Full wwPDB EM Validation Report ⓘ

Aug 15, 2024 – 06:35 PM JST

PDB ID	:	8ZHD
EMDB ID	:	EMD-60099
Title	:	SARS-CoV-2 spike trimer (6P) in complex with two R1-26 Fabs
Authors	:	Yan, Q.; Gao, X.; Liu, B.; Hou, R.; He, P.; Li, Z.; Chen, Q.; Wang, J.; He, J.; Chen, L.; Zhao, J.; Xiong, X.
Deposited on	:	2024-05-10
Resolution	:	3.41 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:

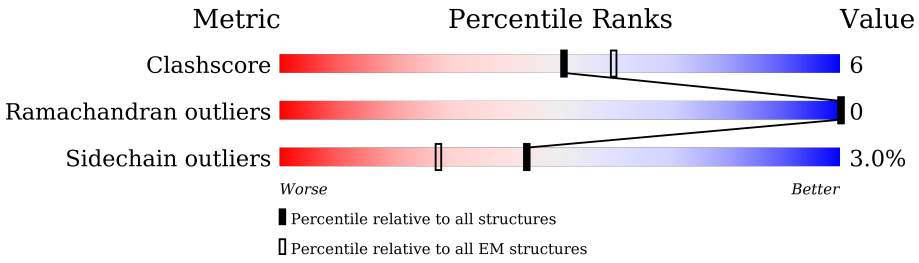
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.41 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	1278	6% 72% 11% 17%
1	B	1278	• 68% 15% 17%
1	C	1278	9% 68% 14% • 17%
2	F	243	33% 40% 9% 51%
2	H	243	24% 41% 8% 51%
3	G	240	31% 36% 10% 54%
3	L	240	24% 36% 8% • 54%
4	D	2	50% 100%

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Mol	Chain	Length	Quality of chain
4	E	2	100%
4	I	2	100%
4	J	2	100%
4	K	2	100%
4	M	2	100%
4	N	2	100%
4	O	2	100%
4	P	2	100%
4	Q	2	100%
4	R	2	100%
4	S	2	50% 50%
4	T	2	100%
4	U	2	100%
4	V	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29306 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,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1066	Total	C	N	O	S	0	0
			8326	5312	1388	1588	38		
1	B	1066	Total	C	N	O	S	0	0
			8326	5312	1388	1588	38		
1	C	1066	Total	C	N	O	S	0	0
			8326	5312	1388	1588	38		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of R1-26 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	119	Total	C	N	O	S	0	0
			920	583	158	175	4		
2	F	119	Total	C	N	O	S	0	0
			920	583	158	175	4		

- Molecule 3 is a protein called Light chain of R1-26 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	110	Total	C	N	O	S	0	0
			824	506	136	179	3		
3	G	110	Total	C	N	O	S	0	0
			824	506	136	179	3		

- 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	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		

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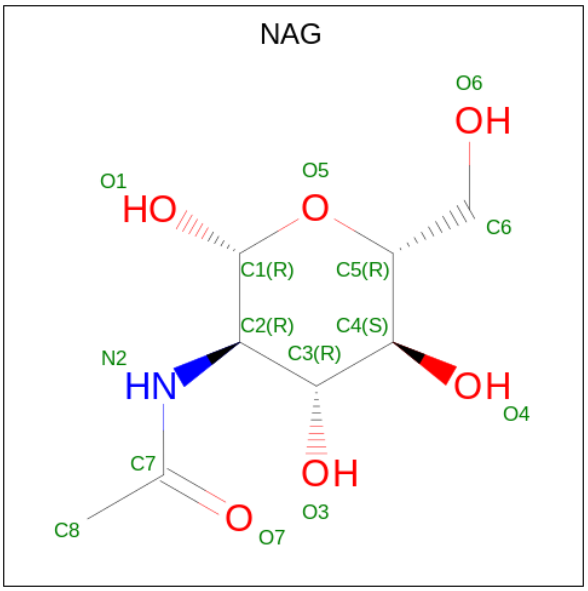
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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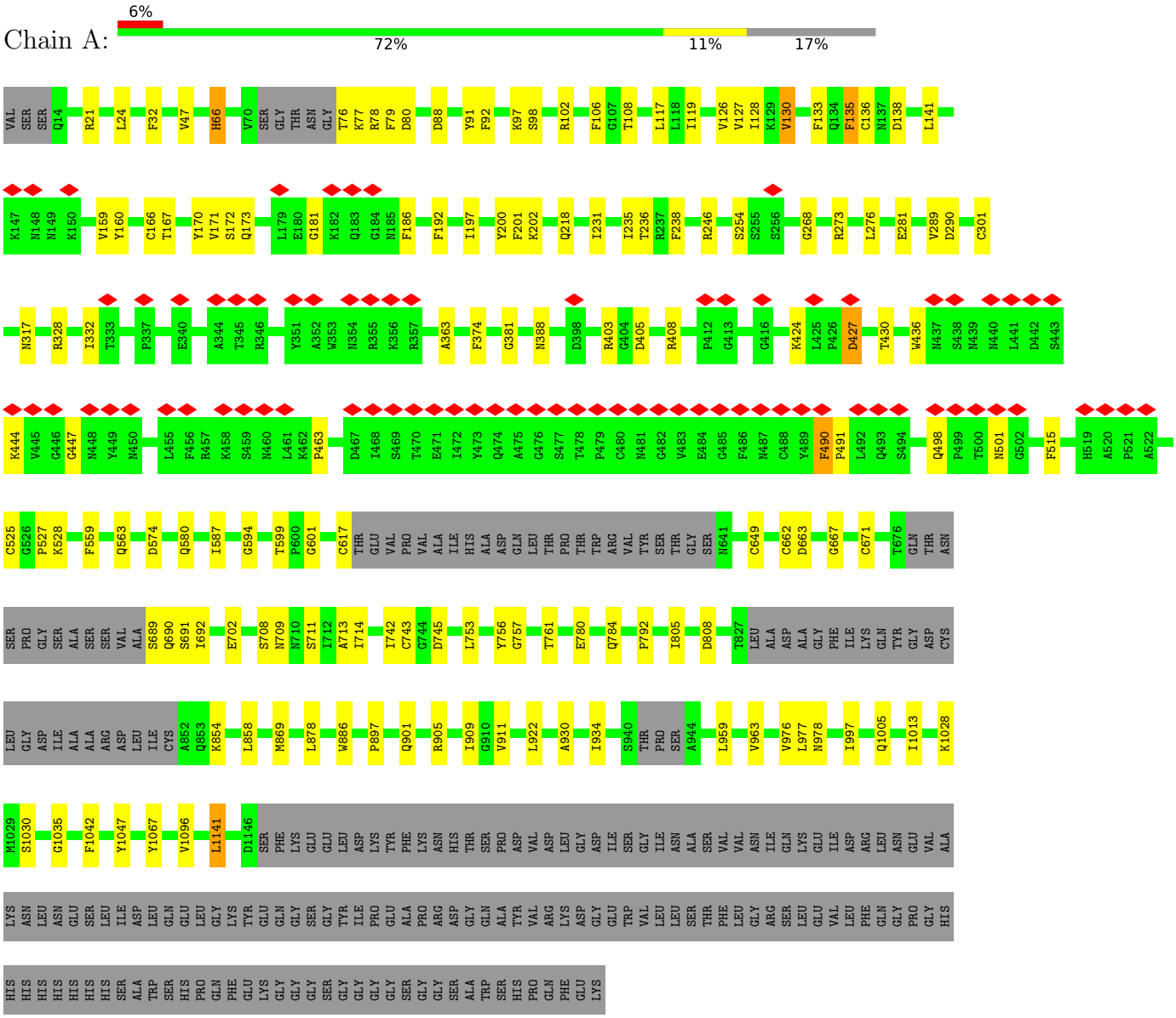
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0

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.

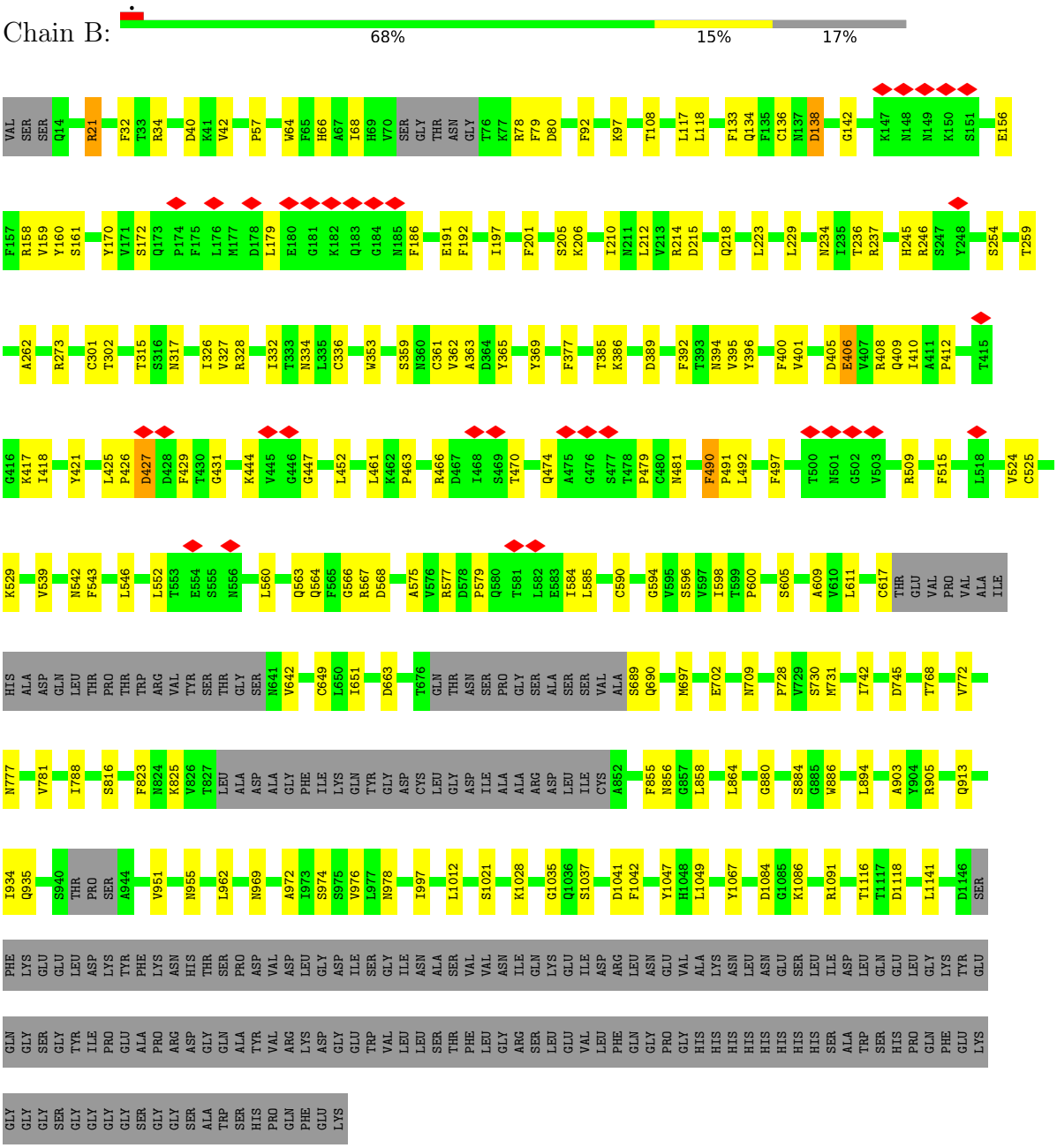
• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag

Chain A:



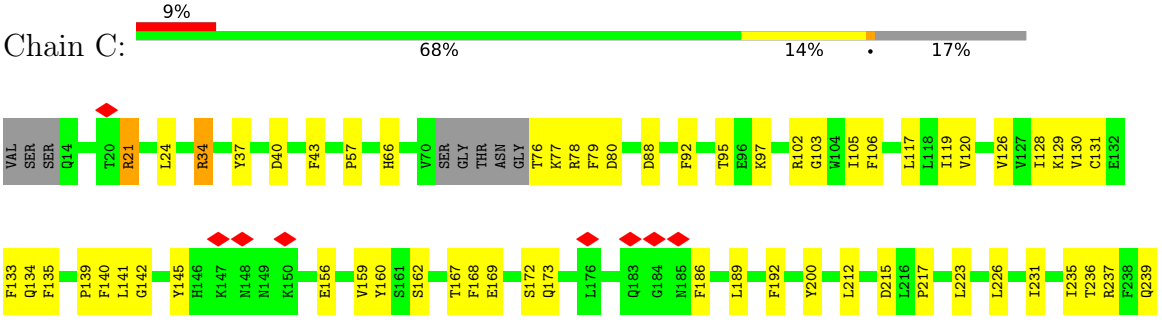
• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag

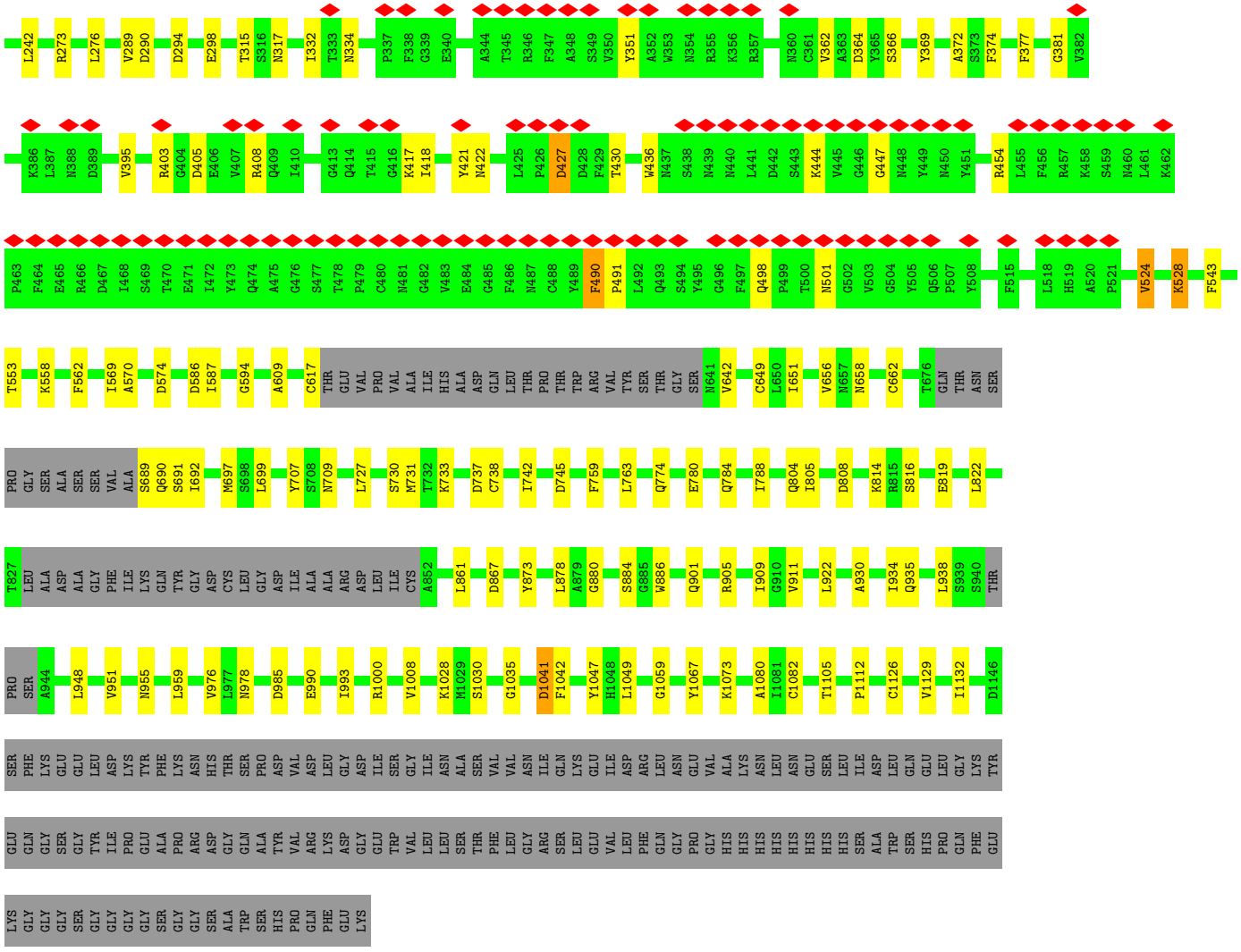
Chain B:



• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag

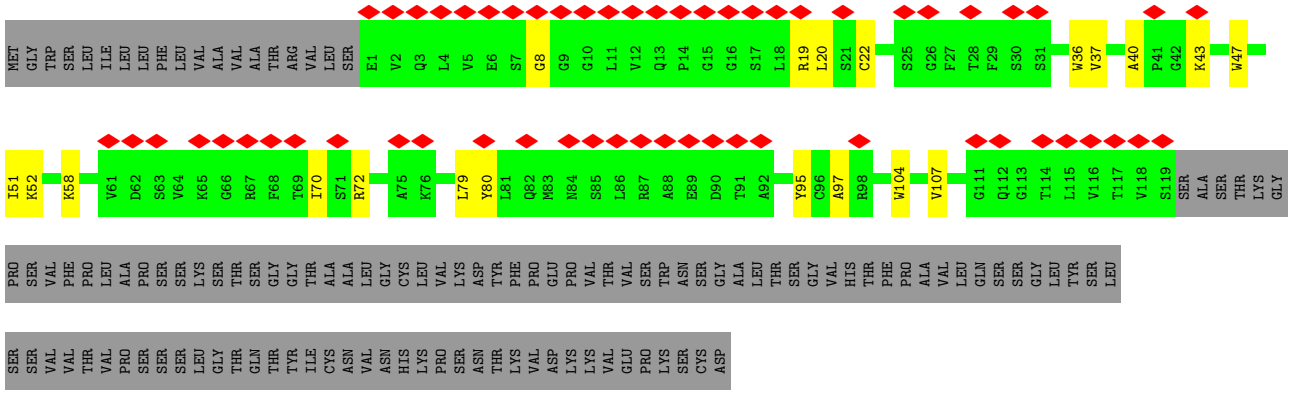
Chain C:





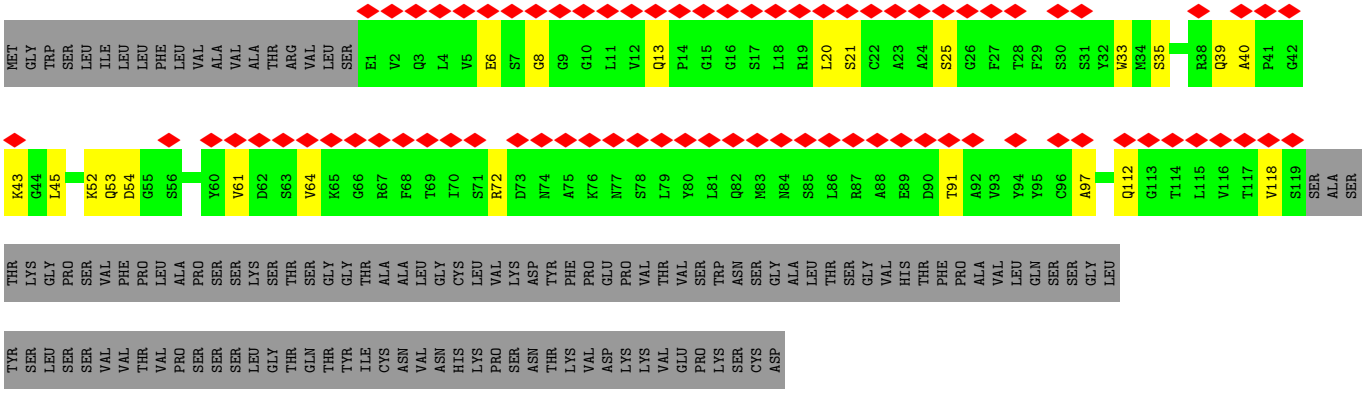
• Molecule 2: Heavy chain of R1-26 Fab

Chain H:



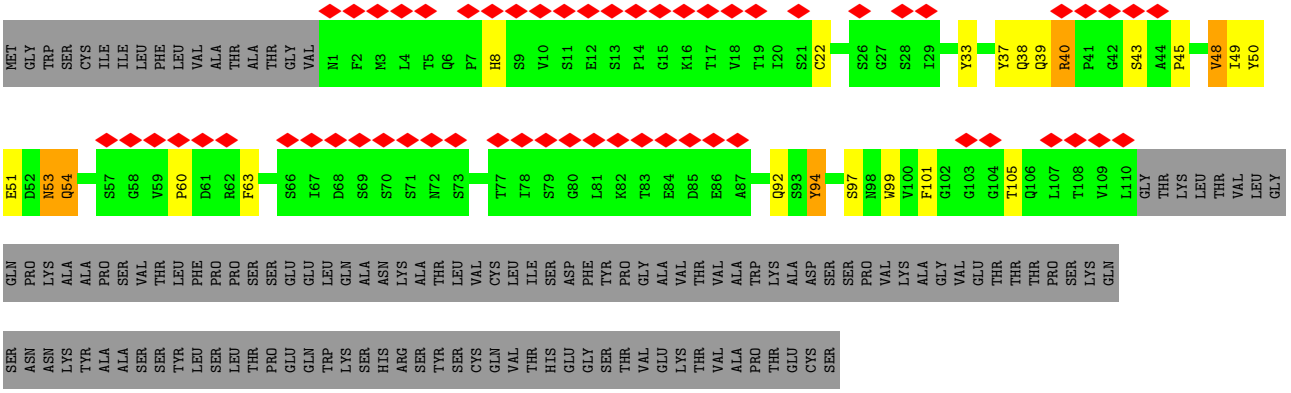
• Molecule 2: Heavy chain of R1-26 Fab

Chain F:



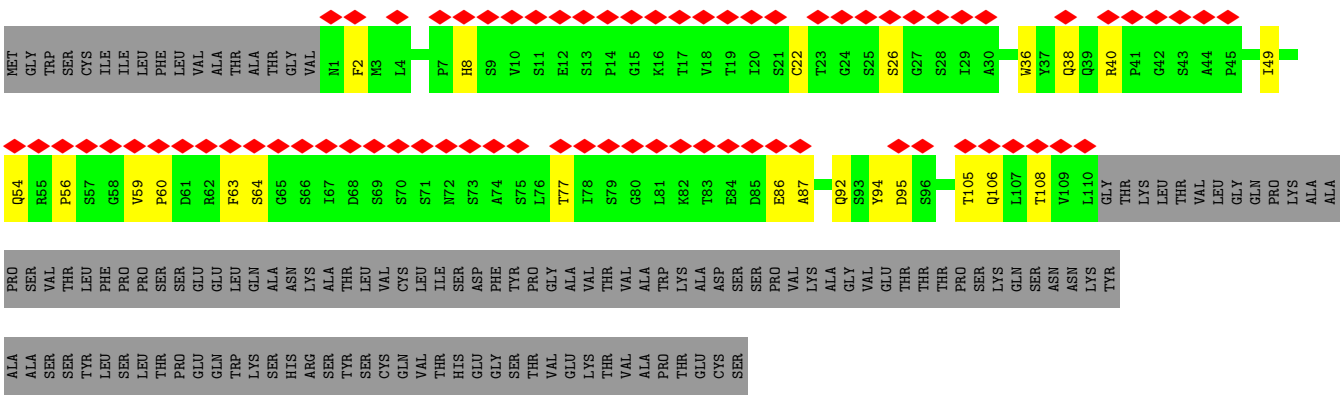
• Molecule 3: Light chain of R1-26 Fab

Chain L:



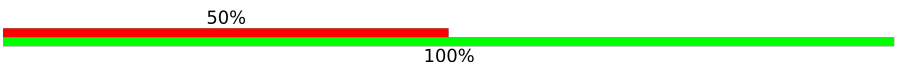
• Molecule 3: Light chain of R1-26 Fab

Chain G:



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

Chain D:



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

Chain E: 100%

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

Chain I: 100%

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

Chain J: 100%

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

Chain K: 100%

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

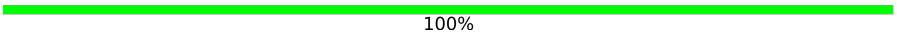
Chain M: 100%

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

Chain N: 100%

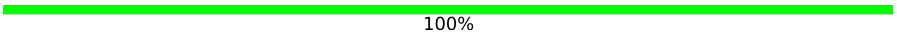
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



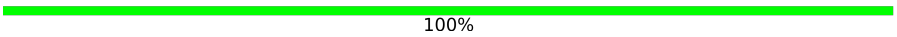
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



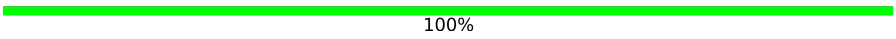
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:

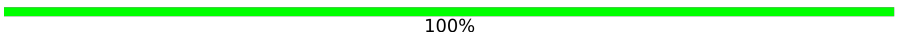


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

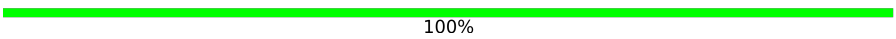
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

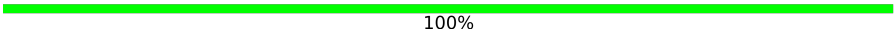


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 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	110522	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.265	Depositor
Minimum map value	-0.533	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	350.4128, 350.4128, 350.4128	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3688, 1.3688, 1.3688	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/8522	0.50	0/11605
1	B	0.29	0/8522	0.53	0/11605
1	C	0.26	0/8522	0.50	0/11605
2	F	0.25	0/942	0.57	0/1277
2	H	0.26	0/942	0.57	0/1277
3	G	0.26	0/843	0.51	0/1151
3	L	0.33	0/843	0.52	0/1151
All	All	0.27	0/29136	0.51	0/39671

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8326	0	8079	84	0
1	B	8326	0	8079	111	0
1	C	8326	0	8079	112	0
2	F	920	0	887	11	0
2	H	920	0	887	15	0
3	G	824	0	755	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	824	0	755	16	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
5	A	140	0	130	1	0
5	B	140	0	130	0	0
5	C	140	0	130	0	0
All	All	29306	0	28286	338	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 6.

