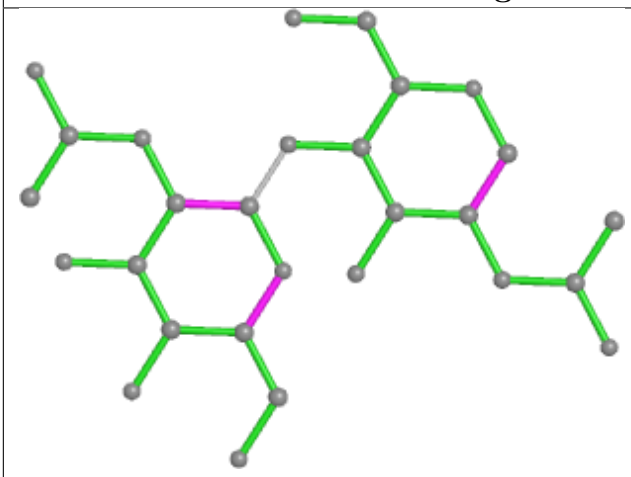


Torsions

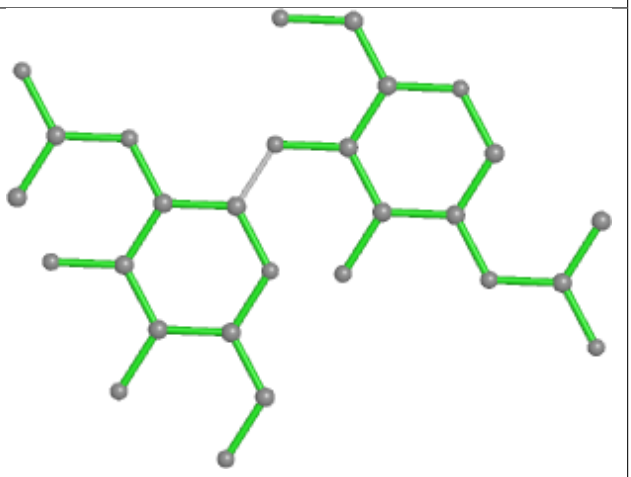


Rings

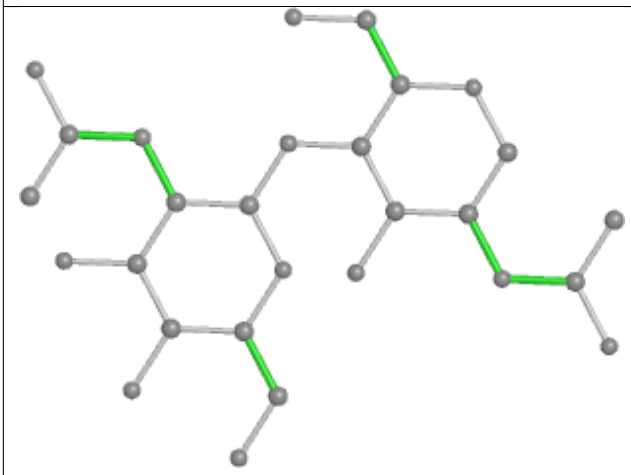
Oligosaccharide Chain R



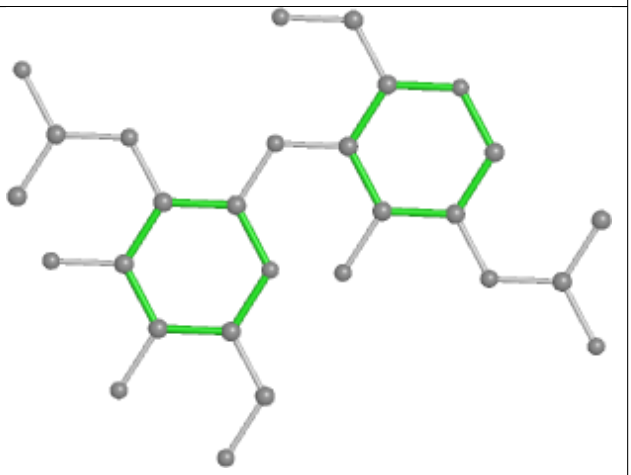
Bond lengths



Bond angles

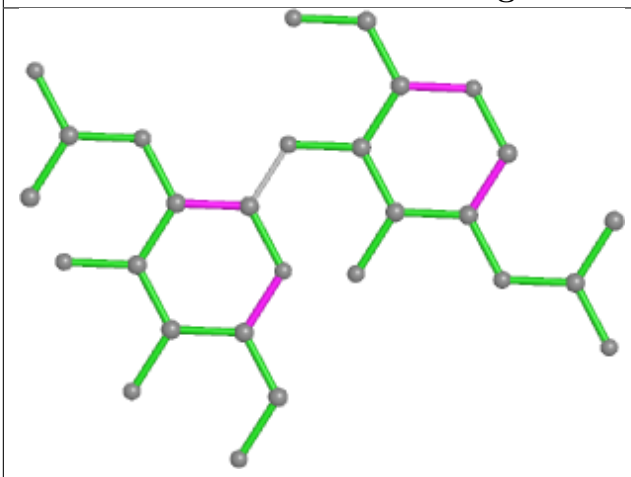


Torsions

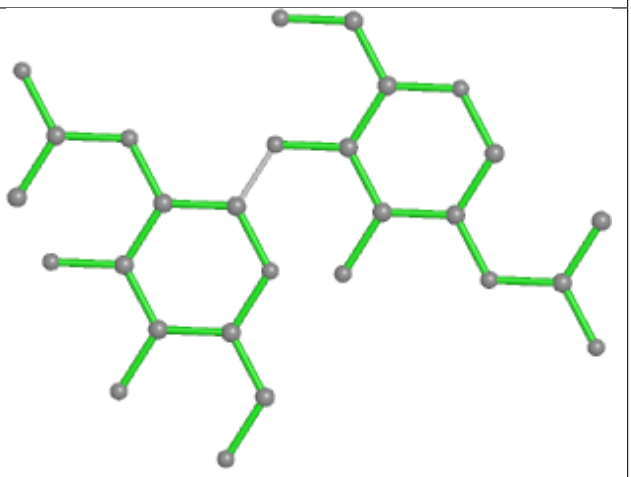


Rings

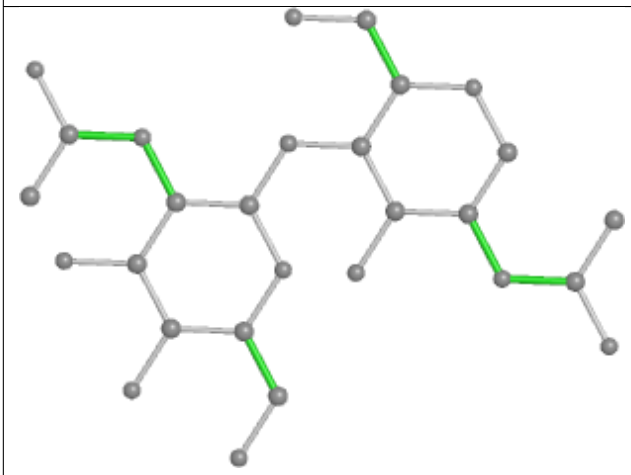
Oligosaccharide Chain S



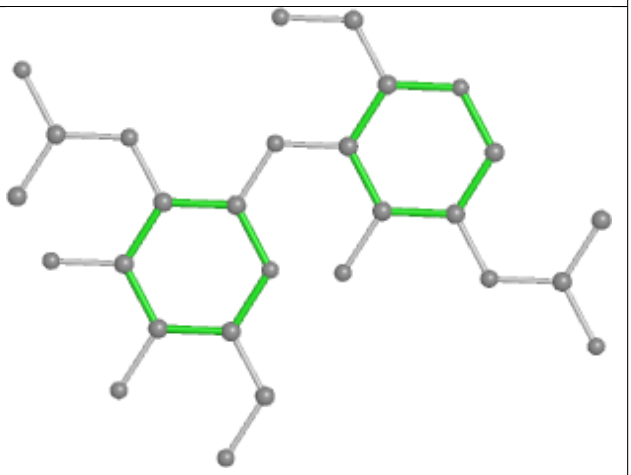
Bond lengths



Bond angles

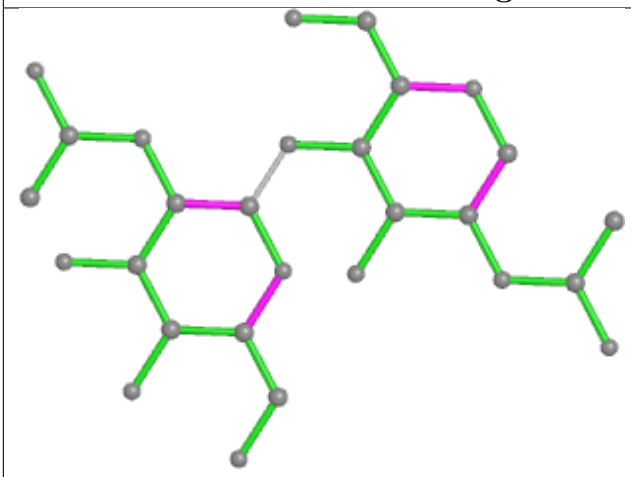


Torsions

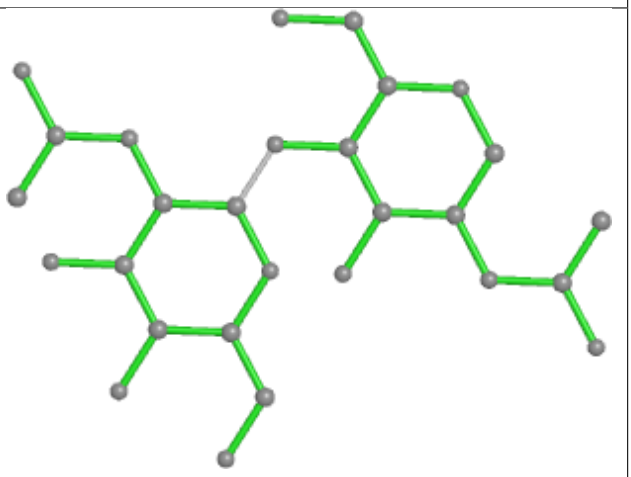


Rings

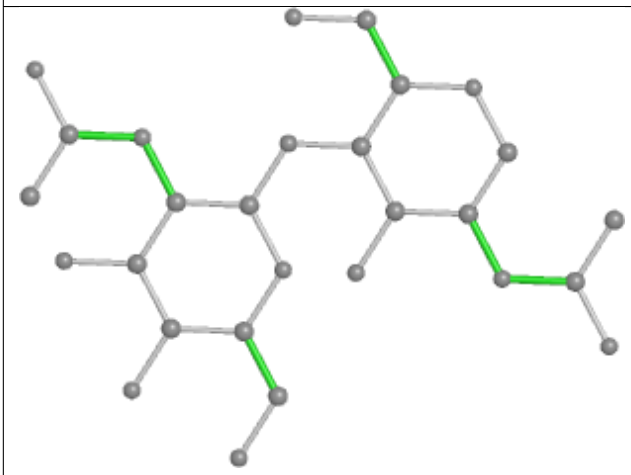
Oligosaccharide Chain T



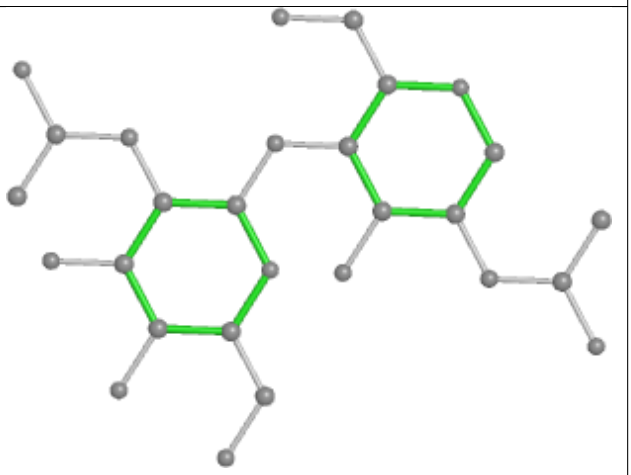
Bond lengths



Bond angles

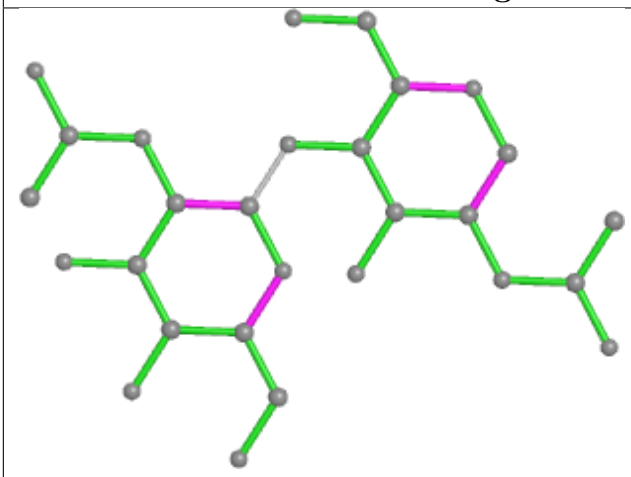


Torsions

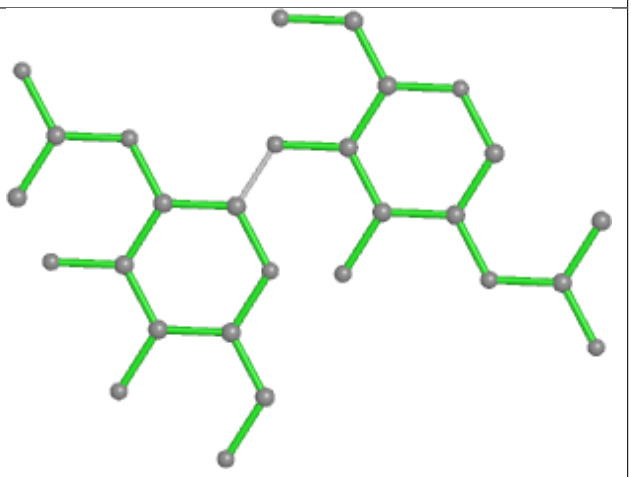


Rings

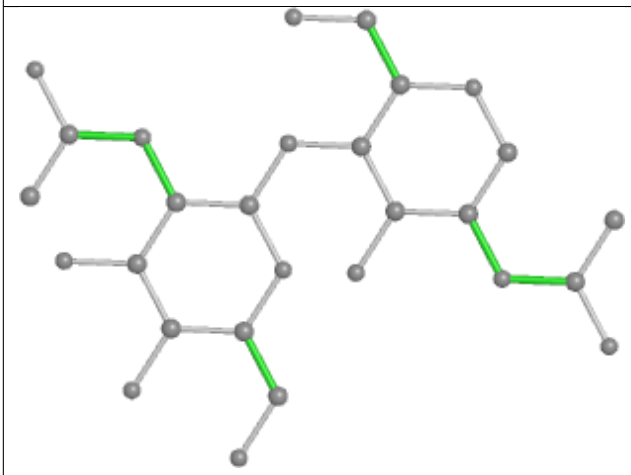
Oligosaccharide Chain V



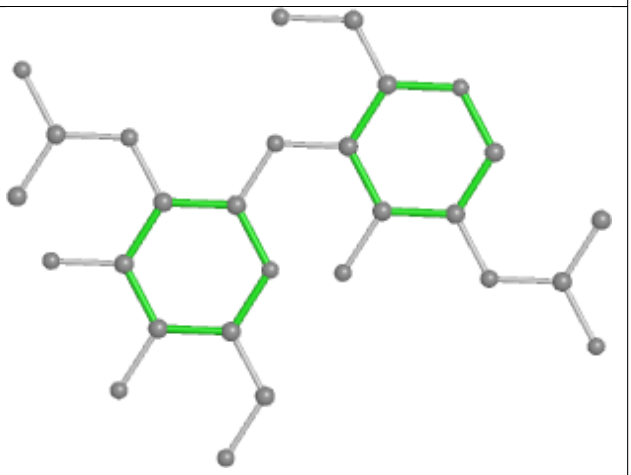
Bond lengths



Bond angles

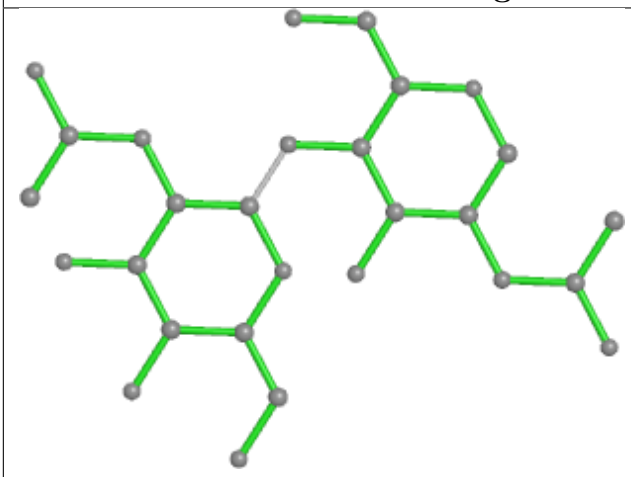


Torsions

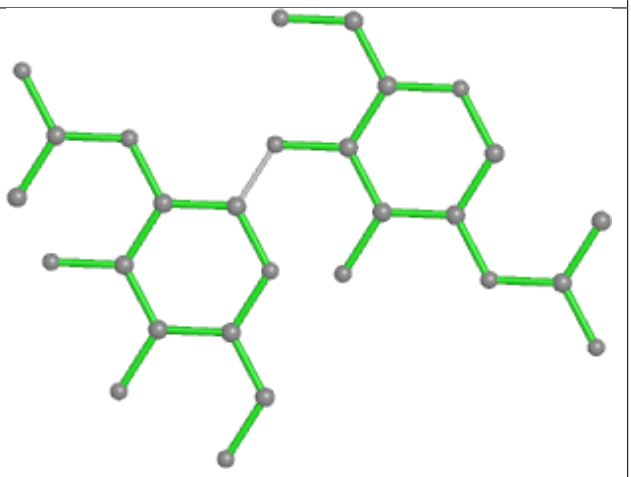


Rings

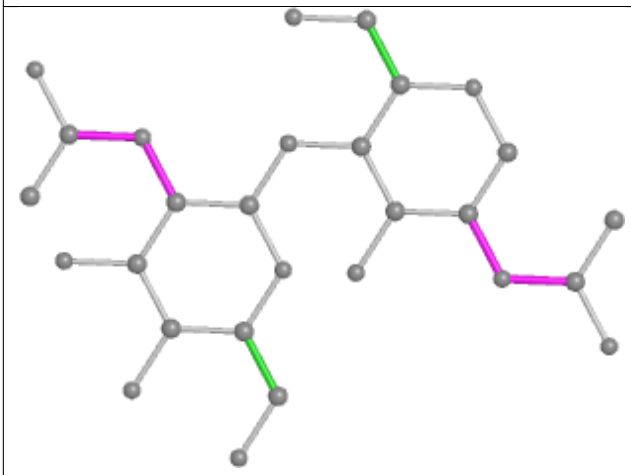
Oligosaccharide Chain Y



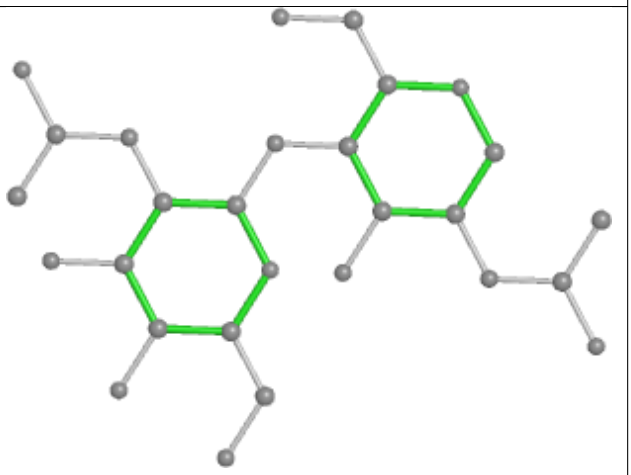
Bond lengths



Bond angles

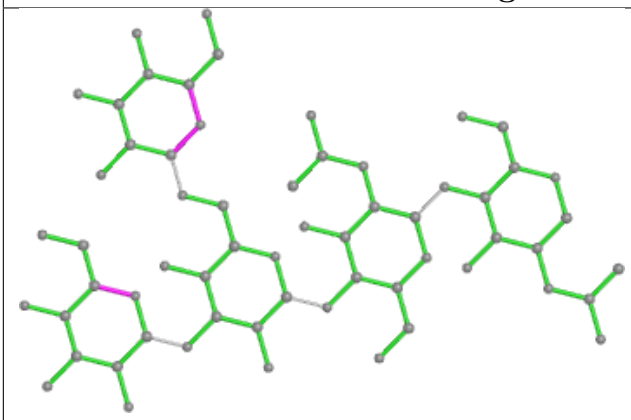


Torsions

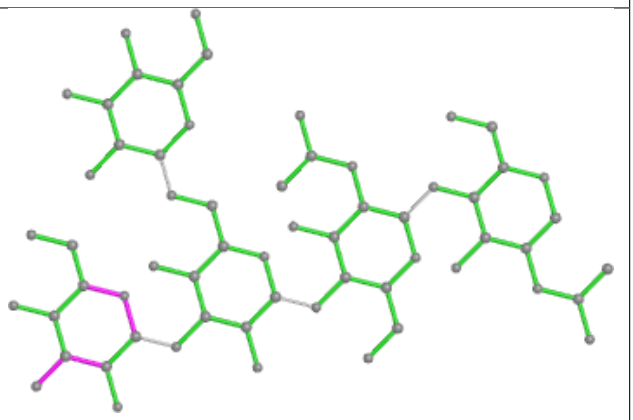


Rings

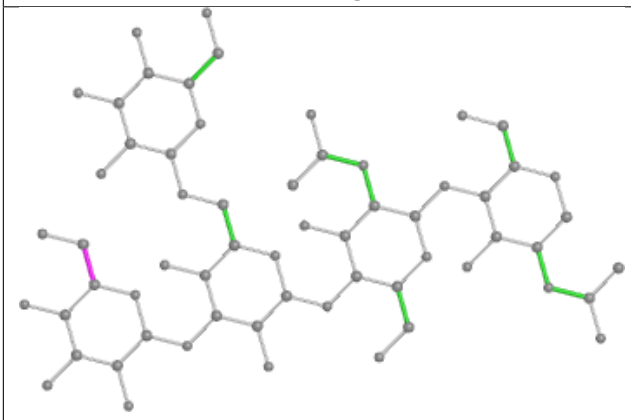
Oligosaccharide Chain J



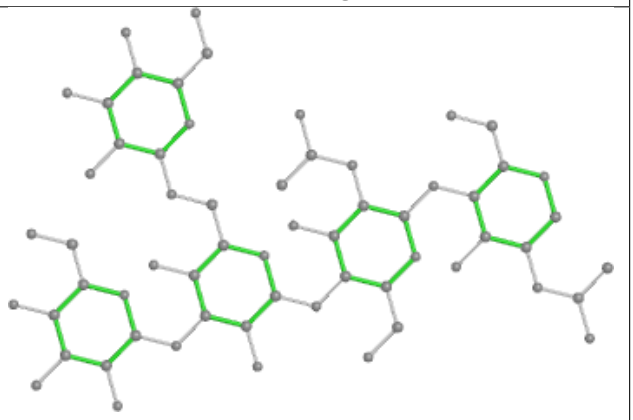
Bond lengths



Bond angles

