



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2021 – 04:12 PM EDT

PDB ID : 7MSG
Title : The crystal structure of LIGHT in complex with HVEM and CD160
Authors : Liu, W.; Ramagopal, U.; Garrett-Thompson, S.C.; Fedorov, E.; Bonanno, J.B.; Almo, S.C.
Deposited on : 2021-05-11
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

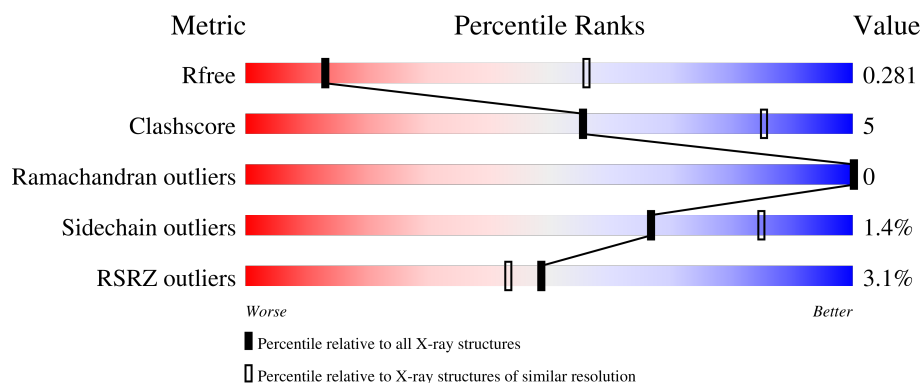
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	<div> <div>8%</div> <div>76%</div> <div>10%</div> <div>14%</div> </div>
1	B	165	<div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
1	C	165	<div> <div>79%</div> <div>7%</div> <div>14%</div> </div>
2	D	250	<div> <div>2%</div> <div>70%</div> <div>12%</div> <div>18%</div> </div>
2	E	250	<div> <div>8%</div> <div>69%</div> <div>12%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	250	
3	H	2	
3	J	2	
3	L	2	
4	I	3	
4	K	3	
4	M	3	

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
3	NAG	H	1	-	-	-	X
3	NAG	H	2	-	-	-	X
3	NAG	J	1	-	-	-	X
3	NAG	J	2	-	-	-	X
3	NAG	L	1	-	-	-	X
4	NAG	I	1	-	-	-	X
4	NAG	I	2	-	-	-	X
4	BMA	I	3	-	-	-	X
4	NAG	K	2	-	-	-	X
4	BMA	K	3	-	-	-	X
4	NAG	M	2	-	-	-	X
4	BMA	M	3	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8130 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Tumor necrosis factor ligand superfamily member 14, membrane form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1093	698	189	203	3			
1	B	142	Total	C	N	O	S	0	0	0
			1093	698	189	203	3			
1	C	142	Total	C	N	O	S	0	0	0
			1093	698	189	203	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	HIS	-	expression tag	UNP O43557
A	77	HIS	-	expression tag	UNP O43557
A	78	HIS	-	expression tag	UNP O43557
A	79	HIS	-	expression tag	UNP O43557
A	80	HIS	-	expression tag	UNP O43557
A	81	HIS	-	expression tag	UNP O43557
A	82	GLY	-	expression tag	UNP O43557
A	214	GLU	LYS	variant	UNP O43557
B	76	HIS	-	expression tag	UNP O43557
B	77	HIS	-	expression tag	UNP O43557
B	78	HIS	-	expression tag	UNP O43557
B	79	HIS	-	expression tag	UNP O43557
B	80	HIS	-	expression tag	UNP O43557
B	81	HIS	-	expression tag	UNP O43557
B	82	GLY	-	expression tag	UNP O43557
B	214	GLU	LYS	variant	UNP O43557
C	76	HIS	-	expression tag	UNP O43557
C	77	HIS	-	expression tag	UNP O43557
C	78	HIS	-	expression tag	UNP O43557
C	79	HIS	-	expression tag	UNP O43557
C	80	HIS	-	expression tag	UNP O43557
C	81	HIS	-	expression tag	UNP O43557

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Chain	Residue	Modelled	Actual	Comment	Reference
C	82	GLY	-	expression tag	UNP O43557
C	214	GLU	LYS	variant	UNP O43557

- Molecule 2 is a protein called CD160 antigen, soluble form, Tumor necrosis factor receptor superfamily member 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	206	Total	C	N	O	S	0	0	0
			1550	951	278	297	24			
2	E	206	Total	C	N	O	S	0	0	0
			1550	951	278	297	24			
2	F	206	Total	C	N	O	S	0	0	0
			1550	951	278	297	24			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1019	GLY	-	linker	UNP O95971
D	1020	GLY	-	linker	UNP O95971
D	1021	GLY	-	linker	UNP O95971
D	1022	GLY	-	linker	UNP O95971
D	1023	SER	-	linker	UNP O95971
D	1024	GLY	-	linker	UNP O95971
D	1025	GLY	-	linker	UNP O95971
D	1026	GLY	-	linker	UNP O95971
D	1027	GLY	-	linker	UNP O95971
D	1028	SER	-	linker	UNP O95971
D	1029	GLY	-	linker	UNP O95971
D	1030	GLY	-	linker	UNP O95971
D	1031	GLY	-	linker	UNP O95971
D	1032	GLY	-	linker	UNP O95971
D	1033	SER	-	linker	UNP O95971
D	1034	GLY	-	linker	UNP O95971
D	1035	GLY	-	linker	UNP O95971
D	1036	GLY	-	linker	UNP O95971
D	1037	GLY	-	linker	UNP O95971
D	1038	SER	-	linker	UNP O95971
D	1144	GLY	-	expression tag	UNP Q92956
D	1145	HIS	-	expression tag	UNP Q92956
D	1146	HIS	-	expression tag	UNP Q92956
D	1147	HIS	-	expression tag	UNP Q92956
D	1148	HIS	-	expression tag	UNP Q92956

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1149	HIS	-	expression tag	UNP Q92956
D	1150	HIS	-	expression tag	UNP Q92956
E	1019	GLY	-	linker	UNP O95971
E	1020	GLY	-	linker	UNP O95971
E	1021	GLY	-	linker	UNP O95971
E	1022	GLY	-	linker	UNP O95971
E	1023	SER	-	linker	UNP O95971
E	1024	GLY	-	linker	UNP O95971
E	1025	GLY	-	linker	UNP O95971
E	1026	GLY	-	linker	UNP O95971
E	1027	GLY	-	linker	UNP O95971
E	1028	SER	-	linker	UNP O95971
E	1029	GLY	-	linker	UNP O95971
E	1030	GLY	-	linker	UNP O95971
E	1031	GLY	-	linker	UNP O95971
E	1032	GLY	-	linker	UNP O95971
E	1033	SER	-	linker	UNP O95971
E	1034	GLY	-	linker	UNP O95971
E	1035	GLY	-	linker	UNP O95971
E	1036	GLY	-	linker	UNP O95971
E	1037	GLY	-	linker	UNP O95971
E	1038	SER	-	linker	UNP O95971
E	1144	GLY	-	expression tag	UNP Q92956
E	1145	HIS	-	expression tag	UNP Q92956
E	1146	HIS	-	expression tag	UNP Q92956
E	1147	HIS	-	expression tag	UNP Q92956
E	1148	HIS	-	expression tag	UNP Q92956
E	1149	HIS	-	expression tag	UNP Q92956
E	1150	HIS	-	expression tag	UNP Q92956
F	1019	GLY	-	linker	UNP O95971
F	1020	GLY	-	linker	UNP O95971
F	1021	GLY	-	linker	UNP O95971
F	1022	GLY	-	linker	UNP O95971
F	1023	SER	-	linker	UNP O95971
F	1024	GLY	-	linker	UNP O95971
F	1025	GLY	-	linker	UNP O95971
F	1026	GLY	-	linker	UNP O95971
F	1027	GLY	-	linker	UNP O95971
F	1028	SER	-	linker	UNP O95971
F	1029	GLY	-	linker	UNP O95971
F	1030	GLY	-	linker	UNP O95971
F	1031	GLY	-	linker	UNP O95971

