



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:20 AM UTC

PDB ID : 6HGB / pdb_00006hgb
Title : Influenza A virus N6 neuraminidase native structure (Duck/England/56).
Authors : Salinger, M.T.; Hobbs, J.R.; Murray, J.W.; Laver, W.G.; Kuhn, P.; Garman, E.F.
Deposited on : 2018-08-23
Resolution : 1.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

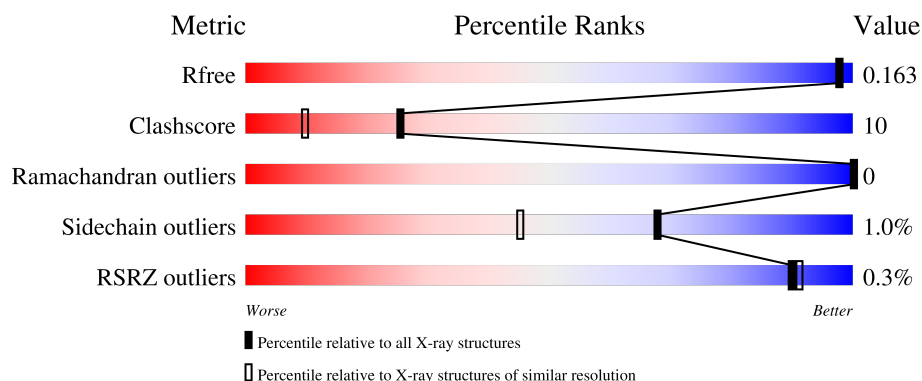
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	389	 88% 11% .
1	B	389	 89% 10% .
1	C	389	 87% 12% .
1	D	389	 90% 9% .
2	E	2	 100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	H	2	 100%
2	J	2	 50% 50%
2	K	2	 100%
2	N	2	 100%
3	G	8	 100%
4	I	7	 71% 29%
5	L	6	 100%
5	M	6	 17% 83%

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
6	GOL	C	517	-	-	X	-
9	PEG	A	522	-	-	X	-
9	PEG	B	520	-	-	X	-
9	PEG	B	523[B]	-	-	X	-
9	PEG	B	526	-	-	X	-
9	PEG	C	520	-	-	X	-
9	PEG	C	521	-	-	X	-
9	PEG	D	517	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 15249 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	389	Total	C	N	O	S	0	29	0
			3203	2003	563	604	33			
1	B	389	Total	C	N	O	S	0	24	0
			3197	1988	565	611	33			
1	C	389	Total	C	N	O	S	0	27	0
			3193	1998	562	601	32			
1	D	389	Total	C	N	O	S	0	29	0
			3206	2004	568	604	30			

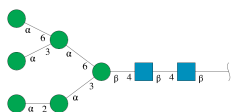
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

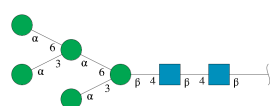
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

-acetamido-2-deoxy-beta-D-glucopyranose.



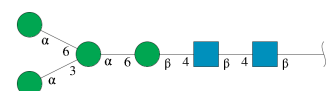
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is an oligosaccharide called 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
5	L	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			12	6	6		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	1
			12	6	6		
6	A	1	Total	C	O	0	1
			12	6	6		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 12 6 6	0	1
6	C	1	Total C O 12 6 6	0	1
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

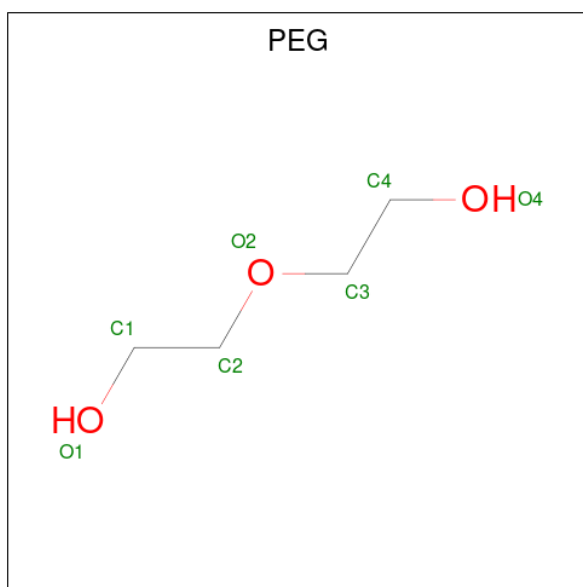
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 14 8 6	0	1
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

