



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:39 AM BST

PDB ID : 2B8H
Title : A/NWS/whale/Maine/1/84 (H1N9) reassortant influenza virus neuraminidase
Authors : Smith, B.J.; Platis, D.; Cox, M.M.J.; Huyton, T.; Joosten, R.P.; McKimm-Breschkin, J.L.; Zhang, J.-G.; Luo, C.S.; Lou, M.-Z.; Garrett, T.P.J.; Labrou, N.E.
Deposited on : 2005-10-07
Resolution : 2.20 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 : 2.13.1
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) : 2.13.1

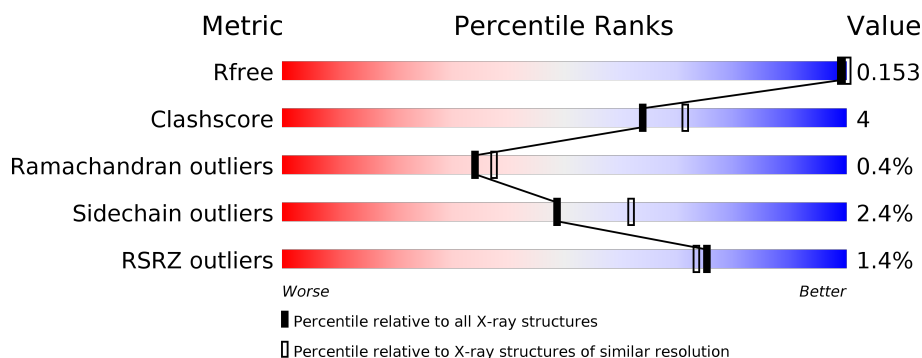
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.




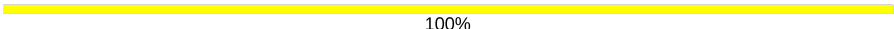
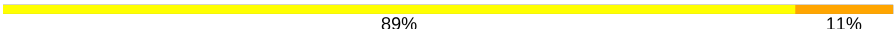
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	388	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	388	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	388	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	388	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	G	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	K	2	 50% 50%
3	F	9	 100%
3	J	9	 89% 11%
3	L	9	 78% 22%
4	H	10	 90% 10%

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
2	NAG	I	2	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14424 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	4	0
			3069	1910	539	595	25			
1	B	388	Total	C	N	O	S	0	4	0
			3067	1908	540	594	25			
1	C	388	Total	C	N	O	S	0	4	0
			3067	1909	540	593	25			
1	D	388	Total	C	N	O	S	0	6	0
			3082	1919	544	594	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	VAL	ILE	conflict	UNP P05803
B	368	VAL	ILE	conflict	UNP P05803
C	368	VAL	ILE	conflict	UNP P05803
D	368	VAL	ILE	conflict	UNP P05803

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



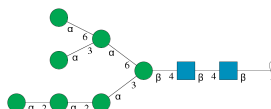
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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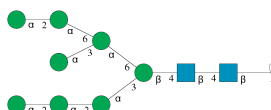
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	9	Total	C	N	O	0	0	0
			105	58	2	45			
3	J	9	Total	C	N	O	0	0	0
			105	58	2	45			
3	L	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

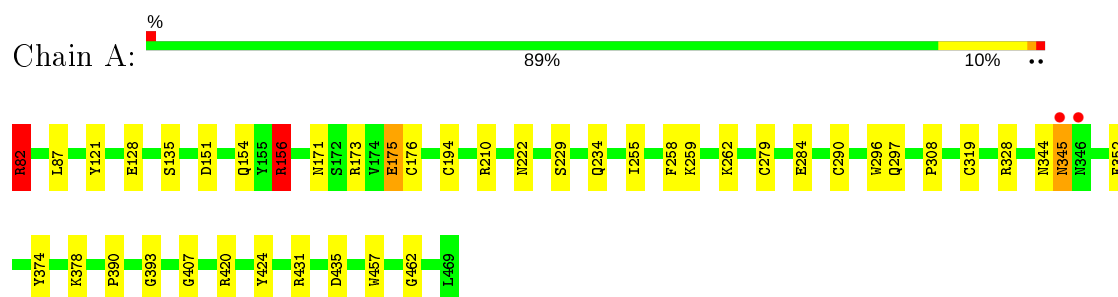
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	369	Total	O	0	0
			369	369		
9	B	315	Total	O	0	0
			315	315		
9	C	324	Total	O	0	0
			324	324		
9	D	365	Total	O	0	0
			365	365		

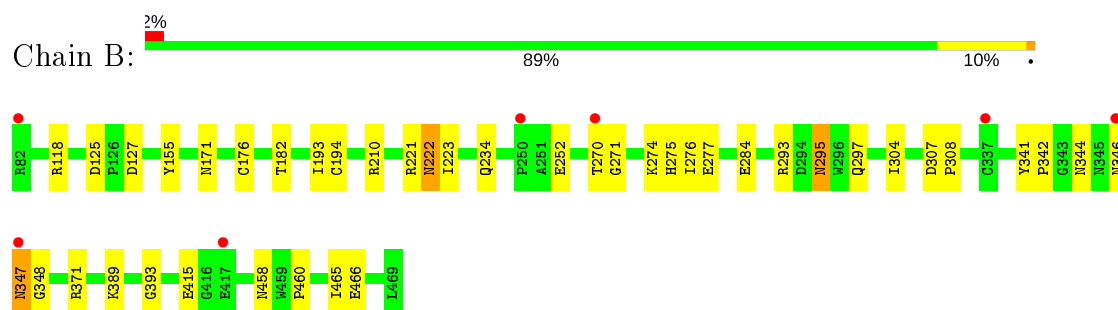
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

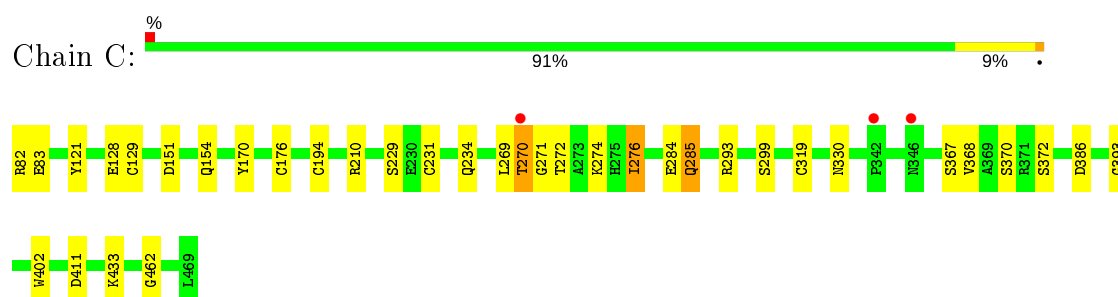
- Molecule 1: Neuraminidase



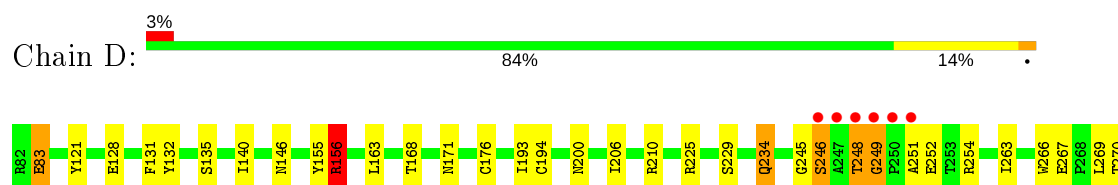
- Molecule 1: Neuraminidase

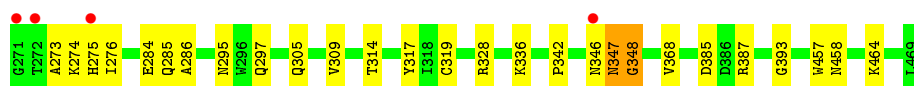


- Molecule 1: Neuraminidase



- Molecule 1: Neuraminidase





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

Chain E:  100%



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

Chain G:  50% 50%



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

Chain I:  100%



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

Chain K:  50% 50%




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

Chain F:  100%




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

Chain J:  89% 11%

MAN1
MAN2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

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

Chain L:  78% 22%

MAN1
MAN2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

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

Chain H:  90% 10%

MAN1
MAN2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.52Å 107.52Å 338.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.20) 99.7 (19.95-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.139 , 0.189 0.152 , 0.153	Depositor DCC
R_{free} test set	5837 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14424	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CL, SO4, MAN

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	1.11	7/3169 (0.2%)	0.99	9/4316 (0.2%)
1	B	1.10	2/3167 (0.1%)	0.98	7/4314 (0.2%)
1	C	1.13	5/3169 (0.2%)	0.98	8/4315 (0.2%)
1	D	1.15	8/3195 (0.3%)	1.02	7/4352 (0.2%)
All	All	1.12	22/12700 (0.2%)	0.99	31/17297 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLU	CD-OE2	8.05	1.34	1.25
1	D	319	CYS	CB-SG	-7.90	1.68	1.82
1	A	128	GLU	CG-CD	7.25	1.62	1.51
1	C	128	GLU	CD-OE2	6.97	1.33	1.25
1	C	319	CYS	CB-SG	-6.88	1.70	1.82
1	D	128	GLU	CD-OE2	6.47	1.32	1.25
1	B	252	GLU	CB-CG	6.30	1.64	1.52
1	A	156	ARG	CD-NE	-6.05	1.36	1.46
1	A	319	CYS	CB-SG	-6.00	1.72	1.81
1	D	83	GLU	CB-CG	-5.99	1.40	1.52
1	D	286	ALA	CA-CB	5.78	1.64	1.52
1	A	259	LYS	CE-NZ	5.73	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	CYS	CB-SG	5.70	1.92	1.82
1	D	267	GLU	CB-CG	-5.69	1.41	1.52
1	D	252	GLU	CB-CG	5.64	1.62	1.52
1	D	156	ARG	CD-NE	-5.44	1.37	1.46
1	A	171	ASN	CB-CG	5.42	1.63	1.51
1	C	129[A]	CYS	CB-SG	5.18	1.91	1.82
1	C	129[B]	CYS	CB-SG	5.18	1.91	1.82
1	A	175	GLU	CD-OE2	5.06	1.31	1.25
1	D	132	TYR	CE1-CZ	-5.02	1.32	1.38
1	B	341	TYR	CD2-CE2	5.01	1.46	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH2	-14.08	113.26	120.30
1	D	156	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	D	156	ARG	NE-CZ-NH2	-11.53	114.54	120.30
1	A	156	ARG	NE-CZ-NH1	11.17	125.88	120.30
1	C	293	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	D	348	GLY	N-CA-C	8.69	134.83	113.10
1	A	151	ASP	CB-CG-OD1	7.92	125.42	118.30
1	D	225	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	C	411	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	C	210	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	127	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	151	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	A	420	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	431	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	82	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	435	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	411	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	210	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	C	386	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	D	387	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	293	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	328	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	210	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	151	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	151	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	385	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	328	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	371	ARG	NE-CZ-NH2	-5.22	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	118	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	118	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	270	THR	Peptide
1	D	246	SER	Peptide