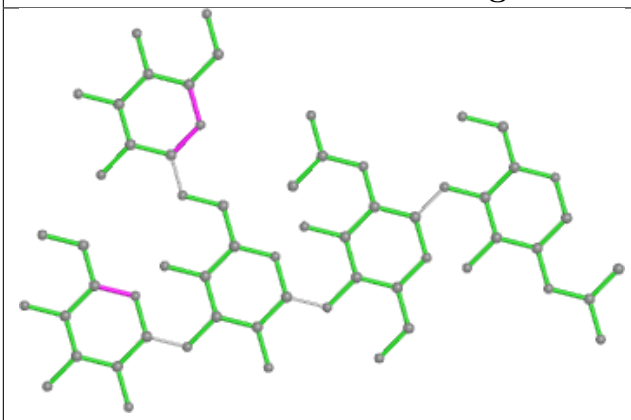


Torsions

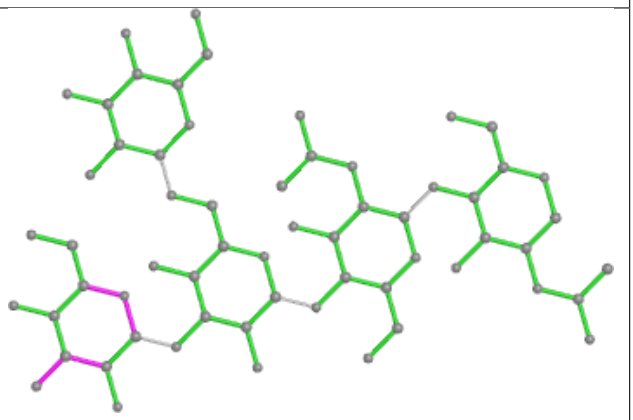


Rings

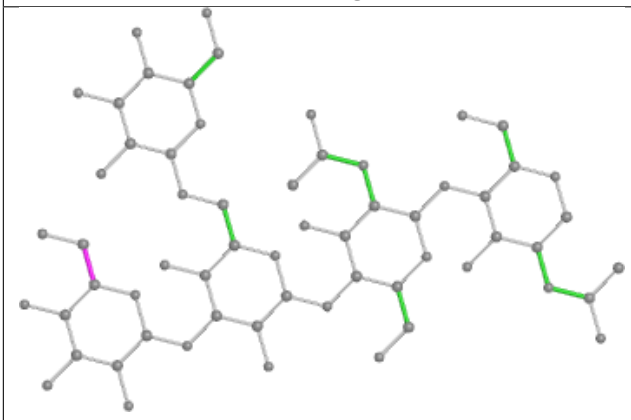
Oligosaccharide Chain W



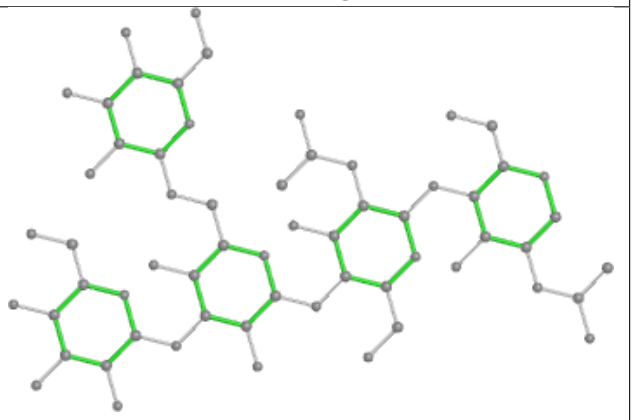
Bond lengths



Bond angles

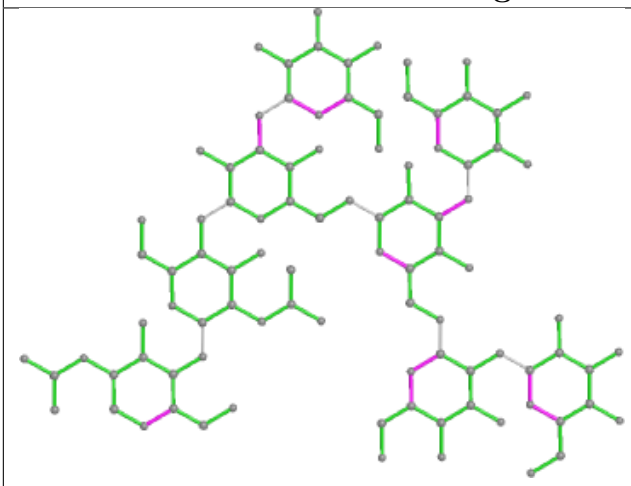


Torsions

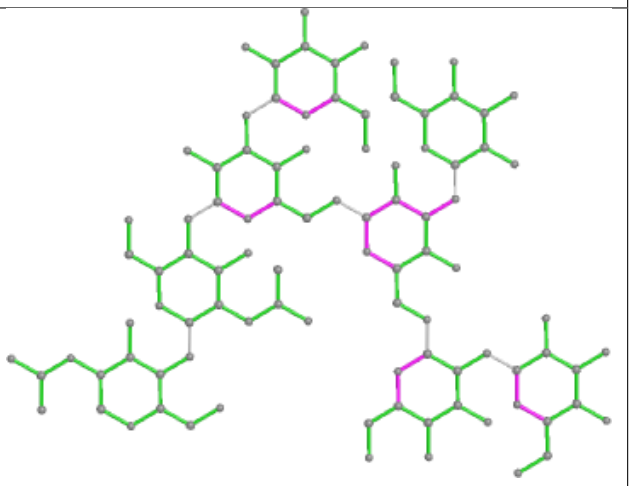


Rings

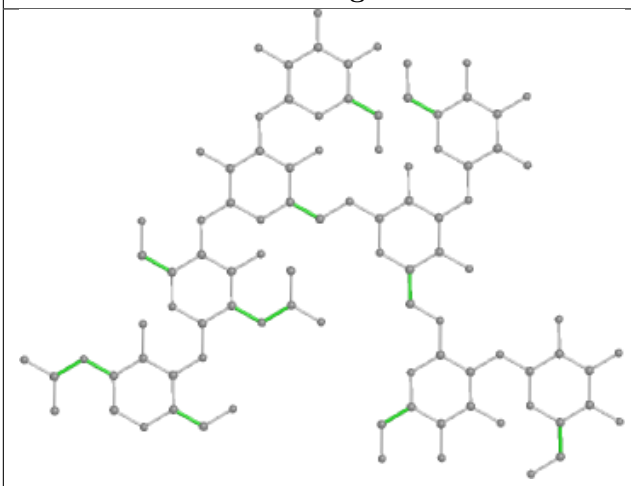
Oligosaccharide Chain N



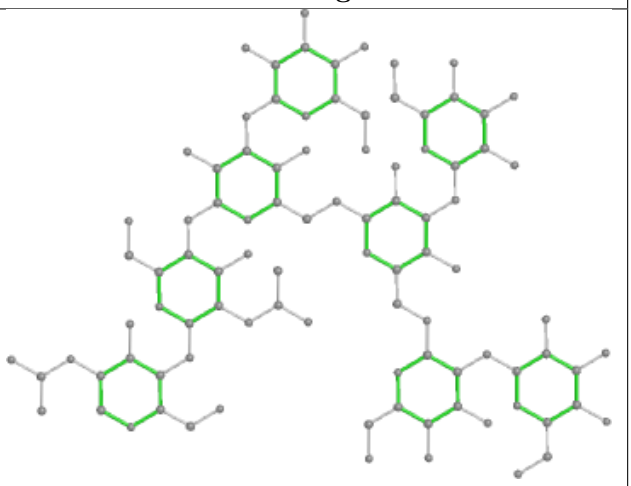
Bond lengths



Bond angles

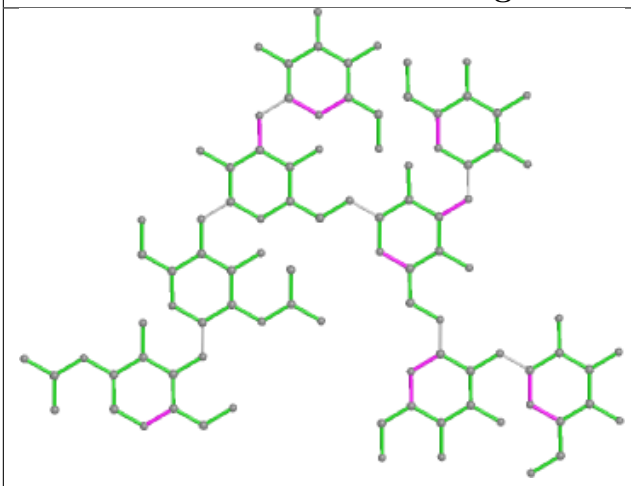


Torsions

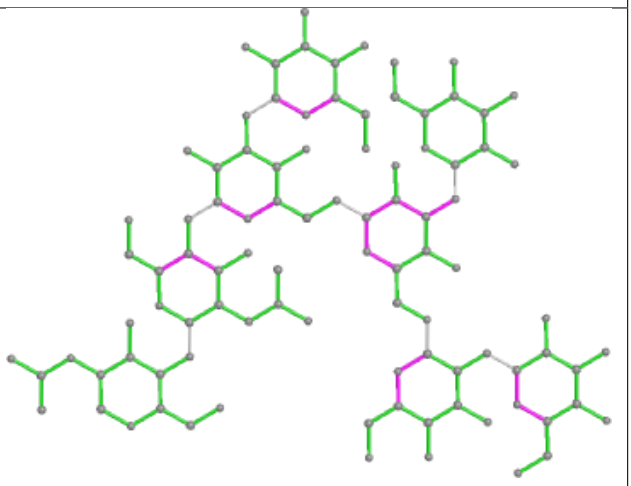


Rings

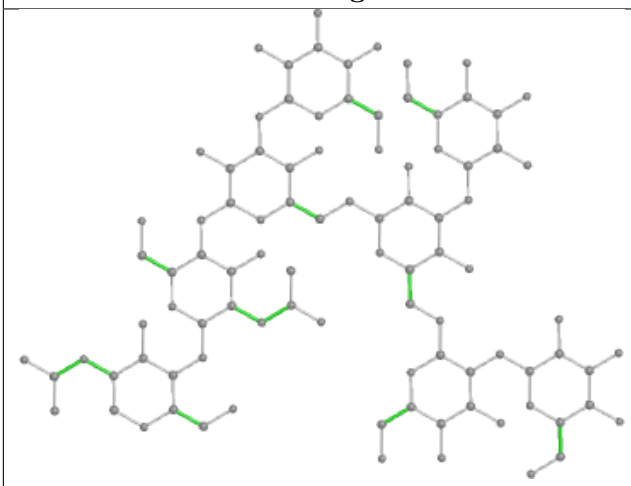
Oligosaccharide Chain X



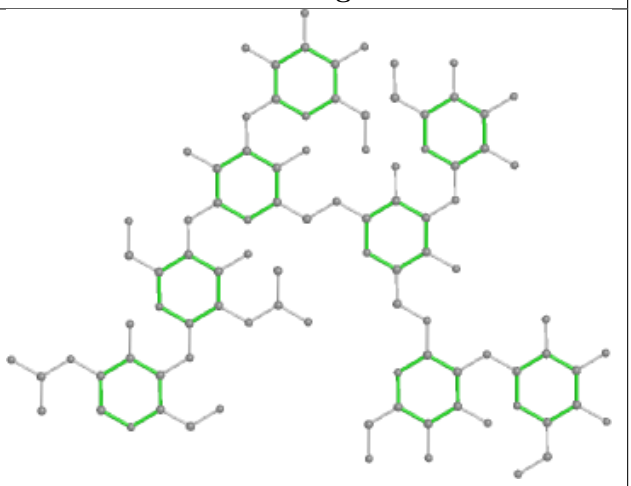
Bond lengths



Bond angles

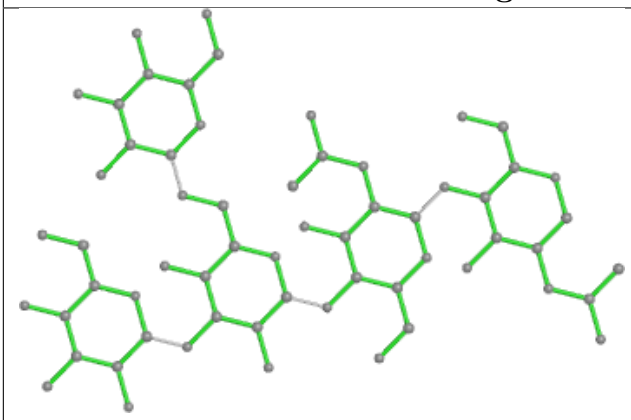


Torsions

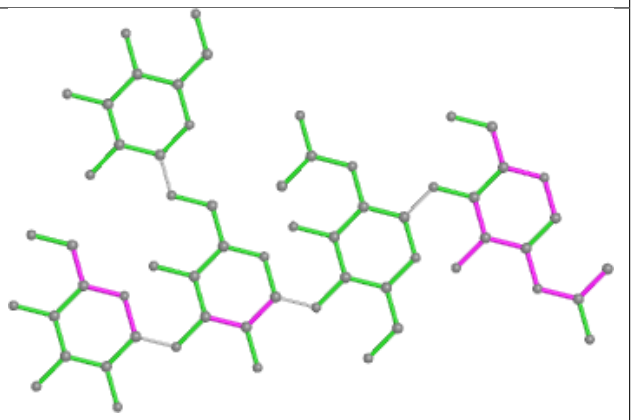


Rings

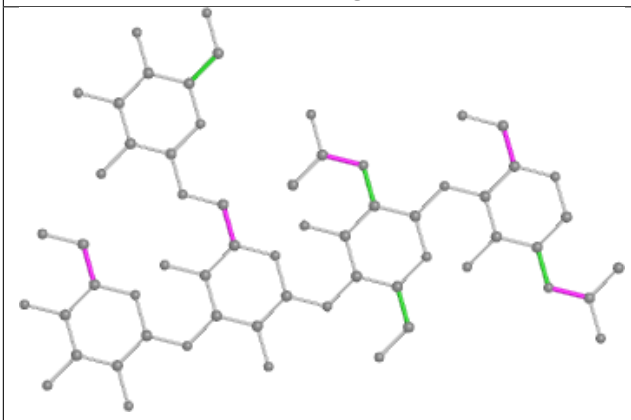
Oligosaccharide Chain P



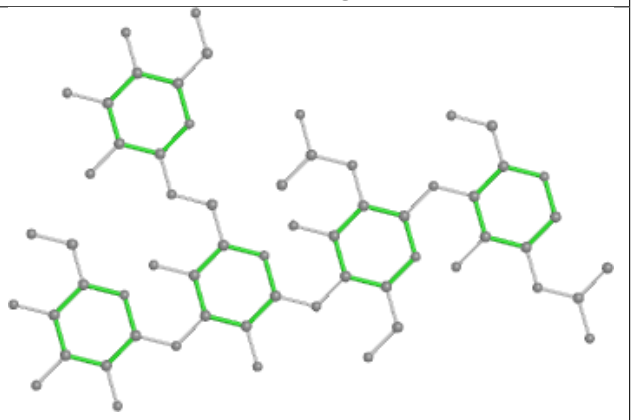
Bond lengths



Bond angles

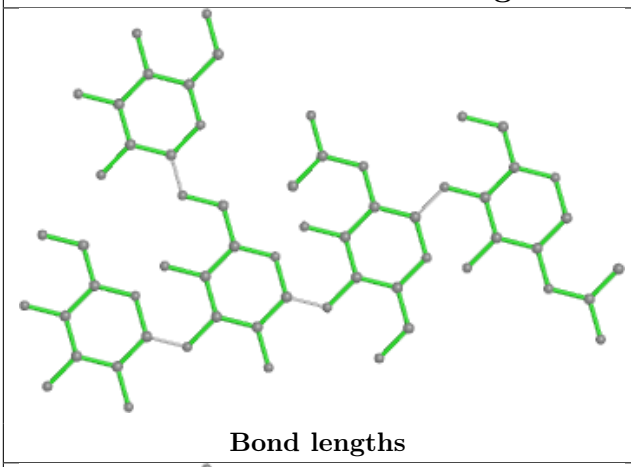


Torsions

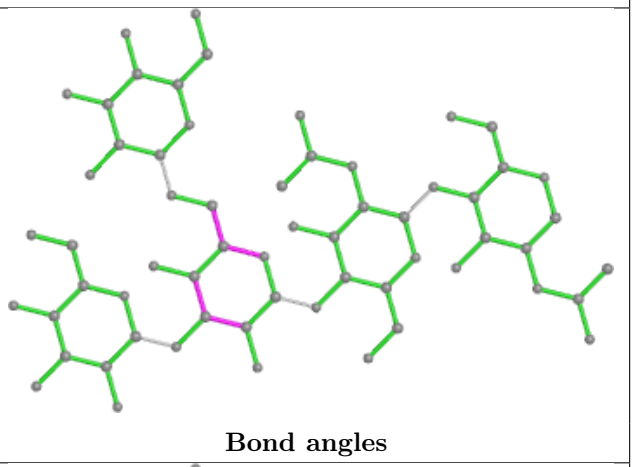


Rings

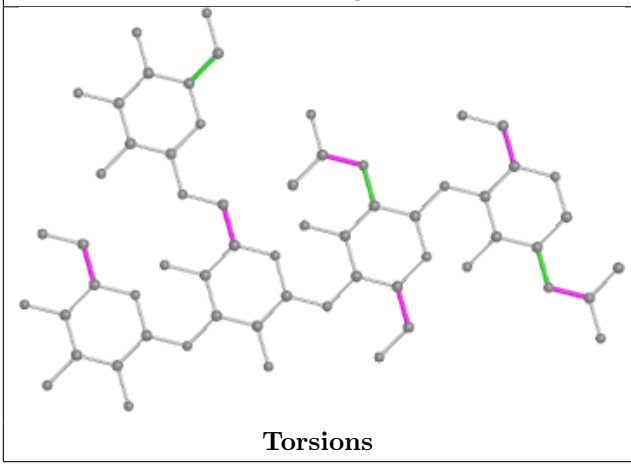
Oligosaccharide Chain U



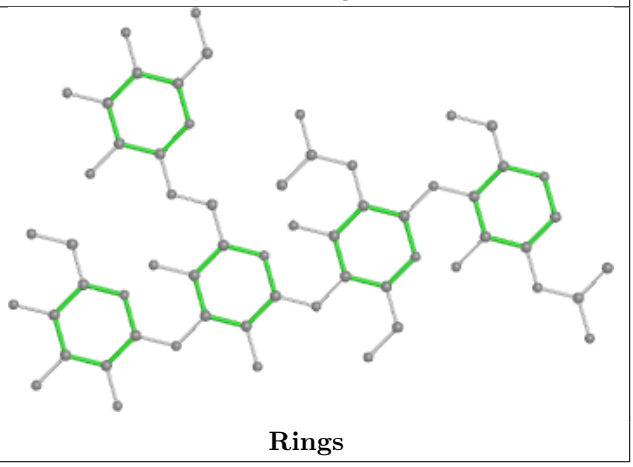
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

25 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	$\#\|Z\| > 2$
8	NAG	B	1304	-	14,14,15	1.53	2 (14%)	17,19,21	0.64	0
8	NAG	C	1201	1	14,14,15	1.54	2 (14%)	17,19,21	0.76	0
8	NAG	A	1302	-	14,14,15	1.57	2 (14%)	17,19,21	0.70	0