All (338) 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)
3:L:92:GLN:HE22	3:L:99:TRP:HB3	1.47	0.80
1:A:200:TYR:HB3	1:A:202:LYS:HE3	1.70	0.73
1:C:273:ARG:NH2	1:C:290:ASP:OD2	2.26	0.68
1:B:577:ARG:HG3	1:B:584:ILE:HD13	1.76	0.67
1:B:206:LYS:HG2	1:B:223:LEU:HD12	1.77	0.67
1:B:425:LEU:HD12	1:B:426:PRO:HD2	1.76	0.66
1:C:131:CYS:SG	1:C:167:THR:N	2.63	0.66
1:B:394:ASN:HD22	1:B:396:TYR:HE1	1.45	0.64
1:A:574:ASP:HA	1:A:587:ILE:HB	1.80	0.64
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.63	0.62
1:A:119:ILE:HG12	1:A:128:ILE:HG23	1.81	0.62
1:B:1116:THR:HG23	1:B:1118:ASP:H	1.65	0.62
1:A:1141:LEU:HD11	1:B:1141:LEU:HD12	1.81	0.62
1:A:667:GLY:HA2	1:B:864:LEU:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLY:HA3	1:C:156:GLU:HB2	1.83	0.61
1:B:642:VAL:HG22	1:B:651:ILE:HG13	1.83	0.61
1:C:126:VAL:HB	1:C:172:SER:HB3	1.82	0.61
3:L:94:TYR:HE1	3:L:97:SER:H	1.49	0.60
3:G:36:TRP:HB2	3:G:49:ILE:HB	1.81	0.60
1:B:97:LYS:HB2	1:B:186:PHE:HA	1.83	0.60
1:C:738:CYS:HB3	1:C:742:ILE:HD12	1.84	0.60
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.34	0.60
3:G:86:GLU:HB2	3:G:108:THR:HA	1.83	0.59
1:A:128:ILE:HG13	1:A:170:TYR:HD2	1.66	0.59
1:C:951:VAL:O	1:C:955:ASN:ND2	2.36	0.59
1:C:1082:CYS:HB2	1:C:1132:ILE:HG12	1.84	0.59
1:B:142:GLY:HA3	1:B:156:GLU:HB2	1.85	0.59
1:B:425:LEU:HD11	1:B:429:PHE:CD1	2.38	0.59
1:C:130:VAL:O	1:C:167:THR:OG1	2.21	0.58
1:C:901:GLN:HG2	1:C:905:ARG:HE	1.68	0.58
1:B:596:SER:HB2	1:B:611:LEU:HB3	1.86	0.58
1:B:21:ARG:NH2	1:B:79:PHE:O	2.37	0.57
1:C:66:HIS:HB3	1:C:78:ARG:HG2	1.85	0.57
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.85	0.57
1:A:32:PHE:HB3	1:A:218:GLN:HG3	1.85	0.57
1:B:474:GLN:OE1	1:B:474:GLN:N	2.36	0.57
1:B:236:THR:HG23	1:B:237:ARG:HG3	1.86	0.57
1:B:566:GLY:HA3	1:B:575:ALA:HB3	1.87	0.57
1:A:126:VAL:HB	1:A:172:SER:HB3	1.85	0.57
1:B:317:ASN:HA	1:B:594:GLY:HA2	1.87	0.57
2:H:19:ARG:NH1	2:H:20:LEU:O	2.38	0.57
1:A:780:GLU:O	1:A:784:GLN:NE2	2.39	0.56
1:A:714:ILE:HD11	1:A:1096:VAL:HG11	1.87	0.56
1:A:753:LEU:HD23	1:A:756:TYR:HB2	1.87	0.56
1:B:138:ASP:OD1	1:B:138:ASP:N	2.38	0.56
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.86	0.56
1:B:32:PHE:HB3	1:B:218:GLN:HG3	1.87	0.56
1:C:21:ARG:NH2	1:C:79:PHE:O	2.39	0.56
1:A:108:THR:HA	1:A:236:THR:HG22	1.88	0.56
1:B:170:TYR:CE2	1:B:172:SER:HB3	2.41	0.56
1:B:134:GLN:HB2	1:B:161:SER:HB2	1.88	0.56
1:C:117:LEU:HB2	1:C:130:VAL:HG13	1.88	0.56
1:A:97:LYS:HB2	1:A:186:PHE:HA	1.88	0.55
1:B:395:VAL:HG12	1:B:524:VAL:HG21	1.88	0.55
1:C:780:GLU:O	1:C:784:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HG23	1:C:160:TYR:HD1	1.72	0.55
1:C:317:ASN:HA	1:C:594:GLY:HA2	1.89	0.55
1:C:731:MET:HG2	1:C:774:GLN:HE22	1.70	0.55
1:C:617:CYS:N	1:C:649:CYS:SG	2.80	0.55
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.39	0.54
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.90	0.54
1:C:444:LYS:NZ	1:C:447:GLY:O	2.36	0.54
1:A:246:ARG:HH22	1:A:254:SER:HB3	1.73	0.54
1:A:708:SER:HB3	1:A:711:SER:HB3	1.90	0.54
1:B:444:LYS:NZ	1:B:447:GLY:O	2.38	0.54
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.89	0.54
3:L:48:VAL:HG22	3:L:49:ILE:HG12	1.88	0.54
1:B:426:PRO:HD3	1:B:463:PRO:HB3	1.89	0.53
1:A:976:VAL:HG22	1:A:978:ASN:H	1.73	0.53
1:B:1049:LEU:HD11	1:B:1067:TYR:HB2	1.90	0.53
2:H:51:ILE:HD12	2:H:70:ILE:HG23	1.90	0.53
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.90	0.53
1:B:479:PRO:HD2	3:G:54:GLN:HA	1.90	0.53
1:B:976:VAL:HG22	1:B:978:ASN:H	1.74	0.53
1:C:40:ASP:N	1:C:40:ASP:OD1	2.41	0.53
1:C:102:ARG:HG3	1:C:141:LEU:HG	1.91	0.53
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.42	0.52
1:C:990:GLU:HA	1:C:993:ILE:HD12	1.91	0.52
1:B:969:ASN:ND2	1:B:972:ALA:O	2.43	0.52
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.43	0.52
1:B:552:LEU:HD13	1:B:585:LEU:HD13	1.91	0.52
2:H:52:LYS:O	2:H:72:ARG:NH1	2.43	0.52
1:A:133:PHE:HB2	1:A:135:PHE:CE1	2.45	0.52
1:B:566:GLY:HA2	1:C:43:PHE:CD2	2.44	0.52
1:A:78:ARG:HE	1:A:80:ASP:HB2	1.74	0.52
1:A:1030:SER:HB3	1:C:1041:ASP:HB3	1.92	0.52
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.90	0.52
2:F:52:LYS:HG2	2:F:53:GLN:OE1	2.09	0.52
1:C:976:VAL:HG22	1:C:978:ASN:H	1.74	0.52
1:A:858:LEU:HD13	1:A:959:LEU:HG	1.90	0.52
1:B:702:GLU:HG2	1:C:788:ILE:HD11	1.90	0.52
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.43	0.51
2:H:51:ILE:HD11	2:H:58:LYS:HE3	1.92	0.51
1:A:47:VAL:HG22	1:C:569:ILE:HD13	1.93	0.51
1:C:34:ARG:NH1	1:C:217:PRO:O	2.44	0.51
1:C:498:GLN:HB2	1:C:501:ASN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:691:SER:OG	1:C:692:ILE:N	2.43	0.51
1:C:97:LYS:HB2	1:C:186:PHE:HA	1.92	0.51
1:C:574:ASP:HA	1:C:587:ILE:HB	1.93	0.51
1:A:444:LYS:NZ	1:A:447:GLY:O	2.36	0.51
1:A:792:PRO:HG3	1:C:707:TYR:HD2	1.75	0.51
1:A:897:PRO:HA	1:C:707:TYR:HE1	1.76	0.51
1:C:80:ASP:OD1	1:C:80:ASP:N	2.44	0.51
2:F:39:GLN:HB3	2:F:45:LEU:HD23	1.93	0.51
2:H:104:TRP:HB3	3:L:33:TYR:HD1	1.75	0.51
1:A:617:CYS:N	1:A:649:CYS:SG	2.84	0.50
1:C:1080:ALA:HB3	1:C:1129:VAL:HG11	1.94	0.50
1:B:689:SER:OG	1:B:690:GLN:N	2.44	0.50
1:B:425:LEU:HD12	1:B:426:PRO:CD	2.41	0.50
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.44	0.50
1:C:129:LYS:NZ	1:C:169:GLU:HG3	2.27	0.50
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.94	0.50
1:C:922:LEU:HD11	4:S:1:NAG:H3	1.93	0.50
1:C:298:GLU:HG2	1:C:315:THR:HB	1.94	0.50
3:G:2:PHE:HD1	3:G:26:SER:HB3	1.76	0.50
1:B:334:ASN:HA	1:B:362:VAL:HB	1.93	0.49
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.94	0.49
1:A:130:VAL:HG11	1:A:231:ILE:HD12	1.93	0.49
1:B:66:HIS:HB2	1:B:78:ARG:HG2	1.95	0.49
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.93	0.49
1:A:88:ASP:N	1:A:88:ASP:OD1	2.42	0.49
1:C:372:ALA:HB2	2:F:33:TRP:HH2	1.77	0.49
1:B:903:ALA:HB1	1:B:913:GLN:HB2	1.94	0.49
2:F:52:LYS:O	2:F:72:ARG:NH1	2.45	0.49
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.78	0.49
1:B:327:VAL:HA	1:B:542:ASN:HB2	1.95	0.49
1:B:777:ASN:O	1:B:781:VAL:HG12	2.12	0.49
1:C:92:PHE:O	1:C:192:PHE:N	2.43	0.49
1:A:363:ALA:N	1:A:525:CYS:O	2.44	0.49
1:C:172:SER:OG	1:C:173:GLN:N	2.46	0.49
1:B:406:GLU:HG3	1:B:418:ILE:HG13	1.95	0.48
1:B:431:GLY:HA2	1:B:515:PHE:CD1	2.48	0.48
1:C:212:LEU:HD21	1:C:215:ASP:HB3	1.95	0.48
1:C:381:GLY:HA3	1:C:430:THR:HA	1.95	0.48
1:C:805:ILE:HB	1:C:878:LEU:HD11	1.94	0.48
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.45	0.48
1:B:481:ASN:ND2	3:G:63:PHE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:LEU:HD21	1:C:938:LEU:HD21	1.94	0.48
1:A:332:ILE:HD13	1:A:528:LYS:H	1.78	0.48
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.42	0.48
1:A:381:GLY:HA3	1:A:430:THR:HA	1.95	0.48
1:A:689:SER:OG	1:A:690:GLN:N	2.45	0.48
1:B:880:GLY:O	1:B:884:SER:OG	2.25	0.48
2:H:37:VAL:HG13	2:H:95:TYR:HB2	1.94	0.48
3:L:51:GLU:C	3:L:53:ASN:H	2.17	0.48
3:G:8:HIS:O	3:G:106:GLN:N	2.47	0.48
1:B:80:ASP:N	1:B:80:ASP:OD1	2.47	0.47
1:B:394:ASN:OD1	1:B:394:ASN:N	2.47	0.47
1:B:206:LYS:HD2	1:B:223:LEU:HA	1.97	0.47
1:B:552:LEU:HD22	1:B:585:LEU:HB3	1.96	0.47
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.96	0.47
1:A:138:ASP:N	1:A:138:ASP:OD1	2.47	0.47
1:B:855:PHE:HB2	1:B:858:LEU:HD12	1.96	0.47
1:C:334:ASN:OD1	1:C:334:ASN:N	2.48	0.47
1:B:560:LEU:O	1:B:577:ARG:NH2	2.48	0.47
1:B:663:ASP:OD1	1:B:663:ASP:N	2.48	0.47
1:B:951:VAL:O	1:B:955:ASN:ND2	2.48	0.47
1:C:609:ALA:HB2	1:C:692:ILE:HD12	1.96	0.47
1:C:985:ASP:OD1	1:C:985:ASP:N	2.47	0.47
1:B:709:ASN:OD1	1:B:709:ASN:N	2.44	0.47
1:C:909:ILE:HD13	1:C:1049:LEU:HD21	1.97	0.47
1:C:909:ILE:HG13	1:C:911:VAL:HG23	1.96	0.47
2:H:97:ALA:HB1	2:H:107:VAL:HG13	1.95	0.47
1:B:64:TRP:CZ2	1:B:214:ARG:HD3	2.50	0.47
3:G:95:ASP:OD1	3:G:95:ASP:N	2.39	0.47
1:A:197:ILE:HG13	1:A:202:LYS:HZ1	1.80	0.47
1:B:159:VAL:HG23	1:B:160:TYR:CD2	2.50	0.46
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.96	0.46
1:A:963:VAL:HG11	1:C:570:ALA:HB1	1.97	0.46
1:C:105:ILE:HG13	1:C:239:GLN:HB3	1.97	0.46
1:B:412:PRO:HB3	1:B:425:LEU:HG	1.97	0.46
1:B:92:PHE:O	1:B:192:PHE:N	2.41	0.46
1:C:403:ARG:HG3	1:C:405:ASP:H	1.81	0.46
1:B:566:GLY:HA2	1:C:43:PHE:HD2	1.79	0.46
2:F:8:GLY:HA3	2:F:20:LEU:HG	1.97	0.46
1:A:92:PHE:O	1:A:192:PHE:N	2.41	0.46
1:C:689:SER:OG	1:C:690:GLN:N	2.48	0.46
1:C:886:TRP:HB3	1:C:1035:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:SER:HB2	2:F:97:ALA:HB3	1.98	0.46
1:B:108:THR:HA	1:B:236:THR:HG22	1.98	0.46
1:C:236:THR:HG23	1:C:237:ARG:HG3	1.98	0.46
1:A:869:MET:HB3	1:C:699:LEU:HD21	1.97	0.46
1:A:91:TYR:O	1:A:268:GLY:N	2.41	0.46
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.49	0.45
2:H:104:TRP:HB3	3:L:33:TYR:CD1	2.52	0.45
1:A:424:LYS:HG3	1:A:463:PRO:HG3	1.98	0.45
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.99	0.45
1:C:332:ILE:HD12	1:C:362:VAL:HG11	1.98	0.45
1:A:427:ASP:N	1:A:427:ASP:OD1	2.50	0.45
1:B:742:ILE:HD11	1:B:997:ILE:HG23	1.99	0.45
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.50	0.45
1:A:98:SER:HB3	1:A:181:GLY:HA2	1.99	0.45
1:A:901:GLN:HG2	1:A:905:ARG:HE	1.82	0.45
1:C:808:ASP:OD1	1:C:808:ASP:N	2.50	0.45
1:A:24:LEU:HB2	1:A:78:ARG:HH11	1.80	0.45
1:A:374:PHE:O	3:L:94:TYR:OH	2.35	0.45
1:A:281:GLU:HG3	5:A:1305:NAG:H62	1.98	0.44
1:A:742:ILE:HD11	1:A:997:ILE:HA	1.99	0.44
1:A:930:ALA:O	1:A:934:ILE:HG22	2.17	0.44
1:C:730:SER:OG	1:C:731:MET:N	2.51	0.44
1:B:326:ILE:HG23	1:B:539:VAL:HG11	1.97	0.44
1:B:452:LEU:HD12	1:B:492:LEU:HG	1.99	0.44
1:B:369:TYR:HB3	1:B:377:PHE:HE1	1.81	0.44
1:C:117:LEU:HD11	1:C:119:ILE:HG13	1.98	0.44
2:F:6:GLU:OE1	2:F:112:GLN:NE2	2.51	0.44
1:A:808:ASP:OD1	1:A:808:ASP:N	2.41	0.44
1:B:461:LEU:HD12	1:B:461:LEU:HA	1.88	0.44
1:C:427:ASP:OD1	1:C:427:ASP:N	2.50	0.44
2:H:8:GLY:HA3	2:H:20:LEU:HA	1.98	0.44
3:L:38:GLN:HE21	3:L:40:ARG:HH22	1.66	0.44
1:B:179:LEU:HD23	1:B:179:LEU:HA	1.87	0.44
3:G:40:ARG:HE	3:G:87:ALA:HB2	1.82	0.44
1:B:490:PHE:HD1	1:B:491:PRO:HD2	1.82	0.44
1:C:366:SER:HA	1:C:369:TYR:CZ	2.53	0.44
3:L:8:HIS:HA	3:L:105:THR:HA	1.99	0.44
1:B:567:ARG:HG3	1:B:568:ASP:H	1.83	0.44
1:B:617:CYS:N	1:B:649:CYS:SG	2.90	0.44
3:L:39:GLN:HA	3:L:45:PRO:HA	1.99	0.44
1:B:406:GLU:HA	1:B:409:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:ASN:OD1	1:C:709:ASN:N	2.50	0.43
1:C:867:ASP:N	1:C:867:ASP:OD1	2.51	0.43
3:G:38:GLN:N	3:G:38:GLN:OE1	2.51	0.43
1:B:427:ASP:OD1	1:B:427:ASP:N	2.51	0.43
1:B:600:PRO:HG2	1:B:605:SER:HB2	2.00	0.43
1:B:728:PRO:O	1:B:1021:SER:OG	2.30	0.43
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	2.01	0.43
1:B:353:TRP:CZ2	1:B:466:ARG:HB3	2.53	0.43
2:F:91:THR:HG22	2:F:118:VAL:H	1.83	0.43
1:C:930:ALA:O	1:C:934:ILE:HG22	2.19	0.43
1:A:403:ARG:HG3	1:A:405:ASP:H	1.83	0.43
1:B:417:LYS:O	1:B:421:TYR:HB2	2.18	0.43
1:C:642:VAL:HG22	1:C:651:ILE:HG12	2.00	0.43
3:G:60:PRO:HD2	3:G:63:PHE:HE2	1.84	0.43
1:C:528:LYS:HA	1:C:528:LYS:HD3	1.68	0.43
1:C:959:LEU:HD12	1:C:959:LEU:HA	1.86	0.43
1:A:66:HIS:HB3	1:A:78:ARG:HG2	2.01	0.43
1:A:490:PHE:HD1	1:A:491:PRO:HD2	1.84	0.43
1:A:1013:ILE:HD13	1:B:1012:LEU:HD13	2.01	0.43
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.99	0.43
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.88	0.43
1:B:768:THR:O	1:B:772:VAL:HG23	2.18	0.43
2:H:40:ALA:HB3	2:H:43:LYS:HB2	2.00	0.43
1:A:691:SER:OG	1:A:692:ILE:N	2.52	0.43
1:C:816:SER:OG	1:C:819:GLU:OE2	2.29	0.43
1:A:127:VAL:HG12	1:A:171:VAL:HG22	2.01	0.43
1:B:1086:LYS:HB2	1:B:1086:LYS:HE2	1.80	0.43
1:C:95:THR:HA	1:C:189:LEU:HA	2.01	0.43
1:C:139:PRO:HB3	1:C:159:VAL:HA	2.00	0.43
1:C:697:MET:H	1:C:697:MET:HG2	1.57	0.43
2:H:47:TRP:HB2	3:L:101:PHE:HE1	1.84	0.43
3:G:56:PRO:HD2	3:G:59:VAL:HG21	2.00	0.43
1:A:24:LEU:HB2	1:A:78:ARG:HD3	2.01	0.42
1:A:498:GLN:HB2	1:A:501:ASN:HB3	2.01	0.42
1:B:470:THR:HG21	1:B:492:LEU:HD22	2.01	0.42
1:B:1041:ASP:HB3	1:C:1030:SER:HB3	2.01	0.42
1:A:117:LEU:HD21	1:A:119:ILE:HG13	2.01	0.42
1:B:245:HIS:HB2	1:B:259:THR:HG23	2.01	0.42
1:B:363:ALA:N	1:B:525:CYS:O	2.50	0.42
1:A:106:PHE:HB2	1:A:117:LEU:HB3	2.00	0.42
1:B:962:LEU:HD23	1:B:962:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:HH22	1:C:217:PRO:HD2	1.83	0.42
1:C:490:PHE:HD1	1:C:491:PRO:HD2	1.84	0.42
1:B:825:LYS:HD2	1:B:825:LYS:HA	1.81	0.42
1:A:276:LEU:HB3	1:A:289:VAL:HG23	2.01	0.42
1:A:713:ALA:HB3	1:B:894:LEU:HB3	2.01	0.42
1:B:886:TRP:HB3	1:B:1035:GLY:HA2	2.01	0.42
1:C:133:PHE:HB2	1:C:135:PHE:CZ	2.54	0.42
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.78	0.42
1:C:805:ILE:HD12	1:C:878:LEU:HD21	2.00	0.42
1:B:197:ILE:HD12	1:B:197:ILE:HA	1.87	0.42
1:C:119:ILE:HG12	1:C:128:ILE:HG12	2.02	0.42
1:C:727:LEU:HD23	1:C:727:LEU:HA	1.91	0.42
1:A:662:CYS:HB2	1:A:671:CYS:HB2	1.74	0.42
1:A:709:ASN:OD1	1:A:709:ASN:N	2.51	0.42
1:B:332:ILE:HG23	1:B:362:VAL:HG22	2.00	0.42
1:B:730:SER:OG	1:B:731:MET:N	2.53	0.42
1:C:364:ASP:OD1	1:C:366:SER:OG	2.33	0.42
3:L:37:TYR:HE2	3:L:92:GLN:HG3	1.85	0.42
1:A:886:TRP:HB3	1:A:1035:GLY:HA2	2.01	0.42
1:A:663:ASP:OD1	1:A:663:ASP:N	2.44	0.42
1:C:418:ILE:HA	1:C:422:ASN:HB2	2.01	0.42
2:H:36:TRP:HE1	2:H:79:LEU:HD22	1.85	0.42
1:C:24:LEU:HD12	1:C:78:ARG:HD3	2.02	0.41
2:H:22:CYS:HB3	2:H:79:LEU:HD13	2.01	0.41
1:A:388:ASN:HB3	1:A:527:PRO:HD2	2.02	0.41
1:A:106:PHE:HB3	1:A:235:ILE:HD12	2.02	0.41
1:B:156:GLU:OE1	1:B:158:ARG:NE	2.43	0.41
1:C:57:PRO:HB3	1:C:273:ARG:NH1	2.35	0.41
3:L:60:PRO:HD2	3:L:63:PHE:HE2	1.84	0.41
1:B:336:CYS:N	1:B:361:CYS:HB2	2.36	0.41
1:C:37:TYR:HB3	1:C:223:LEU:HB2	2.02	0.41
2:H:19:ARG:NH1	2:H:80:TYR:HA	2.34	0.41
1:A:909:ILE:HG13	1:A:911:VAL:HG12	2.03	0.41
1:B:934:ILE:HG13	1:B:935:GLN:N	2.36	0.41
1:C:92:PHE:HB3	1:C:192:PHE:HB2	2.02	0.41
1:C:351:TYR:HA	1:C:454:ARG:NH2	2.35	0.41
1:C:553:THR:OG1	1:C:586:ASP:OD2	2.39	0.41
1:C:733:LYS:HB2	1:C:861:LEU:HB2	2.03	0.41
1:B:57:PRO:HB3	1:B:273:ARG:HH22	1.86	0.41
1:C:417:LYS:O	1:C:421:TYR:HB2	2.21	0.41
1:A:76:THR:OG1	1:A:77:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:ILE:HB	1:B:609:ALA:HB3	2.02	0.41
1:C:656:VAL:HG12	1:C:658:ASN:H	1.86	0.41
1:B:418:ILE:H	1:B:418:ILE:HG12	1.75	0.41
1:B:745:ASP:OD2	1:B:745:ASP:N	2.54	0.41
1:C:76:THR:OG1	1:C:77:LYS:N	2.53	0.41
1:C:130:VAL:HG11	1:C:231:ILE:HG12	2.02	0.41
1:C:1105:THR:HG22	1:C:1112:PRO:HA	2.03	0.41
1:A:599:THR:HG22	1:A:601:GLY:H	1.86	0.41
1:A:757:GLY:O	1:A:761:THR:OG1	2.34	0.41
1:C:134:GLN:HB3	1:C:162:SER:H	1.86	0.41
1:C:276:LEU:HD23	1:C:289:VAL:HB	2.03	0.41
1:C:369:TYR:HB3	1:C:377:PHE:HE2	1.85	0.41
3:L:92:GLN:NE2	3:L:99:TRP:HB3	2.26	0.41
3:G:8:HIS:HA	3:G:105:THR:HA	2.02	0.41
3:G:64:SER:HB2	3:G:77:THR:OG1	2.21	0.41
1:A:102:ARG:HG3	1:A:141:LEU:HD12	2.02	0.40
1:A:173:GLN:H	1:A:173:GLN:HG3	1.70	0.40
1:B:564:GLN:HG2	1:B:577:ARG:HB3	2.02	0.40
2:F:54:ASP:OD1	2:F:54:ASP:N	2.52	0.40
1:A:563:GLN:NE2	1:B:42:VAL:O	2.54	0.40
1:A:805:ILE:HB	1:A:878:LEU:HD11	2.02	0.40
1:A:959:LEU:HA	1:A:959:LEU:HD12	1.87	0.40
1:B:210:ILE:HD12	1:B:210:ILE:HA	2.00	0.40
1:B:302:THR:HG21	1:B:315:THR:HG22	2.02	0.40
1:B:564:GLN:HG3	1:B:579:PRO:HG3	2.04	0.40
3:L:50:TYR:CE1	3:L:54:GLN:HB3	2.56	0.40
2:F:61:VAL:HG22	2:F:64:VAL:HG22	2.03	0.40
1:B:117:LEU:HD12	1:B:118:LEU:N	2.36	0.40
1:A:201:PHE:C	1:A:202:LYS:HD3	2.41	0.40
1:A:702:GLU:HG2	1:B:788:ILE:HD11	2.03	0.40
1:A:743:CYS:SG	1:A:753:LEU:HD12	2.61	0.40
1:B:246:ARG:HH22	1:B:254:SER:HB3	1.86	0.40
1:C:1073:LYS:HB3	1:C:1073:LYS:HE2	1.75	0.40
1:B:68:ILE:HG13	1:B:262:ALA:HA	2.04	0.40
1:C:759:PHE:O	1:C:763:LEU:HG	2.22	0.40
1:C:880:GLY:O	1:C:884:SER:OG	2.28	0.40
2:H:47:TRP:CG	3:L:99:TRP:HB2	2.56	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	1054/1278 (82%)	1020 (97%)	34 (3%)	0	100	100
1	B	1054/1278 (82%)	1019 (97%)	35 (3%)	0	100	100
1	C	1054/1278 (82%)	1016 (96%)	38 (4%)	0	100	100
2	F	117/243 (48%)	110 (94%)	7 (6%)	0	100	100
2	H	117/243 (48%)	109 (93%)	8 (7%)	0	100	100
3	G	108/240 (45%)	98 (91%)	10 (9%)	0	100	100
3	L	108/240 (45%)	100 (93%)	8 (7%)	0	100	100
All	All	3612/4800 (75%)	3472 (96%)	140 (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	930/1106 (84%)	909 (98%)	21 (2%)	50	77
1	B	930/1106 (84%)	893 (96%)	37 (4%)	31	63
1	C	930/1106 (84%)	906 (97%)	24 (3%)	46	74
2	F	96/203 (47%)	93 (97%)	3 (3%)	40	70
2	H	96/203 (47%)	96 (100%)	0	100	100
3	G	95/206 (46%)	92 (97%)	3 (3%)	39	69
3	L	95/206 (46%)	88 (93%)	7 (7%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3172/4136 (77%)	3077 (97%)	95 (3%)	44 71

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	66	HIS
1	A	79	PHE
1	A	130	VAL
1	A	135	PHE
1	A	136	CYS
1	A	166	CYS
1	A	167	THR
1	A	238	PHE
1	A	301	CYS
1	A	408	ARG
1	A	427	ASP
1	A	490	PHE
1	A	515	PHE
1	A	559	PHE
1	A	745	ASP
1	A	854	LYS
1	A	922	LEU
1	A	977	LEU
1	A	1005	GLN
1	A	1141	LEU
1	B	21	ARG
1	B	40	ASP
1	B	133	PHE
1	B	136	CYS
1	B	138	ASP
1	B	201	PHE
1	B	205	SER
1	B	215	ASP
1	B	229	LEU
1	B	234	ASN
1	B	301	CYS
1	B	328	ARG
1	B	359	SER
1	B	365	TYR
1	B	385	THR
1	B	386	LYS

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Mol	Chain	Res	Type
1	B	389	ASP
1	B	392	PHE
1	B	400	PHE
1	B	405	ASP
1	B	406	GLU
1	B	408	ARG
1	B	410	ILE
1	B	427	ASP
1	B	490	PHE
1	B	497	PHE
1	B	529	LYS
1	B	543	PHE
1	B	546	LEU
1	B	563	GLN
1	B	590	CYS
1	B	697	MET
1	B	816	SER
1	B	823	PHE
1	B	856	ASN
1	B	974	SER
1	B	1037	SER
1	C	21	ARG
1	C	34	ARG
1	C	88	ASP
1	C	140	PHE
1	C	145	TYR
1	C	168	PHE
1	C	200	TYR
1	C	242	LEU
1	C	294	ASP
1	C	408	ARG
1	C	427	ASP
1	C	490	PHE
1	C	524	VAL
1	C	528	LYS
1	C	543	PHE
1	C	558	LYS
1	C	562	PHE
1	C	662	CYS
1	C	737	ASP
1	C	745	ASP
1	C	814	LYS

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Mol	Chain	Res	Type
1	C	873	TYR
1	C	1041	ASP
1	C	1126	CYS
3	L	22	CYS
3	L	40	ARG
3	L	43	SER
3	L	48	VAL
3	L	53	ASN
3	L	54	GLN
3	L	94	TYR
2	F	13	GLN
2	F	21	SER
2	F	25	SER
3	G	22	CYS
3	G	92	GLN
3	G	94	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	804	GLN
1	A	935	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)

30 monosaccharides are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.41	0	17,19,21	0.69	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	E	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	I	1	4,1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	I	2	4	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	J	1	4,1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	J	2	4	14,14,15	0.29	0	17,19,21	0.41	0
4	NAG	K	1	4,1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	M	1	4,1	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	M	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	N	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	N	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	O	1	4,1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	P	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	P	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	Q	1	4,1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	Q	2	4	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	R	1	4,1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	R	2	4	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	S	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	S	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	T	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	T	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	U	1	4,1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	U	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	V	1	4,1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	V	2	4	14,14,15	0.25	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	K	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

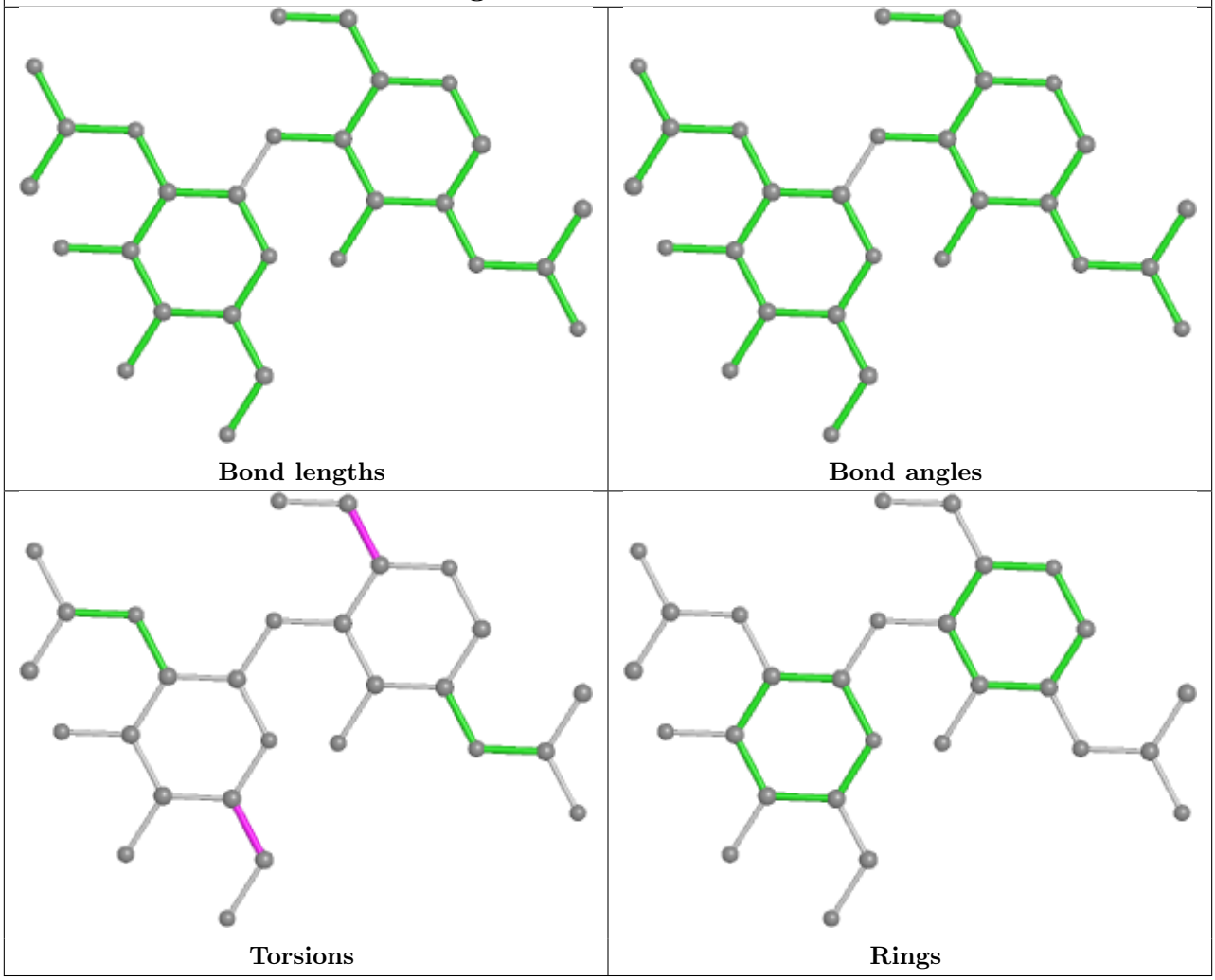
There are no ring outliers.