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	3069	0	2880	23	0
1	B	3067	0	2878	21	0
1	C	3067	0	2878	20	0
1	D	3082	0	2891	37	0
2	E	28	0	25	0	0
2	G	28	0	25	1	0
2	I	28	0	25	0	0
2	K	28	0	25	1	0
3	F	105	0	87	1	0
3	J	105	0	88	1	0
3	L	105	0	88	2	0
4	H	116	0	97	1	0
5	A	14	0	13	1	0
5	B	14	0	13	1	0
5	C	14	0	13	1	0
5	D	14	0	13	0	0
6	A	40	0	0	1	0
6	B	30	0	0	1	0
6	C	45	0	0	3	0
6	D	30	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	18	0	24	1	0
9	A	369	0	0	3	1
9	B	315	0	0	5	0
9	C	324	0	0	4	0
9	D	365	0	0	10	1
All	All	14424	0	12063	105	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 4.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:HIS:HB3	1:B:295[A]:ASN:HD21	1.04	1.16
1:B:275:HIS:HB3	1:B:295[A]:ASN:ND2	1.78	0.98
6:A:2516:SO4:O1	9:A:5368:HOH:O	1.84	0.93
1:B:271:GLY:O	1:B:274:LYS:NZ	2.02	0.93
6:B:3516:SO4:O4	9:B:3772:HOH:O	1.86	0.93
1:C:368:VAL:HG22	6:C:3521:SO4:O3	1.71	0.89
1:A:176:CYS:SG	1:A:194[B]:CYS:HB2	2.18	0.84
1:D:176:CYS:SG	1:D:194[B]:CYS:HB2	2.23	0.78
1:A:82:ARG:HB2	1:A:82:ARG:HH11	1.50	0.75
6:C:3520:SO4:O2	9:C:4826:HOH:O	2.05	0.74
1:B:276:ILE:HD13	1:B:304:ILE:HD11	1.70	0.73
1:C:176:CYS:SG	1:C:194[B]:CYS:HB2	2.28	0.73
1:D:305:GLN:HB3	1:D:314:THR:HG22	1.71	0.72
1:D:270:THR:HG23	9:D:4723:HOH:O	1.89	0.72
1:C:271:GLY:H	1:C:274:LYS:NZ	1.87	0.72
1:A:222:ASN:HD21	8:A:5003:GOL:H32	1.55	0.72
1:A:82:ARG:CB	1:A:82:ARG:HH11	2.03	0.72
7:B:2522:CL:CL	9:B:3822:HOH:O	2.46	0.71
1:D:285:GLN:HG3	9:D:4741:HOH:O	1.88	0.71
1:D:347:ASN:C	1:D:347:ASN:HD22	1.94	0.71
1:D:368:VAL:HG23	9:D:4886:HOH:O	1.91	0.70
1:D:295:ASN:O	1:D:346:ASN:HA	1.92	0.69
1:C:402:TRP:CZ3	1:C:433:LYS:HD3	2.28	0.69
1:B:176:CYS:SG	1:B:194[B]:CYS:HB2	2.33	0.68
1:D:269:LEU:O	9:D:4623:HOH:O	2.13	0.67
1:D:248:THR:O	1:D:249:GLY:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:HIS:CB	1:B:295[A]:ASN:ND2	2.59	0.63
1:D:245:GLY:HA3	1:D:251:ALA:HA	1.80	0.63
1:D:314:THR:HG23	9:D:4679:HOH:O	1.97	0.63
1:C:271:GLY:H	1:C:274:LYS:HZ3	1.49	0.60
1:D:273:ALA:HA	1:D:317:TYR:CE1	2.36	0.59
1:C:270:THR:HG23	9:C:4801:HOH:O	2.00	0.59
1:D:135:SER:O	1:D:156:ARG:HD2	2.02	0.59
1:B:276:ILE:CD1	1:B:304:ILE:HD11	2.33	0.58
1:D:336:LYS:NZ	9:D:4838:HOH:O	2.36	0.58
1:D:464:LYS:NZ	1:D:464:LYS:HB3	2.21	0.56
6:C:4516:SO4:O3	9:C:4712:HOH:O	2.18	0.55
1:D:269:LEU:HB3	9:D:4623:HOH:O	2.08	0.55
1:B:270:THR:HG22	9:B:3682:HOH:O	2.08	0.54
1:B:297:GLN:OE1	1:B:342:PRO:HA	2.08	0.53
5:A:500:NAG:H83	9:A:5140:HOH:O	2.07	0.53
1:D:210[B]:ARG:NE	9:D:4865:HOH:O	2.40	0.53
1:B:344:ASN:ND2	1:B:347:ASN:OD1	2.42	0.53
1:B:415:GLU:OE1	1:B:415:GLU:HA	2.09	0.52
1:B:234:GLN:HG2	1:B:308:PRO:HG2	1.91	0.52
1:A:175:GLU:OE1	9:A:5220:HOH:O	2.19	0.51
1:C:402:TRP:CZ3	1:C:433:LYS:CD	2.94	0.51
1:A:234[A]:GLN:HG2	1:A:308:PRO:HG2	1.93	0.51
1:B:171[A]:ASN:HD21	1:C:170:TYR:HB3	1.76	0.50
1:C:402:TRP:CH2	1:C:433:LYS:HD3	2.46	0.50
1:D:464:LYS:HB3	1:D:464:LYS:HZ3	1.77	0.49
5:C:500:NAG:H61	9:C:4718:HOH:O	2.11	0.49
9:B:3715:HOH:O	2:G:2:NAG:O4	2.20	0.49
1:A:378:LYS:O	1:A:390:PRO:HA	2.12	0.49
1:A:344:ASN:C	1:A:345:ASN:HD22	2.15	0.48
1:D:210[A]:ARG:HD3	9:D:4865:HOH:O	2.13	0.48
1:A:352:PHE:HE1	1:A:374:TYR:HH	1.62	0.48
1:D:121:TYR:CG	1:D:229:SER:HA	2.48	0.47
1:C:121:TYR:CG	1:C:229:SER:HA	2.50	0.47
1:D:131:PHE:CE1	1:D:163:LEU:HD12	2.49	0.47
1:C:271:GLY:H	1:C:274:LYS:HZ1	1.59	0.47
1:B:347:ASN:N	1:B:347:ASN:OD1	2.47	0.47
1:A:87:LEU:H	1:A:234[B]:GLN:HG2	1.79	0.46
1:D:193:ILE:HG12	1:D:206:ILE:HG13	1.96	0.46
1:A:154:GLN:HG2	1:D:458:ASN:O	2.15	0.46
1:D:275:HIS:O	1:D:276:ILE:CG1	2.64	0.45
1:A:255:ILE:HD12	1:A:255:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:500:NAG:H61	9:B:3709:HOH:O	2.15	0.45
1:A:173:ARG:NE	1:A:210:ARG:NH2	2.65	0.45
1:A:135:SER:O	1:A:156:ARG:HD2	2.16	0.45
1:B:222:ASN:HD22	1:B:223:ILE:HG13	1.82	0.45
1:A:121:TYR:CG	1:A:229:SER:HA	2.52	0.44
1:D:263:ILE:HG21	1:D:266[B]:TRP:CE3	2.53	0.44
1:A:135:SER:O	1:A:156:ARG:CD	2.65	0.44
1:D:347:ASN:C	1:D:347:ASN:ND2	2.67	0.44
1:A:407:GLY:HA3	1:A:424:TYR:CE1	2.53	0.43
1:D:234[A]:GLN:HE22	1:D:309:VAL:HG22	1.83	0.43
1:D:297:GLN:NE2	1:D:342:PRO:HA	2.33	0.43
1:A:279:CYS:HB3	1:A:290:CYS:HB3	1.99	0.43
1:A:393:GLY:HA3	4:H:3:BMA:O2	2.18	0.43
1:D:135:SER:O	1:D:156:ARG:CD	2.65	0.43
1:C:393:GLY:HA3	3:L:3:BMA:O2	2.19	0.42
1:A:82:ARG:NH1	1:A:82:ARG:HB2	2.28	0.42
1:D:393:GLY:HA3	3:F:3:BMA:O2	2.18	0.42
1:C:271:GLY:N	1:C:274:LYS:HZ3	2.15	0.42
1:C:367:SER:HB3	1:C:372:SER:HB2	2.01	0.42
1:D:263:ILE:HG21	1:D:266[B]:TRP:CZ3	2.54	0.42
1:D:146:ASN:ND2	2:K:1:NAG:O7	2.53	0.42
1:B:182:THR:HG22	1:B:193:ILE:HB	2.00	0.42
1:A:296:TRP:CG	1:A:297:GLN:HG3	2.54	0.42
1:C:276:ILE:HD12	1:C:276:ILE:HA	1.80	0.42
1:D:254:ARG:HD3	1:D:266[A]:TRP:CE3	2.55	0.41
1:C:462:GLY:HA3	1:D:155:TYR:CE1	2.55	0.41
1:B:458:ASN:O	1:C:154:GLN:HG2	2.21	0.41
1:D:464:LYS:NZ	1:D:464:LYS:CB	2.83	0.41
1:C:330:ASN:HA	3:L:6:MAN:O3	2.19	0.41
1:D:140:ILE:HD11	9:D:4619:HOH:O	2.20	0.41
1:B:307:ASP:C	1:B:307:ASP:OD1	2.59	0.41
1:B:393:GLY:HA3	3:J:3:BMA:O2	2.21	0.41
1:A:258:PHE:HA	1:A:262:LYS:O	2.21	0.41
1:A:462:GLY:HA3	1:B:155:TYR:CE1	2.56	0.41
1:B:465:ILE:HG23	1:B:465:ILE:HD12	1.79	0.40
1:D:168:THR:OG1	1:D:171[A]:ASN:OD1	2.38	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)
9:A:5115:HOH:O	9:D:4752:HOH:O[4_565]	2.19	0.01

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 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	390/388 (100%)	374 (96%)	16 (4%)	0	100	100
1	B	390/388 (100%)	369 (95%)	19 (5%)	2 (0%)	29	31
1	C	390/388 (100%)	366 (94%)	24 (6%)	0	100	100
1	D	392/388 (101%)	365 (93%)	23 (6%)	4 (1%)	15	14
All	All	1562/1552 (101%)	1474 (94%)	82 (5%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	249	GLY
1	B	348	GLY
1	D	348	GLY
1	D	246	SER
1	B	347	ASN
1	D	248	THR

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 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	343/340 (101%)	338 (98%)	5 (2%)	65	78
1	B	343/340 (101%)	333 (97%)	10 (3%)	42	54
1	C	343/340 (101%)	332 (97%)	11 (3%)	39	50
1	D	345/340 (102%)	336 (97%)	9 (3%)	46	58
All	All	1374/1360 (101%)	1339 (98%)	35 (2%)	49	60

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	156	ARG
1	A	284	GLU
1	A	345	ASN
1	A	457	TRP
1	B	221	ARG
1	B	222	ASN
1	B	277	GLU
1	B	284	GLU
1	B	295[A]	ASN
1	B	295[B]	ASN
1	B	346	ASN
1	B	389	LYS
1	B	460	PRO
1	B	466	GLU
1	C	82	ARG
1	C	83	GLU
1	C	234	GLN
1	C	269	LEU
1	C	272	THR
1	C	276	ILE
1	C	284	GLU
1	C	285[A]	GLN
1	C	285[B]	GLN
1	C	299	SER
1	C	370	SER
1	D	83	GLU
1	D	156	ARG
1	D	200	ASN
1	D	234[A]	GLN
1	D	234[B]	GLN
1	D	274	LYS
1	D	284	GLU

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Mol	Chain	Res	Type
1	D	347	ASN
1	D	457	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	381	ASN
1	B	222	ASN
1	B	235	ASN
1	C	95	ASN
1	C	234	GLN
1	C	326	ASN
1	D	200	ASN
1	D	297	GLN
1	D	347	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

45 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	1.26	2 (14%)	17,19,21	1.80	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.76	0	17,19,21	1.29	2 (11%)
3	NAG	F	1	1,3	14,14,15	1.12	1 (7%)	17,19,21	1.48	3 (17%)
3	NAG	F	2	3	14,14,15	1.21	1 (7%)	17,19,21	1.82	6 (35%)
3	BMA	F	3	3	11,11,12	0.92	0	15,15,17	0.93	0
3	MAN	F	4	3	11,11,12	0.73	0	15,15,17	1.87	5 (33%)
3	MAN	F	5	3	11,11,12	1.36	1 (9%)	15,15,17	1.63	3 (20%)
3	MAN	F	6	3	11,11,12	0.90	0	15,15,17	1.49	3 (20%)
3	MAN	F	7	3	11,11,12	1.12	1 (9%)	15,15,17	1.51	2 (13%)
3	MAN	F	8	3	11,11,12	1.19	1 (9%)	15,15,17	1.56	3 (20%)
3	MAN	F	9	3	11,11,12	0.86	0	15,15,17	2.61	7 (46%)
2	NAG	G	1	1,2	14,14,15	1.06	1 (7%)	17,19,21	1.82	4 (23%)
2	NAG	G	2	2	14,14,15	0.71	0	17,19,21	1.73	2 (11%)
4	NAG	H	1	1,4	14,14,15	1.26	2 (14%)	17,19,21	1.86	7 (41%)
4	MAN	H	10	4	11,11,12	0.68	0	15,15,17	1.57	3 (20%)
4	NAG	H	2	4	14,14,15	0.93	0	17,19,21	1.66	3 (17%)
4	BMA	H	3	4	11,11,12	1.02	1 (9%)	15,15,17	1.44	2 (13%)
4	MAN	H	4	4	11,11,12	1.31	2 (18%)	15,15,17	2.04	3 (20%)
4	MAN	H	5	4	11,11,12	0.97	0	15,15,17	1.41	4 (26%)
4	MAN	H	6	4	11,11,12	0.58	0	15,15,17	1.12	1 (6%)
4	MAN	H	7	4	11,11,12	0.96	1 (9%)	15,15,17	1.37	3 (20%)
4	MAN	H	8	4	11,11,12	0.84	0	15,15,17	1.12	1 (6%)
4	MAN	H	9	4	11,11,12	0.78	0	15,15,17	1.44	1 (6%)
2	NAG	I	1	1,2	14,14,15	1.41	2 (14%)	17,19,21	2.28	5 (29%)
2	NAG	I	2	2	14,14,15	1.17	1 (7%)	17,19,21	2.95	3 (17%)
3	NAG	J	1	1,3	14,14,15	0.89	0	17,19,21	1.62	6 (35%)
3	NAG	J	2	3	14,14,15	1.18	1 (7%)	17,19,21	1.35	2 (11%)
3	BMA	J	3	3	11,11,12	1.33	2 (18%)	15,15,17	1.59	3 (20%)
3	MAN	J	4	3	11,11,12	1.10	1 (9%)	15,15,17	2.31	6 (40%)
3	MAN	J	5	3	11,11,12	1.11	1 (9%)	15,15,17	1.23	2 (13%)
3	MAN	J	6	3	11,11,12	1.08	0	15,15,17	1.43	1 (6%)
3	MAN	J	7	3	11,11,12	1.20	2 (18%)	15,15,17	0.96	1 (6%)
3	MAN	J	8	3	11,11,12	0.76	0	15,15,17	1.37	1 (6%)
3	MAN	J	9	3	11,11,12	1.06	0	15,15,17	2.27	4 (26%)
2	NAG	K	1	1,2	14,14,15	0.99	1 (7%)	17,19,21	2.16	6 (35%)
2	NAG	K	2	2	14,14,15	0.82	0	17,19,21	1.68	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	L	1	1,3	14,14,15	1.16	2 (14%)	17,19,21	1.43	3 (17%)
3	NAG	L	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.89	6 (35%)
3	BMA	L	3	3	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
3	MAN	L	4	3	11,11,12	1.37	1 (9%)	15,15,17	1.84	4 (26%)
3	MAN	L	5	3	11,11,12	0.91	1 (9%)	15,15,17	1.69	4 (26%)
3	MAN	L	6	3	11,11,12	0.89	0	15,15,17	1.21	1 (6%)
3	MAN	L	7	3	11,11,12	0.87	0	15,15,17	1.26	1 (6%)
3	MAN	L	8	3	11,11,12	0.72	0	15,15,17	1.45	1 (6%)
3	MAN	L	9	3	11,11,12	1.04	1 (9%)	15,15,17	1.44	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
3	MAN	F	8	3	-	2/2/19/22	0/1/1/1
3	MAN	F	9	3	-	1/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	H	10	4	-	0/2/19/22	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	MAN	H	6	4	-	0/2/19/22	0/1/1/1
4	MAN	H	7	4	-	0/2/19/22	0/1/1/1
4	MAN	H	8	4	-	0/2/19/22	0/1/1/1
4	MAN	H	9	4	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	0/2/19/22	0/1/1/1
3	MAN	J	5	3	-	0/2/19/22	0/1/1/1
3	MAN	J	6	3	-	0/2/19/22	0/1/1/1
3	MAN	J	7	3	-	0/2/19/22	0/1/1/1
3	MAN	J	8	3	-	0/2/19/22	0/1/1/1
3	MAN	J	9	3	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	MAN	L	4	3	-	1/2/19/22	0/1/1/1
3	MAN	L	5	3	-	0/2/19/22	0/1/1/1
3	MAN	L	6	3	-	0/2/19/22	0/1/1/1
3	MAN	L	7	3	-	0/2/19/22	0/1/1/1
3	MAN	L	8	3	-	0/2/19/22	0/1/1/1
3	MAN	L	9	3	-	0/2/19/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	NAG	O5-C1	-3.72	1.37	1.43
2	I	2	NAG	C1-C2	3.60	1.57	1.52
2	I	1	NAG	O5-C1	-3.52	1.38	1.43
3	F	5	MAN	O3-C3	-3.48	1.34	1.43
2	E	1	NAG	O5-C1	-3.42	1.38	1.43
3	F	2	NAG	O5-C1	-3.34	1.38	1.43
3	L	4	MAN	O5-C1	-3.31	1.38	1.43
3	F	8	MAN	O5-C1	-3.19	1.38	1.43
3	J	3	BMA	C2-C3	3.10	1.57	1.52
4	H	4	MAN	C2-C3	2.96	1.56	1.52
3	F	1	NAG	C1-C2	2.80	1.56	1.52
3	L	1	NAG	C1-C2	2.78	1.56	1.52
4	H	7	MAN	O2-C2	-2.71	1.37	1.43
3	F	7	MAN	O5-C1	-2.68	1.39	1.43
2	K	1	NAG	O7-C7	2.68	1.29	1.23
2	G	1	NAG	O7-C7	2.62	1.29	1.23
4	H	1	NAG	C1-C2	2.58	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-2.57	1.39	1.43
3	J	4	MAN	O5-C1	-2.46	1.39	1.43
3	J	7	MAN	O5-C1	-2.46	1.39	1.43
2	I	1	NAG	C3-C2	2.45	1.57	1.52
2	E	1	NAG	O7-C7	2.44	1.28	1.23
4	H	3	BMA	O3-C3	-2.36	1.37	1.43
3	L	9	MAN	C1-C2	2.34	1.57	1.52
3	J	5	MAN	O5-C1	-2.30	1.40	1.43
3	J	7	MAN	O2-C2	-2.23	1.38	1.43
3	L	2	NAG	O5-C1	-2.20	1.40	1.43
3	L	1	NAG	C4-C5	2.18	1.57	1.53
3	L	5	MAN	O5-C1	-2.15	1.40	1.43
4	H	4	MAN	O5-C1	-2.10	1.40	1.43
3	J	3	BMA	O3-C3	-2.05	1.38	1.43