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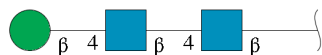
Chain	Residue	Modelled	Actual	Comment	Reference
F	1032	GLY	-	linker	UNP O95971
F	1033	SER	-	linker	UNP O95971
F	1034	GLY	-	linker	UNP O95971
F	1035	GLY	-	linker	UNP O95971
F	1036	GLY	-	linker	UNP O95971
F	1037	GLY	-	linker	UNP O95971
F	1038	SER	-	linker	UNP O95971
F	1144	GLY	-	expression tag	UNP Q92956
F	1145	HIS	-	expression tag	UNP Q92956
F	1146	HIS	-	expression tag	UNP Q92956
F	1147	HIS	-	expression tag	UNP Q92956
F	1148	HIS	-	expression tag	UNP Q92956
F	1149	HIS	-	expression tag	UNP Q92956
F	1150	HIS	-	expression tag	UNP Q92956

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



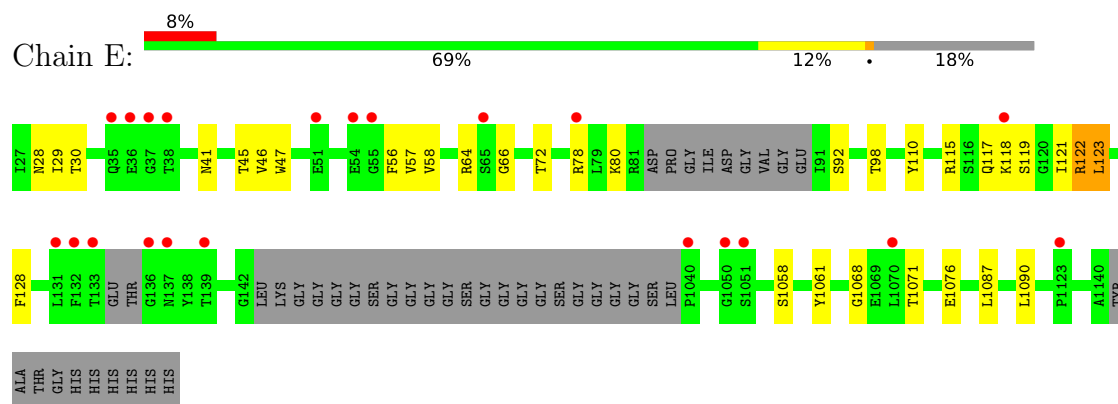
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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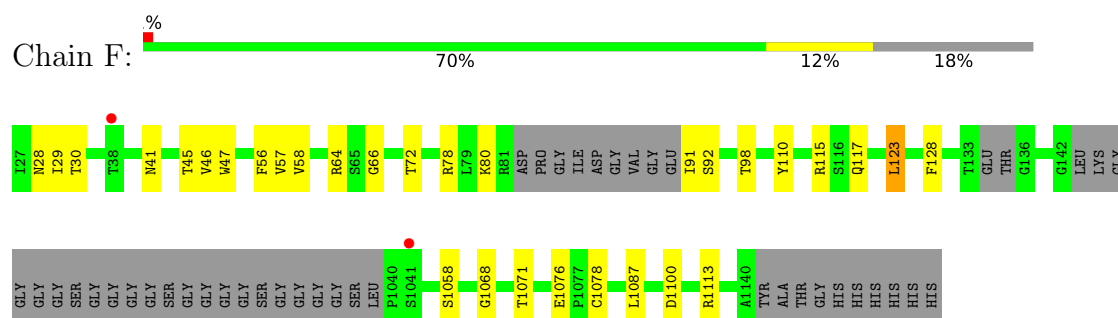
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 2: CD160 antigen, soluble form,Tumor necrosis factor receptor superfamily member 14



- Molecule 2: CD160 antigen, soluble form,Tumor necrosis factor receptor superfamily member 14



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



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



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



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

Chain I:  33% 67%



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

Chain K:  33% 67%



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

Chain M:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	214.69Å 214.69Å 214.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 3.50 19.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.93-3.50) 100.0 (19.93-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.257 , 0.285 0.254 , 0.281	Depositor DCC
R_{free} test set	1005 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	114.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8130	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/1118	0.72	0/1516
1	B	0.69	0/1118	0.74	0/1516
1	C	0.67	0/1118	0.72	0/1516
2	D	0.70	1/1577 (0.1%)	0.81	3/2123 (0.1%)
2	E	0.78	2/1577 (0.1%)	1.04	5/2123 (0.2%)
2	F	0.71	0/1577	0.82	3/2123 (0.1%)
All	All	0.71	3/8085 (0.0%)	0.83	11/10917 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	115	ARG	CZ-NH2	-8.31	1.22	1.33
2	E	115	ARG	CZ-NH1	-7.82	1.22	1.33
2	D	115	ARG	CZ-NH2	-5.19	1.26	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	115	ARG	NE-CZ-NH2	20.94	130.77	120.30
2	E	115	ARG	NE-CZ-NH1	17.50	129.05	120.30
2	E	115	ARG	NH1-CZ-NH2	-17.48	100.17	119.40
2	F	115	ARG	NE-CZ-NH2	10.04	125.32	120.30
2	D	115	ARG	NE-CZ-NH1	9.19	124.89	120.30
2	D	115	ARG	NE-CZ-NH2	9.14	124.87	120.30
2	F	115	ARG	NE-CZ-NH1	8.51	124.56	120.30
2	F	115	ARG	NH1-CZ-NH2	-8.48	110.08	119.40
2	D	115	ARG	NH1-CZ-NH2	-8.33	110.23	119.40
2	E	122	ARG	NE-CZ-NH1	-6.47	117.06	120.30
2	E	118	LYS	N-CA-CB	5.40	120.32	110.60

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	1093	0	1074	12	0
1	B	1093	0	1074	9	0
1	C	1093	0	1074	6	0
2	D	1550	0	1490	22	0
2	E	1550	0	1490	22	1
2	F	1550	0	1490	20	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
4	I	39	0	34	0	0
4	K	39	0	34	0	0
4	M	39	0	34	0	0
All	All	8130	0	7869	81	1

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 5.