1 monomer is involved in 1 short contact:

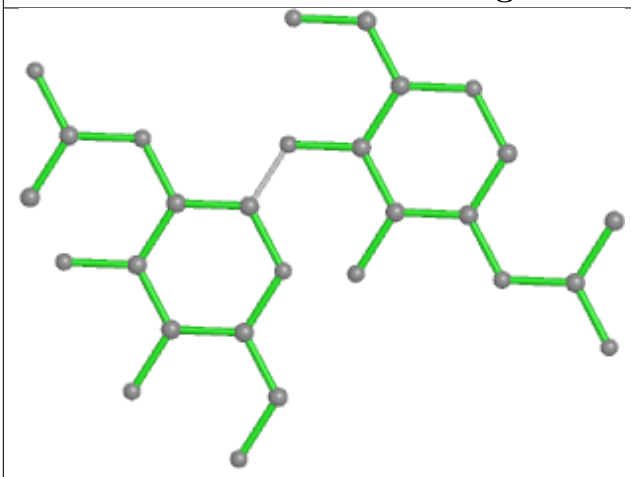
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	1	0

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

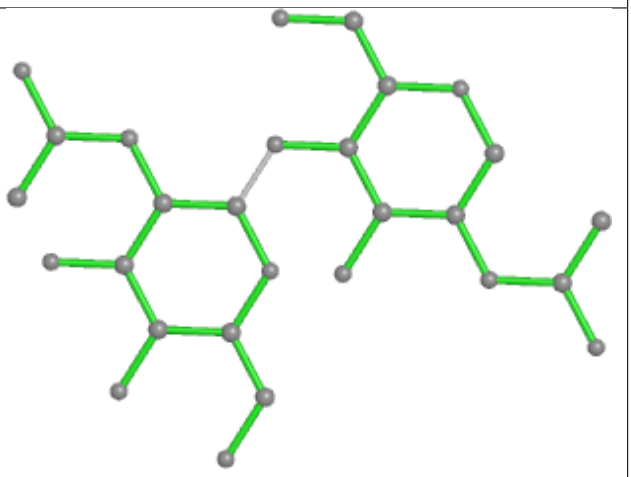
Oligosaccharide Chain D



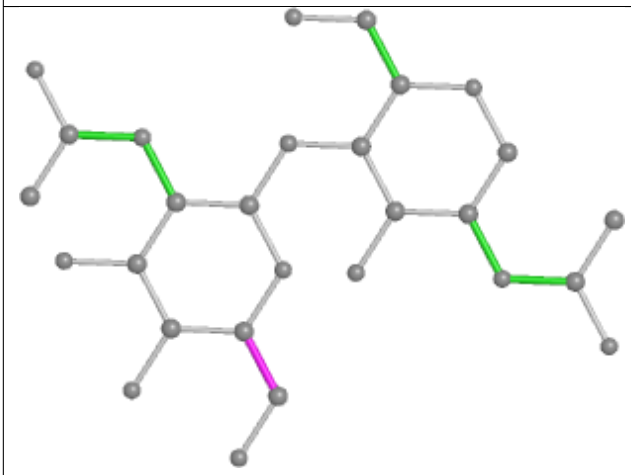
Oligosaccharide Chain E



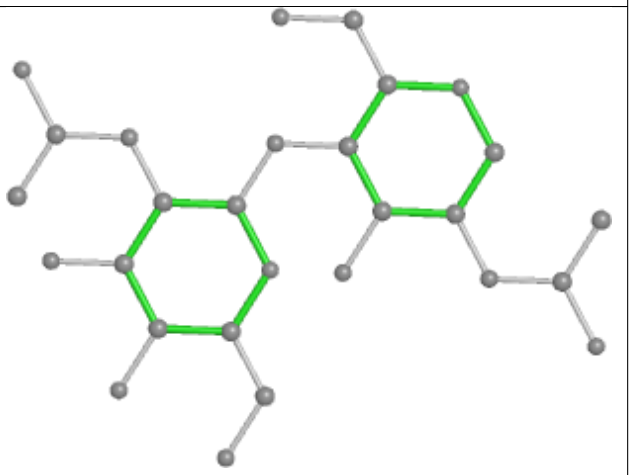
Bond lengths



Bond angles

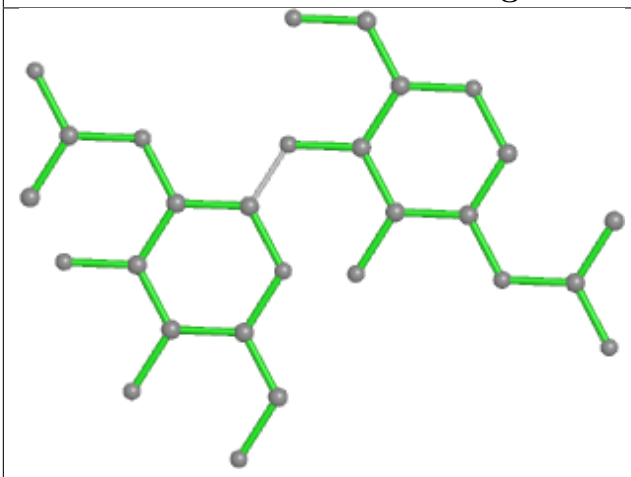


Torsions

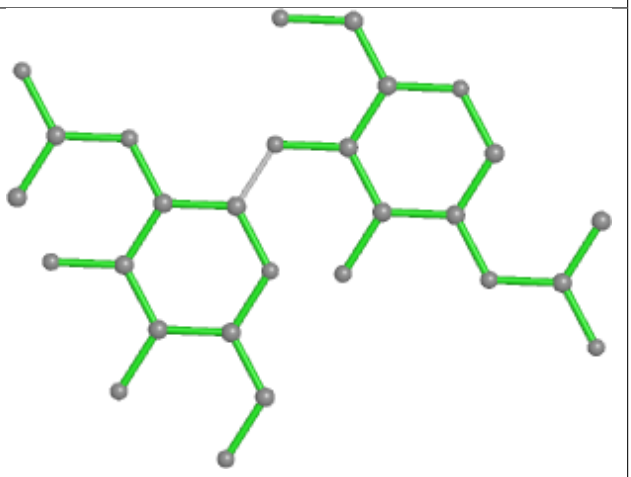


Rings

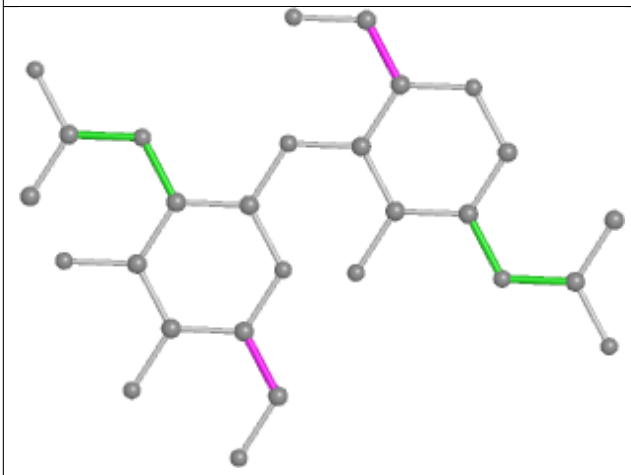
Oligosaccharide Chain I



Bond lengths



Bond angles



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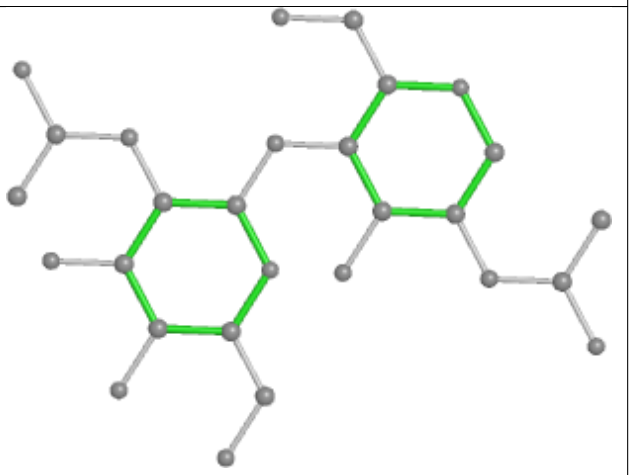
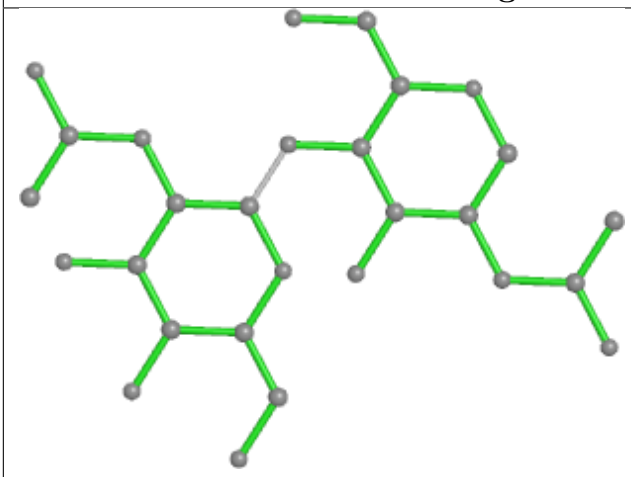
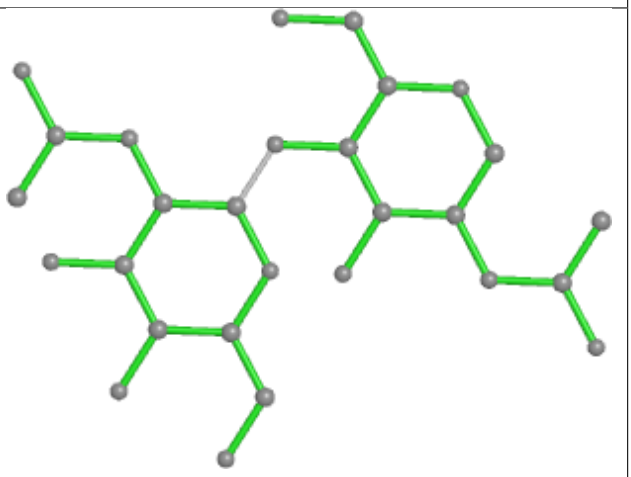