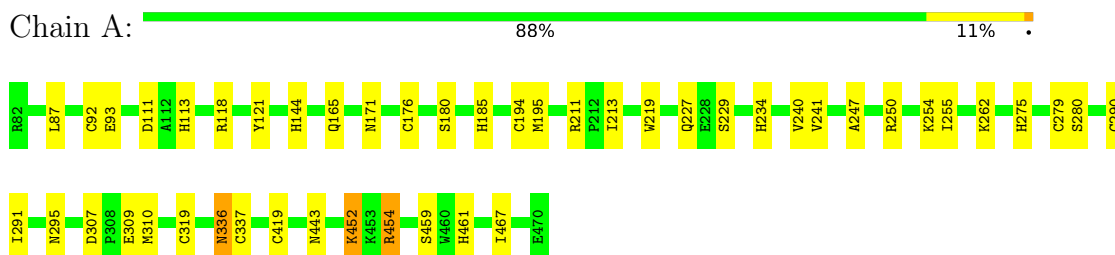
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	391	Total	O	0	1
			392	392		
11	B	407	Total	O	0	0
			407	407		
11	C	405	Total	O	0	4
			409	409		
11	D	384	Total	O	0	2
			386	386		

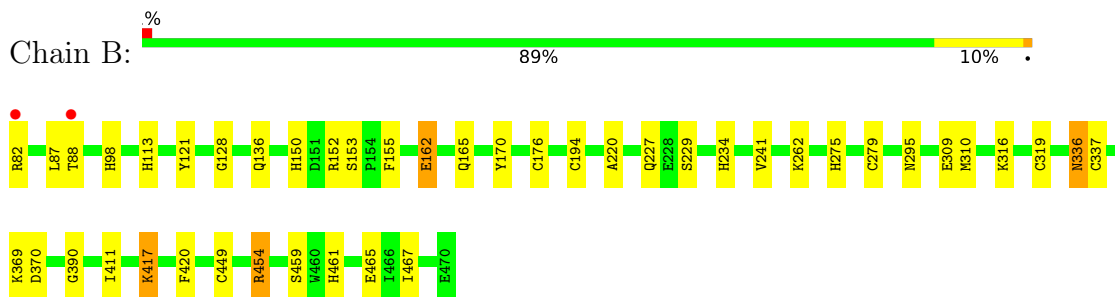
3 Residue-property plots

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.

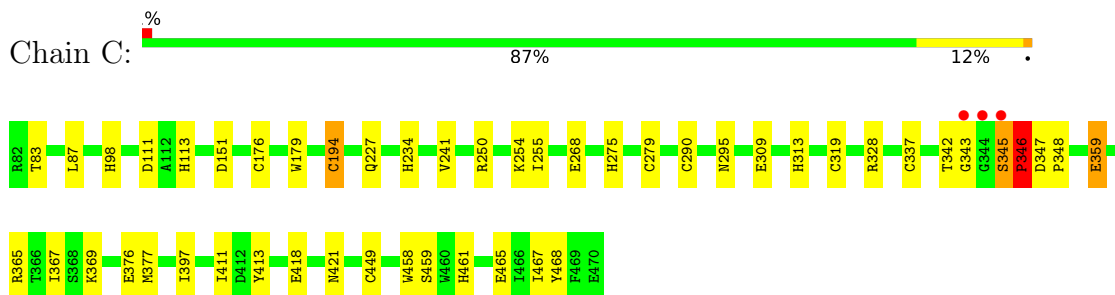
• Molecule 1: Neuraminidase



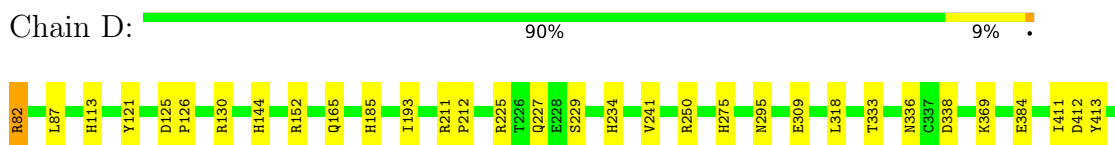
• Molecule 1: Neuraminidase

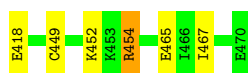


• Molecule 1: Neuraminidase



• 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 F:  100%



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

Chain H:  100%



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

Chain J:  50% 50%



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

Chain K:  100%

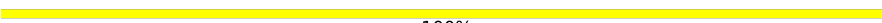


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%



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

Chain G:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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