All (81) 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)
2:D:47:TRP:CZ3	2:D:92:SER:HB2	2.09	0.88
2:E:47:TRP:CZ3	2:E:92:SER:HB2	2.09	0.87
2:F:47:TRP:CZ3	2:F:92:SER:HB2	2.10	0.87
2:E:30:THR:OG1	2:E:45:THR:HB	1.92	0.69
2:F:30:THR:OG1	2:F:45:THR:HB	1.93	0.69
1:B:117:GLN:O	2:D:1092:LYS:NZ	2.22	0.68
2:D:30:THR:OG1	2:D:45:THR:HB	1.93	0.68
2:E:57:VAL:HG22	2:E:78:ARG:HG3	1.81	0.62
2:E:122:ARG:HG2	2:E:1061:TYR:CE2	2.35	0.62
2:F:117:GLN:HA	2:F:117:GLN:OE1	2.02	0.59
2:F:57:VAL:HG22	2:F:78:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:VAL:HG22	2:D:78:ARG:HG3	1.86	0.57
1:B:196:VAL:HG23	2:D:1128:ILE:HG21	1.86	0.56
2:F:117:GLN:OE1	2:F:117:GLN:CA	2.54	0.55
2:D:78:ARG:HH12	2:D:80:LYS:HG2	1.74	0.53
2:E:1068:GLY:N	2:E:1071:THR:OG1	2.37	0.53
1:B:173:TYR:CD1	2:E:1090:LEU:HD11	2.44	0.53
2:E:78:ARG:HH12	2:E:80:LYS:HG2	1.73	0.52
2:F:78:ARG:HH12	2:F:80:LYS:HG2	1.73	0.52
2:D:1068:GLY:N	2:D:1071:THR:OG1	2.37	0.51
2:F:41:ASN:ND2	2:F:98:THR:OG1	2.46	0.49
2:E:41:ASN:ND2	2:E:98:THR:OG1	2.45	0.49
1:B:173:TYR:HB2	2:E:1090:LEU:HD21	1.95	0.49
2:E:119:SER:HB3	2:E:121:ILE:HD12	1.95	0.48
2:D:41:ASN:ND2	2:D:98:THR:OG1	2.45	0.48
1:A:106:THR:HG21	1:A:110:GLY:HA3	1.96	0.47
1:A:163:THR:HB	1:A:220:LEU:HB2	1.97	0.47
1:A:173:TYR:HE1	2:D:1084:ILE:HG23	1.78	0.47
2:E:110:TYR:HB2	2:E:128:PHE:CE2	2.50	0.47
2:F:110:TYR:HB2	2:F:128:PHE:CE2	2.49	0.47
2:F:47:TRP:CE3	2:F:92:SER:HB2	2.50	0.47
2:E:119:SER:HB3	2:E:121:ILE:CD1	2.44	0.46
1:C:104:SER:HB2	1:C:227:LEU:HD11	1.97	0.46
1:B:163:THR:HB	1:B:220:LEU:HB2	1.98	0.46
2:D:47:TRP:CE3	2:D:92:SER:HB2	2.49	0.46
2:F:64:ARG:HE	2:F:72:THR:HB	1.81	0.46
1:A:104:SER:HB2	1:A:227:LEU:HD11	1.98	0.46
2:D:110:TYR:HB2	2:D:128:PHE:CE2	2.50	0.46
2:F:1068:GLY:N	2:F:1071:THR:OG1	2.38	0.46
1:B:135:VAL:HG21	1:B:209:LEU:HB3	1.98	0.46
2:D:29:ILE:HG21	2:D:123:LEU:HD22	1.98	0.46
2:D:64:ARG:HE	2:D:72:THR:HB	1.80	0.46
2:E:29:ILE:HG21	2:E:123:LEU:HD22	1.98	0.46
2:E:64:ARG:HE	2:E:72:THR:HB	1.80	0.45
1:C:135:VAL:HG21	1:C:209:LEU:HB3	1.98	0.45
2:E:117:GLN:HA	2:E:117:GLN:OE1	2.16	0.45
2:F:46:VAL:HG21	2:F:58:VAL:HB	1.97	0.45
2:F:29:ILE:HG21	2:F:123:LEU:HD22	1.99	0.44
1:A:226:ARG:HH21	2:F:1100:ASP:CG	2.21	0.44
2:D:46:VAL:HG21	2:D:58:VAL:HB	1.99	0.44
1:C:163:THR:HB	1:C:220:LEU:HB2	1.98	0.44
2:E:47:TRP:CE3	2:E:92:SER:HB2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:121:ILE:HG22	2:E:122:ARG:O	2.17	0.44
1:C:169:ARG:HB2	1:C:214:GLU:HB2	1.99	0.44
1:A:135:VAL:HG21	1:A:209:LEU:HB3	1.99	0.44
1:B:106:THR:HG21	1:B:110:GLY:HA3	1.98	0.44
1:B:169:ARG:HB2	1:B:214:GLU:HB2	2.00	0.44
2:D:66:GLY:HA3	2:D:1087:LEU:HD11	2.00	0.44
1:A:173:TYR:CD2	1:A:177:LEU:HD11	2.53	0.43
2:E:46:VAL:HG21	2:E:58:VAL:HB	2.00	0.43
1:A:169:ARG:HB2	1:A:214:GLU:HB2	2.01	0.43
2:F:66:GLY:HA3	2:F:1087:LEU:HD11	2.00	0.43
1:B:173:TYR:CD2	1:B:177:LEU:HD11	2.54	0.42
2:D:28:ASN:H	2:D:47:TRP:HB2	1.85	0.42
2:F:46:VAL:HG11	2:F:56:PHE:CE1	2.55	0.42
2:E:28:ASN:H	2:E:47:TRP:HB2	1.85	0.42
2:E:66:GLY:HA3	2:E:1087:LEU:HD11	2.00	0.42
2:F:28:ASN:CB	2:F:47:TRP:CD1	3.03	0.41
1:C:173:TYR:CD2	1:C:177:LEU:HD11	2.55	0.41
2:D:47:TRP:CH2	2:D:92:SER:HB2	2.53	0.41
2:F:28:ASN:H	2:F:47:TRP:HB2	1.85	0.41
2:D:46:VAL:HG11	2:D:56:PHE:CE1	2.56	0.41
2:E:28:ASN:CB	2:E:47:TRP:CD1	3.03	0.41
2:F:1078:CYS:O	2:F:1113:ARG:HD2	2.21	0.41
1:A:174:PRO:CG	2:D:1086:HIS:CG	3.04	0.41
2:E:46:VAL:HG11	2:E:56:PHE:CE1	2.55	0.41
1:A:174:PRO:HG2	2:D:1086:HIS:CG	2.56	0.41
1:A:234:TYR:CE2	1:C:180:LEU:HD22	2.56	0.41
2:F:47:TRP:HE3	2:F:91:ILE:HD12	1.86	0.41
1:A:173:TYR:CD1	2:D:1090:LEU:HD11	2.56	0.40
2:D:29:ILE:HG21	2:D:123:LEU:CD2	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:78:ARG:CD	2:E:78:ARG:CD[2_555]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	136/165 (82%)	132 (97%)	4 (3%)	0	100	100
1	B	136/165 (82%)	132 (97%)	4 (3%)	0	100	100
1	C	136/165 (82%)	132 (97%)	4 (3%)	0	100	100
2	D	198/250 (79%)	192 (97%)	6 (3%)	0	100	100
2	E	198/250 (79%)	191 (96%)	7 (4%)	0	100	100
2	F	198/250 (79%)	192 (97%)	6 (3%)	0	100	100
All	All	1002/1245 (80%)	971 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	116/135 (86%)	115 (99%)	1 (1%)	78	90
1	B	116/135 (86%)	115 (99%)	1 (1%)	78	90
1	C	116/135 (86%)	115 (99%)	1 (1%)	78	90
2	D	177/200 (88%)	174 (98%)	3 (2%)	60	82
2	E	177/200 (88%)	174 (98%)	3 (2%)	60	82
2	F	177/200 (88%)	174 (98%)	3 (2%)	60	82
All	All	879/1005 (88%)	867 (99%)	12 (1%)	67	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LEU
1	B	203	LEU
1	C	203	LEU
2	D	123	LEU
2	D	1058	SER
2	D	1076	GLU
2	E	123	LEU
2	E	1058	SER
2	E	1076	GLU
2	F	123	LEU
2	F	1058	SER
2	F	1076	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	B	184	GLN
1	C	184	GLN
2	D	41	ASN
2	E	41	ASN
2	F	41	ASN

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](#)