Rings

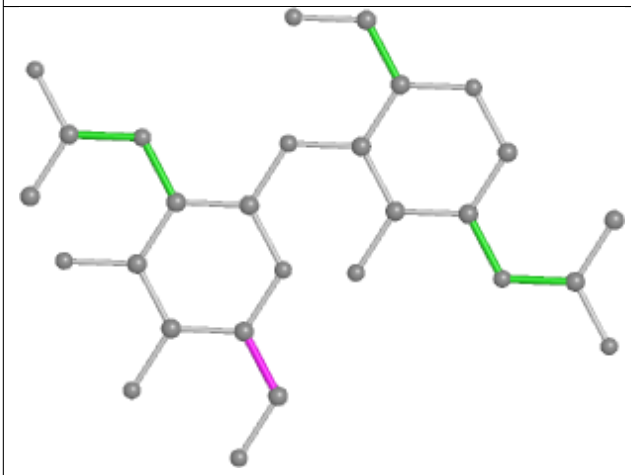
Oligosaccharide Chain J



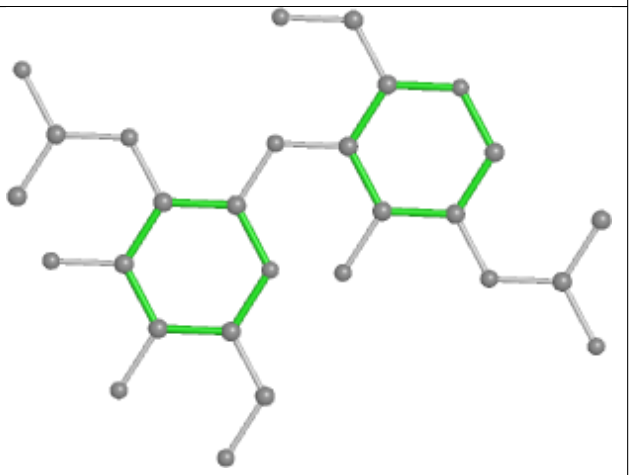
Bond lengths



Bond angles

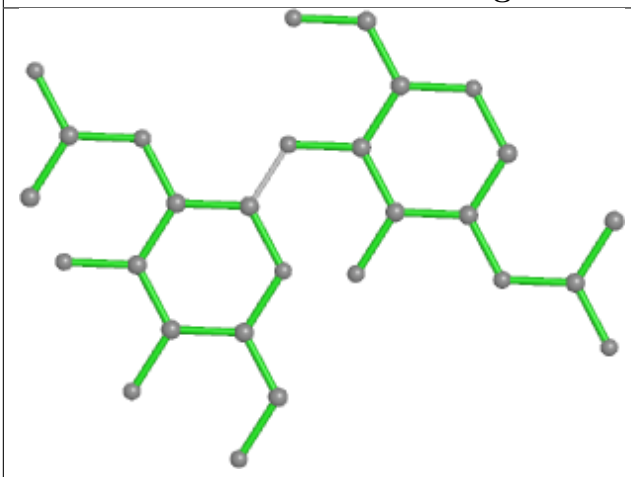


Torsions

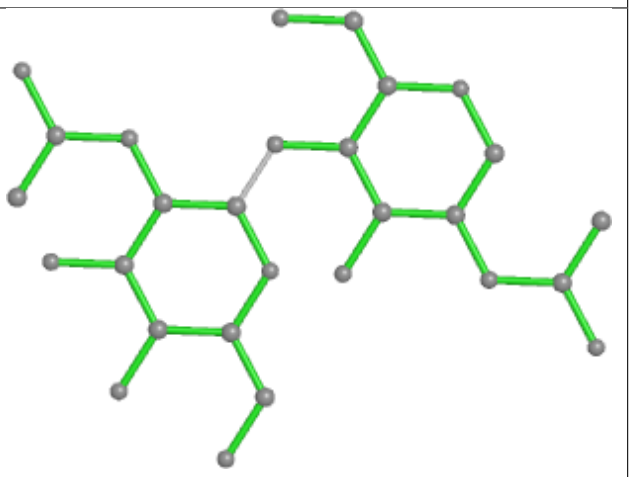


Rings

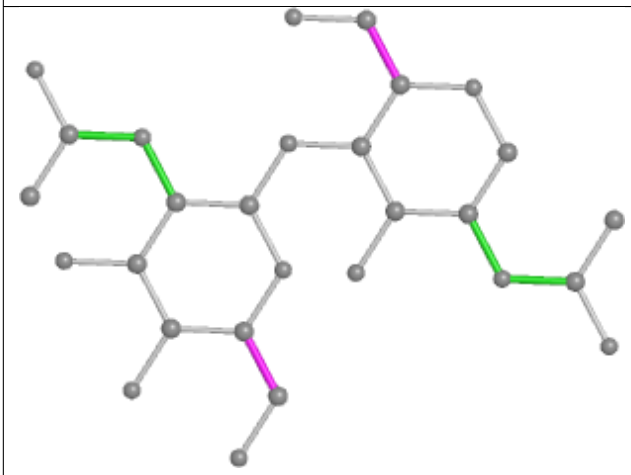
Oligosaccharide Chain K



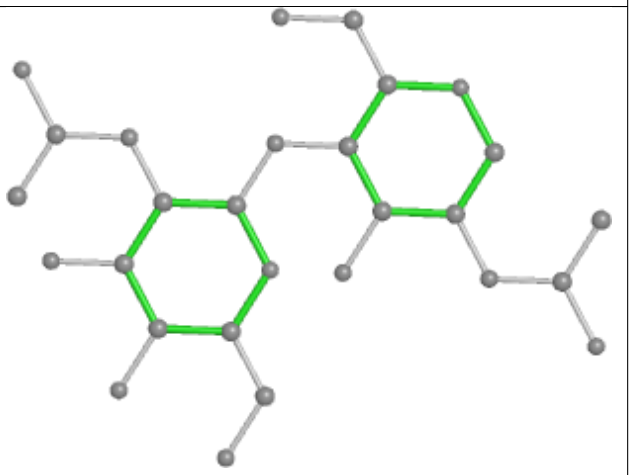
Bond lengths



Bond angles

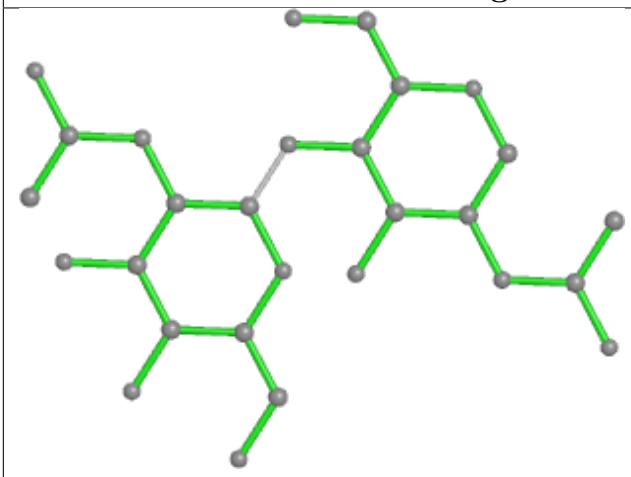


Torsions

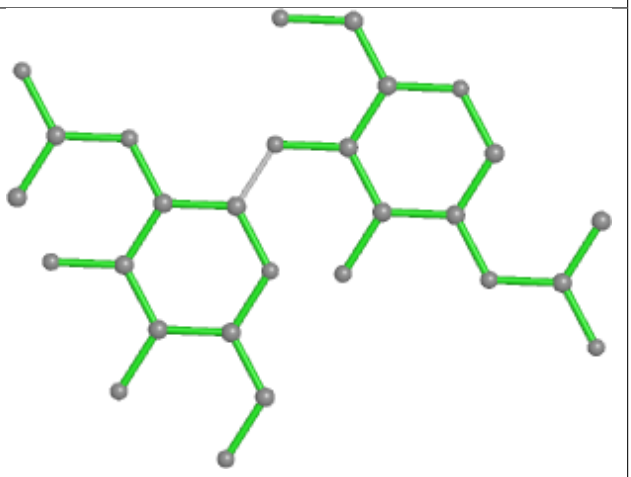


Rings

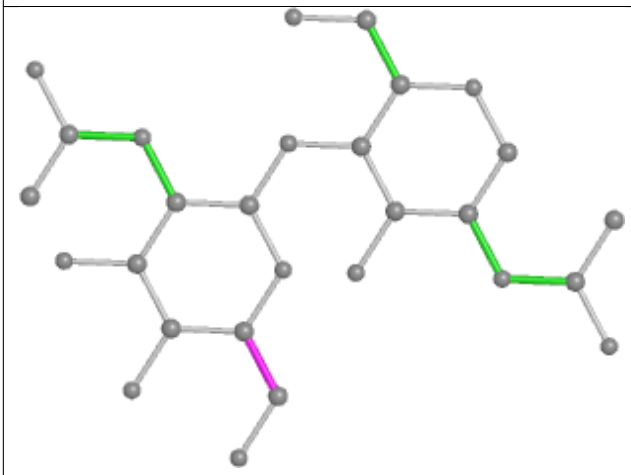
Oligosaccharide Chain M



Bond lengths



Bond angles



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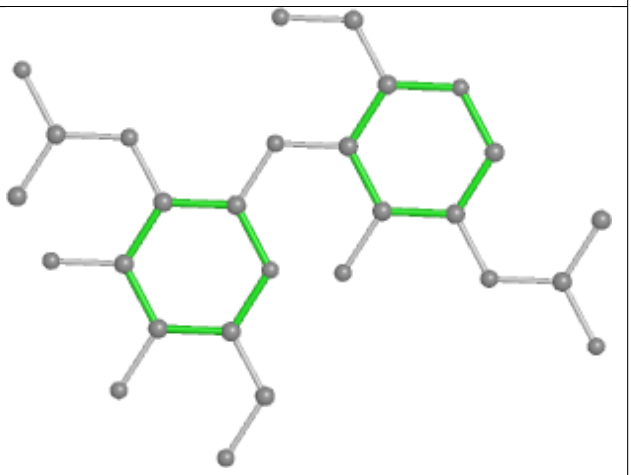
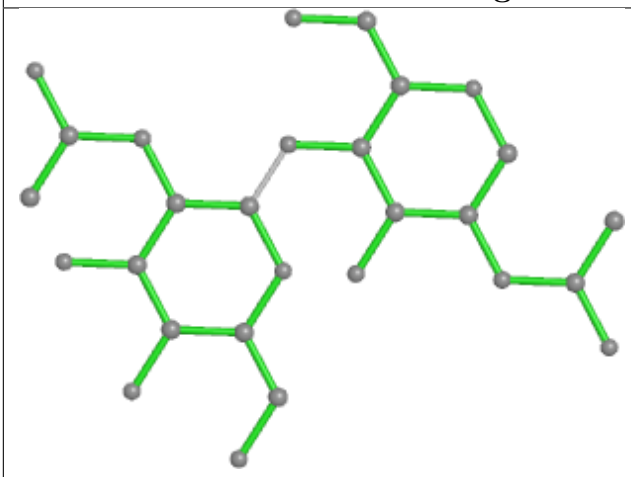
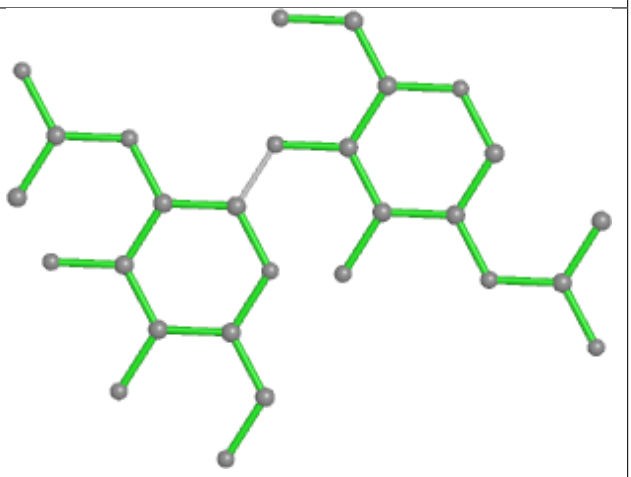


Rings

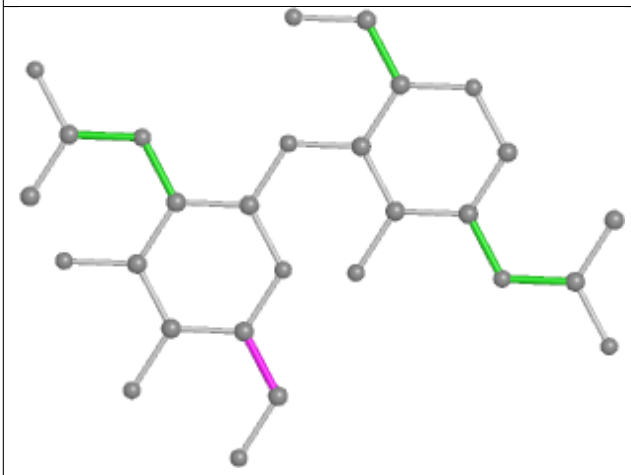
Oligosaccharide Chain N



Bond lengths



Bond angles



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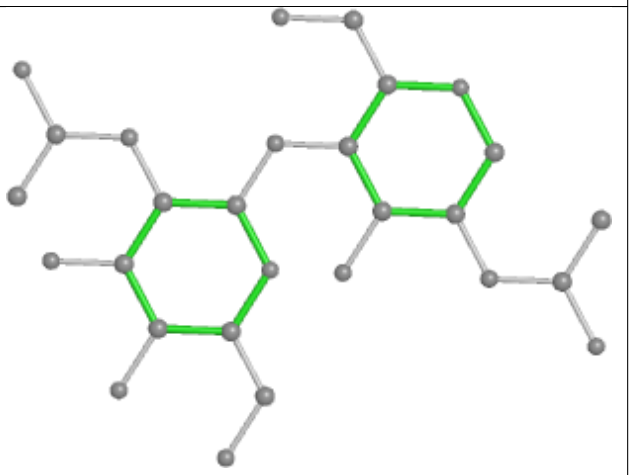
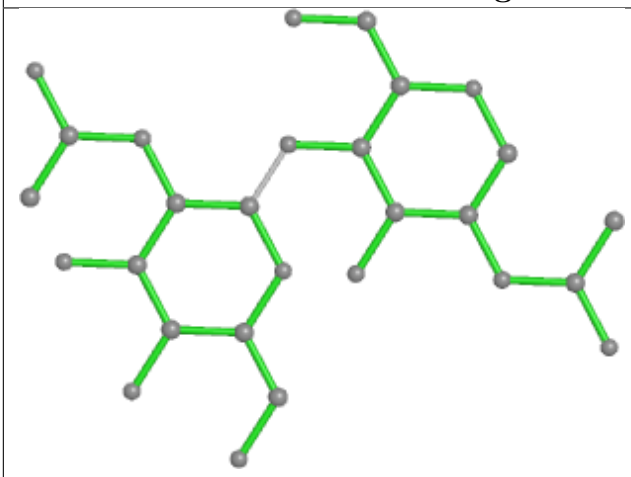
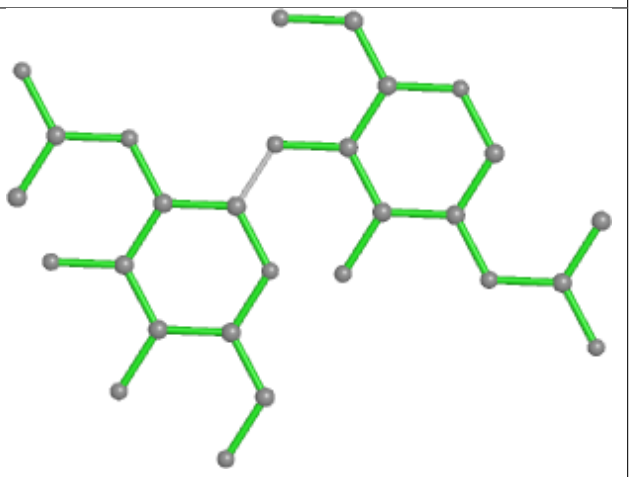


Rings

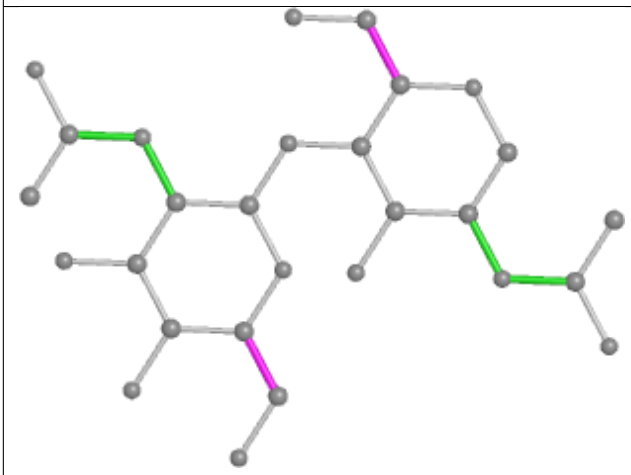
Oligosaccharide Chain O



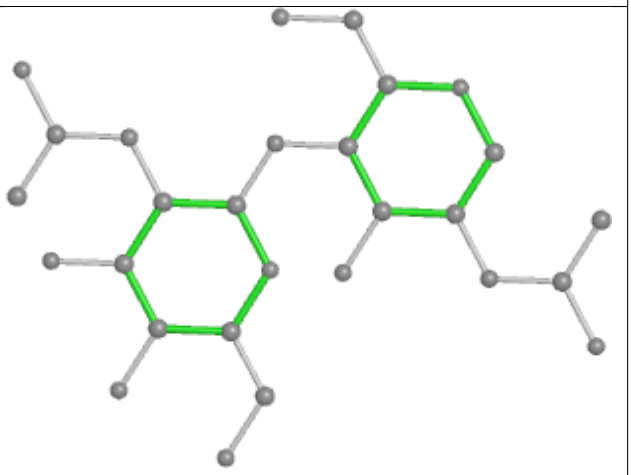
Bond lengths



Bond angles

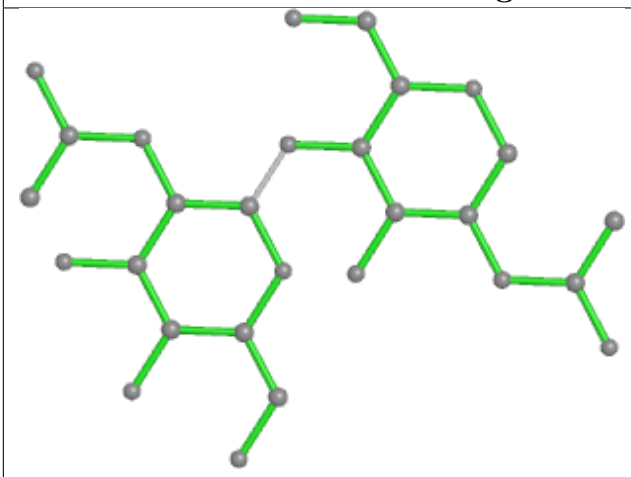


Torsions

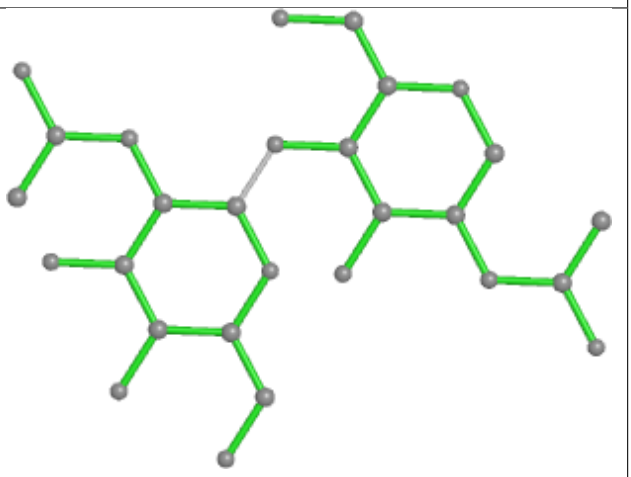


Rings

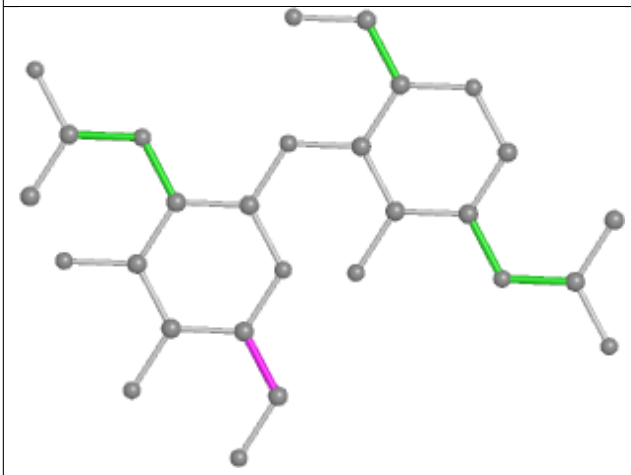
Oligosaccharide Chain P



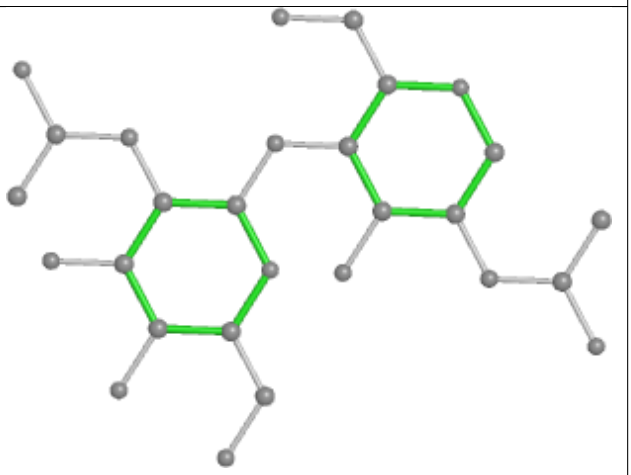
Bond lengths



Bond angles

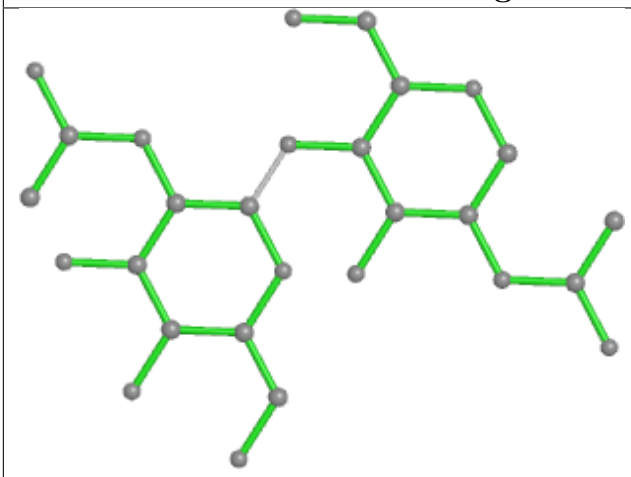


Torsions



Rings

Oligosaccharide Chain Q



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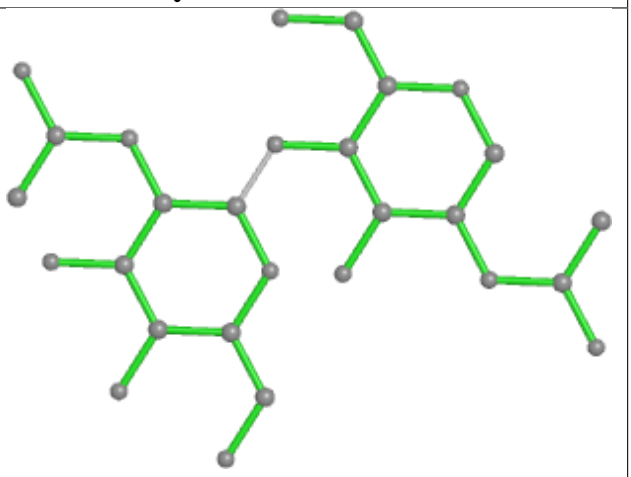
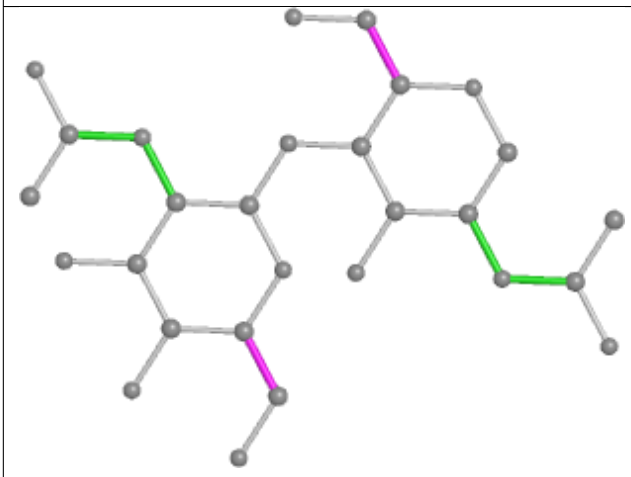
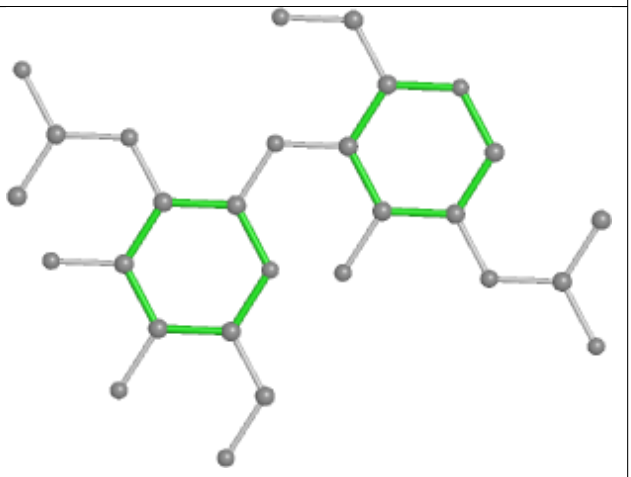