8	NAG	B	1305	1	14,14,15	1.43	1 (7%)	17,19,21	0.73	0
8	NAG	B	1301	1	14,14,15	1.51	2 (14%)	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	B	1306	-	14,14,15	0.30	0	17,19,21	0.72	0
8	NAG	A	1308	-	14,14,15	0.29	0	17,19,21	0.67	0
8	NAG	C	1204	-	14,14,15	1.51	2 (14%)	17,19,21	0.72	0
8	NAG	C	1208	1	14,14,15	1.48	2 (14%)	17,19,21	0.71	0
8	NAG	B	1303	-	14,14,15	1.50	2 (14%)	17,19,21	0.73	0
8	NAG	C	1202	1	14,14,15	1.44	2 (14%)	17,19,21	0.72	0
8	NAG	A	1305	-	14,14,15	1.42	1 (7%)	17,19,21	0.74	0
8	NAG	A	1306	-	14,14,15	0.29	0	17,19,21	0.72	0
8	NAG	B	1302	-	14,14,15	1.57	2 (14%)	17,19,21	0.72	0
8	NAG	A	1303	-	14,14,15	1.51	2 (14%)	17,19,21	0.72	0
8	NAG	A	1301	1	14,14,15	1.52	2 (14%)	17,19,21	0.63	0
8	NAG	C	1205	-	14,14,15	1.57	2 (14%)	17,19,21	0.69	0
8	NAG	C	1207	1	14,14,15	1.54	2 (14%)	17,19,21	0.65	0
8	NAG	B	1309	-	14,14,15	0.24	0	17,19,21	0.63	0
8	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.73	0
8	NAG	C	1203	-	14,14,15	1.53	2 (14%)	17,19,21	0.63	0
8	NAG	A	1304	-	14,14,15	1.55	2 (14%)	17,19,21	0.64	0
8	NAG	B	1308	-	14,14,15	0.28	0	17,19,21	0.66	0
8	NAG	B	1307	1	14,14,15	0.24	0	17,19,21	0.73	0
8	NAG	C	1206	-	14,14,15	1.51	2 (14%)	17,19,21	0.73	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
8	NAG	B	1304	-	-	1/6/23/26	0/1/1/1
8	NAG	C	1201	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1302	-	-	0/6/23/26	0/1/1/1
8	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
8	NAG	A	1308	-	-	3/6/23/26	0/1/1/1
8	NAG	C	1204	-	-	0/6/23/26	0/1/1/1