15 monosaccharides are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	H	1	2,3	14,14,15	0.54	0	17,19,21	1.43	2 (11%)
3	NAG	H	2	3	14,14,15	0.46	0	17,19,21	1.23	3 (17%)
4	NAG	I	1	2,4	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
4	NAG	I	2	4	14,14,15	0.65	0	17,19,21	0.91	0
4	BMA	I	3	4	11,11,12	0.44	0	15,15,17	1.16	2 (13%)
3	NAG	J	1	2,3	14,14,15	0.54	0	17,19,21	1.42	2 (11%)
3	NAG	J	2	3	14,14,15	0.47	0	17,19,21	1.21	3 (17%)
4	NAG	K	1	2,4	14,14,15	0.54	0	17,19,21	1.16	2 (11%)
4	NAG	K	2	4	14,14,15	0.67	0	17,19,21	0.91	0
4	BMA	K	3	4	11,11,12	0.47	0	15,15,17	1.14	2 (13%)
3	NAG	L	1	2,3	14,14,15	0.53	0	17,19,21	1.40	2 (11%)
3	NAG	L	2	3	14,14,15	0.47	0	17,19,21	1.21	3 (17%)
4	NAG	M	1	2,4	14,14,15	0.55	0	17,19,21	1.13	2 (11%)
4	NAG	M	2	4	14,14,15	0.65	0	17,19,21	0.91	0
4	BMA	M	3	4	11,11,12	0.45	0	15,15,17	1.15	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
3	NAG	J	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
4	NAG	K	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
3	NAG	L	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
4	NAG	M	1	2,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	O5-C1-C2	4.16	117.86	111.29
3	L	1	NAG	O5-C1-C2	4.16	117.85	111.29
3	J	1	NAG	O5-C1-C2	4.11	117.77	111.29
3	J	1	NAG	C1-O5-C5	3.33	116.71	112.19
4	I	1	NAG	O5-C1-C2	3.32	116.53	111.29
3	H	1	NAG	C1-O5-C5	3.30	116.66	112.19
4	K	1	NAG	O5-C1-C2	3.26	116.44	111.29
4	M	1	NAG	O5-C1-C2	3.14	116.25	111.29
3	L	1	NAG	C1-O5-C5	3.06	116.34	112.19
3	J	2	NAG	C4-C3-C2	2.80	115.12	111.02
3	H	2	NAG	C4-C3-C2	2.79	115.10	111.02
3	L	2	NAG	C4-C3-C2	2.78	115.08	111.02
4	I	1	NAG	C1-C2-N2	2.66	115.03	110.49
4	K	3	BMA	C1-C2-C3	2.64	112.91	109.67
4	K	1	NAG	C1-C2-N2	2.60	114.92	110.49
4	M	1	NAG	C1-C2-N2	2.57	114.88	110.49
4	I	3	BMA	C1-C2-C3	2.53	112.78	109.67
4	M	3	BMA	C1-C2-C3	2.38	112.59	109.67
3	H	2	NAG	C1-C2-N2	2.26	114.34	110.49
3	L	2	NAG	C1-C2-N2	2.25	114.34	110.49
3	J	2	NAG	C1-C2-N2	2.24	114.32	110.49
4	M	3	BMA	O5-C1-C2	2.22	114.20	110.77
3	L	2	NAG	O5-C1-C2	2.16	114.70	111.29
3	H	2	NAG	O5-C1-C2	2.16	114.69	111.29
4	K	3	BMA	O5-C1-C2	2.12	114.05	110.77
3	J	2	NAG	O5-C1-C2	2.10	114.60	111.29
4	I	3	BMA	O5-C1-C2	2.03	113.90	110.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	3	BMA	C4-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6

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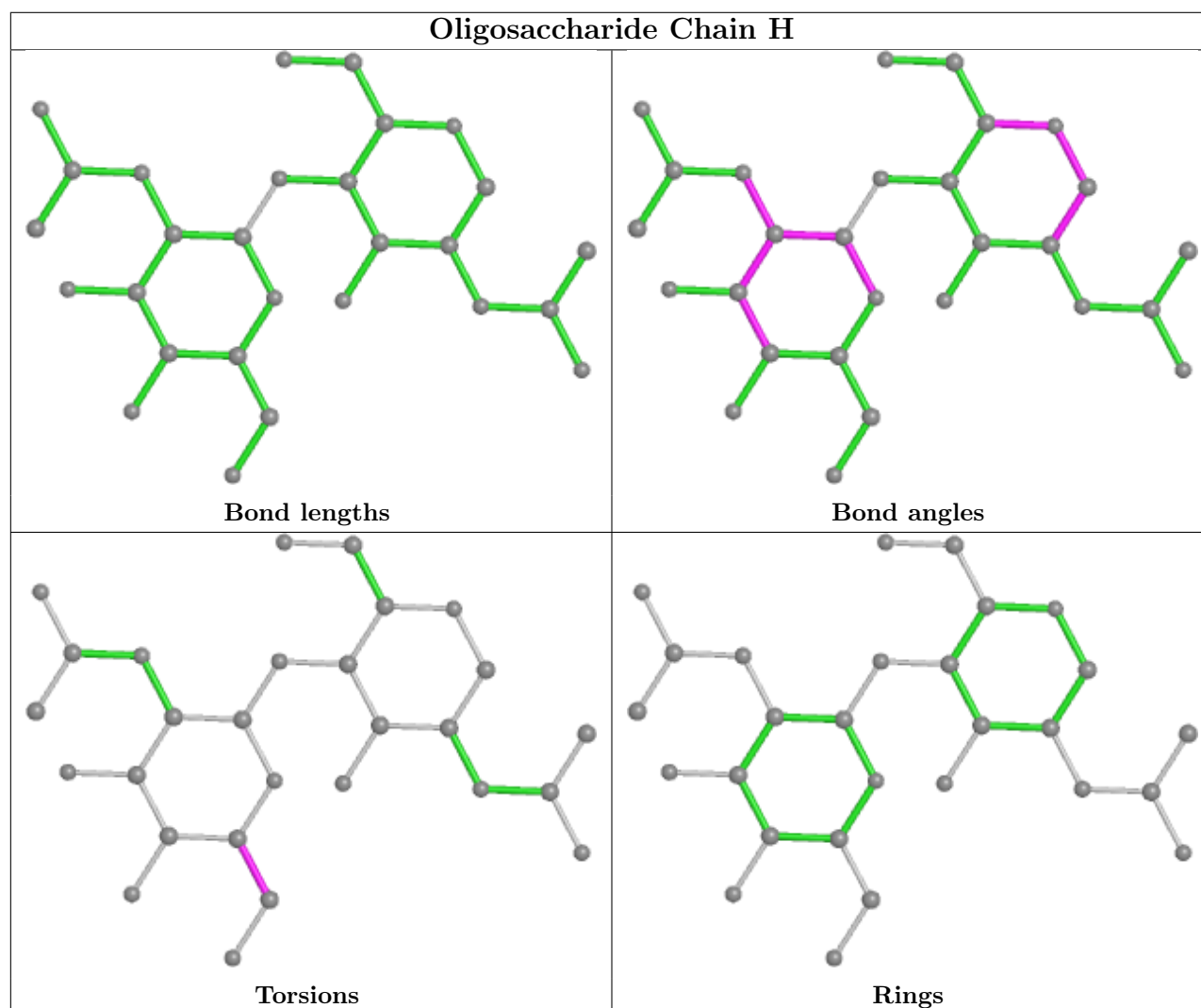
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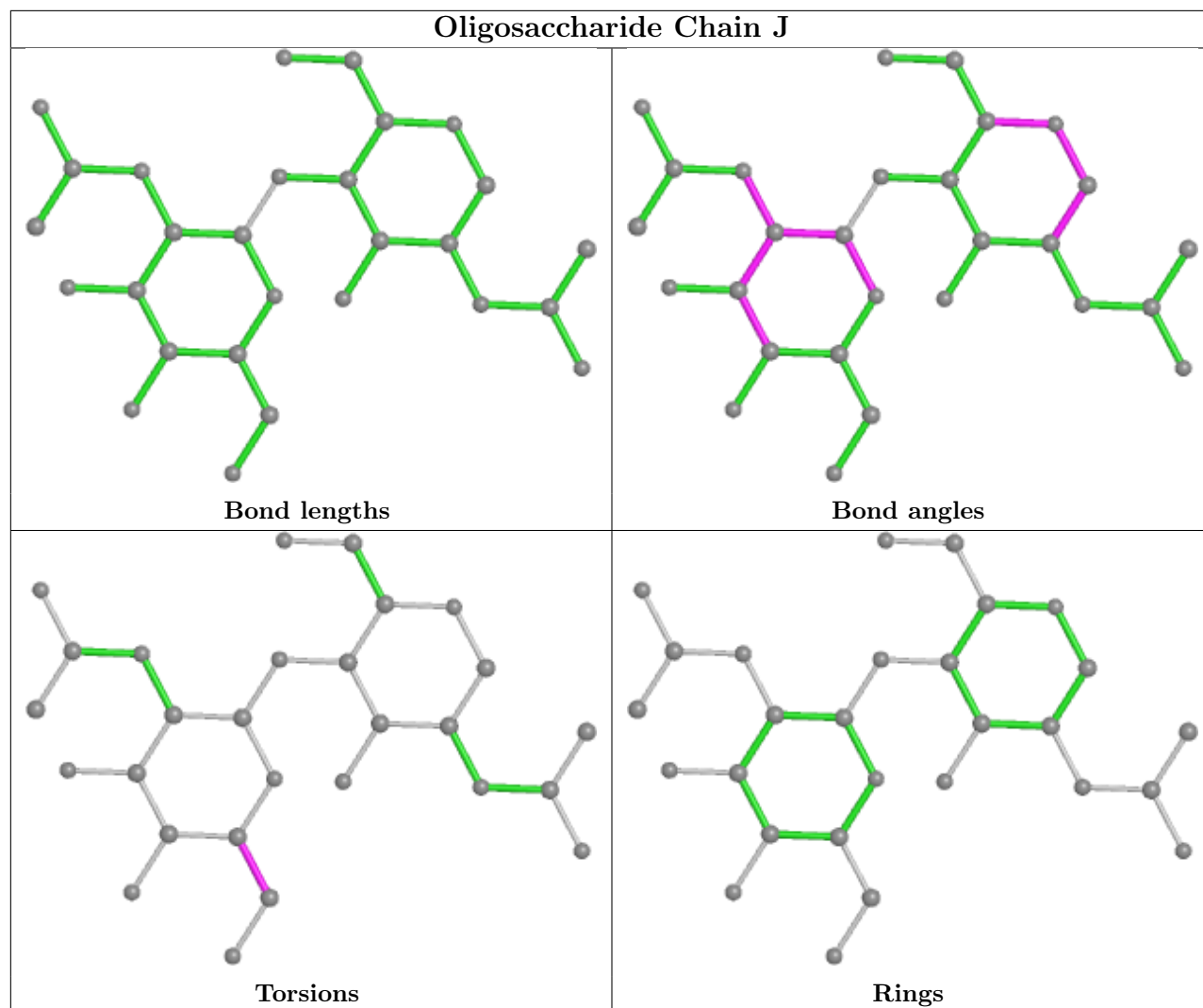
Mol	Chain	Res	Type	Atoms
4	M	3	BMA	C4-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6