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C1-O5-C5	10.67	126.65	112.19
3	J	9	MAN	O2-C2-C1	5.54	120.48	109.15
3	J	4	MAN	C1-O5-C5	5.40	119.50	112.19
3	F	9	MAN	O3-C3-C2	5.28	120.11	109.99
3	F	4	MAN	O2-C2-C1	-4.98	98.96	109.15
2	G	2	NAG	C1-O5-C5	4.89	118.82	112.19
4	H	4	MAN	O2-C2-C1	-4.80	99.33	109.15
2	E	1	NAG	O5-C1-C2	-4.77	103.76	111.29
3	J	4	MAN	O2-C2-C1	-4.76	99.42	109.15
2	I	1	NAG	O3-C3-C4	4.72	121.25	110.35
2	I	1	NAG	C3-C4-C5	-4.42	102.35	110.24
2	I	1	NAG	O4-C4-C3	4.40	120.53	110.35
3	L	5	MAN	C1-O5-C5	4.39	118.14	112.19
4	H	4	MAN	C1-O5-C5	4.36	118.10	112.19
3	F	5	MAN	C1-C2-C3	-4.24	104.45	109.67
2	G	1	NAG	C2-N2-C7	-4.18	116.95	122.90
3	L	4	MAN	O2-C2-C1	-4.15	100.67	109.15
3	F	6	MAN	C1-O5-C5	4.07	117.70	112.19
2	E	2	NAG	C2-N2-C7	-4.05	117.14	122.90
2	K	1	NAG	C2-N2-C7	-4.02	117.18	122.90
2	K	1	NAG	O4-C4-C3	-3.98	101.14	110.35
3	J	3	BMA	O5-C5-C6	3.92	113.35	107.20
3	F	9	MAN	O2-C2-C1	3.87	117.07	109.15
3	L	7	MAN	O2-C2-C1	3.86	117.05	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	8	MAN	O5-C5-C6	3.86	113.25	107.20
3	F	9	MAN	O4-C4-C3	-3.82	101.52	110.35
3	L	2	NAG	C1-C2-N2	3.72	116.85	110.49
4	H	2	NAG	O6-C6-C5	-3.69	98.64	111.29
3	F	2	NAG	C8-C7-N2	3.65	122.29	116.10
3	F	9	MAN	O2-C2-C3	3.64	117.44	110.14
3	L	9	MAN	O2-C2-C1	3.60	116.52	109.15
3	L	6	MAN	C1-O5-C5	3.55	117.00	112.19
3	J	9	MAN	O6-C6-C5	-3.54	99.13	111.29
2	K	1	NAG	O5-C1-C2	-3.51	105.75	111.29
3	L	2	NAG	O5-C5-C6	3.47	112.64	107.20
3	F	9	MAN	C1-C2-C3	-3.46	105.41	109.67
3	J	2	NAG	O3-C3-C4	3.45	118.32	110.35
4	H	2	NAG	O3-C3-C4	3.44	118.31	110.35
2	G	1	NAG	C1-O5-C5	3.39	116.78	112.19
3	J	1	NAG	O7-C7-N2	3.33	128.07	121.95
3	F	8	MAN	C1-O5-C5	3.32	116.68	112.19
4	H	1	NAG	C1-O5-C5	3.26	116.60	112.19
3	L	1	NAG	O5-C5-C6	3.24	112.28	107.20
2	K	1	NAG	O7-C7-C8	3.22	128.05	122.06
3	F	9	MAN	O5-C5-C6	3.22	112.25	107.20
2	K	1	NAG	C8-C7-N2	-3.18	110.71	116.10
3	L	2	NAG	O6-C6-C5	-3.18	100.39	111.29
4	H	1	NAG	O4-C4-C3	-3.14	103.09	110.35
3	J	9	MAN	C1-C2-C3	-3.13	105.82	109.67
2	G	1	NAG	O5-C1-C2	-3.12	106.36	111.29
2	K	2	NAG	C8-C7-N2	3.11	121.37	116.10
2	K	2	NAG	C2-N2-C7	-3.11	118.47	122.90
2	I	2	NAG	O5-C5-C4	3.08	118.32	110.83
3	F	2	NAG	O4-C4-C3	-3.07	103.25	110.35
4	H	6	MAN	C1-O5-C5	3.06	116.33	112.19
4	H	1	NAG	O5-C1-C2	-2.99	106.57	111.29
2	K	2	NAG	O5-C5-C6	2.98	111.87	107.20
4	H	5	MAN	O5-C5-C6	2.95	111.83	107.20
3	F	7	MAN	O4-C4-C3	-2.93	103.57	110.35
3	J	6	MAN	C1-O5-C5	2.92	116.14	112.19
3	J	4	MAN	O2-C2-C3	2.92	115.98	110.14
3	L	4	MAN	O6-C6-C5	-2.90	101.35	111.29
3	J	5	MAN	O4-C4-C3	-2.89	103.66	110.35
4	H	7	MAN	O5-C1-C2	-2.87	106.34	110.77
3	F	1	NAG	O7-C7-N2	2.84	127.18	121.95
3	F	6	MAN	C3-C4-C5	-2.75	105.34	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	9	MAN	O6-C6-C5	-2.71	101.99	111.29
4	H	10	MAN	O2-C2-C3	2.70	115.54	110.14
4	H	10	MAN	O3-C3-C4	2.67	116.52	110.35
2	I	1	NAG	C1-C2-N2	-2.67	105.93	110.49
4	H	3	BMA	C1-C2-C3	-2.64	106.43	109.67
3	J	1	NAG	O5-C5-C6	2.63	111.33	107.20
3	J	9	MAN	O4-C4-C3	-2.63	104.27	110.35
3	L	2	NAG	O5-C1-C2	-2.62	107.15	111.29
3	J	2	NAG	O6-C6-C5	-2.59	102.41	111.29
4	H	10	MAN	C1-C2-C3	-2.58	106.49	109.67
3	F	1	NAG	C2-N2-C7	2.57	126.57	122.90
3	L	2	NAG	C3-C4-C5	-2.57	105.65	110.24
2	G	1	NAG	O4-C4-C3	-2.56	104.42	110.35
3	F	6	MAN	O2-C2-C1	2.54	114.35	109.15
3	L	1	NAG	O5-C1-C2	-2.52	107.31	111.29
3	F	2	NAG	C6-C5-C4	2.52	118.90	113.00
2	E	1	NAG	O4-C4-C3	-2.51	104.55	110.35
3	F	4	MAN	O2-C2-C3	2.51	115.16	110.14
3	L	4	MAN	C1-O5-C5	2.49	115.57	112.19
4	H	2	NAG	C3-C4-C5	-2.48	105.81	110.24
2	E	1	NAG	C2-N2-C7	-2.47	119.39	122.90
2	G	2	NAG	C2-N2-C7	2.46	126.40	122.90
3	J	3	BMA	C6-C5-C4	-2.45	107.26	113.00
3	F	2	NAG	C2-N2-C7	-2.44	119.43	122.90
3	J	5	MAN	O2-C2-C1	-2.42	104.21	109.15
3	F	2	NAG	O7-C7-C8	-2.39	117.61	122.06
4	H	1	NAG	O7-C7-N2	2.39	126.34	121.95
3	F	2	NAG	O3-C3-C4	2.37	115.84	110.35
3	J	4	MAN	O4-C4-C3	2.37	115.83	110.35
4	H	3	BMA	O3-C3-C2	-2.37	105.47	109.99
3	J	1	NAG	C1-O5-C5	2.34	115.36	112.19
3	L	4	MAN	O5-C5-C4	2.33	116.50	110.83
4	H	7	MAN	C2-C3-C4	2.33	114.93	110.89
2	I	1	NAG	C4-C3-C2	-2.33	107.60	111.02
4	H	4	MAN	O3-C3-C2	2.32	114.43	109.99
3	F	7	MAN	O5-C1-C2	-2.31	107.20	110.77
4	H	5	MAN	C1-C2-C3	-2.31	106.83	109.67
3	F	5	MAN	O5-C5-C6	2.30	110.81	107.20
3	J	8	MAN	O5-C5-C6	2.29	110.80	107.20
2	K	2	NAG	O7-C7-C8	-2.28	117.82	122.06
4	H	1	NAG	C3-C4-C5	-2.26	106.21	110.24
3	F	9	MAN	O6-C6-C5	-2.24	103.61	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	O3-C3-C4	-2.22	105.21	110.35
3	J	4	MAN	O6-C6-C5	-2.21	103.71	111.29
3	L	5	MAN	O6-C6-C5	2.20	118.85	111.29
4	H	5	MAN	C1-O5-C5	2.20	115.17	112.19
2	K	1	NAG	C1-O5-C5	2.19	115.16	112.19
3	F	4	MAN	C1-C2-C3	2.18	112.34	109.67
3	J	3	BMA	O2-C2-C1	2.18	113.61	109.15
2	E	1	NAG	C8-C7-N2	-2.18	112.41	116.10
3	F	1	NAG	C8-C7-N2	-2.18	112.42	116.10
2	E	2	NAG	O6-C6-C5	-2.17	103.84	111.29
3	F	4	MAN	O3-C3-C2	2.17	114.14	109.99
3	F	8	MAN	O3-C3-C2	-2.17	105.85	109.99
3	F	8	MAN	O5-C5-C6	-2.16	103.82	107.20
3	L	3	BMA	C3-C4-C5	-2.16	106.39	110.24
2	I	2	NAG	O3-C3-C2	2.16	113.93	109.47
3	J	4	MAN	C3-C4-C5	-2.16	106.39	110.24
3	J	1	NAG	C2-N2-C7	-2.15	119.84	122.90
3	J	1	NAG	O4-C4-C3	-2.14	105.41	110.35
4	H	1	NAG	O5-C5-C6	2.13	110.55	107.20
3	L	2	NAG	O3-C3-C4	2.12	115.26	110.35
3	L	9	MAN	C6-C5-C4	-2.12	108.03	113.00
4	H	5	MAN	O2-C2-C1	2.12	113.49	109.15
3	L	9	MAN	O6-C6-C5	-2.11	104.03	111.29
3	J	1	NAG	O7-C7-C8	-2.11	118.14	122.06
3	F	5	MAN	O3-C3-C4	-2.09	105.51	110.35
3	J	7	MAN	C1-C2-C3	2.09	112.23	109.67
3	F	4	MAN	C1-O5-C5	2.09	115.02	112.19
3	L	1	NAG	O7-C7-N2	2.09	125.79	121.95
3	L	5	MAN	O4-C4-C3	2.05	115.09	110.35
3	L	5	MAN	O3-C3-C2	-2.05	106.08	109.99
4	H	8	MAN	C1-O5-C5	2.02	114.93	112.19
4	H	7	MAN	O2-C2-C1	-2.02	105.02	109.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	9	MAN	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	J	9	MAN	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C8-C7-N2-C2