Bond angles

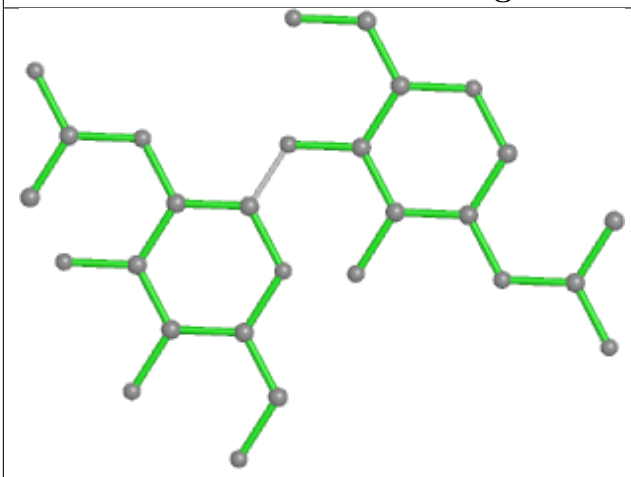


Torsions

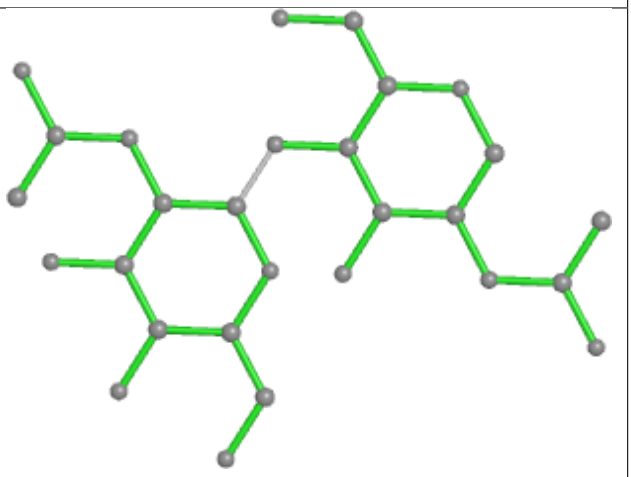


Rings

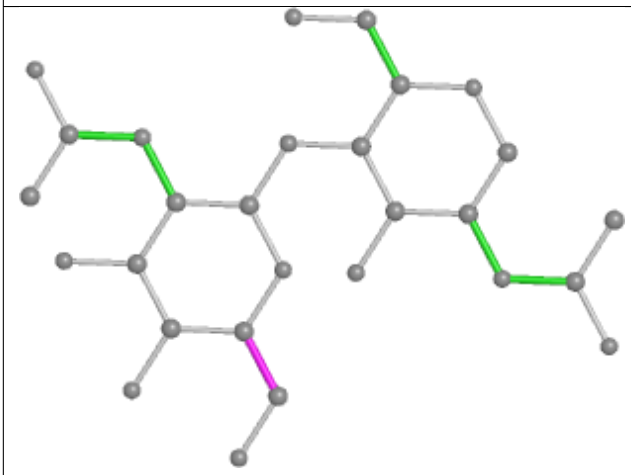
Oligosaccharide Chain R



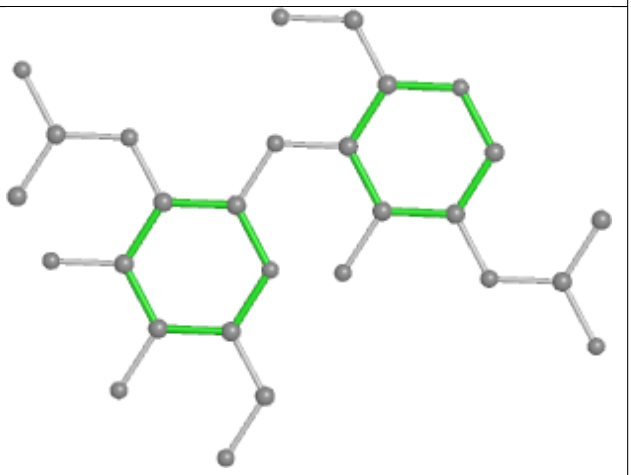
Bond lengths



Bond angles

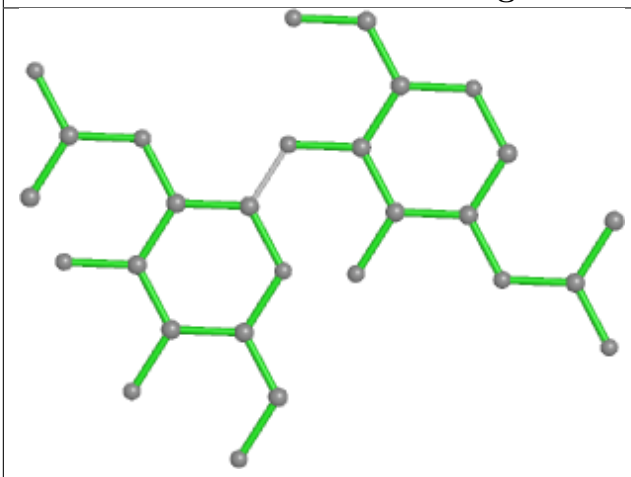


Torsions

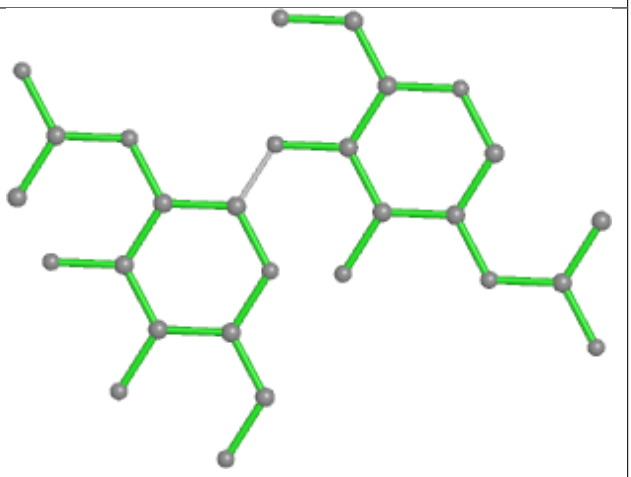


Rings

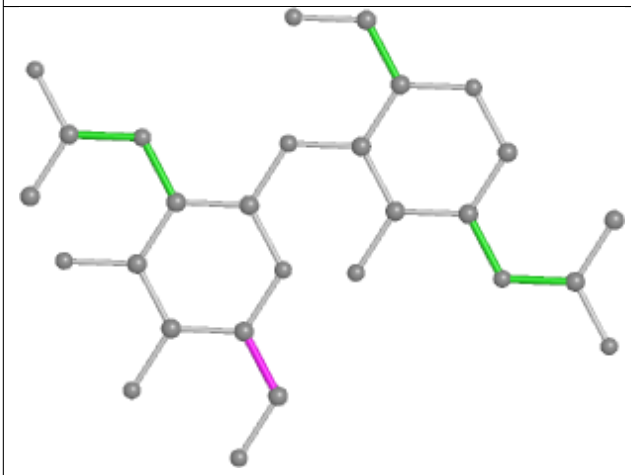
Oligosaccharide Chain S



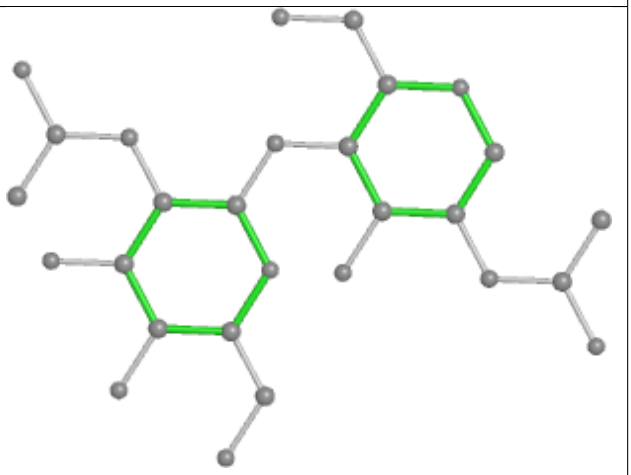
Bond lengths



Bond angles

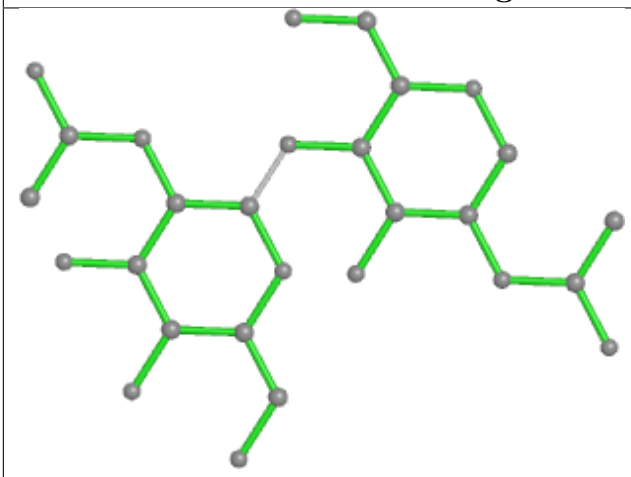


Torsions

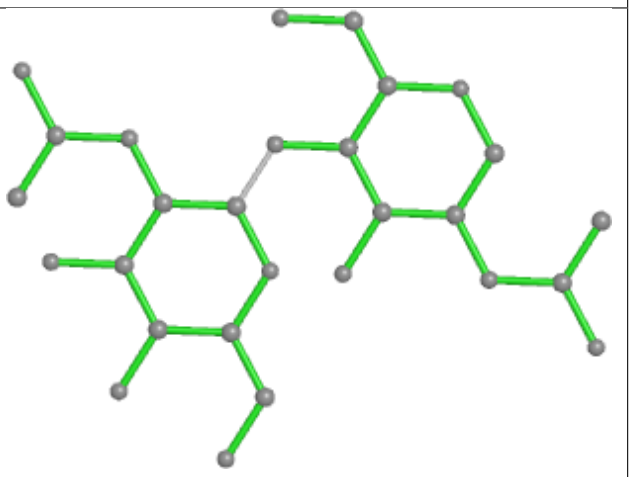


Rings

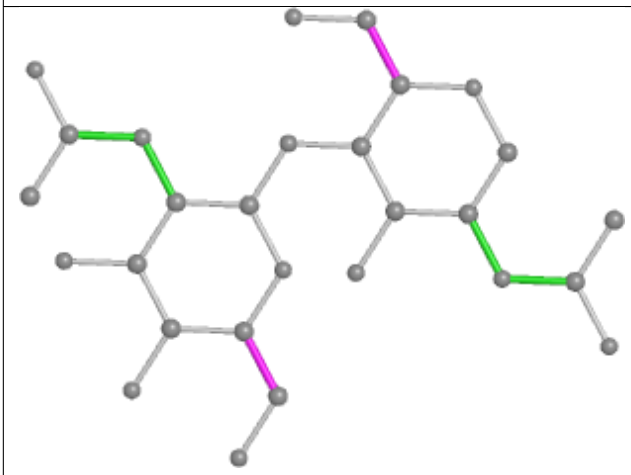
Oligosaccharide Chain T



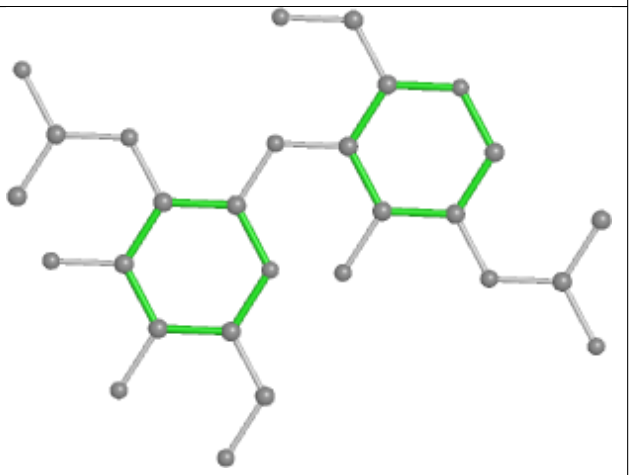
Bond lengths



Bond angles

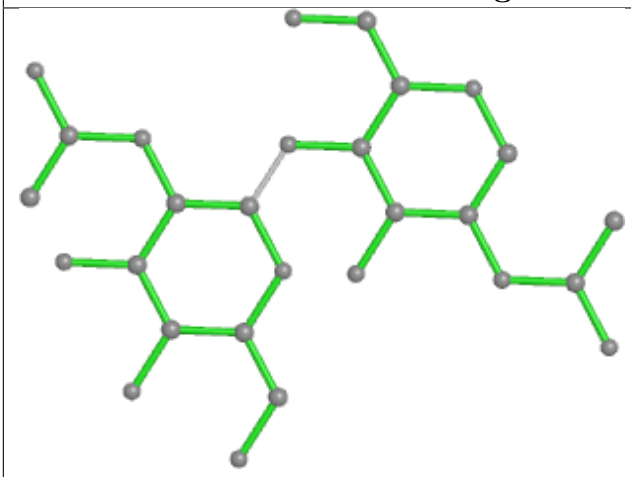


Torsions

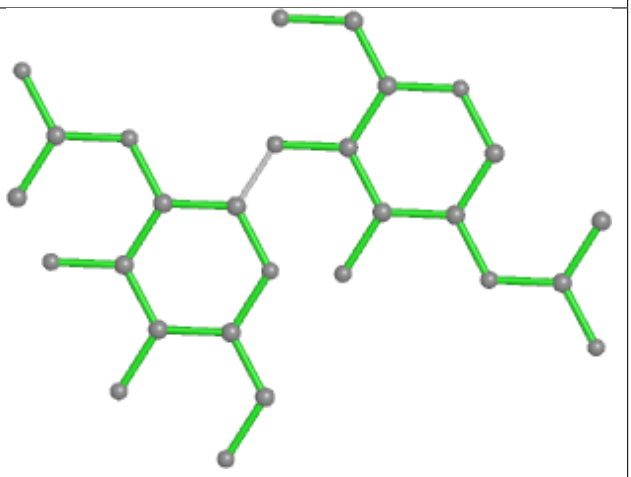


Rings

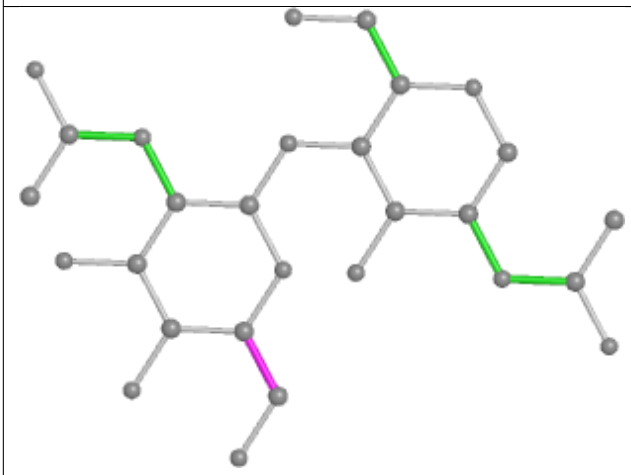
Oligosaccharide Chain U



Bond lengths



Bond angles



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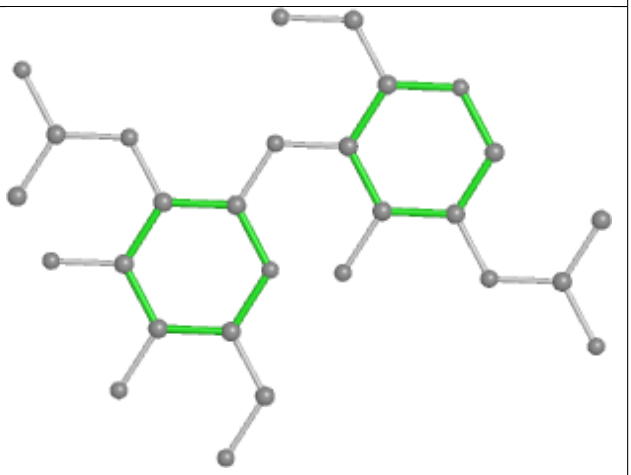
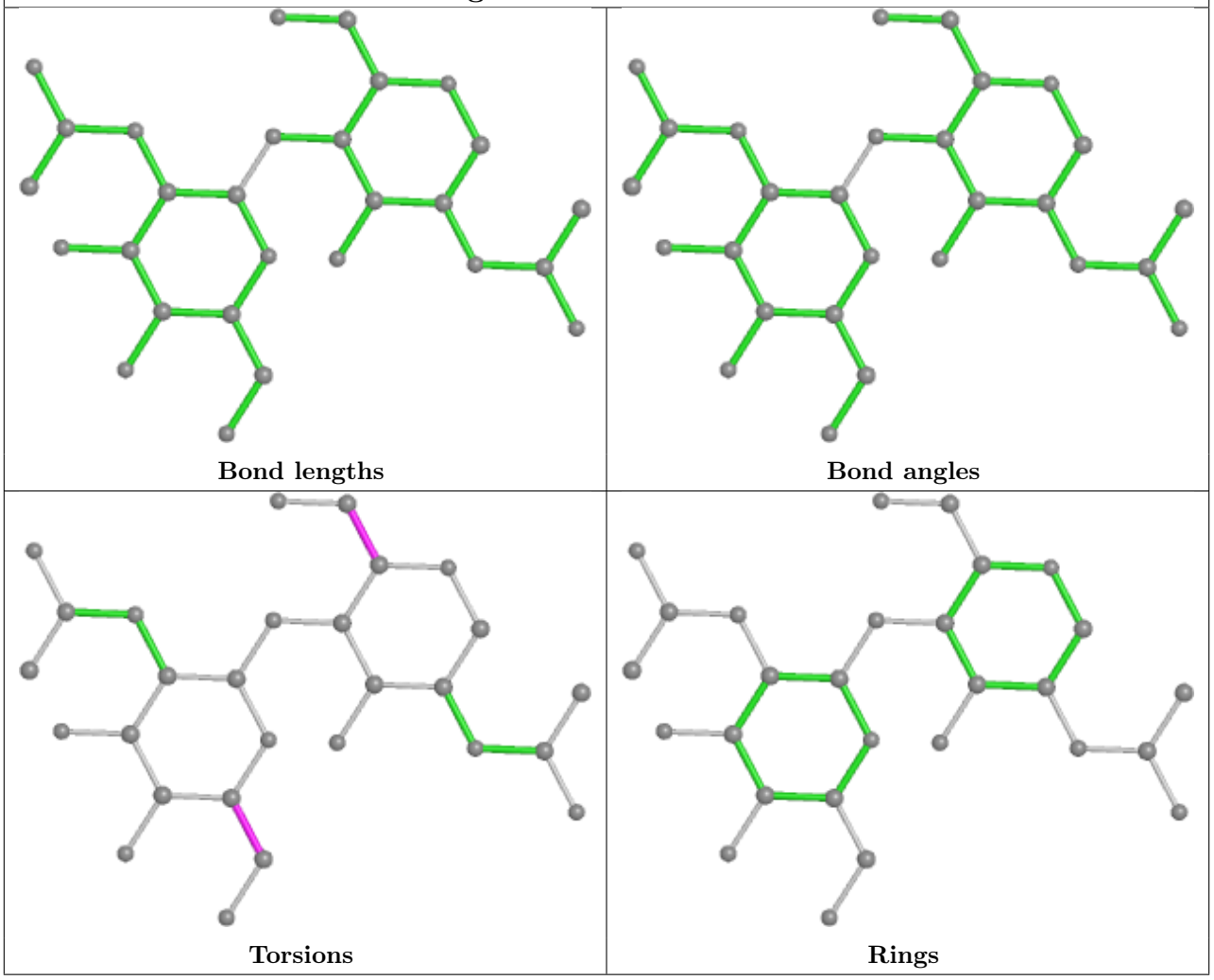


Rings

Oligosaccharide Chain V



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	$\#\|Z\| > 2$
5	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	B	1307	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	B	1301	1	14,14,15	0.45	0	17,19,21	0.44	0
5	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	A	1307	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	C	1309	1	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	C	1301	1	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	C	1305	1	14,14,15	0.30	0	17,19,21	0.48	0
5	NAG	B	1309	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	C	1310	1	14,14,15	0.45	0	17,19,21	0.40	0
5	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.49	0
5	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.38	0
5	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	A	1303	1	14,14,15	0.45	0	17,19,21	0.46	0
5	NAG	A	1309	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	A	1301	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	C	1304	1	14,14,15	0.29	0	17,19,21	0.43	0
5	NAG	B	1306	1	14,14,15	0.41	0	17,19,21	0.63	1 (5%)
5	NAG	B	1308	1	14,14,15	0.56	0	17,19,21	0.51	0
5	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.37	0
5	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	C	1302	1	14,14,15	0.54	0	17,19,21	0.42	0

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

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1306	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	C4-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1305	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

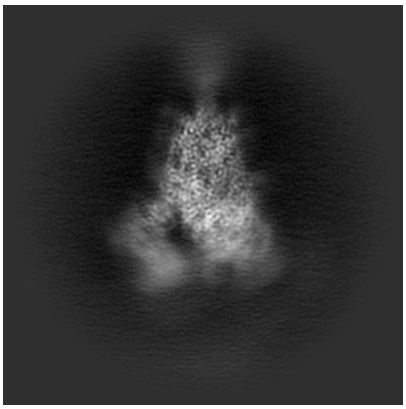
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60099. These allow visual inspection of the internal detail of the map and identification of artifacts.