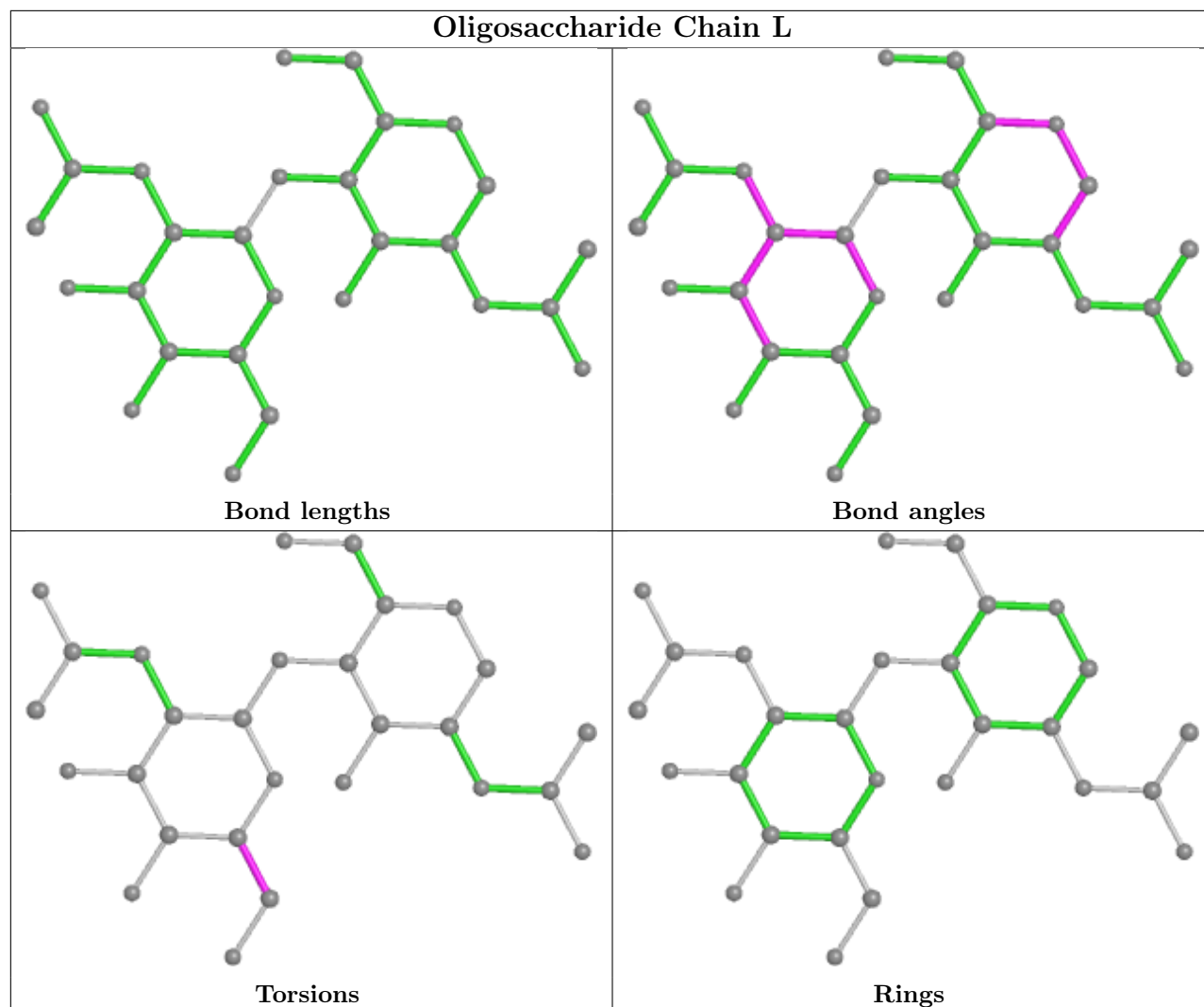
There are no ring outliers.