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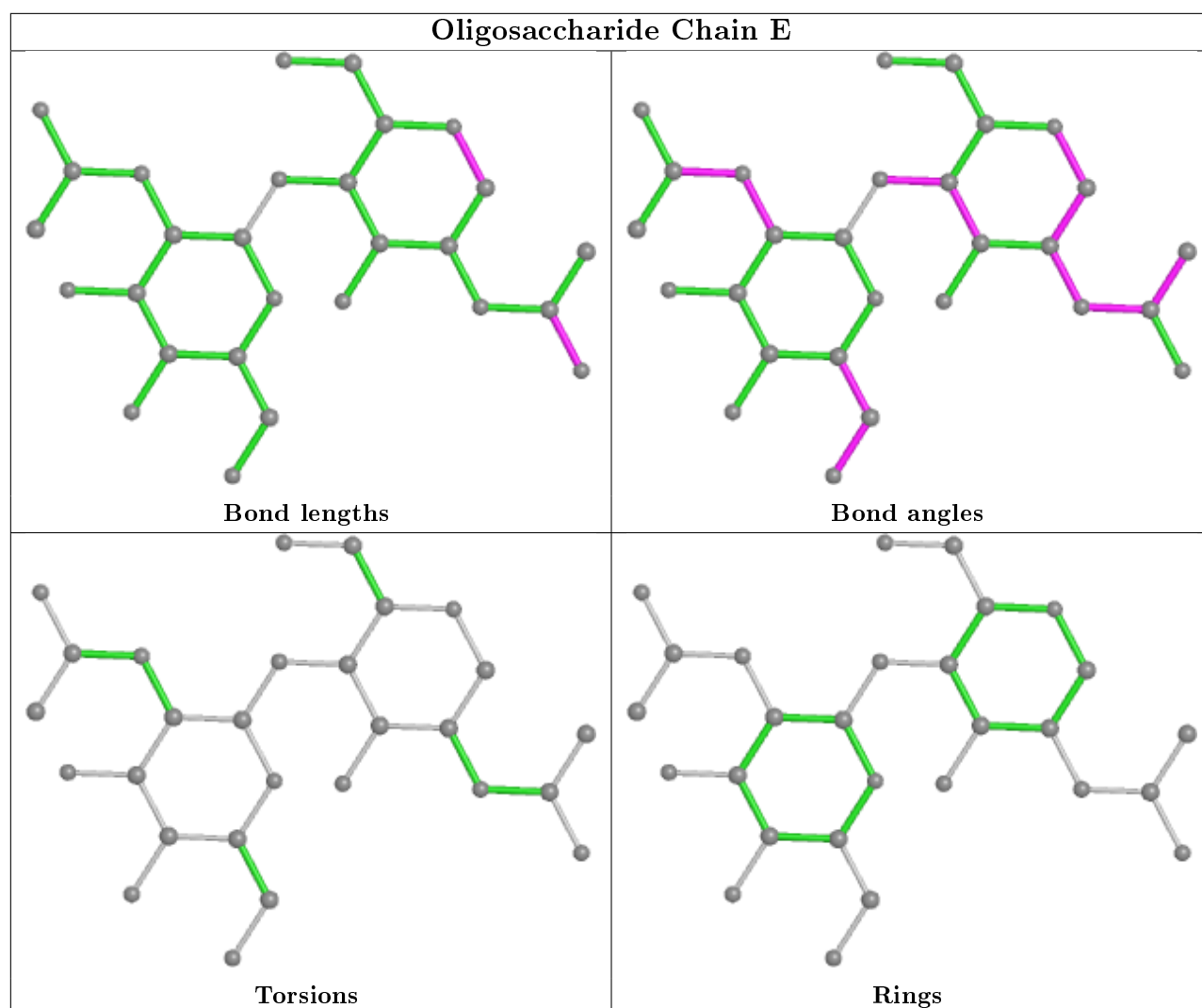
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	F	8	MAN	C4-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6
3	F	9	MAN	O5-C5-C6-O6
3	L	4	MAN	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6

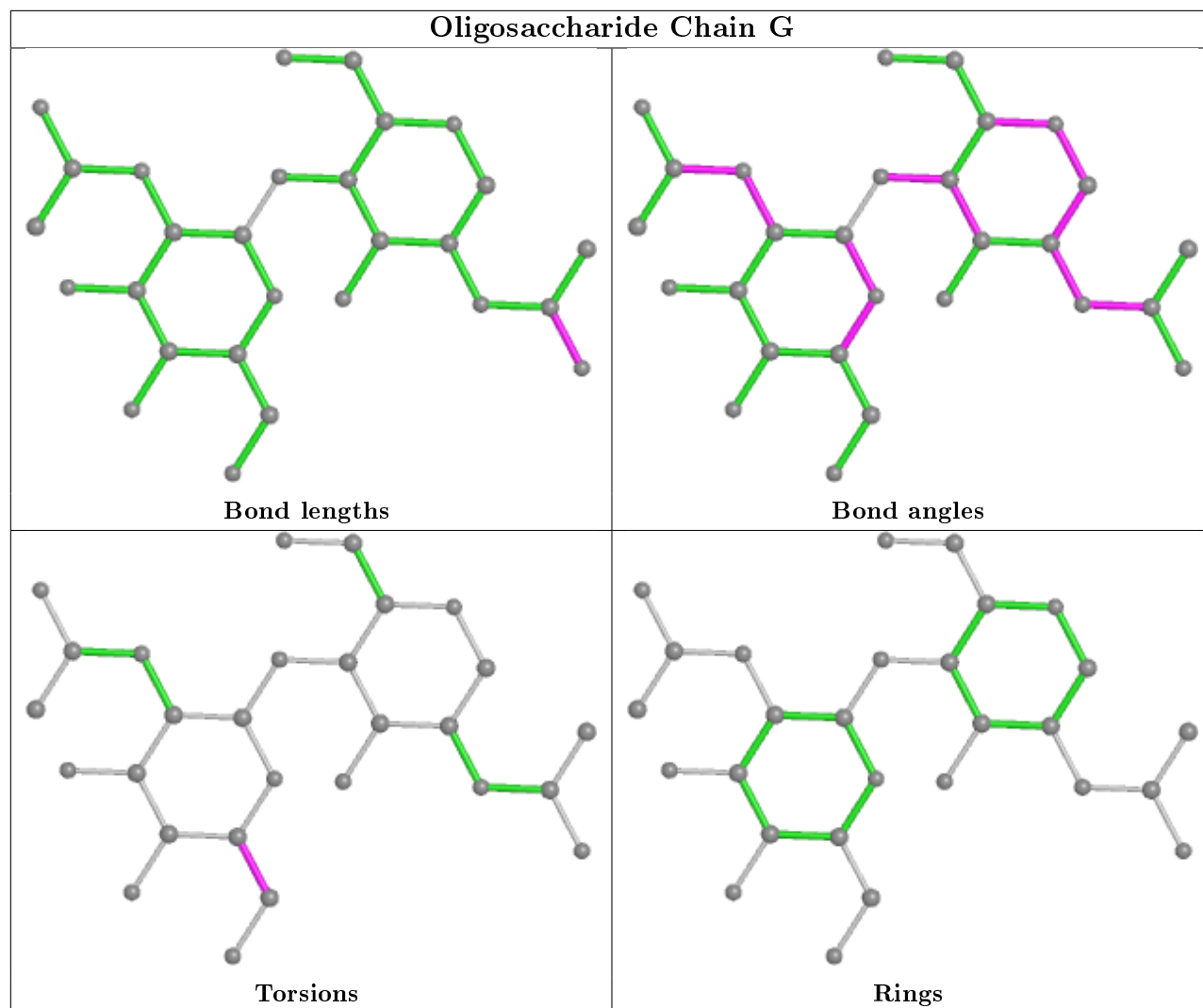
There are no ring outliers.

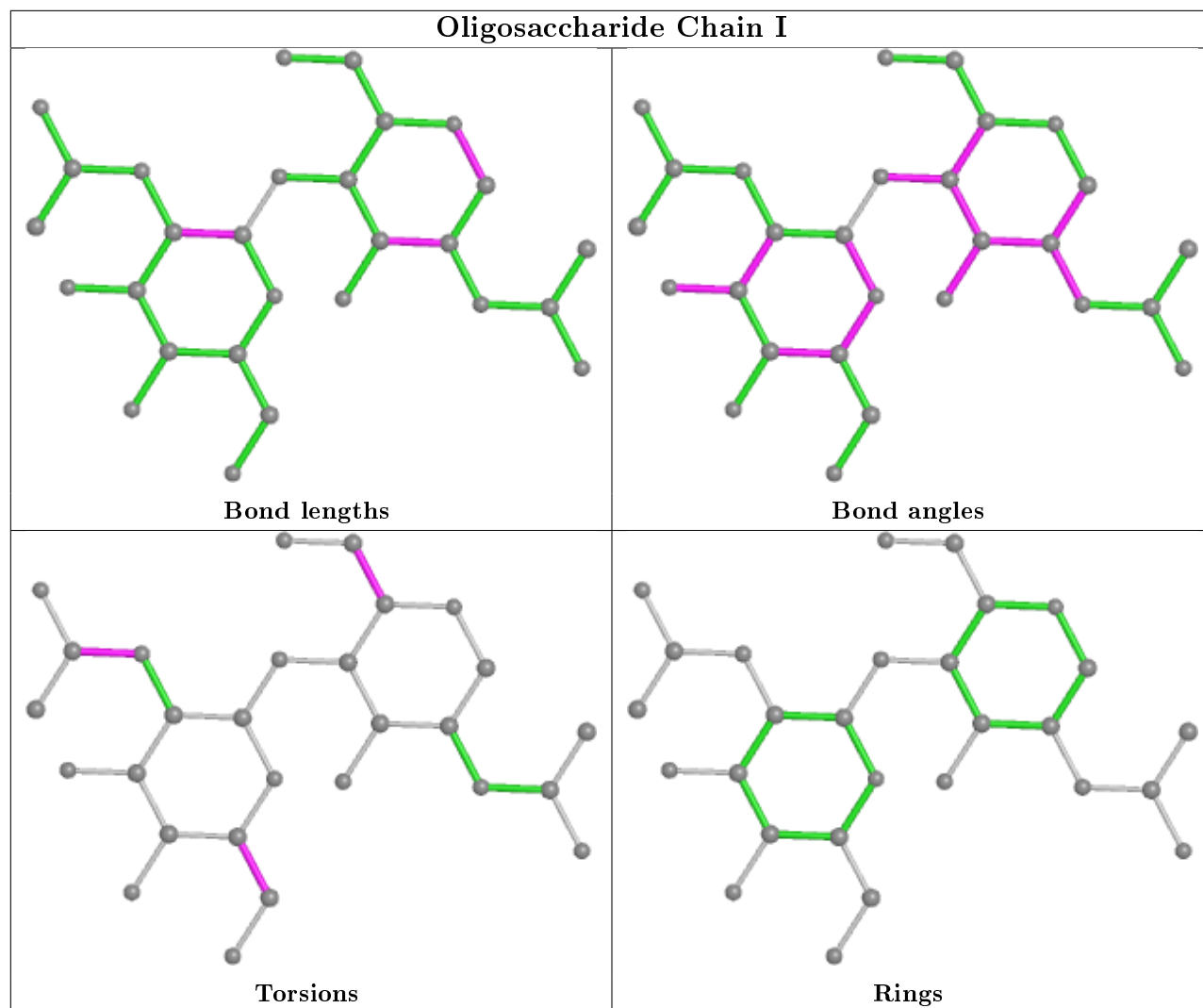
7 monomers are involved in 7 short contacts:

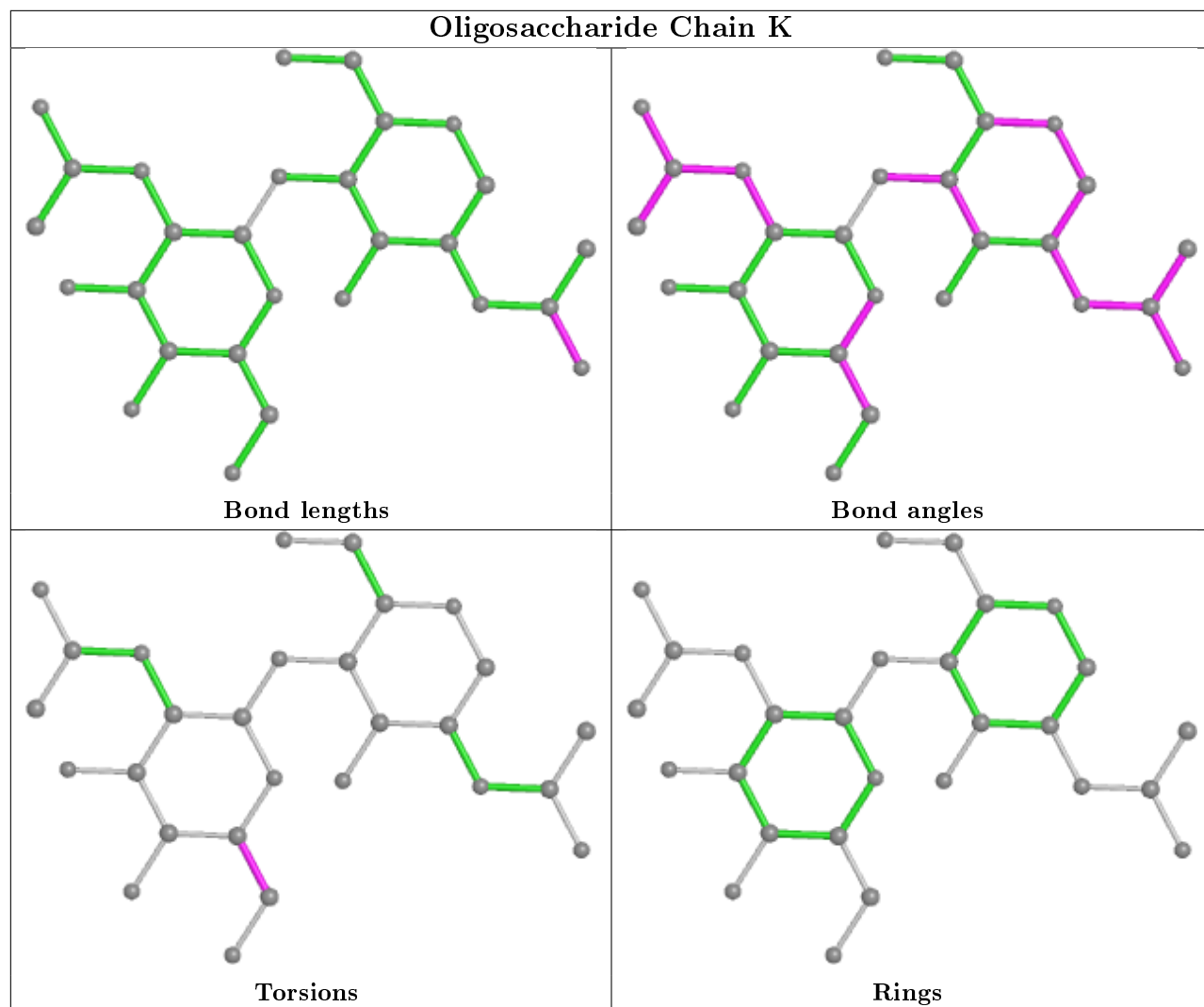
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3	BMA	1	0
2	G	2	NAG	1	0
3	J	3	BMA	1	0
3	L	6	MAN	1	0
2	K	1	NAG	1	0
3	L	3	BMA	1	0
3	F	3	BMA	1	0

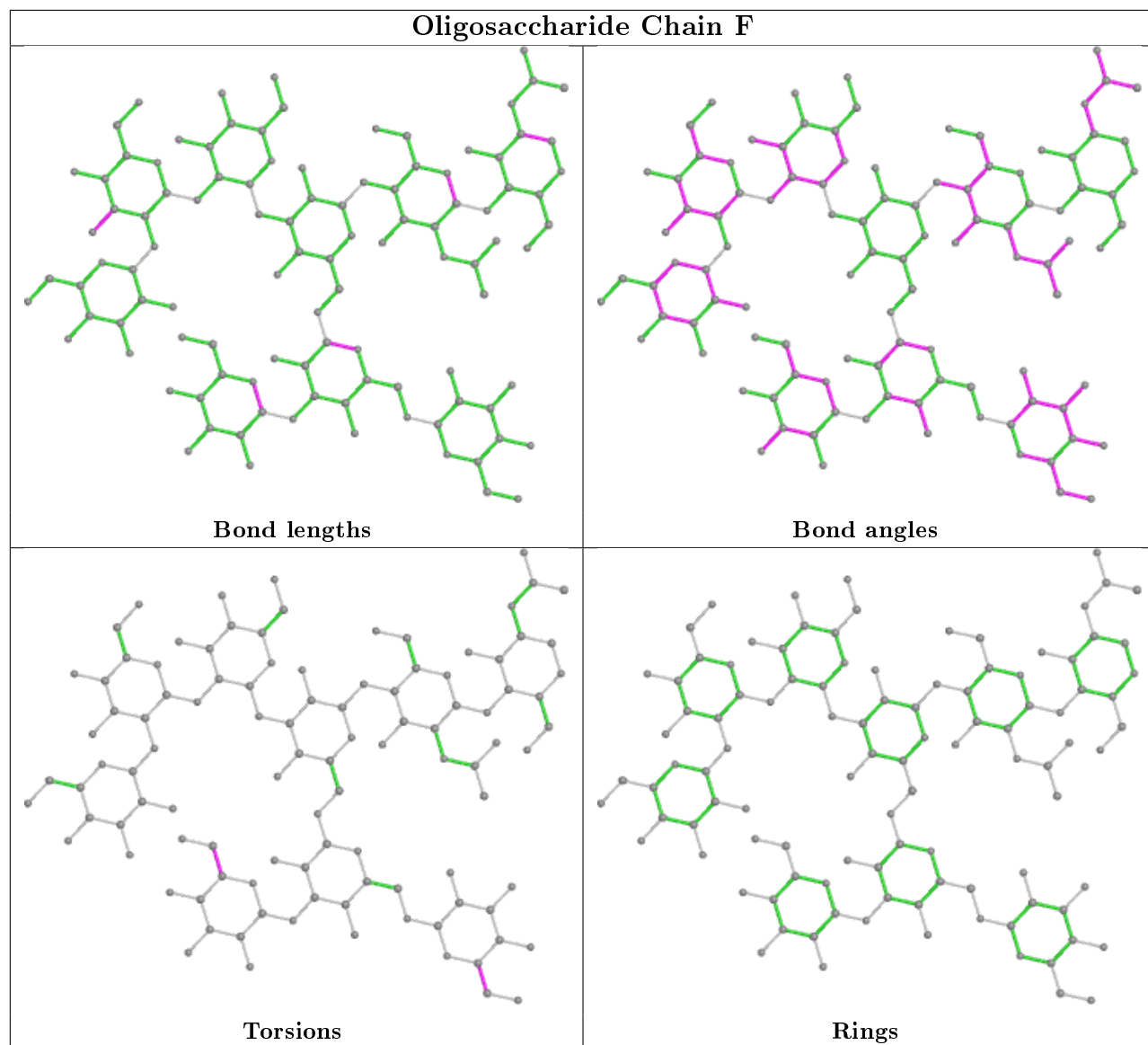
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

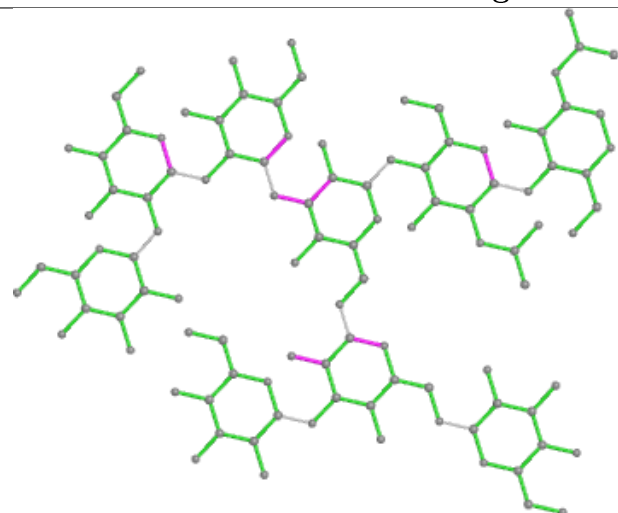
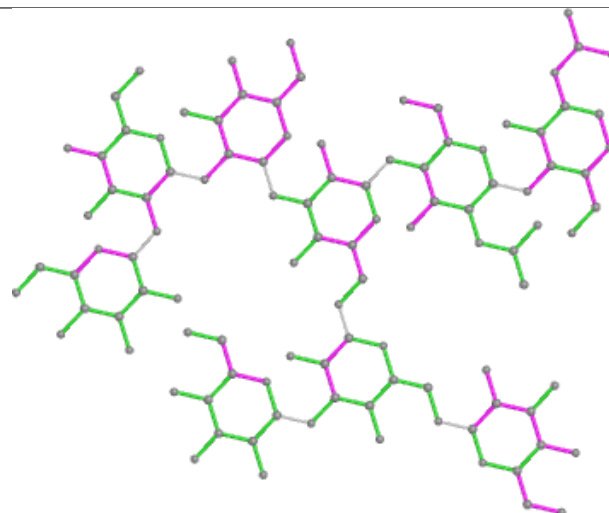
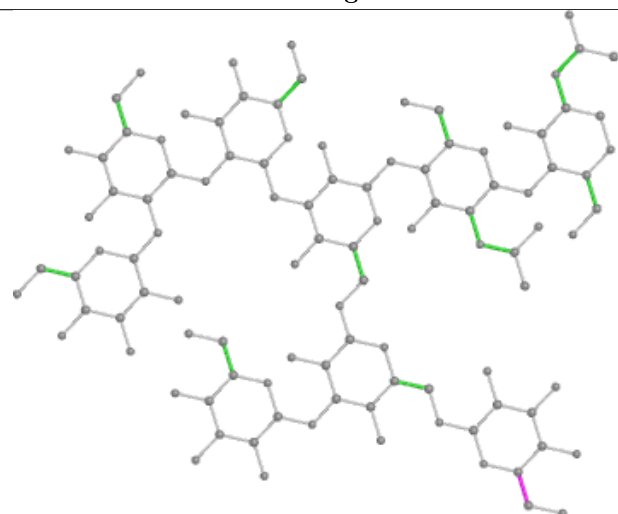
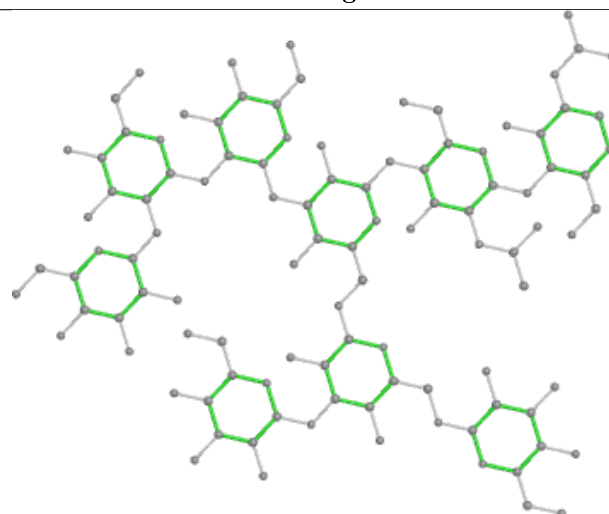