8	NAG	C	1208	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
8	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1305	-	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1306	-	-	2/6/23/26	0/1/1/1
8	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1303	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1205	-	-	0/6/23/26	0/1/1/1
8	NAG	C	1207	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1309	-	-	4/6/23/26	0/1/1/1
8	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1203	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1304	-	-	1/6/23/26	0/1/1/1
8	NAG	B	1308	-	-	3/6/23/26	0/1/1/1
8	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1206	-	-	0/6/23/26	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1302	NAG	C1-C2	4.33	1.58	1.52
8	C	1205	NAG	C1-C2	4.32	1.58	1.52
8	A	1302	NAG	C1-C2	4.28	1.58	1.52
8	C	1201	NAG	C1-C2	4.26	1.58	1.52
8	C	1203	NAG	C1-C2	4.18	1.58	1.52
8	A	1301	NAG	C1-C2	4.15	1.58	1.52
8	B	1301	NAG	C1-C2	4.11	1.58	1.52
8	A	1304	NAG	C1-C2	4.10	1.58	1.52
8	C	1207	NAG	C1-C2	4.08	1.58	1.52
8	B	1304	NAG	C1-C2	4.07	1.58	1.52
8	A	1303	NAG	C1-C2	4.04	1.58	1.52
8	C	1204	NAG	C1-C2	4.04	1.58	1.52
8	C	1208	NAG	C1-C2	4.03	1.58	1.52
8	C	1206	NAG	C1-C2	4.03	1.58	1.52
8	B	1303	NAG	C1-C2	4.00	1.58	1.52
8	C	1202	NAG	C1-C2	3.96	1.58	1.52
8	B	1305	NAG	C1-C2	3.92	1.58	1.52
8	A	1305	NAG	C1-C2	3.88	1.58	1.52
8	A	1302	NAG	O5-C5	2.48	1.48	1.43
8	B	1302	NAG	O5-C5	2.44	1.48	1.43
8	C	1205	NAG	O5-C5	2.41	1.48	1.43