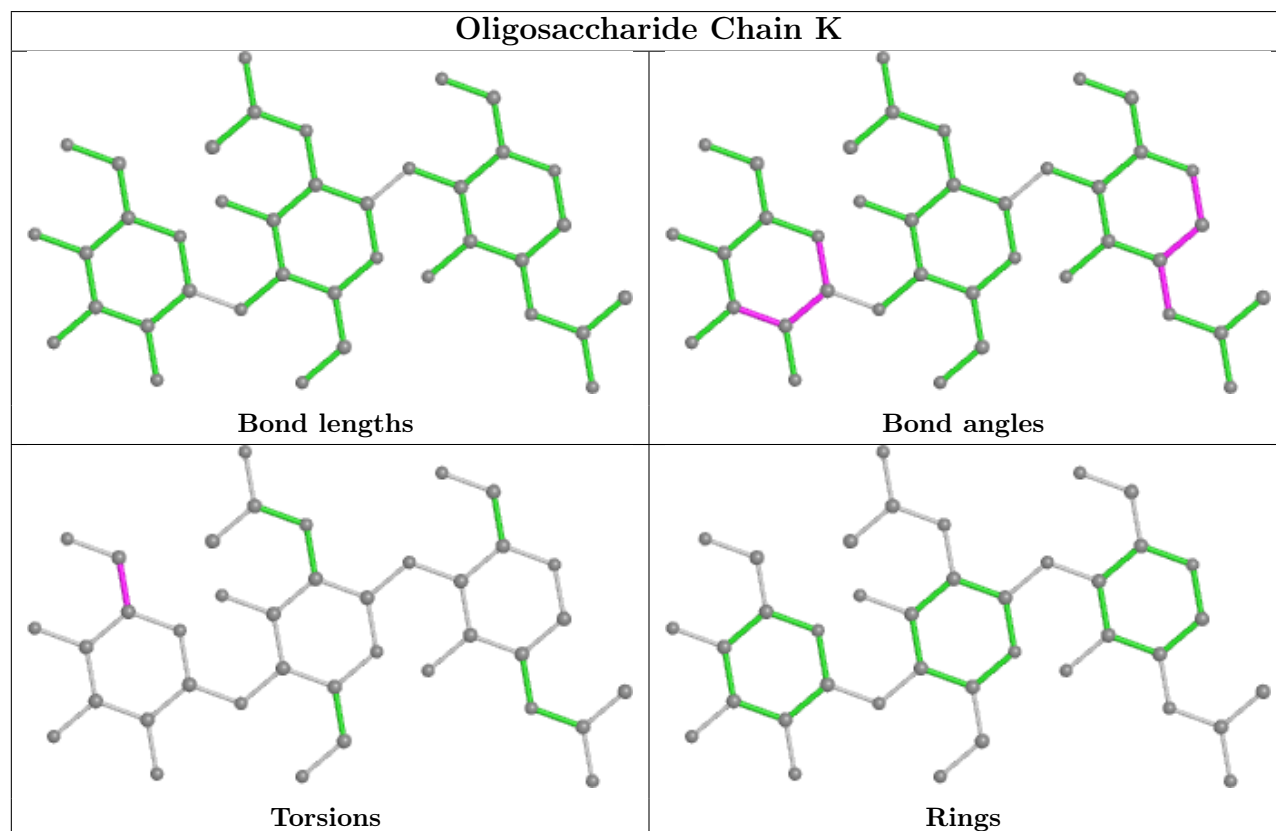
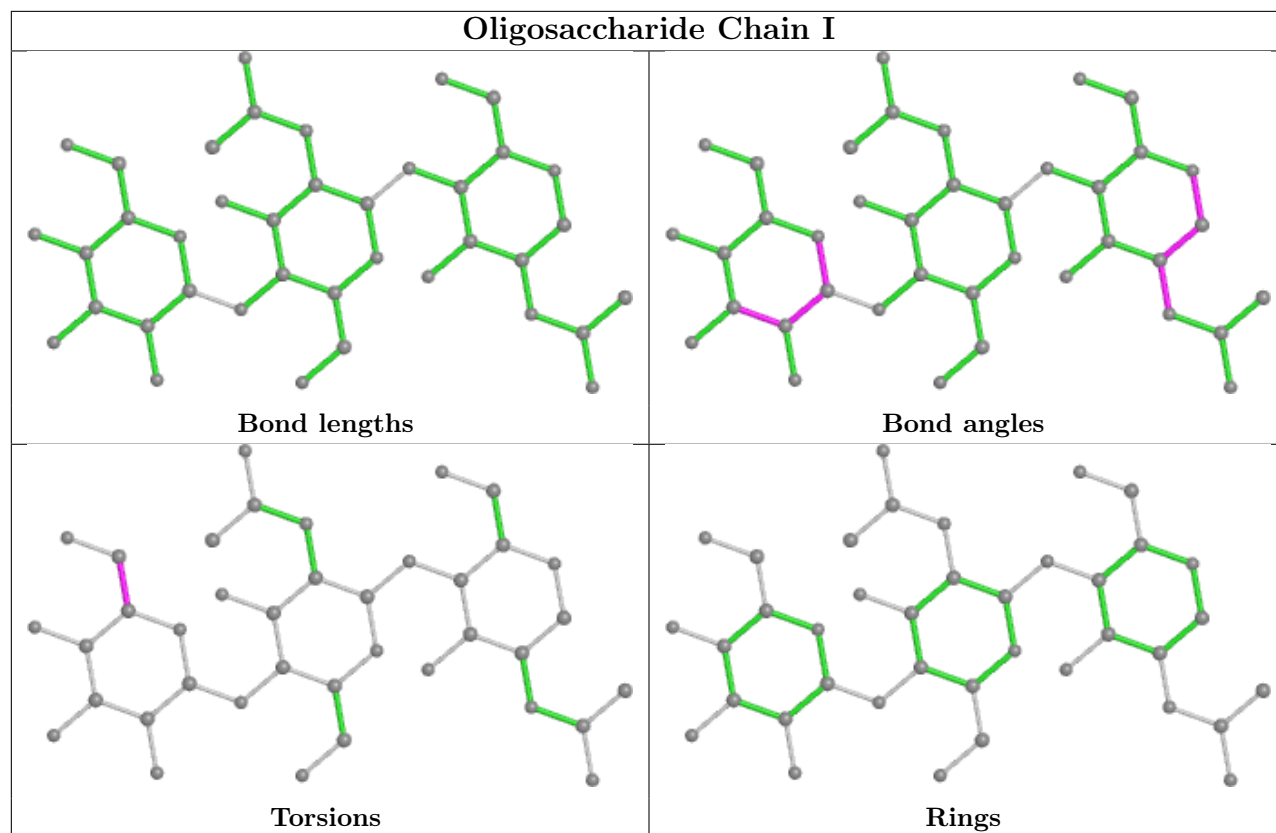
No monomer is involved in short contacts.

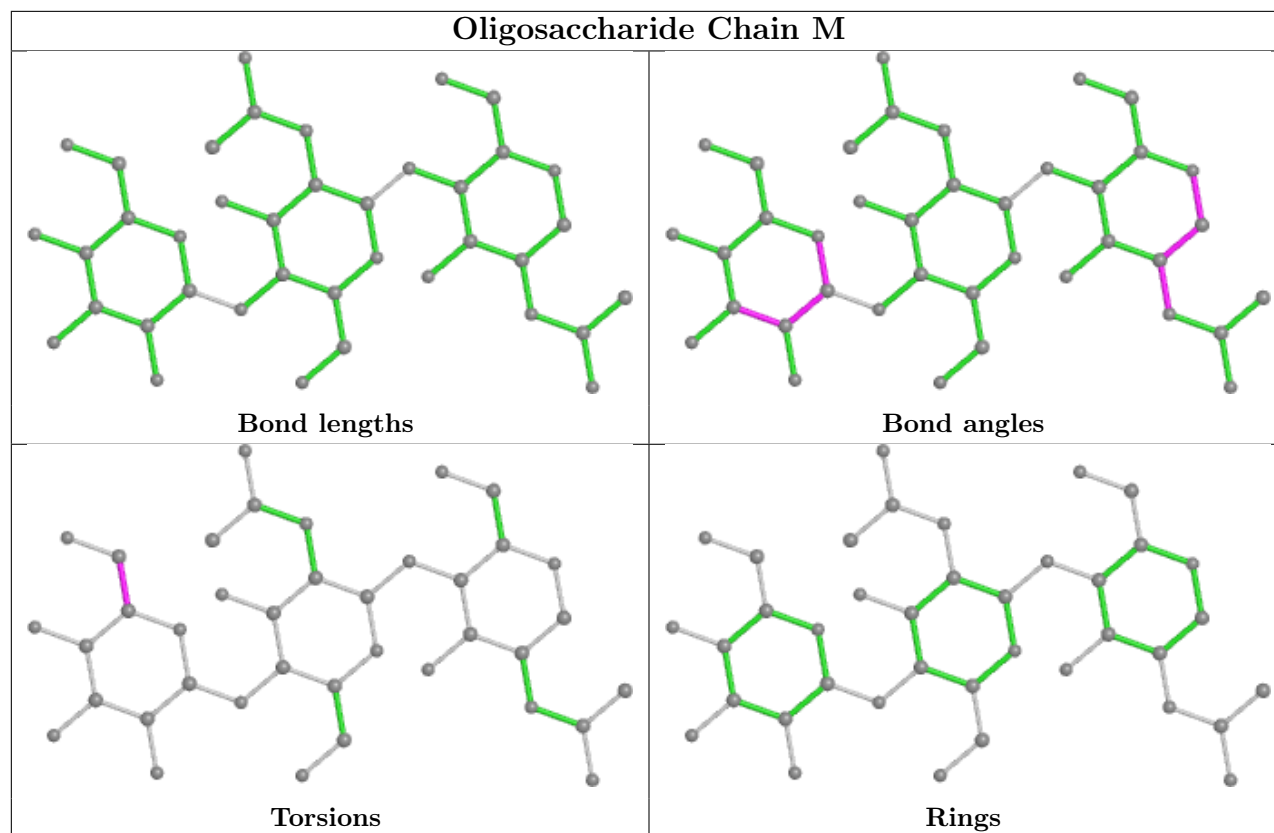
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	142/165 (86%)	-0.34	2 (1%) 75 69	81, 105, 189, 215	0
1	B	142/165 (86%)	-0.29	1 (0%) 87 83	97, 130, 189, 231	0
1	C	142/165 (86%)	-0.38	1 (0%) 87 83	84, 115, 187, 220	0
2	D	206/250 (82%)	-0.01	5 (2%) 59 53	89, 155, 225, 249	0
2	E	206/250 (82%)	0.25	21 (10%) 6 7	125, 197, 251, 275	0
2	F	206/250 (82%)	-0.15	2 (0%) 82 77	92, 140, 200, 223	0
All	All	1044/1245 (83%)	-0.12	32 (3%) 49 43	81, 145, 223, 275	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	133	THR	11.1
2	D	1140	ALA	4.1
2	D	1052	GLU	3.8
2	E	137	ASN	3.6
2	E	55	GLY	3.4
2	E	35	GLN	3.1
2	E	131	LEU	3.0
1	A	193	SER	3.0
2	E	65	SER	3.0
2	F	38	THR	3.0
2	E	136	GLY	2.9
2	E	1070	LEU	2.6
2	E	54	GLU	2.6
2	E	36	GLU	2.5
2	E	118	LYS	2.5
2	E	51	GLU	2.5
2	E	1051	SER	2.5
2	E	1050	GLY	2.4
1	C	192	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	132	PHE	2.3
2	E	1123	PRO	2.3
2	E	38	THR	2.2
2	D	1069	GLU	2.2
2	E	139	THR	2.2
2	D	1040	PRO	2.2
2	E	78	ARG	2.1
2	F	1041	SER	2.1
2	E	37	GLY	2.1
1	B	101	ALA	2.1
2	E	1040	PRO	2.1
2	D	1133	ASP	2.1
1	A	102	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