Chain I:  71% 29%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain L:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain M:  17% 83%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.20Å 73.90Å 106.40Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	30.68 – 1.50 30.68 – 1.50	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.68-1.50) 91.9 (30.68-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.139 , 0.161 0.141 , 0.163	Depositor DCC
R_{free} test set	11165 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	9.8	Xtriage
Anisotropy	1.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for l,k,-h 0.016 for h,-k,-l 0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15249	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: PEG, PO4, GOL, MAN, BMA, CA, 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	0.89	3/3313 (0.1%)	0.96	1/4491 (0.0%)
1	B	0.88	1/3285 (0.0%)	0.95	0/4451
1	C	0.88	0/3304	0.95	2/4480 (0.0%)
1	D	0.91	3/3323 (0.1%)	0.96	2/4505 (0.0%)
All	All	0.89	7/13225 (0.1%)	0.95	5/17927 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	D	0	6
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	SER	CA-CB	-6.42	1.44	1.53
1	D	333[A]	THR	CA-C	6.18	1.60	1.52
1	D	333[B]	THR	CA-C	6.18	1.60	1.52
1	D	193	ILE	C-O	-5.75	1.18	1.24
1	A	185	HIS	CE1-NE2	5.54	1.38	1.32
1	A	240	VAL	N-CA	-5.34	1.40	1.46
1	B	370	ASP	C-O	-5.02	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	ASP	CA-CB-CG	9.14	121.74	112.60
1	C	346	PRO	N-CA-CB	-8.24	93.53	102.60
1	D	333[A]	THR	N-CA-C	5.10	117.51	111.33
1	D	333[B]	THR	N-CA-C	5.10	117.51	111.33
1	A	211	ARG	CD-NE-CZ	5.03	131.44	124.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	ARG	Sidechain
1	A	454[A]	ARG	Sidechain
1	B	454	ARG	Sidechain
1	D	152	ARG	Sidechain
1	D	211[A]	ARG	Sidechain
1	D	211[C]	ARG	Sidechain
1	D	250[A]	ARG	Sidechain
1	D	250[B]	ARG	Sidechain
1	D	454	ARG	Sidechain