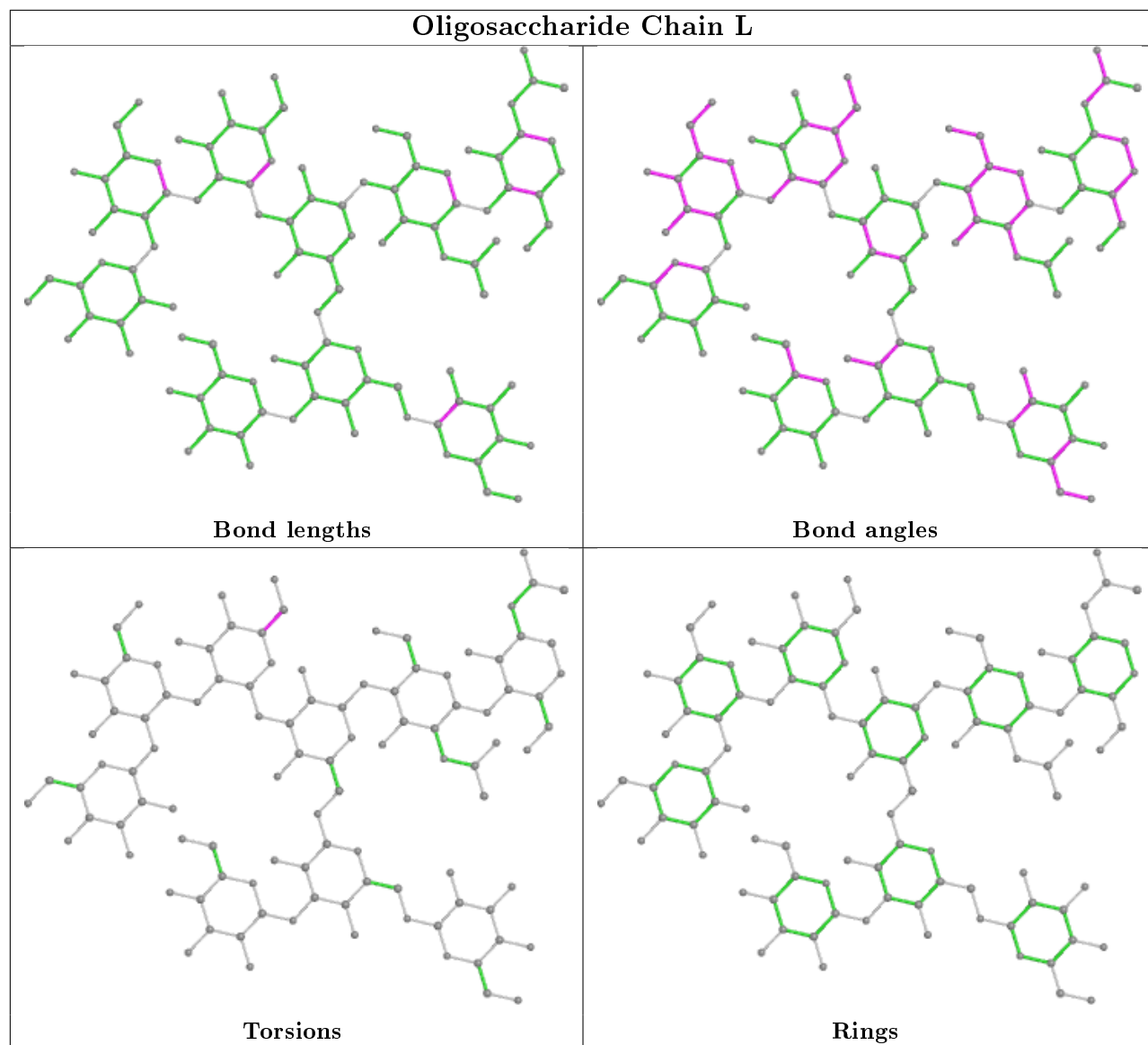


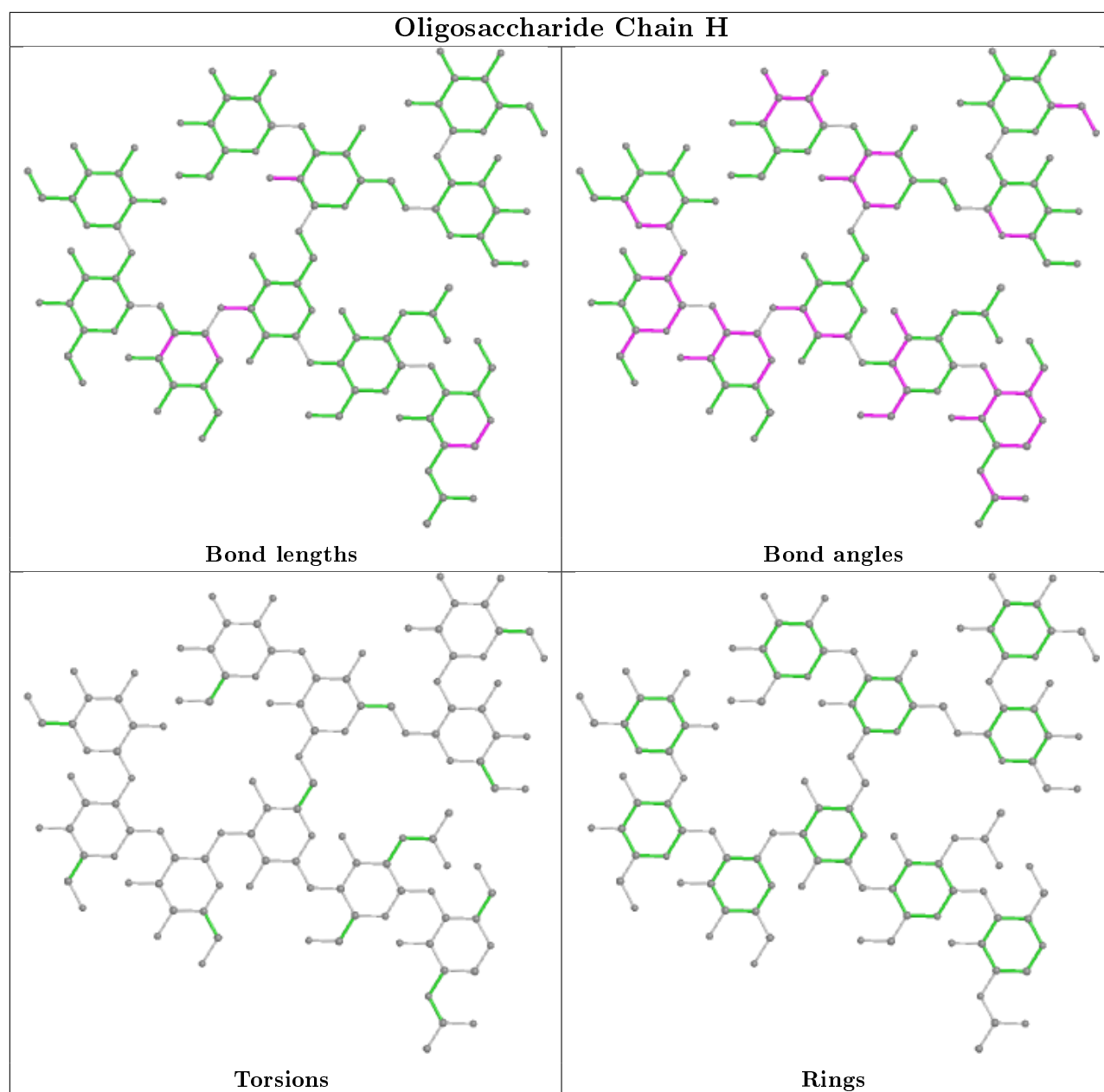






Oligosaccharide Chain J**Bond lengths****Bond angles****Torsions****Rings**





5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 for Mogul analysis.

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
6	SO4	B	2513	-	4,4,4	0.42	0	6,6,6	0.53	0
5	NAG	A	500	1	14,14,15	0.88	0	17,19,21	2.41	9 (52%)
6	SO4	C	3519	-	4,4,4	0.34	0	6,6,6	0.61	0
5	NAG	B	500	1	14,14,15	0.77	0	17,19,21	1.86	2 (11%)
6	SO4	C	3513	-	4,4,4	0.41	0	6,6,6	0.51	0
6	SO4	B	2514	-	4,4,4	0.15	0	6,6,6	0.64	0
6	SO4	B	3516	-	4,4,4	0.20	0	6,6,6	0.82	0
6	SO4	C	3514	-	4,4,4	0.16	0	6,6,6	1.02	0
6	SO4	D	4515	-	4,4,4	0.43	0	6,6,6	0.85	0
6	SO4	B	2520	-	4,4,4	0.09	0	6,6,6	0.72	0
6	SO4	C	3515	-	4,4,4	0.21	0	6,6,6	1.16	0
8	GOL	A	5003	-	5,5,5	0.60	0	5,5,5	0.37	0
6	SO4	A	1517	-	4,4,4	0.23	0	6,6,6	0.51	0
5	NAG	D	500	1	14,14,15	1.05	1 (7%)	17,19,21	2.02	7 (41%)
6	SO4	A	1513	-	4,4,4	0.37	0	6,6,6	0.82	0
6	SO4	A	1518	-	4,4,4	0.23	0	6,6,6	1.06	1 (16%)
5	NAG	C	500	1	14,14,15	0.63	0	17,19,21	1.37	1 (5%)
6	SO4	A	1519	-	4,4,4	0.39	0	6,6,6	0.38	0
6	SO4	D	4513	-	4,4,4	0.56	0	6,6,6	0.63	0
6	SO4	C	3521	-	4,4,4	0.45	0	6,6,6	0.74	0
6	SO4	A	2516	-	4,4,4	0.19	0	6,6,6	0.80	0
6	SO4	D	1516	-	4,4,4	0.25	0	6,6,6	0.66	0
8	GOL	A	5001	-	5,5,5	0.74	0	5,5,5	0.89	0
6	SO4	B	2515	-	4,4,4	0.48	0	6,6,6	0.62	0
6	SO4	D	4519	-	4,4,4	0.65	0	6,6,6	0.83	0
8	GOL	A	5002	-	5,5,5	0.77	0	5,5,5	1.30	1 (20%)
6	SO4	D	4520	-	4,4,4	0.16	0	6,6,6	0.48	0
6	SO4	A	1515	-	4,4,4	0.23	0	6,6,6	0.66	0
6	SO4	A	1520	-	4,4,4	0.12	0	6,6,6	0.91	0
6	SO4	C	4516	-	4,4,4	0.11	0	6,6,6	0.51	0
6	SO4	D	4514	-	4,4,4	0.52	0	6,6,6	0.70	0
6	SO4	C	3520	-	4,4,4	0.22	0	6,6,6	0.62	0
6	SO4	A	1514	-	4,4,4	0.29	0	6,6,6	0.75	0
6	SO4	C	3517	-	4,4,4	0.31	0	6,6,6	0.63	0
6	SO4	C	3518	-	4,4,4	0.29	0	6,6,6	1.20	1 (16%)
6	SO4	B	2519	-	4,4,4	0.49	0	6,6,6	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
8	GOL	A	5003	-	-	0/4/4/4	-
5	NAG	A	500	1	-	2/6/23/26	0/1/1/1
5	NAG	B	500	1	-	4/6/23/26	0/1/1/1
5	NAG	D	500	1	-	2/6/23/26	0/1/1/1
8	GOL	A	5001	-	-	4/4/4/4	-
8	GOL	A	5002	-	-	2/4/4/4	-
5	NAG	C	500	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	500	NAG	C4-C5	2.42	1.58	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	NAG	O5-C5-C6	4.92	114.92	107.20
5	A	500	NAG	O5-C5-C6	4.65	114.50	107.20
5	D	500	NAG	C4-C3-C2	-4.22	104.83	111.02
5	B	500	NAG	C1-C2-N2	-4.04	103.59	110.49
5	A	500	NAG	O3-C3-C4	-3.89	101.36	110.35
5	C	500	NAG	O5-C5-C6	3.47	112.65	107.20
5	D	500	NAG	O5-C1-C2	3.37	116.61	111.29
5	D	500	NAG	C6-C5-C4	3.06	120.17	113.00
5	A	500	NAG	O3-C3-C2	2.98	115.64	109.47
5	A	500	NAG	C1-C2-N2	-2.74	105.81	110.49
5	A	500	NAG	O5-C1-C2	2.65	115.47	111.29
5	A	500	NAG	O4-C4-C3	-2.65	104.23	110.35
5	A	500	NAG	O4-C4-C5	2.61	115.78	109.30
5	A	500	NAG	C2-N2-C7	2.56	126.55	122.90
5	A	500	NAG	O7-C7-N2	2.53	126.61	121.95
5	D	500	NAG	C1-O5-C5	-2.50	108.81	112.19
5	D	500	NAG	C2-N2-C7	2.47	126.42	122.90
8	A	5002	GOL	O2-C2-C3	-2.21	99.41	109.12
5	D	500	NAG	O4-C4-C5	2.15	114.62	109.30
5	D	500	NAG	O4-C4-C3	-2.13	105.42	110.35
6	C	3518	SO4	O4-S-O3	2.13	118.14	109.06
6	A	1518	SO4	O4-S-O3	2.09	117.99	109.06

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	500	NAG	C8-C7-N2-C2
5	A	500	NAG	O7-C7-N2-C2
5	B	500	NAG	C8-C7-N2-C2
5	B	500	NAG	O7-C7-N2-C2
5	D	500	NAG	C8-C7-N2-C2
5	D	500	NAG	O7-C7-N2-C2
5	C	500	NAG	C8-C7-N2-C2
5	C	500	NAG	O7-C7-N2-C2
8	A	5001	GOL	C1-C2-C3-O3
8	A	5002	GOL	O1-C1-C2-O2
8	A	5002	GOL	O1-C1-C2-C3
5	C	500	NAG	O5-C5-C6-O6
5	B	500	NAG	C4-C5-C6-O6
5	B	500	NAG	O5-C5-C6-O6
5	C	500	NAG	C4-C5-C6-O6
8	A	5001	GOL	O1-C1-C2-C3
8	A	5001	GOL	O1-C1-C2-O2
8	A	5001	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	NAG	1	0
5	B	500	NAG	1	0
6	B	3516	SO4	1	0
8	A	5003	GOL	1	0
5	C	500	NAG	1	0
6	C	3521	SO4	1	0
6	A	2516	SO4	1	0
6	C	4516	SO4	1	0
6	C	3520	SO4	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 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	388/388 (100%)	-0.90	2 (0%) 91 90	11, 18, 31, 44	5 (1%)
1	B	388/388 (100%)	-0.75	7 (1%) 68 66	12, 20, 37, 53	5 (1%)
1	C	388/388 (100%)	-0.77	3 (0%) 86 85	12, 20, 43, 58	0
1	D	388/388 (100%)	-0.78	10 (2%) 56 53	11, 18, 38, 58	3 (0%)
All	All	1552/1552 (100%)	-0.80	22 (1%) 75 73	11, 19, 38, 58	13 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	THR	9.2
1	D	250	PRO	5.4
1	D	247	ALA	5.1
1	B	346	ASN	4.5
1	D	249	GLY	4.4
1	D	346	ASN	4.2
1	B	347	ASN	3.8
1	A	346	ASN	3.5
1	C	270	THR	3.3
1	D	246	SER	3.0
1	D	251	ALA	3.0
1	D	272	THR	2.9
1	B	250	PRO	2.7
1	B	270	THR	2.6
1	C	342	PRO	2.5
1	D	275	HIS	2.4
1	A	345	ASN	2.3
1	C	346	ASN	2.2
1	B	82	ARG	2.2
1	B	337	CYS	2.2
1	D	271	GLY	2.1
1	B	417	GLU	2.1

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.