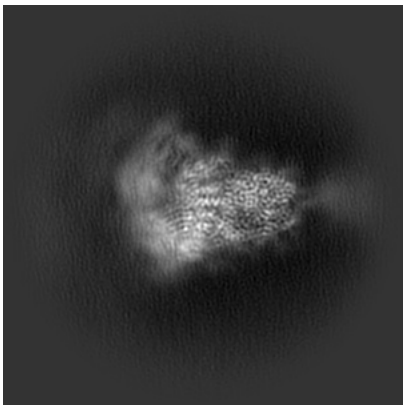
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

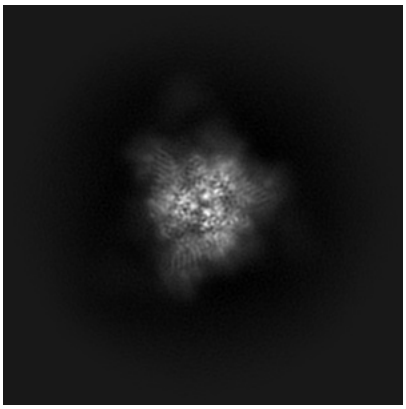
6.1.1 Primary map



X

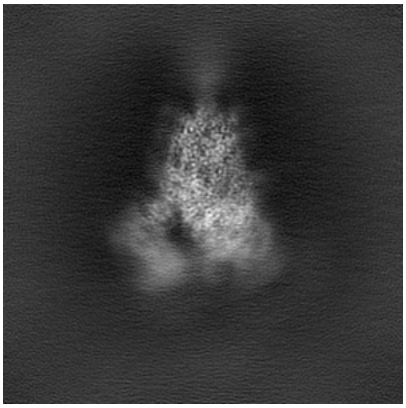


Y

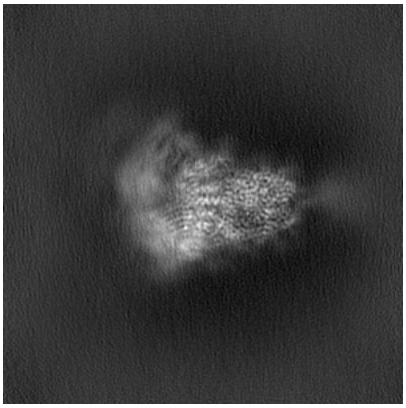


Z

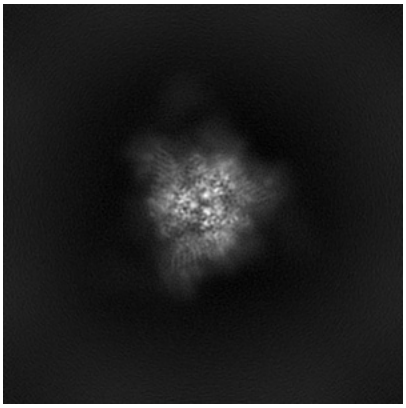
6.1.2 Raw map



X



Y

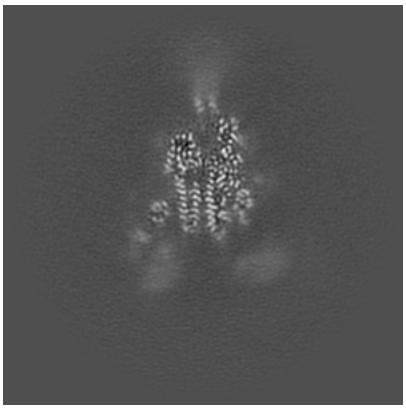


Z

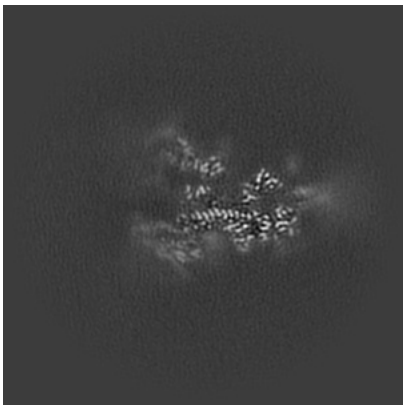
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

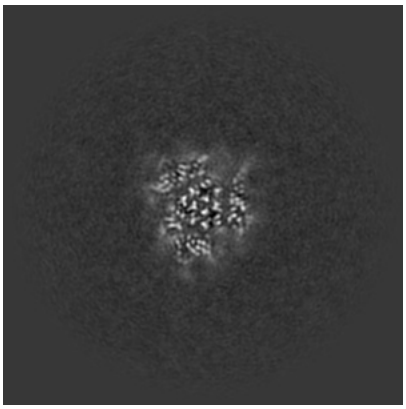
6.2.1 Primary map



X Index: 128

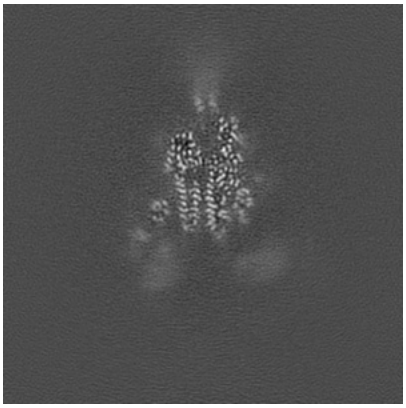


Y Index: 128

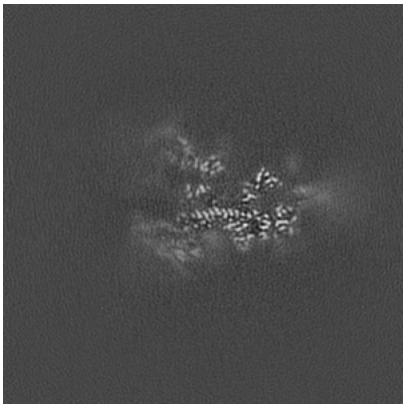


Z Index: 128

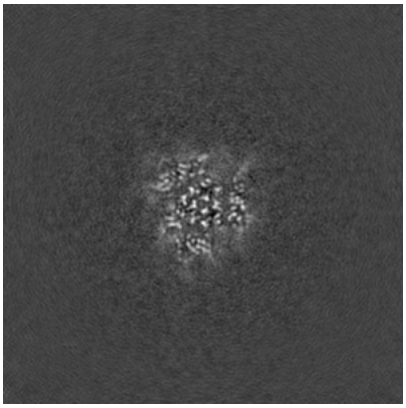
6.2.2 Raw map



X Index: 128



Y Index: 128

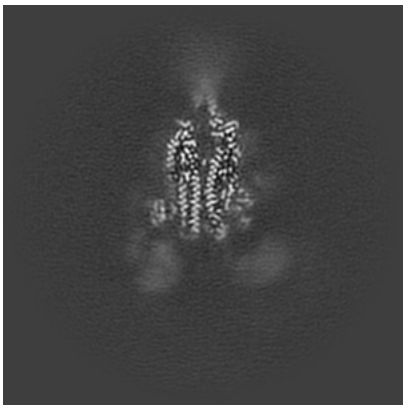


Z Index: 128

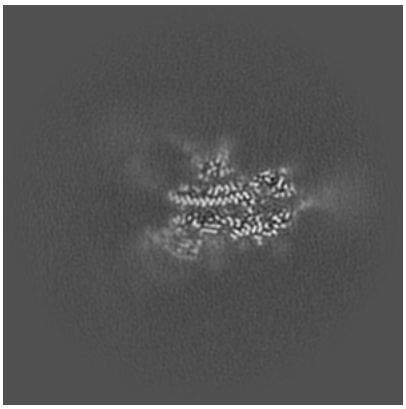
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

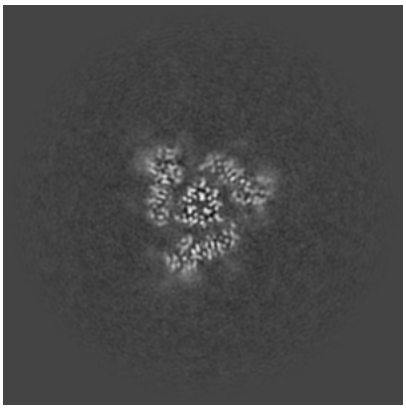
6.3.1 Primary map



X Index: 130

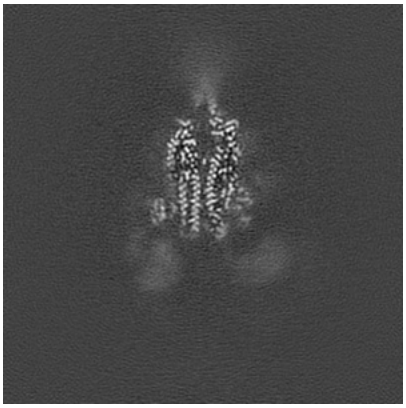


Y Index: 123

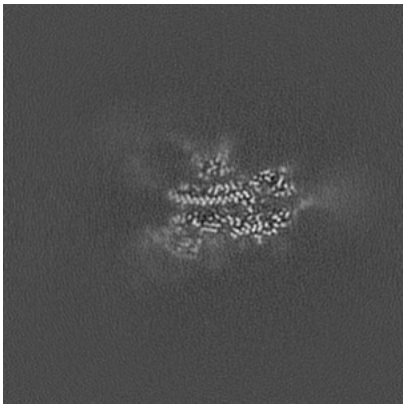


Z Index: 119

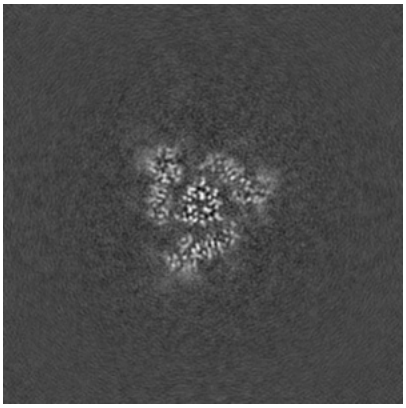
6.3.2 Raw map



X Index: 130



Y Index: 123

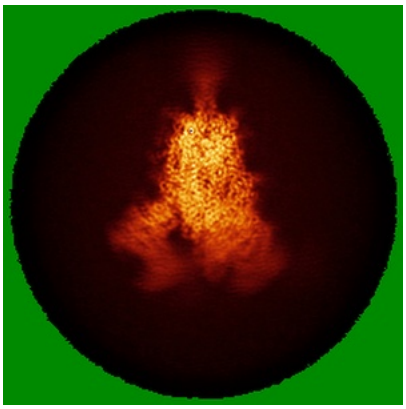


Z Index: 119

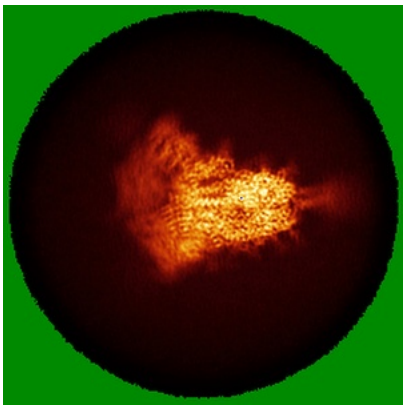
The images above show the largest variance slices of the map in three orthogonal directions.

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

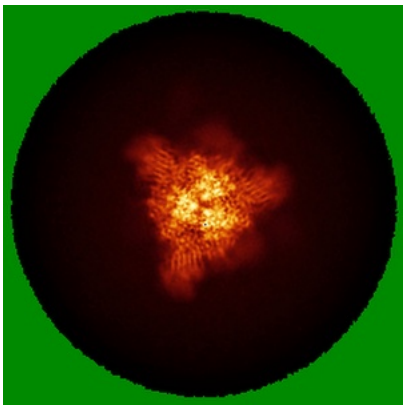
6.4.1 Primary map



X

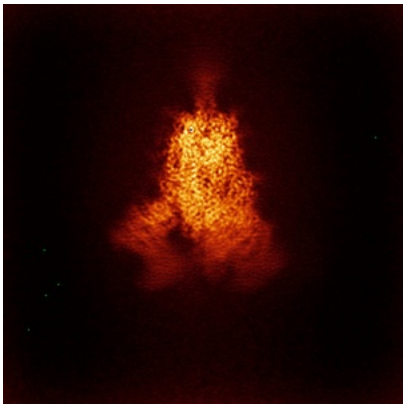


Y

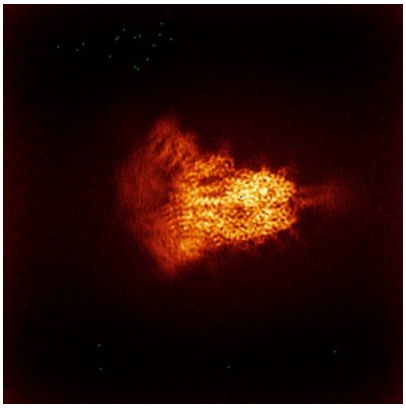


Z

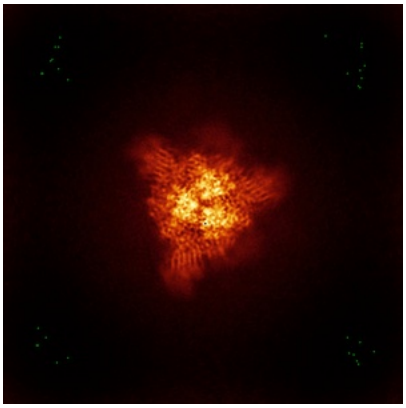
6.4.2 Raw map



X



Y

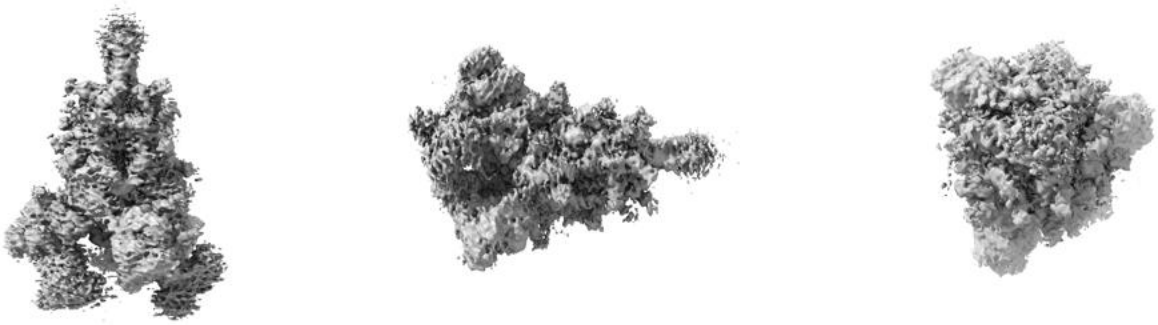


Z

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

6.5 Orthogonal surface views (i)

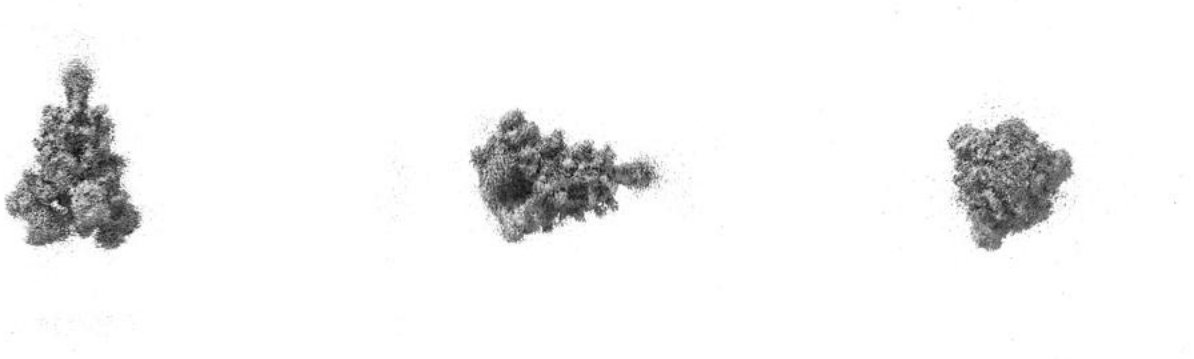
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

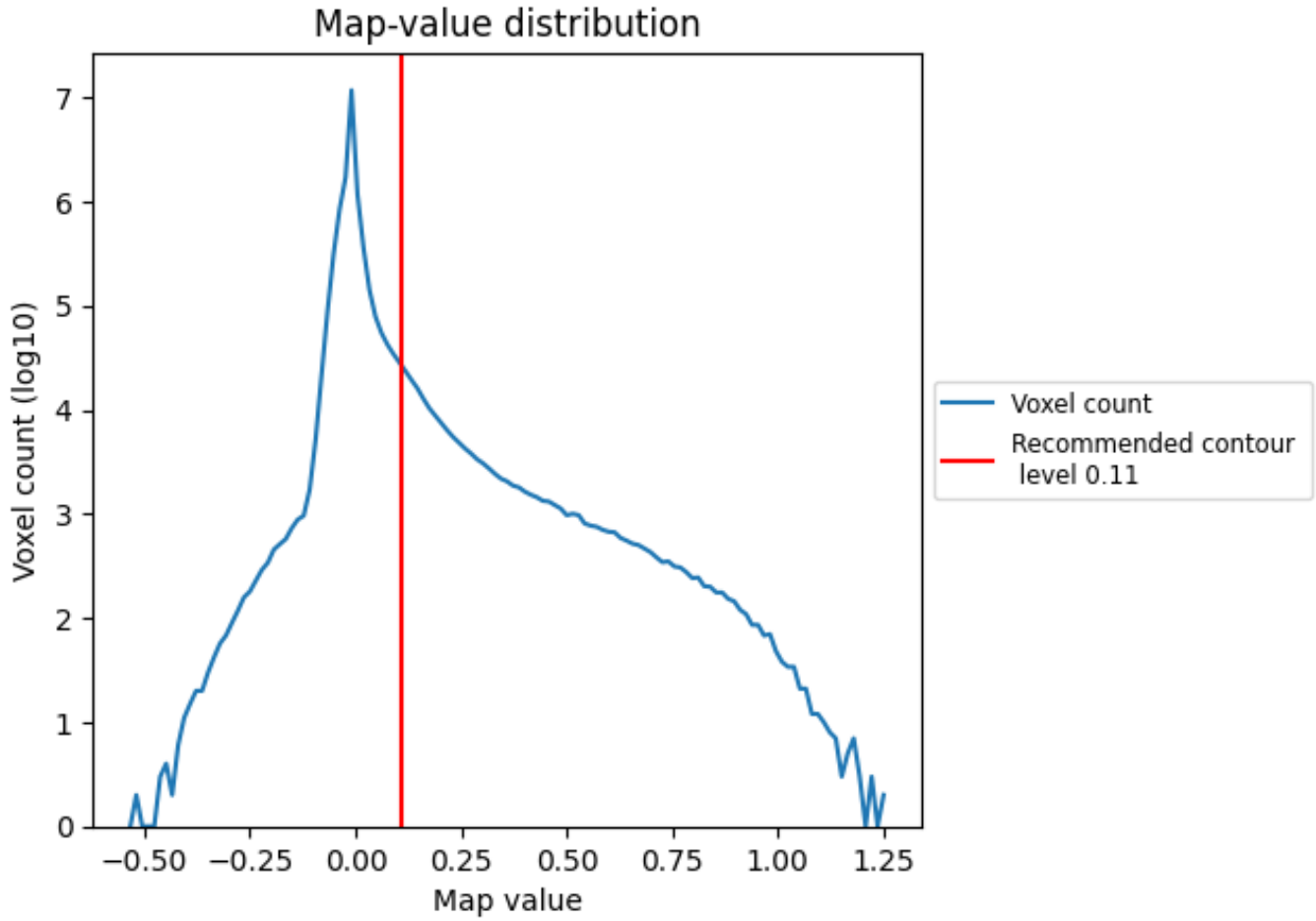
6.6 Mask visualisation (i)