8	A	1304	NAG	O5-C5	2.39	1.48	1.43
8	B	1304	NAG	O5-C5	2.37	1.48	1.43
8	C	1204	NAG	O5-C5	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1207	NAG	O5-C5	2.36	1.48	1.43
8	C	1206	NAG	O5-C5	2.29	1.48	1.43
8	C	1208	NAG	O5-C5	2.27	1.48	1.43
8	A	1303	NAG	O5-C5	2.24	1.48	1.43
8	B	1303	NAG	O5-C5	2.23	1.48	1.43
8	B	1301	NAG	O5-C5	2.20	1.47	1.43
8	C	1201	NAG	O5-C5	2.19	1.47	1.43
8	C	1203	NAG	O5-C5	2.19	1.47	1.43
8	A	1301	NAG	O5-C5	2.17	1.47	1.43
8	C	1202	NAG	O5-C5	2.03	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1307	NAG	C8-C7-N2-C2
8	A	1307	NAG	O7-C7-N2-C2
8	A	1308	NAG	C8-C7-N2-C2
8	A	1308	NAG	O7-C7-N2-C2
8	B	1307	NAG	C8-C7-N2-C2
8	B	1307	NAG	O7-C7-N2-C2
8	B	1308	NAG	C8-C7-N2-C2
8	B	1308	NAG	O7-C7-N2-C2
8	B	1309	NAG	C8-C7-N2-C2
8	B	1309	NAG	O7-C7-N2-C2
8	A	1306	NAG	C8-C7-N2-C2
8	B	1306	NAG	C8-C7-N2-C2
8	A	1307	NAG	C1-C2-N2-C7
8	B	1307	NAG	C1-C2-N2-C7
8	B	1309	NAG	C1-C2-N2-C7
8	A	1306	NAG	O7-C7-N2-C2
8	B	1306	NAG	O7-C7-N2-C2
8	A	1308	NAG	C1-C2-N2-C7
8	B	1308	NAG	C1-C2-N2-C7
8	A	1305	NAG	O5-C5-C6-O6
8	B	1305	NAG	O5-C5-C6-O6
8	C	1202	NAG	O5-C5-C6-O6
8	B	1309	NAG	O5-C5-C6-O6
8	A	1304	NAG	C4-C5-C6-O6
8	B	1304	NAG	C4-C5-C6-O6
8	C	1207	NAG	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1304	NAG	2	0
8	A	1302	NAG	1	0
8	C	1204	NAG	3	0
8	A	1305	NAG	1	0
8	A	1306	NAG	1	0
8	B	1302	NAG	3	0
8	A	1303	NAG	3	0
8	C	1205	NAG	3	0
8	B	1309	NAG	4	0
8	C	1203	NAG	4	0
8	A	1304	NAG	4	0
8	B	1308	NAG	4	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.