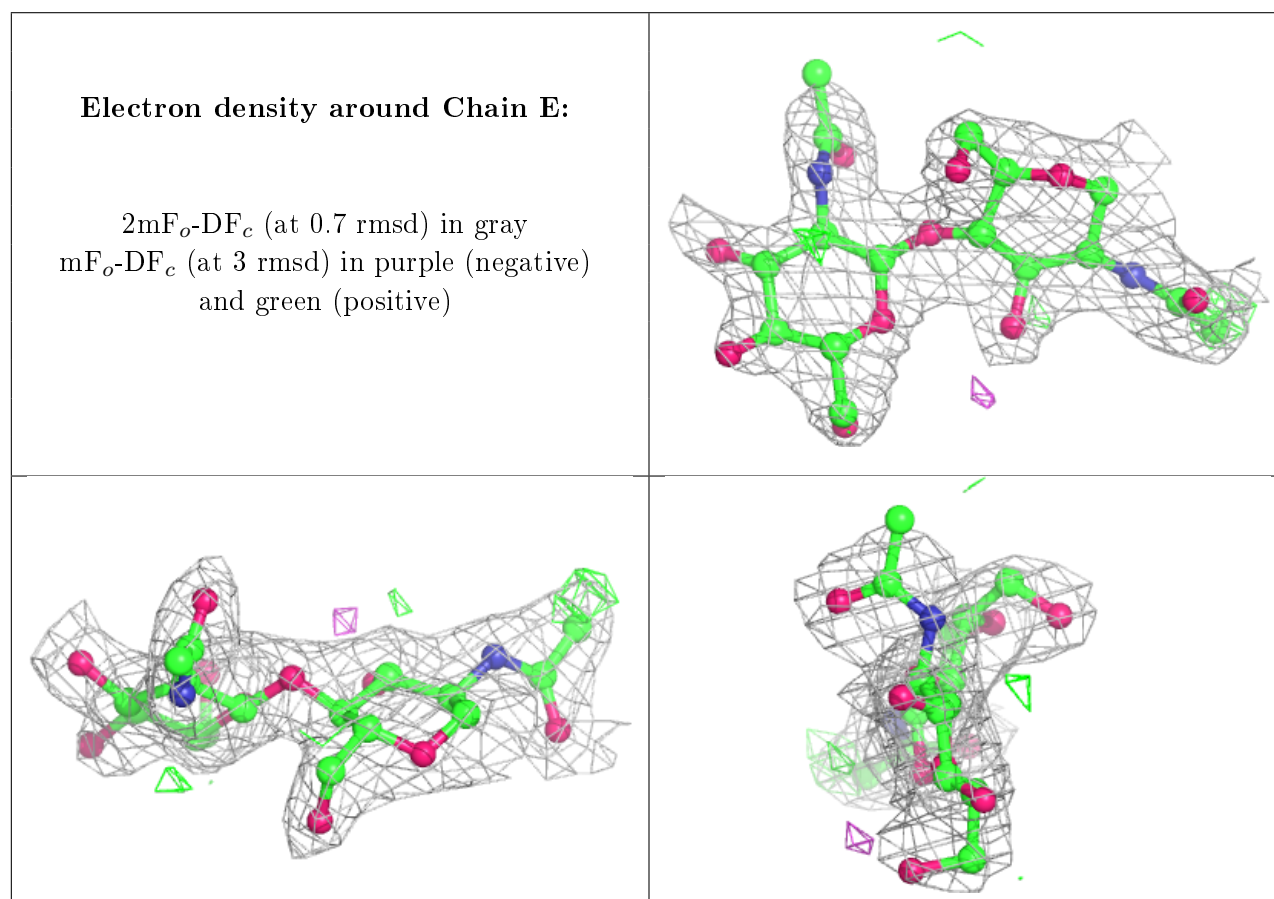
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	I	2	14/15	0.62	0.45	63,67,69,69	0
2	NAG	G	2	14/15	0.81	0.31	44,52,57,59	0
2	NAG	K	2	14/15	0.82	0.33	46,51,55,56	0
3	MAN	J	9	11/12	0.84	0.27	46,51,56,57	0
2	NAG	K	1	14/15	0.85	0.18	25,33,47,47	0
4	MAN	H	9	11/12	0.86	0.32	52,56,57,57	0
2	NAG	E	2	14/15	0.88	0.33	43,51,56,58	0
4	MAN	H	8	11/12	0.88	0.31	44,50,54,56	0
4	MAN	H	10	11/12	0.88	0.24	49,52,53,55	0
2	NAG	I	1	14/15	0.89	0.20	33,44,48,58	0
2	NAG	G	1	14/15	0.89	0.18	33,39,47,48	0
3	MAN	L	9	11/12	0.90	0.15	35,38,41,43	0
3	MAN	F	9	11/12	0.90	0.28	43,48,50,53	0
2	NAG	E	1	14/15	0.90	0.15	30,37,41,45	0
4	MAN	H	7	11/12	0.90	0.14	35,39,44,44	0
3	MAN	J	8	11/12	0.92	0.24	32,39,44,46	0
3	MAN	L	8	11/12	0.93	0.18	32,35,38,39	0
4	NAG	H	2	14/15	0.93	0.10	17,22,26,38	0
3	MAN	J	7	11/12	0.95	0.15	29,35,38,42	0
3	NAG	J	1	14/15	0.95	0.08	20,21,25,26	0
3	MAN	J	4	11/12	0.95	0.12	18,22,24,31	0
3	NAG	F	1	14/15	0.95	0.09	15,18,27,29	0
4	MAN	H	4	11/12	0.95	0.10	16,20,26,33	0
3	NAG	L	2	14/15	0.95	0.08	17,21,25,31	0
3	MAN	J	6	11/12	0.96	0.10	16,19,22,22	0
3	NAG	F	2	14/15	0.96	0.08	15,18,24,24	0
3	MAN	F	4	11/12	0.96	0.09	16,19,25,26	0
4	NAG	H	1	14/15	0.96	0.10	18,22,25,26	0
4	MAN	H	5	11/12	0.96	0.10	22,28,32,33	0
3	MAN	J	5	11/12	0.96	0.11	18,21,26,27	0
3	MAN	F	8	11/12	0.96	0.19	32,36,38,43	0
3	NAG	J	2	14/15	0.96	0.07	17,21,27,32	0

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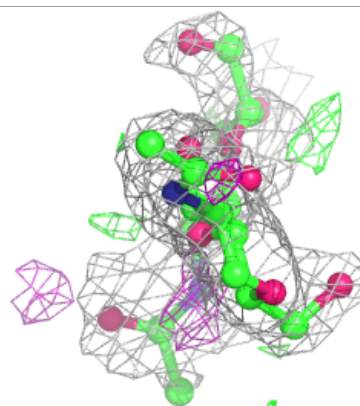
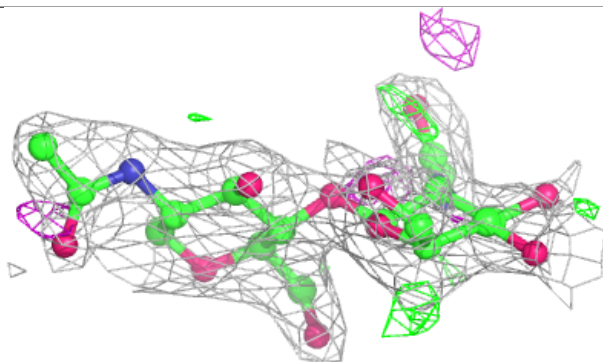
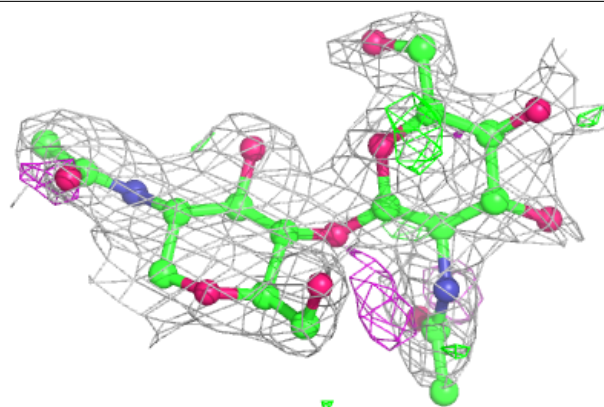
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	L	4	11/12	0.97	0.10	16,21,28,34	0
3	MAN	F	5	11/12	0.97	0.06	18,20,22,24	0
4	MAN	H	6	11/12	0.97	0.09	18,25,26,26	0
3	MAN	L	5	11/12	0.97	0.09	18,20,24,27	0
3	NAG	L	1	14/15	0.97	0.10	17,22,28,30	0
4	BMA	H	3	11/12	0.97	0.07	20,22,28,29	0
3	MAN	L	6	11/12	0.97	0.07	19,21,23,23	0
3	MAN	F	6	11/12	0.98	0.07	15,17,18,21	0
3	BMA	L	3	11/12	0.98	0.06	20,24,26,26	0
3	MAN	L	7	11/12	0.98	0.12	24,27,29,31	0
3	BMA	F	3	11/12	0.98	0.06	14,19,22,23	0
3	MAN	F	7	11/12	0.98	0.15	21,26,32,37	0
3	BMA	J	3	11/12	0.98	0.09	18,23,25,29	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.

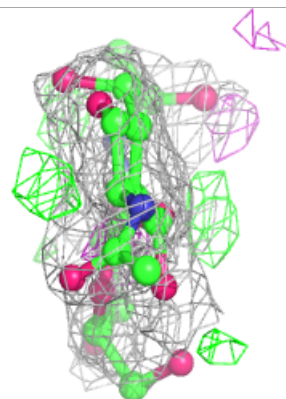
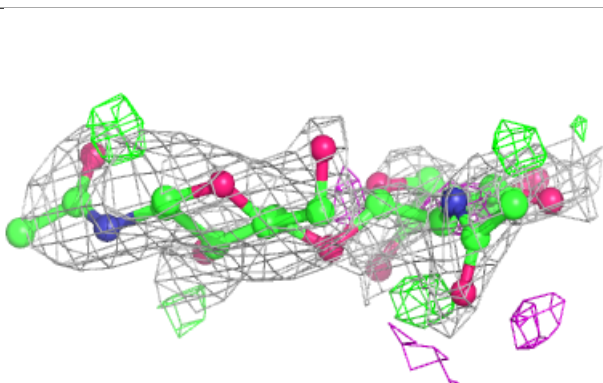
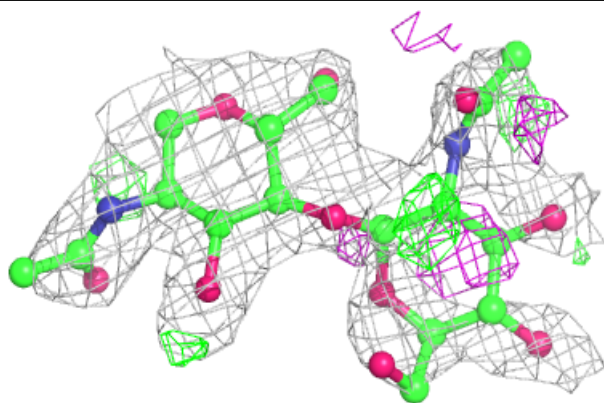


Electron density around Chain G:

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

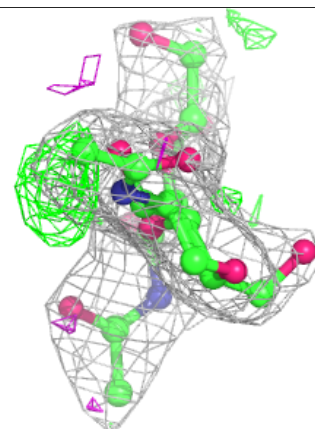
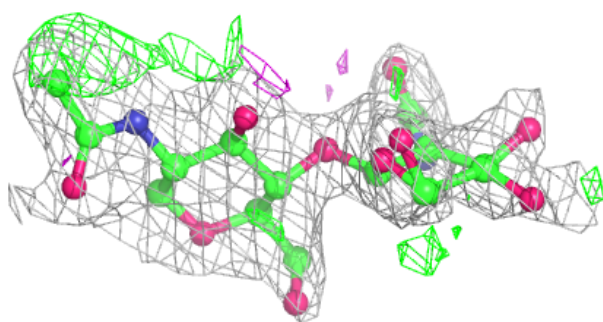
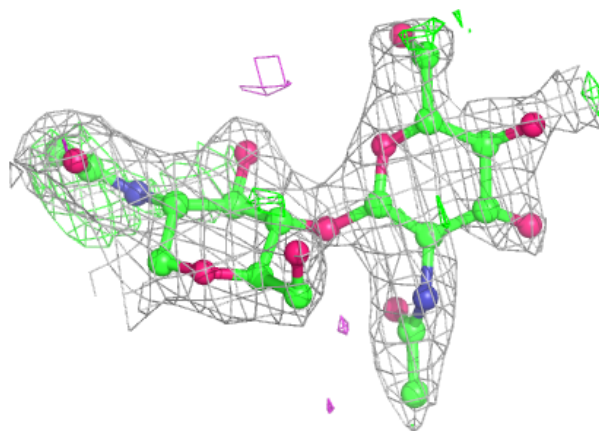
**Electron density around Chain I:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