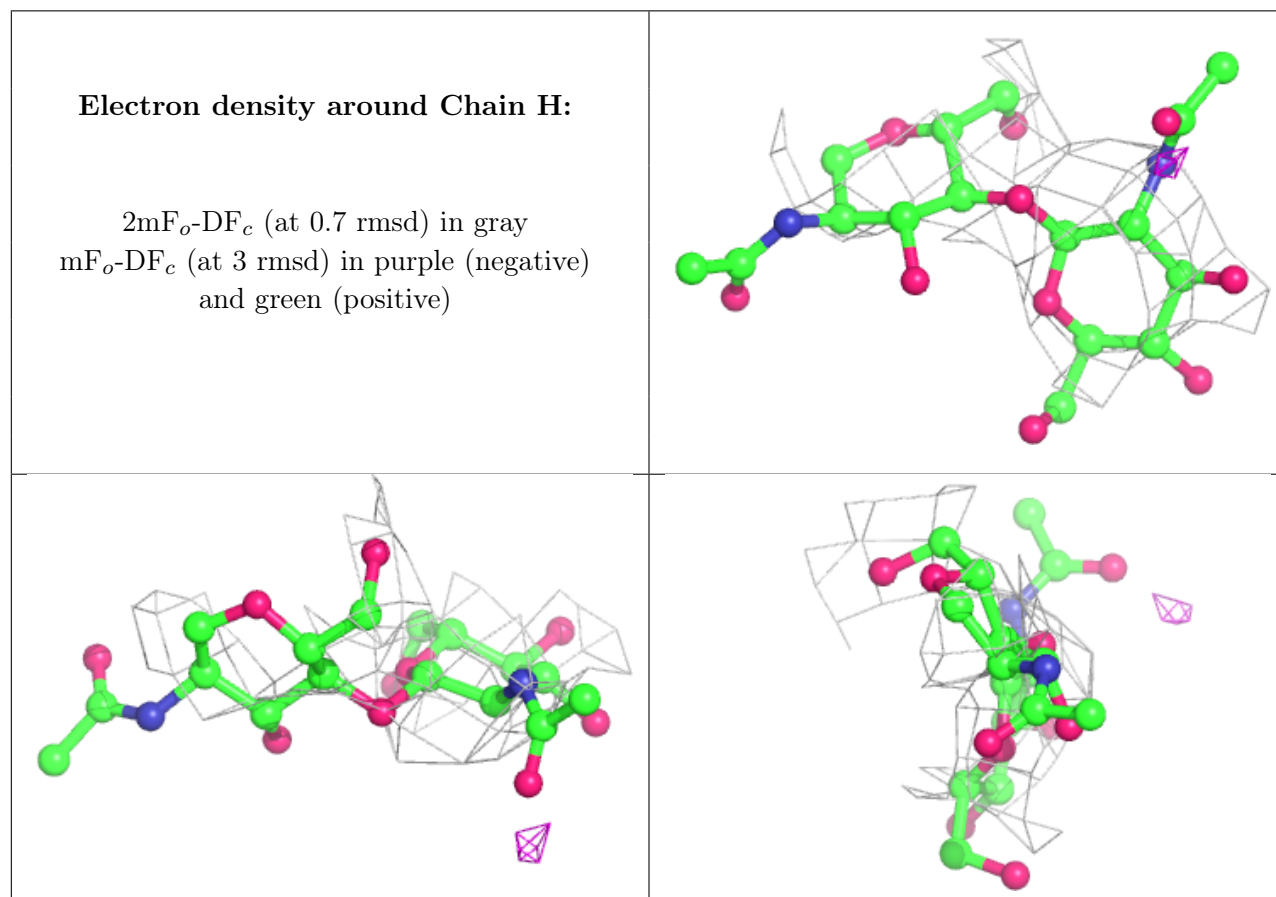
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

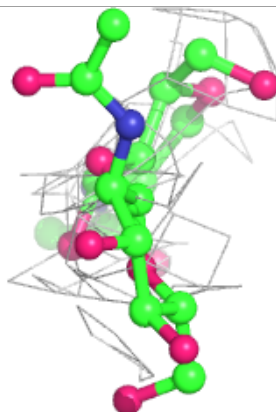
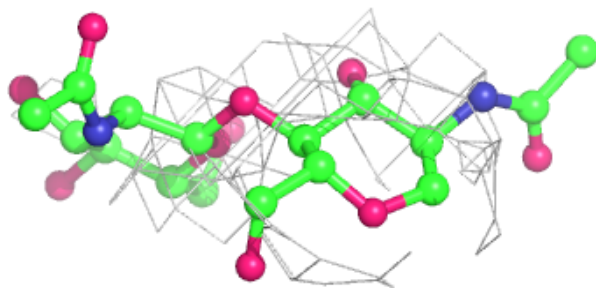
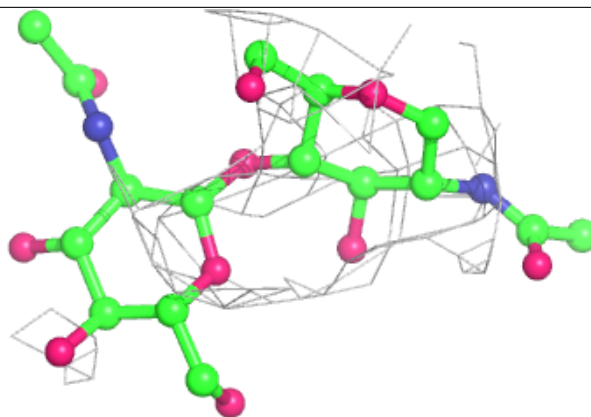
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	I	3	11/12	0.32	0.68	268,284,286,291	0
4	BMA	K	3	11/12	0.35	0.70	284,293,300,308	0
4	NAG	K	2	14/15	0.45	0.67	268,279,288,292	0
4	BMA	M	3	11/12	0.51	0.50	243,258,265,268	0
3	NAG	J	2	14/15	0.56	0.66	261,269,271,271	0
4	NAG	K	1	14/15	0.61	0.33	200,225,237,248	0
3	NAG	J	1	14/15	0.67	0.46	234,248,259,267	0
3	NAG	H	1	14/15	0.68	0.66	227,243,248,249	0
3	NAG	L	1	14/15	0.70	0.45	171,183,191,193	0
3	NAG	L	2	14/15	0.73	0.38	171,182,188,188	0
3	NAG	H	2	14/15	0.74	0.70	241,244,247,253	0
4	NAG	I	2	14/15	0.75	0.71	249,261,273,274	0
4	NAG	M	2	14/15	0.76	0.43	214,234,242,251	0
4	NAG	I	1	14/15	0.76	0.43	202,212,226,235	0
4	NAG	M	1	14/15	0.88	0.25	177,186,195,212	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