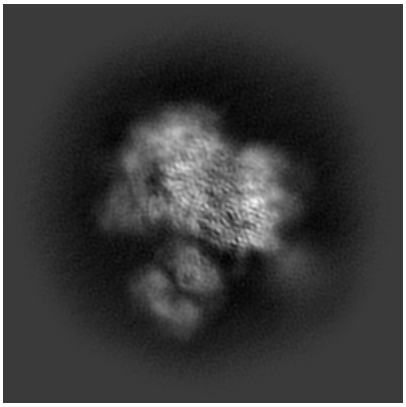
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23095. These allow visual inspection of the internal detail of the map and identification of artifacts.

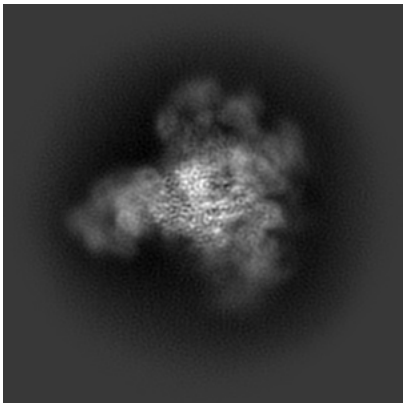
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

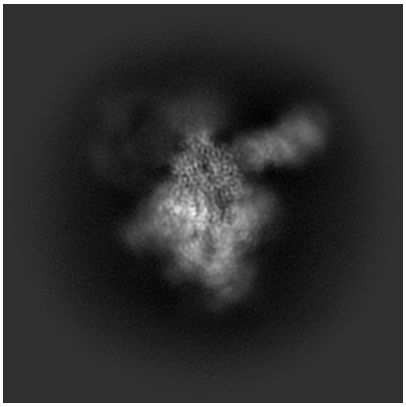
6.1.1 Primary map



X



Y

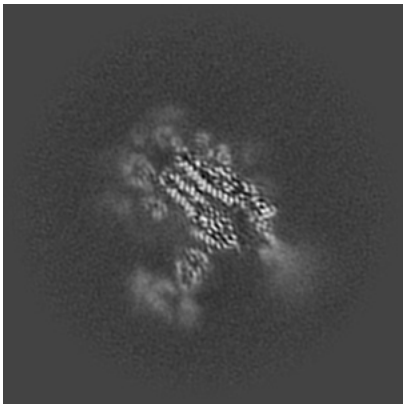


Z

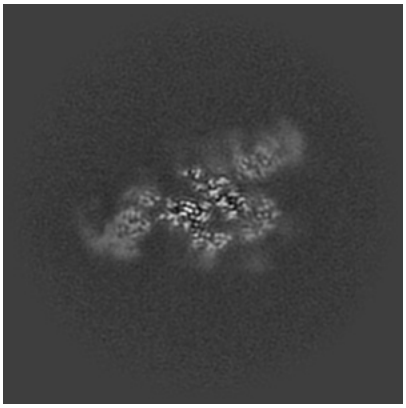
The images above show the map projected in three orthogonal directions.

6.2 Central slices

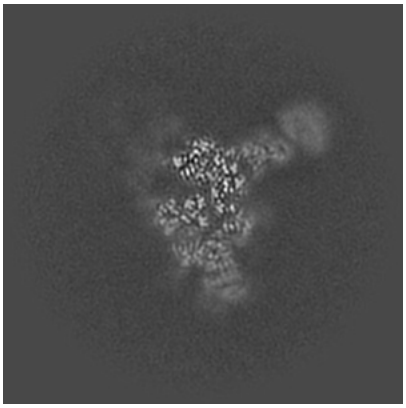
6.2.1 Primary map



X Index: 160



Y Index: 160

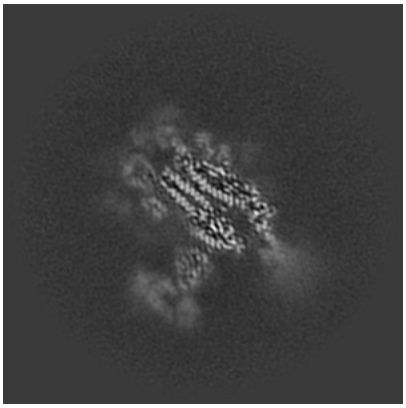


Z Index: 160

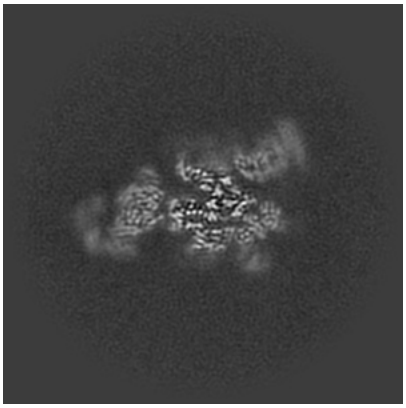
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

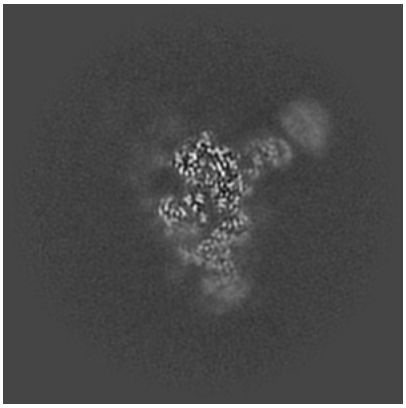
6.3.1 Primary map



X Index: 159



Y Index: 155



Z Index: 157

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 0.204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

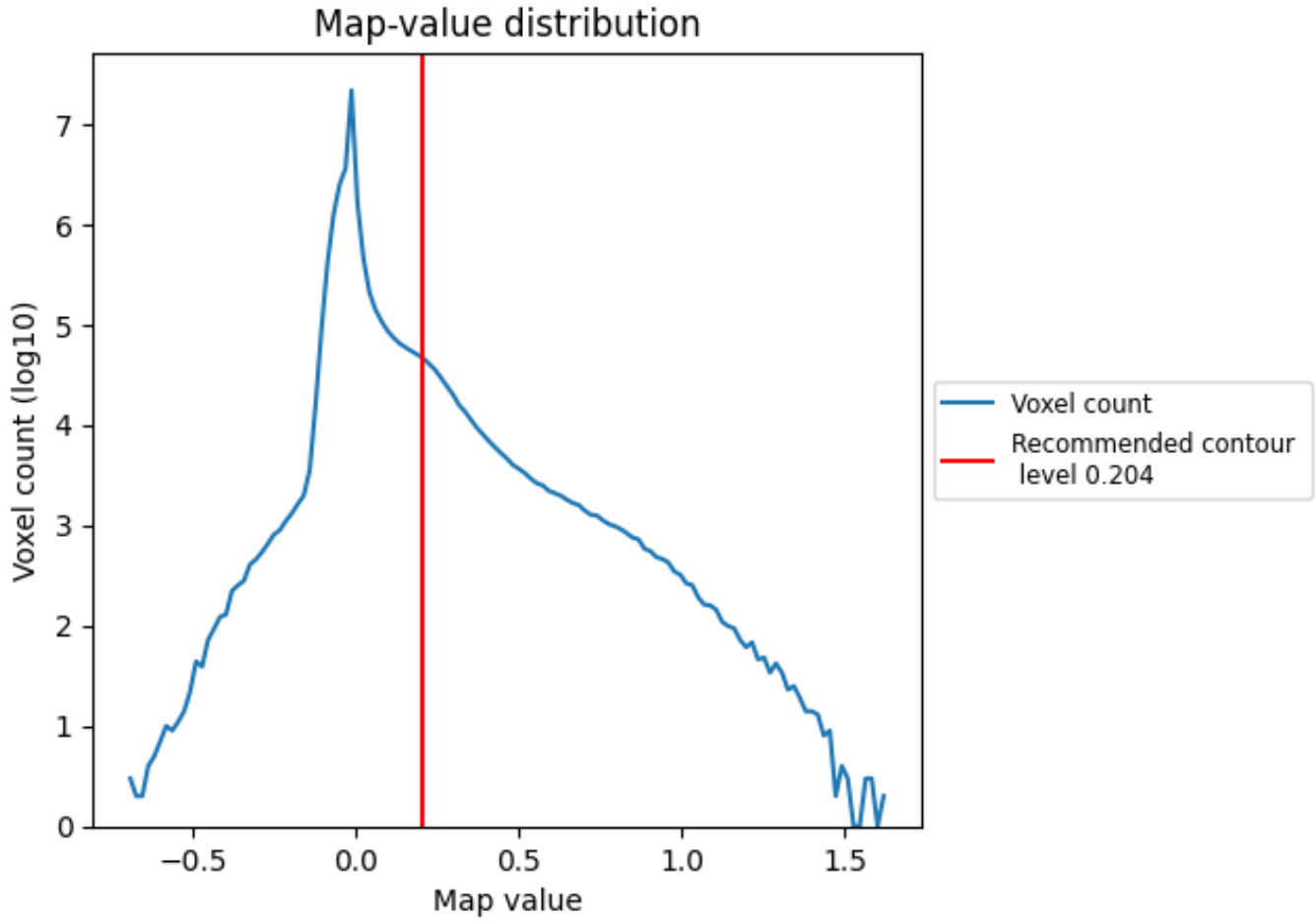
6.5 Mask visualisation (i)