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	3203	0	3109	54	0
1	B	3197	0	3065	64	0
1	C	3193	0	3095	68	0
1	D	3206	0	3111	46	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	3	0
2	K	28	0	25	0	0
2	N	28	0	25	0	0
3	G	94	0	79	0	0
4	I	83	0	70	3	0
5	L	72	0	61	0	0
5	M	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	54	0	72	5	0
6	B	36	0	48	3	0
6	C	60	0	80	22	0
6	D	30	0	40	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0
9	A	7	0	10	5	0
9	B	63	0	90	27	0
9	C	28	0	39	19	0
9	D	42	0	59	14	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	392	0	0	12	0
11	B	407	0	0	21	0
11	C	409	0	0	11	0
11	D	386	0	0	10	0
All	All	15249	0	13265	259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (259) 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:A:213[B]:ILE:HD12	1:A:213[B]:ILE:O	1.32	1.29
9:B:523[B]:PEG:O4	9:B:523[B]:PEG:H12	1.22	1.25
1:B:319:CYS:SG	1:B:337[B]:CYS:HB3	1.84	1.17
9:B:523[B]:PEG:O4	9:B:523[B]:PEG:C1	1.94	1.15
9:A:522:PEG:H32	11:A:627:HOH:O	1.46	1.15
1:C:377:MET:HG2	1:C:397[B]:ILE:HD11	1.18	1.14
1:B:310[B]:MET:HA	1:B:310[B]:MET:HE3	1.34	1.09
9:B:523[B]:PEG:H12	9:B:523[B]:PEG:C4	1.72	1.09
1:B:88[B]:THR:HG22	1:B:88[B]:THR:O	1.57	1.05
1:C:319:CYS:SG	1:C:337[B]:CYS:HB3	1.97	1.04
1:A:319:CYS:SG	1:A:337[B]:CYS:HB3	1.97	1.04
1:B:220:ALA:HB1	9:B:526:PEG:H42	1.42	0.99
1:B:162[A]:GLU:OE2	1:B:165[A]:GLN:NE2	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369[A]:LYS:CE	6:C:517:GOL:O3	2.14	0.95
9:C:520:PEG:H41	11:C:759:HOH:O	1.68	0.93
1:C:87:LEU:H	1:C:234:HIS:HD2	1.16	0.93
11:A:603:HOH:O	9:C:520:PEG:H42	1.70	0.92
9:B:523[B]:PEG:C1	9:B:523[B]:PEG:HO4	1.80	0.91
1:A:454[B]:ARG:CG	1:A:454[B]:ARG:O	2.19	0.90
1:D:82:ARG:N	9:D:518:PEG:HO1	1.71	0.89
1:D:165[A]:GLN:HE22	9:D:521:PEG:H22	1.36	0.89
9:B:520:PEG:H41	11:B:688:HOH:O	1.73	0.88
1:C:319:CYS:SG	1:C:337[B]:CYS:CB	2.56	0.88
1:B:88[B]:THR:O	1:B:88[B]:THR:CG2	2.20	0.87
1:C:83:THR:HG21	2:J:1:NAG:H83	1.57	0.87
1:D:87:LEU:H	1:D:234:HIS:HD2	1.22	0.87
1:B:87:LEU:H	1:B:234:HIS:HD2	1.23	0.86
1:A:144:HIS:HE1	1:C:465[B]:GLU:H	1.26	0.84
1:A:144:HIS:HE1	1:C:465[A]:GLU:H	1.25	0.83
1:B:465[A]:GLU:H	1:D:144:HIS:HE1	1.28	0.81
1:D:465[B]:GLU:HG3	1:D:467[B]:ILE:HG22	1.59	0.81
1:B:176:CYS:SG	1:B:194[B]:CYS:HB2	2.20	0.81
1:D:465[B]:GLU:CG	1:D:467[B]:ILE:HG22	2.11	0.80
1:C:369[A]:LYS:NZ	6:C:517:GOL:O3	2.13	0.79
1:A:213[B]:ILE:O	1:A:213[B]:ILE:CD1	2.24	0.78
1:A:454[B]:ARG:O	1:A:454[B]:ARG:HG2	1.82	0.78
1:B:465[C]:GLU:H	1:D:144:HIS:HE1	1.27	0.78
1:B:319:CYS:SG	1:B:337[B]:CYS:CB	2.56	0.77
1:A:319:CYS:SG	1:A:337[B]:CYS:CB	2.67	0.76
1:C:87:LEU:H	1:C:234:HIS:CD2	2.03	0.76