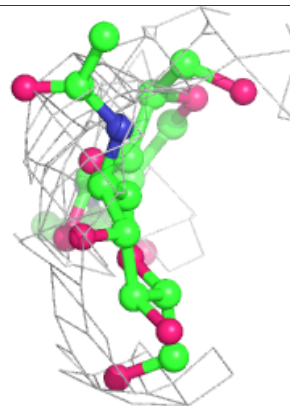
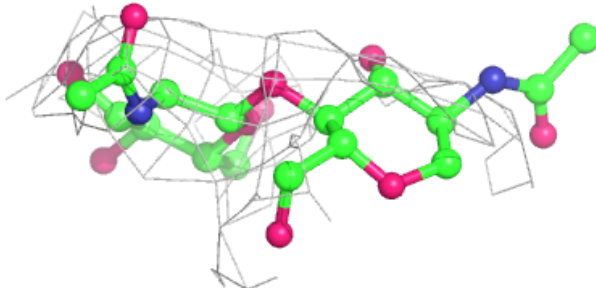
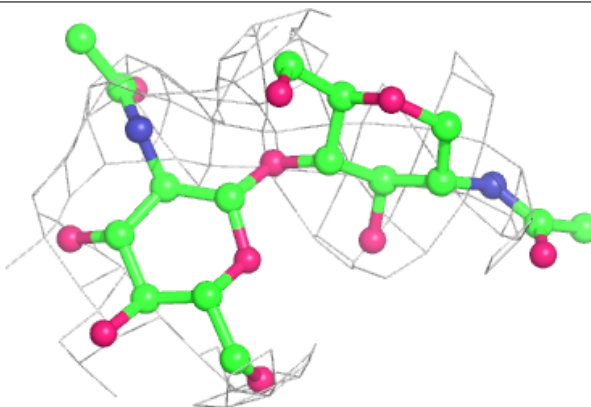


Electron density around Chain J:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

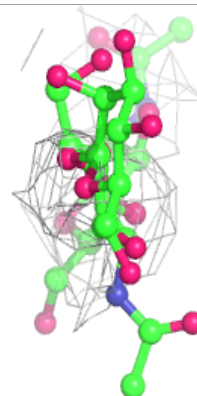
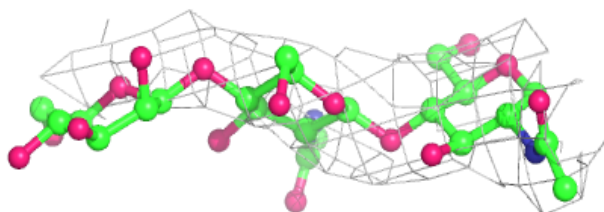
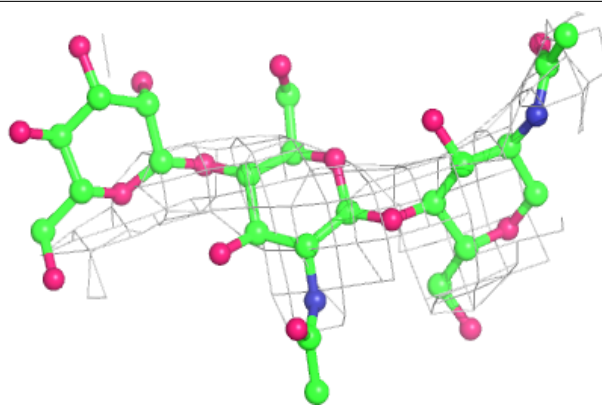
**Electron density around Chain L:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

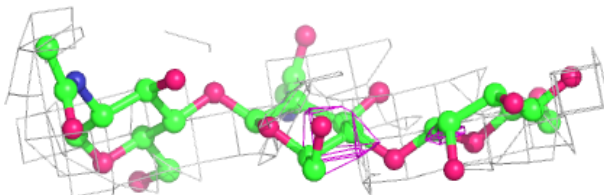
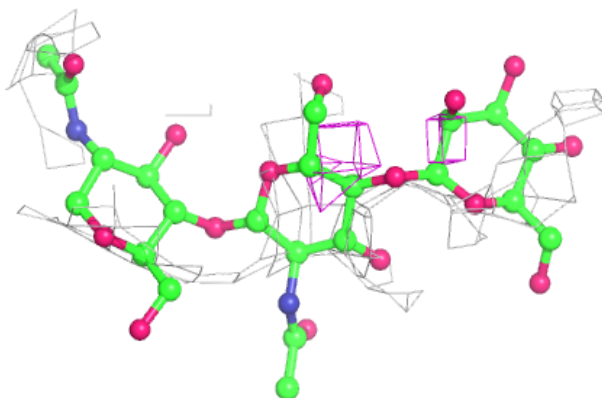


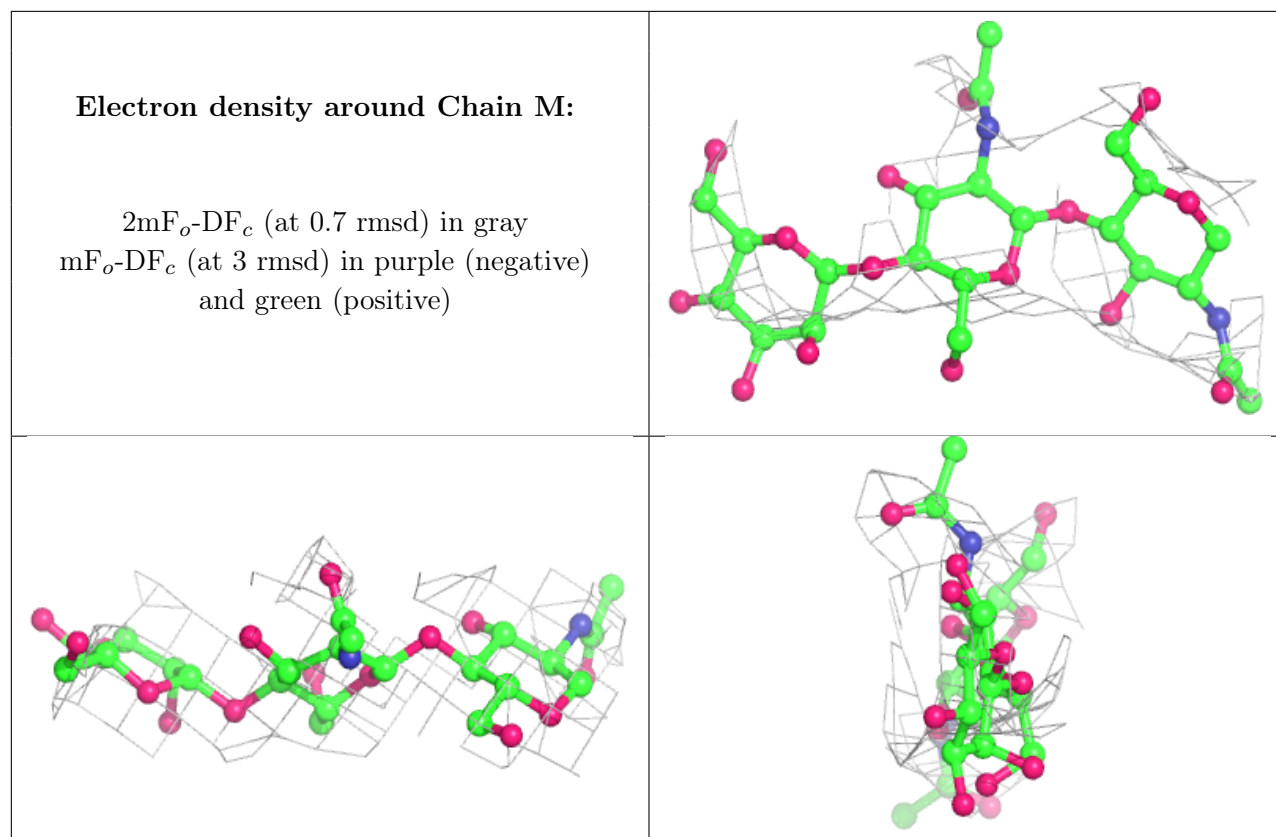
Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain K:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.