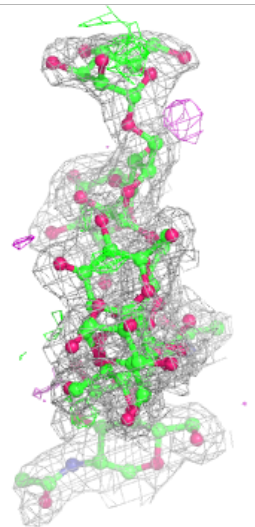
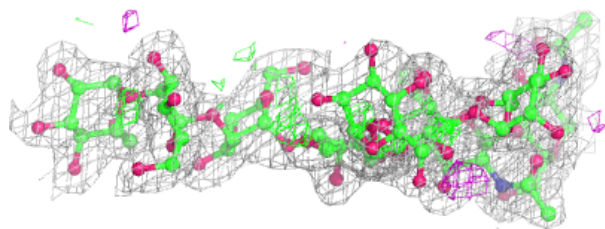
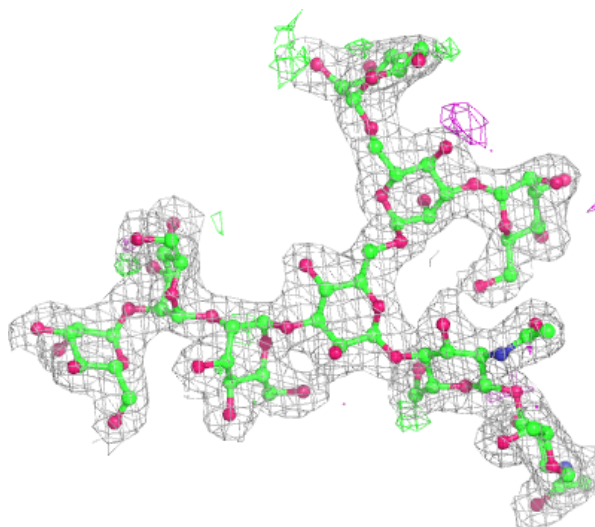
Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



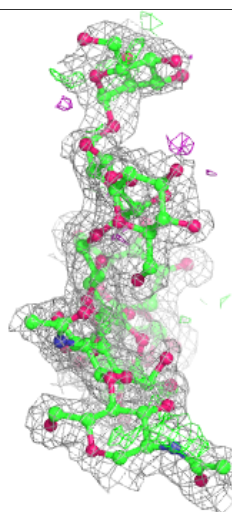
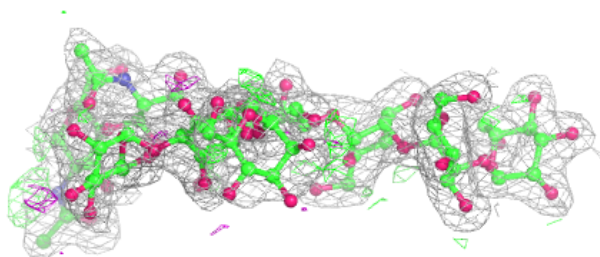
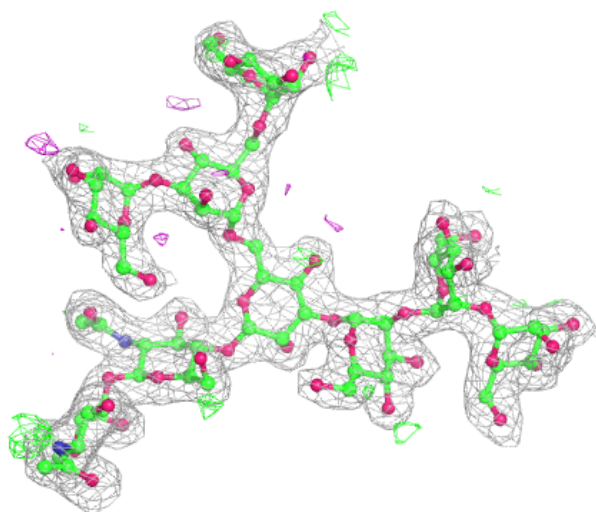
Electron density around Chain F:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



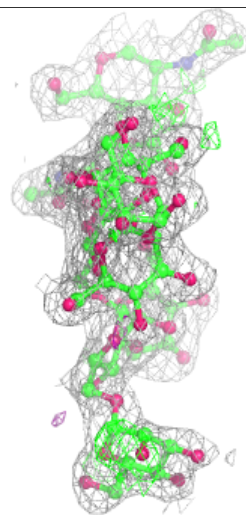
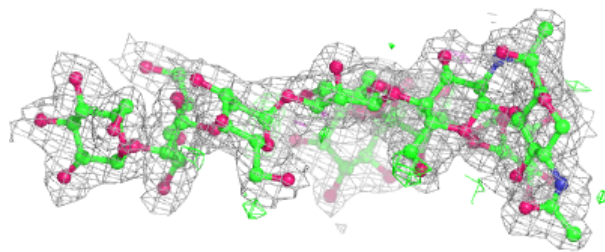
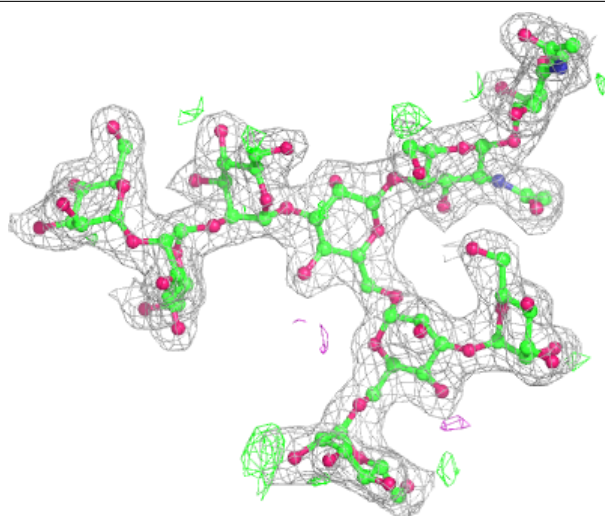
Electron density around Chain J:

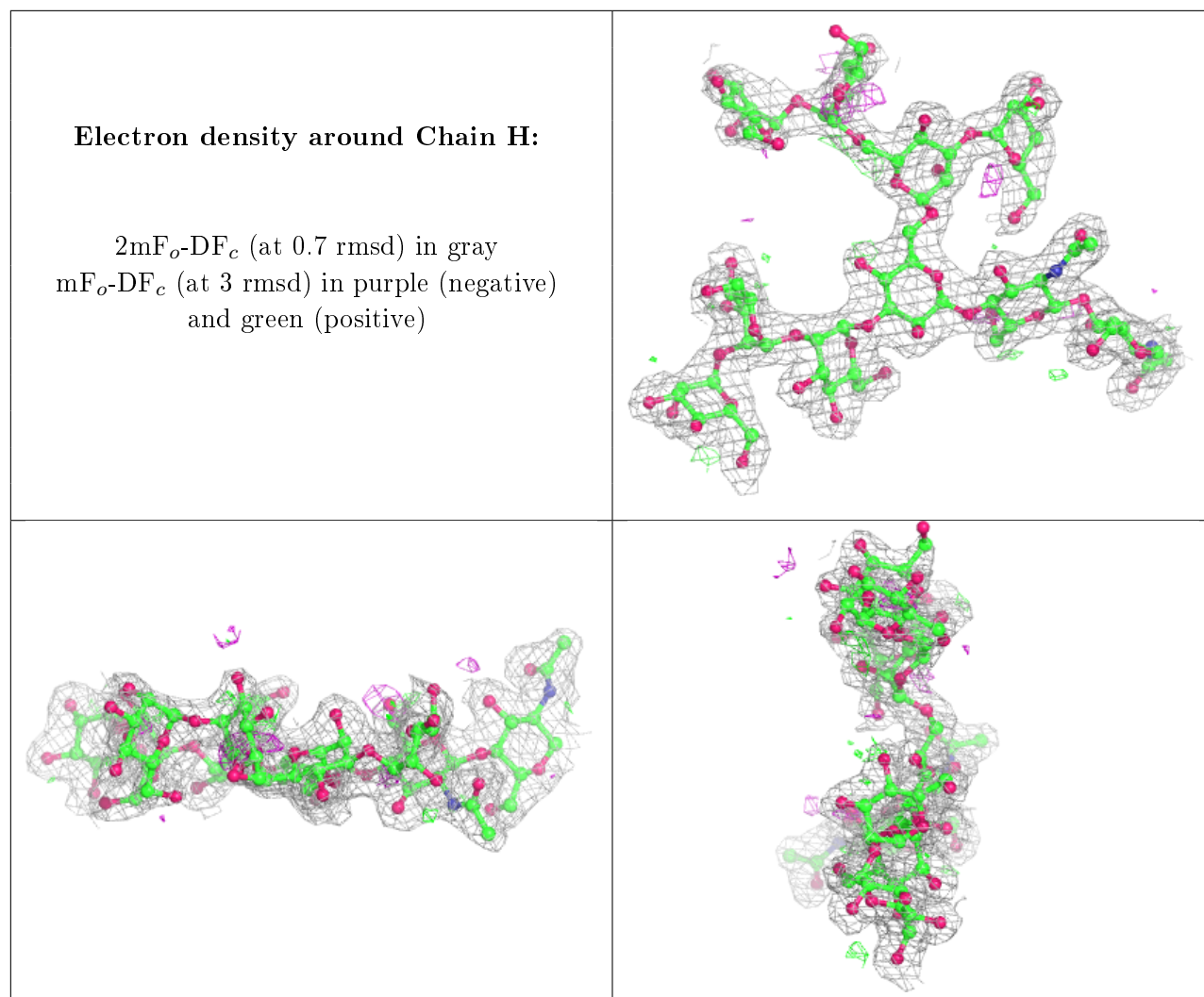
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

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
6	SO4	A	1518	5/5	0.69	0.30	76,77,81,81	0
5	NAG	D	500	14/15	0.84	0.24	45,50,57,58	0
5	NAG	A	500	14/15	0.85	0.24	40,48,52,52	0
8	GOL	A	5003	6/6	0.85	0.21	56,56,58,59	0
5	NAG	C	500	14/15	0.86	0.27	47,55,58,59	0
5	NAG	B	500	14/15	0.87	0.25	45,50,59,61	0
8	GOL	A	5001	6/6	0.89	0.23	55,57,59,59	0
6	SO4	A	1515	5/5	0.89	0.24	50,54,57,60	0
7	CL	A	1522	1/1	0.90	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	D	4515	5/5	0.90	0.23	50,54,58,59	0
6	SO4	B	2513	5/5	0.91	0.25	70,71,73,75	0
6	SO4	C	3515	5/5	0.93	0.28	55,56,58,61	0
6	SO4	C	3513	5/5	0.93	0.27	63,65,66,67	0
8	GOL	A	5002	6/6	0.93	0.13	34,40,43,44	0
6	SO4	D	4513	5/5	0.93	0.19	55,59,62,63	0
6	SO4	B	2515	5/5	0.94	0.27	53,55,57,59	0
7	CL	C	3522	1/1	0.94	0.04	50,50,50,50	0
6	SO4	D	4520	5/5	0.94	0.24	63,64,64,64	0
6	SO4	B	3516	5/5	0.94	0.20	72,73,75,76	0
6	SO4	C	3519	5/5	0.95	0.30	57,61,61,63	0
6	SO4	A	2516	5/5	0.96	0.23	60,61,62,64	0
7	CL	D	4522	1/1	0.96	0.07	46,46,46,46	0
6	SO4	A	1517	5/5	0.96	0.29	53,56,58,59	0
6	SO4	A	1520	5/5	0.96	0.20	60,63,64,65	0
6	SO4	D	4514	5/5	0.96	0.16	35,48,50,52	0
6	SO4	C	3517	5/5	0.96	0.30	59,61,64,66	0
6	SO4	B	2519	5/5	0.96	0.27	46,46,48,52	0
6	SO4	C	3514	5/5	0.97	0.14	32,38,41,43	0
6	SO4	C	3520	5/5	0.97	0.31	63,64,65,67	0
7	CL	B	2522	1/1	0.97	0.05	45,45,45,45	0
6	SO4	D	1516	5/5	0.97	0.21	52,55,57,58	0
6	SO4	A	1513	5/5	0.98	0.13	40,41,47,47	0
6	SO4	D	4519	5/5	0.98	0.24	40,42,44,45	0
6	SO4	B	2520	5/5	0.98	0.25	47,50,52,52	0
6	SO4	C	4516	5/5	0.98	0.12	56,57,58,60	0
6	SO4	A	1514	5/5	0.99	0.07	29,29,32,32	0
6	SO4	A	1519	5/5	0.99	0.25	40,43,45,45	0
6	SO4	C	3518	5/5	0.99	0.08	21,22,24,25	0
6	SO4	B	2514	5/5	0.99	0.15	40,41,45,45	0
6	SO4	C	3521	5/5	1.00	0.08	17,20,21,23	0

6.5 Other polymers

There are no such residues in this entry.