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

7 Map analysis

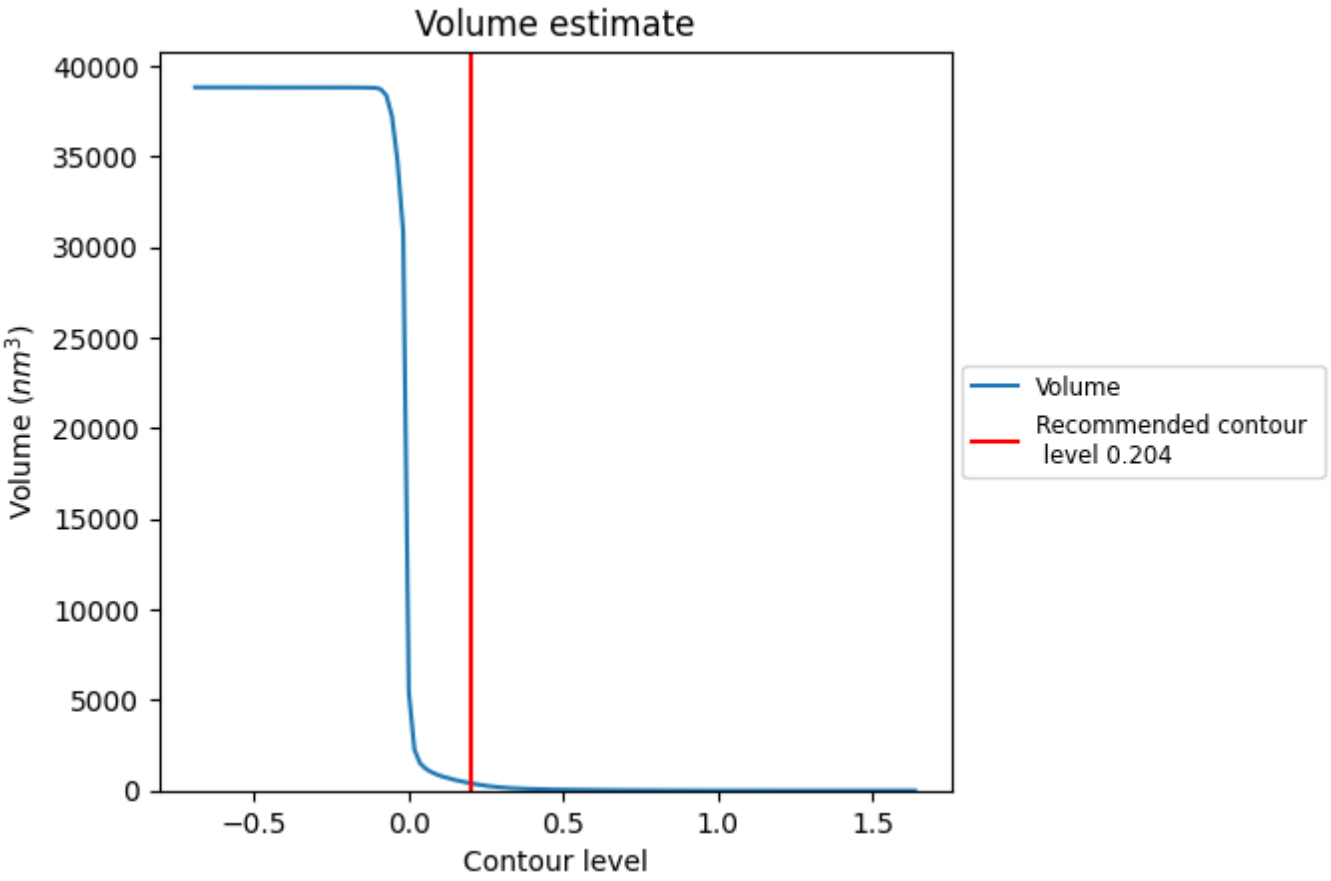
This section contains the results of statistical analysis of the map.

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.

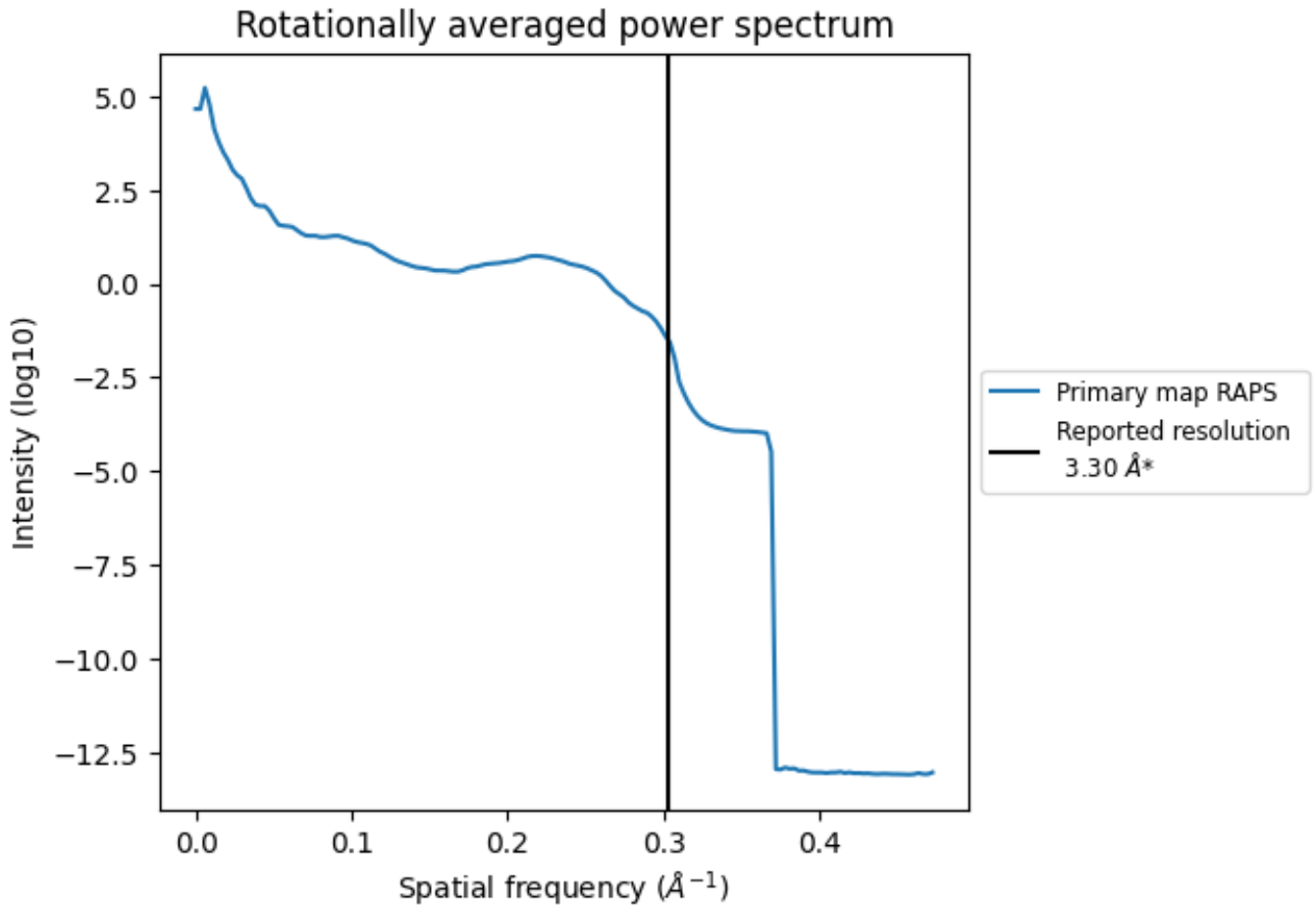
7.2 Volume estimate



The volume at the recommended contour level is 394 nm^3; this corresponds to an approximate mass of 356 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

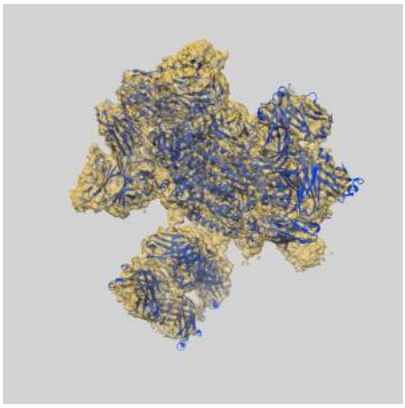
8 Fourier-Shell correlation (i)

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

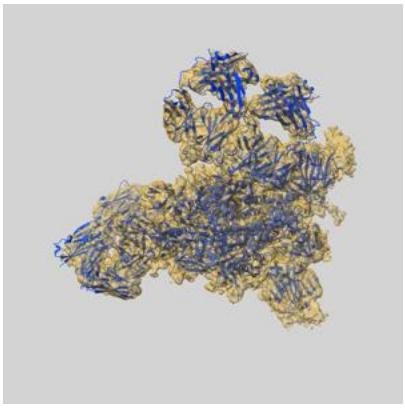
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23095 and PDB model 7L06. Per-residue inclusion information can be found in section 3 on page 9.