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

7 Map analysis

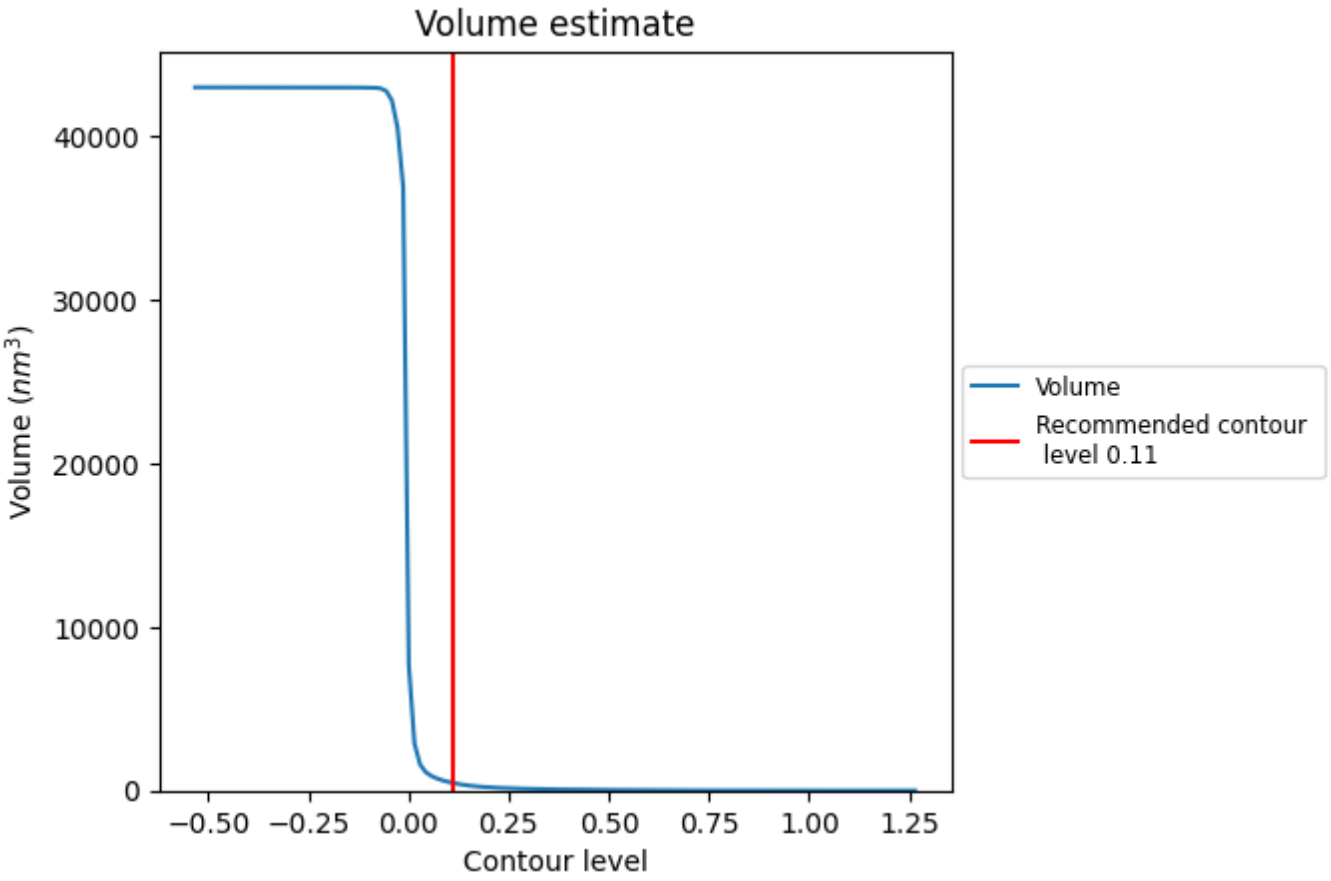
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

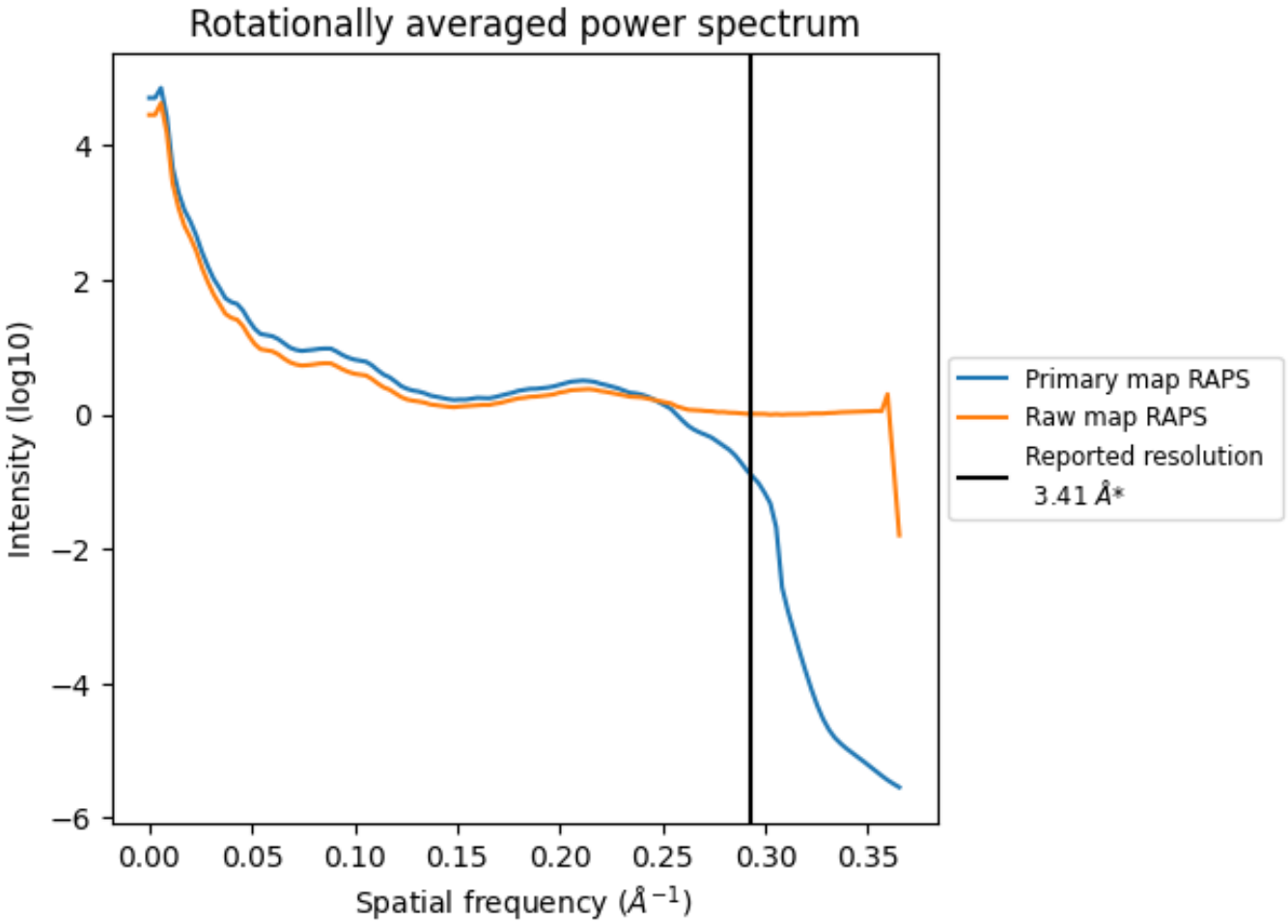
7.2 Volume estimate



The volume at the recommended contour level is 470 nm^3; this corresponds to an approximate mass of 425 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)

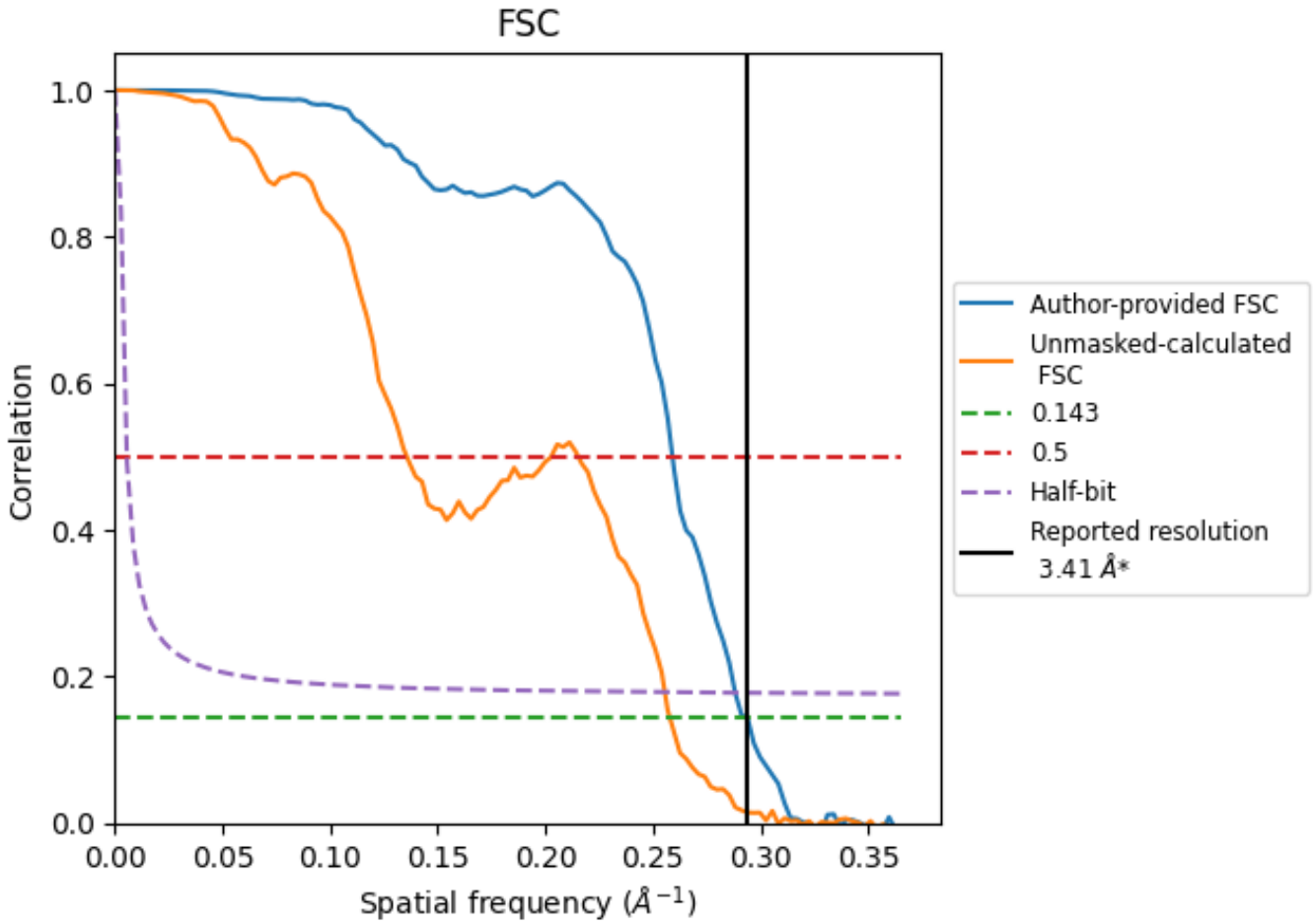


*Reported resolution corresponds to spatial frequency of 0.293 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.293 Å^{-1}

8.2 Resolution estimates (i)

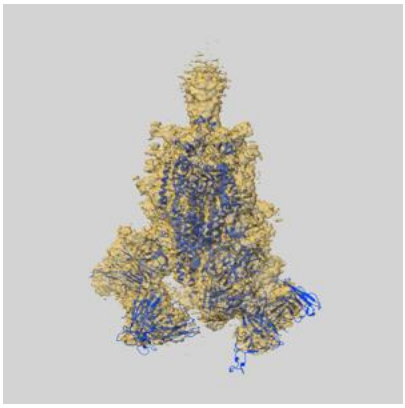
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.41	3.86	3.47
Unmasked-calculated*	3.88	7.37	3.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.41 by more than 10 %

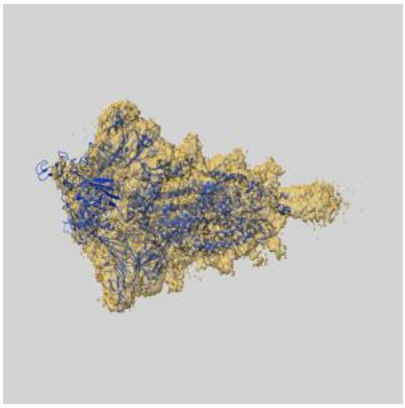
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60099 and PDB model 8ZHD. Per-residue inclusion information can be found in section 3 on page 9.

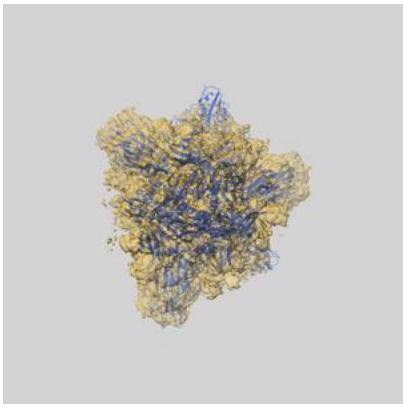
9.1 Map-model overlay



X



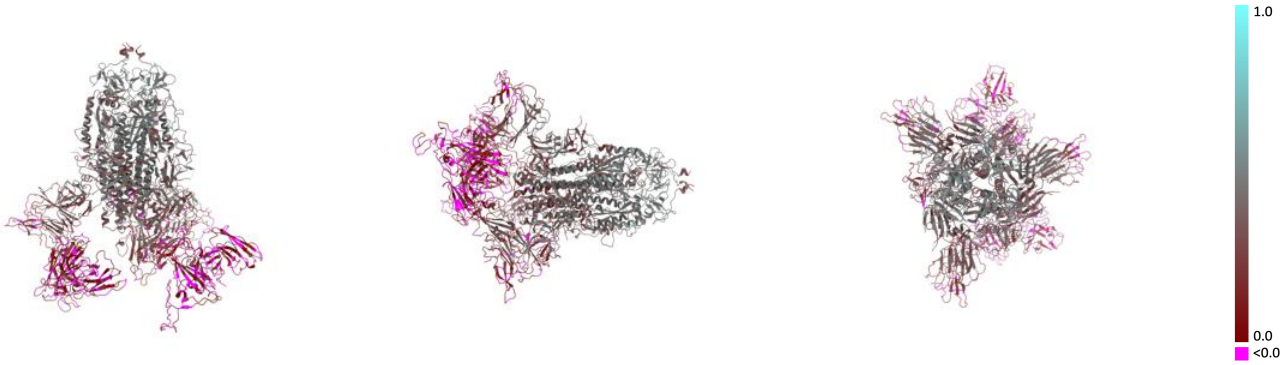
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

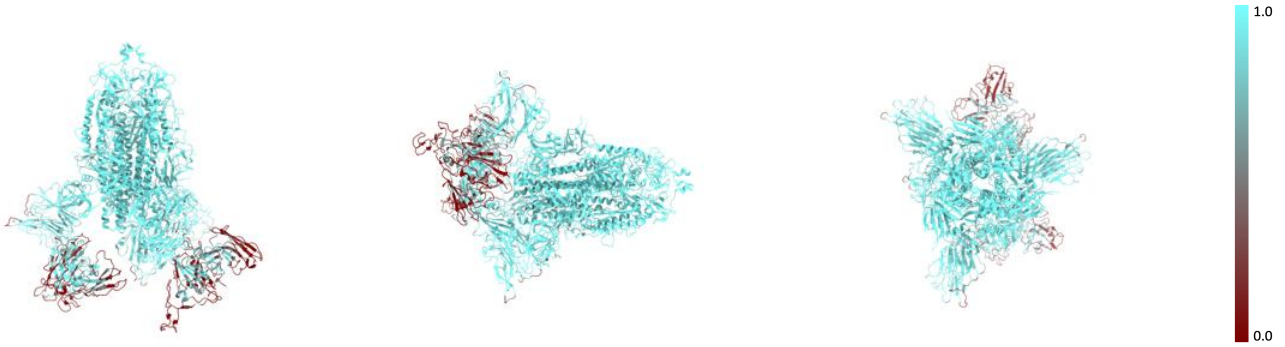
9.2 Q-score mapped to coordinate model



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.

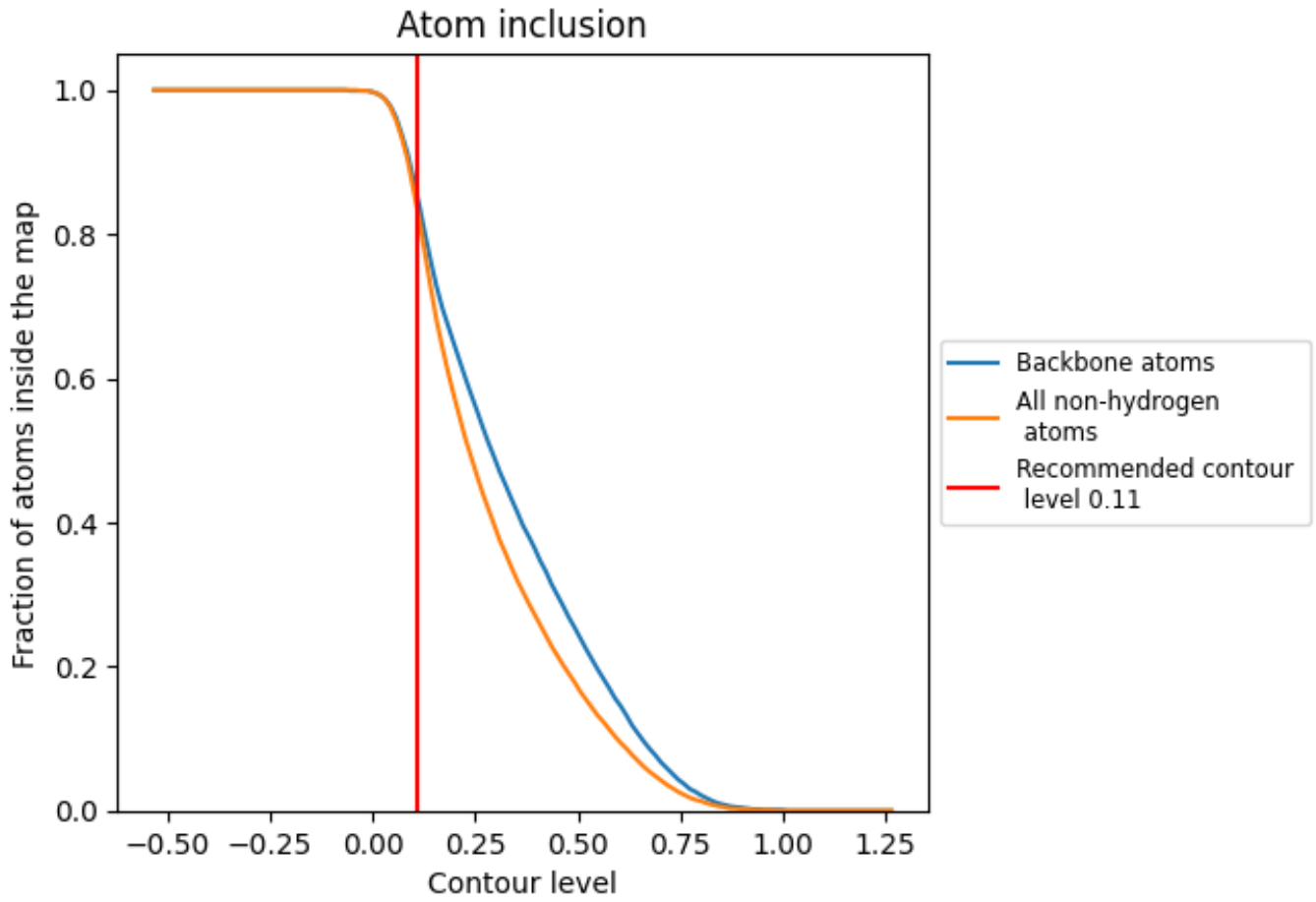
9.3 Atom inclusion mapped to coordinate model



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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.2810
A	0.8870	0.3090
B	0.9200	0.3200
C	0.8590	0.3070
D	0.3930	0.0610
E	0.9290	0.3420
F	0.3390	0.0700
G	0.3160	0.0190
H	0.4900	0.0780
I	0.9290	0.2730
J	0.9290	0.2620
K	0.9640	0.3930
L	0.4540	0.0580
M	0.8570	0.0830
N	0.9640	0.3600
O	1.0000	0.3310
P	1.0000	0.4090
Q	0.9290	0.3730
R	0.6070	0.1390
S	0.9640	0.4430
T	0.8930	0.2770
U	0.9640	0.3600
V	0.9640	0.3910