1:C:369[A]:LYS:HE2	6:C:517:GOL:O3	1.86	0.76
1:A:213[B]:ILE:HD12	1:A:213[B]:ILE:C	2.10	0.76
9:B:523[B]:PEG:C1	9:B:523[B]:PEG:C4	2.40	0.75
1:A:87:LEU:H	1:A:234:HIS:HD2	1.33	0.75
1:A:92:CYS:SG	1:A:419[C]:CYS:HB2	2.27	0.75
1:A:454[A]:ARG:NH1	4:I:2:NAG:O7	2.20	0.75
1:C:465[B]:GLU:HG2	1:C:467[B]:ILE:HD11	1.67	0.75
1:D:418[B]:GLU:CD	1:D:418[B]:GLU:H	1.94	0.74
1:B:87:LEU:H	1:B:234:HIS:CD2	2.06	0.74
1:B:390:GLY:HA3	9:B:523[A]:PEG:H21	1.70	0.73
1:D:82:ARG:N	9:D:518:PEG:O1	2.22	0.72
1:B:465[B]:GLU:H	1:D:144:HIS:HE1	1.37	0.72
1:D:227:GLN:HE21	1:D:241:VAL:H	1.37	0.71
1:A:176:CYS:SG	1:A:194[B]:CYS:HB2	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLN:HE21	1:B:241:VAL:H	1.36	0.71
1:D:87:LEU:H	1:D:234:HIS:CD2	2.06	0.69
1:C:328:ARG:HH21	6:C:517:GOL:H11	1.57	0.69
1:C:176:CYS:SG	1:C:194[A]:CYS:HB2	2.33	0.69
1:C:377:MET:HG2	1:C:397[B]:ILE:CD1	2.10	0.69
1:C:467[B]:ILE:HD12	1:C:468:TYR:N	2.06	0.69
1:C:369[A]:LYS:HG2	6:C:517:GOL:H32	1.75	0.68
1:B:454:ARG:HD3	11:B:777:HOH:O	1.92	0.68
1:B:128:GLY:HA2	11:D:895:HOH:O	1.92	0.68
1:C:377:MET:CG	1:C:397[B]:ILE:HD11	2.10	0.68
1:A:87:LEU:H	1:A:234:HIS:CD2	2.12	0.68
1:A:227:GLN:HE21	1:A:241:VAL:H	1.39	0.67
1:C:98:HIS:NE2	9:C:520:PEG:C3	2.58	0.67
1:C:365:ARG:NH2	6:C:517:GOL:H2	2.10	0.67
1:B:310[B]:MET:HA	1:B:310[B]:MET:CE	2.19	0.66
1:C:465[B]:GLU:CD	1:C:467[B]:ILE:HG13	2.20	0.66
1:C:227:GLN:HE21	1:C:241:VAL:H	1.41	0.66
1:B:310[B]:MET:HE3	1:B:310[B]:MET:CA	2.15	0.66
1:D:454:ARG:NE	11:D:601:HOH:O	2.22	0.66
1:C:254[B]:LYS:NZ	1:C:268[B]:GLU:OE1	2.29	0.65
1:B:88[A]:THR:HG21	11:B:913:HOH:O	1.97	0.65
9:C:522:PEG:H42	11:C:623:HOH:O	1.96	0.65
1:C:111:ASP:O	6:C:515[B]:GOL:H32	1.96	0.64
1:C:83:THR:CG2	2:J:1:NAG:H83	2.28	0.64
1:D:275:HIS:HD2	1:D:295:ASN:H	1.45	0.64
1:A:454[B]:ARG:O	1:A:454[B]:ARG:HG3	1.96	0.64
1:C:459:SER:OG	1:C:461:HIS:HD2	1.81	0.64
1:B:449[B]:CYS:SG	9:B:520:PEG:H22	2.38	0.63
9:C:520:PEG:H12	11:C:676:HOH:O	1.99	0.63
1:C:465[B]:GLU:CG	1:C:467[B]:ILE:CD1	2.76	0.63
6:D:511:GOL:H32	11:D:945:HOH:O	1.99	0.62
1:B:459:SER:OG	1:B:461:HIS:HD2	1.82	0.62
1:A:275:HIS:HD2	1:A:295:ASN:H	1.45	0.62
1:C:328:ARG:NH2	6:C:517:GOL:H11	2.14	0.62
1:C:465[B]:GLU:CG	1:C:467[B]:ILE:HG13	2.29	0.62
1:C:465[B]:GLU:HG3	1:C:467[B]:ILE:CD1	2.30	0.62
1:D:412:ASP:HB2	9:D:517:PEG:H11	1.82	0.62
1:D:449:CYS:HB3	9:D:517:PEG:H41	1.81	0.62
1:A:459:SER:OG	1:A:461:HIS:HD2	1.83	0.61
1:A:234:HIS:HE1	1:A:309:GLU:OE2	1.83	0.61
6:C:516[A]:GOL:O3	6:C:517:GOL:H2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:CE1	1:C:465[B]:GLU:H	2.15	0.61
1:A:454[A]:ARG:HG3	11:B:609:HOH:O	2.01	0.60
1:B:234:HIS:HE1	1:B:309:GLU:OE2	1.84	0.60