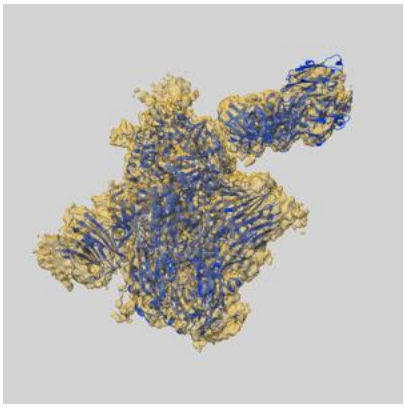
9.1 Map-model overlay



X



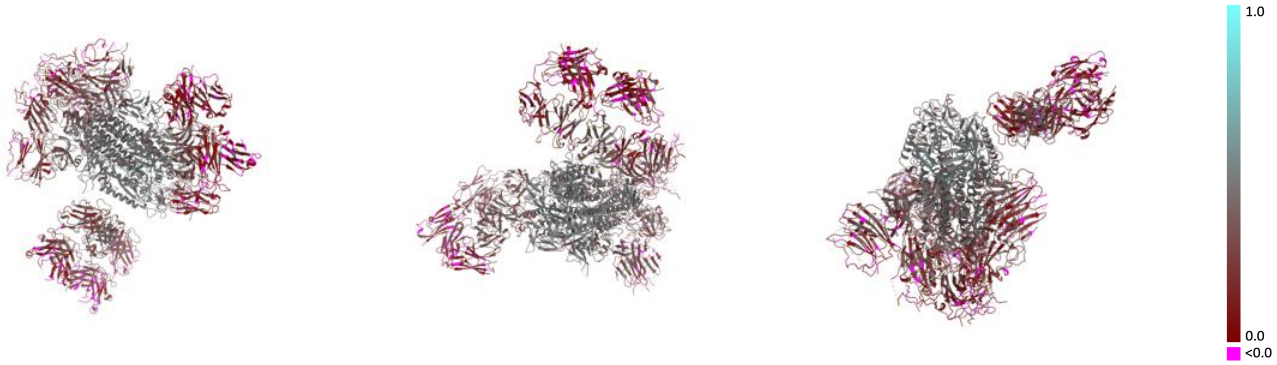
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.204 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.

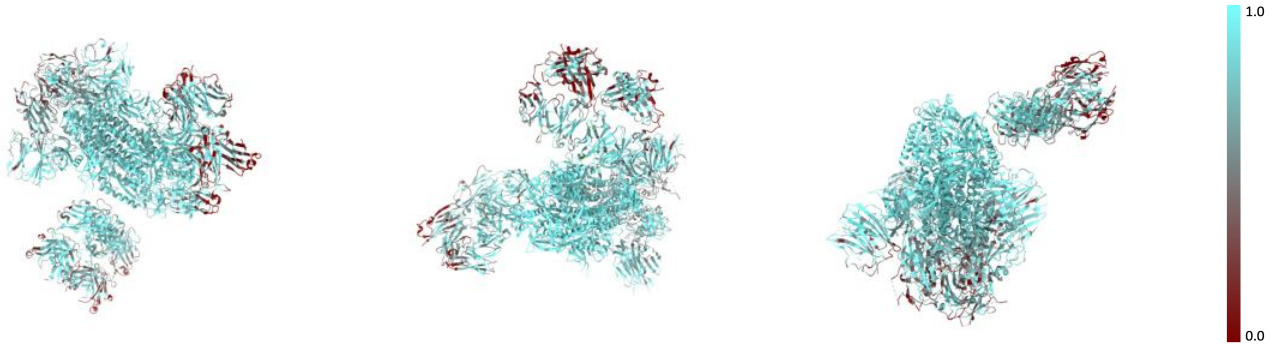
9.2 Q-score mapped to coordinate model



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.

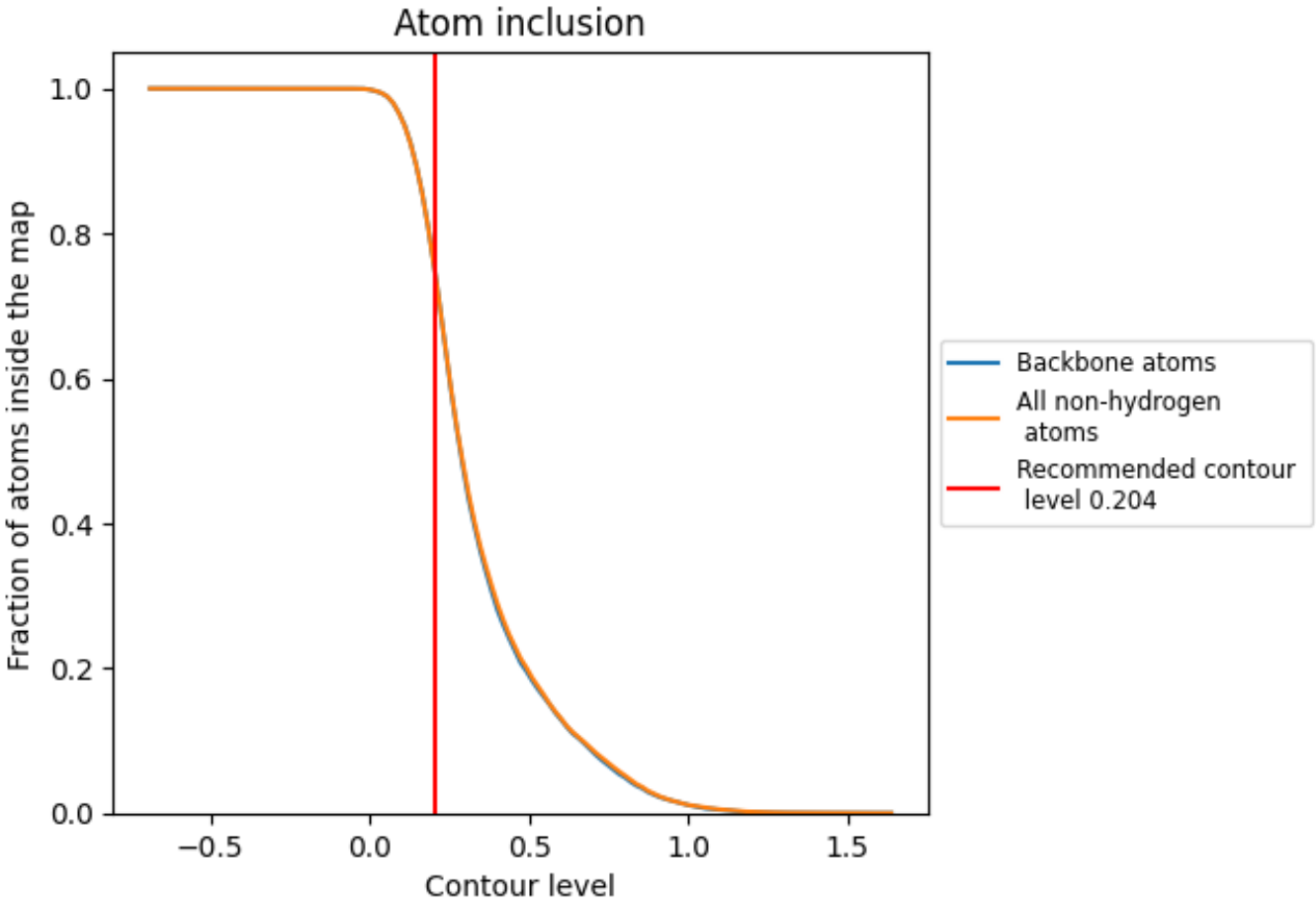
9.3 Atom inclusion mapped to coordinate model



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 (0.204).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7485	0.3030
A	0.8201	0.3570
B	0.8045	0.3540
C	0.8134	0.3450
D	0.6714	0.2270
E	0.6158	0.1540
F	0.5113	0.1520
G	0.6073	0.2480
H	0.7834	0.2620
I	0.7143	0.3660
J	0.9344	0.4440
K	0.7412	0.2320
L	0.6041	0.1260
M	0.6976	0.2800
N	0.8617	0.4490
O	0.9286	0.4210
P	0.6885	0.3770
Q	0.7857	0.4310
R	0.7143	0.2620
S	0.8571	0.3640
T	0.6786	0.2900
U	0.7869	0.3520
V	0.7500	0.3110
W	0.9016	0.4530
X	0.8723	0.4370
Y	0.8214	0.3480