1:C:465[B]:GLU:CG	1:C:467[B]:ILE:HD11	2.31	0.60
1:B:417[B]:LYS:CE	11:B:606:HOH:O	2.49	0.60
1:B:417[B]:LYS:HE3	11:B:606:HOH:O	2.02	0.60
1:D:449:CYS:CB	9:D:517:PEG:H41	2.32	0.60
1:B:275:HIS:HD2	1:B:295:ASN:H	1.48	0.60
1:C:342[A]:THR:HG22	1:C:343:GLY:N	2.16	0.60
1:C:465[B]:GLU:OE1	1:C:467[B]:ILE:HG13	2.01	0.59
1:A:113:HIS:CE1	11:A:884:HOH:O	2.54	0.59
1:B:153:SER:CB	9:B:522:PEG:H32	2.33	0.59
1:C:369[A]:LYS:HZ3	6:C:517:GOL:HO3	1.49	0.59
11:A:884:HOH:O	1:D:113:HIS:CE1	2.55	0.58
9:B:520:PEG:H12	11:B:757:HOH:O	2.02	0.58
1:C:367:ILE:O	6:C:517:GOL:C1	2.51	0.58
9:D:519:PEG:H11	11:D:858:HOH:O	2.02	0.58
6:A:518:GOL:H32	11:A:649:HOH:O	2.03	0.58
1:B:98:HIS:NE2	9:B:520:PEG:H32	2.17	0.58
1:D:449:CYS:SG	9:D:517:PEG:H21	2.43	0.58
9:B:520:PEG:H11	11:B:658:HOH:O	2.04	0.58
1:A:319:CYS:SG	1:A:337[B]:CYS:SG	3.02	0.58
11:C:766:HOH:O	2:J:1:NAG:H82	2.03	0.58
1:C:465[B]:GLU:HG3	1:C:467[B]:ILE:HG13	1.86	0.57
9:C:522:PEG:C4	11:C:623:HOH:O	2.51	0.57
1:C:369[A]:LYS:CD	6:C:517:GOL:O3	2.53	0.57
1:D:234:HIS:HE1	1:D:309:GLU:OE1	1.88	0.57
1:C:376:GLU:OE1	6:C:516[B]:GOL:H31	2.03	0.57
1:D:452[A]:LYS:HE3	11:D:675:HOH:O	2.05	0.57
6:D:512:GOL:H31	11:D:910:HOH:O	2.05	0.57
9:D:517:PEG:C3	11:D:657:HOH:O	2.53	0.57
1:B:454:ARG:CD	11:B:777:HOH:O	2.52	0.56
1:B:467[B]:ILE:HD13	9:B:521:PEG:H32	1.86	0.56
6:B:513:GOL:H11	11:B:961:HOH:O	2.05	0.56
1:C:449:CYS:SG	9:C:520:PEG:H22	2.46	0.56
1:C:275:HIS:HD2	1:C:295:ASN:H	1.54	0.56
11:A:884:HOH:O	1:C:113:HIS:CE1	2.59	0.56
1:C:98:HIS:NE2	9:C:520:PEG:H32	2.20	0.56
1:B:220:ALA:HB1	9:B:526:PEG:C4	2.28	0.55
1:A:93:GLU:HB3	1:A:452:LYS:HD2	1.89	0.55
1:C:369[A]:LYS:CG	6:C:517:GOL:H32	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165[A]:GLN:HE21	1:A:171:ASN:HD22	1.52	0.55
6:C:516[A]:GOL:O3	6:C:517:GOL:C2	2.55	0.55
6:C:517:GOL:H31	11:C:693:HOH:O	2.08	0.54
1:C:234:HIS:HE1	1:C:309:GLU:OE1	1.90	0.54
1:D:336:ASN:HD22	1:D:338:ASP:H	1.55	0.54
1:A:213[B]:ILE:CD1	1:A:213[B]:ILE:C	2.78	0.54
1:D:336:ASN:ND2	1:D:338:ASP:H	2.07	0.53
1:B:279[B]:CYS:SG	11:B:914:HOH:O	2.59	0.53
9:B:520:PEG:C4	11:B:688:HOH:O	2.44	0.53
9:C:521:PEG:H22	1:D:467[B]:ILE:HD13	1.89	0.53
1:B:417[B]:LYS:NZ	11:B:606:HOH:O	2.41	0.53
1:B:162[A]:GLU:CD	11:B:692:HOH:O	2.52	0.52
1:A:275:HIS:CD2	1:A:295:ASN:H	2.28	0.52
1:A:454[B]:ARG:NH2	4:I:1:NAG:H3	2.25	0.52
1:D:185:HIS:HE2	9:D:518:PEG:C4	2.22	0.52
1:B:465[A]:GLU:HG2	9:B:521:PEG:H12	1.92	0.52
9:C:520:PEG:H11	11:C:627:HOH:O	2.09	0.52
1:D:165[A]:GLN:NE2	9:D:521:PEG:H22	2.16	0.52
1:A:461:HIS:H	1:A:461:HIS:CD2	2.28	0.52
9:C:521:PEG:C4	1:D:465[B]:GLU:HG2	2.40	0.51
1:B:390:GLY:C	9:B:523[A]:PEG:H32	2.36	0.51
9:B:520:PEG:H42	1:D:212:PRO:HB2	1.92	0.51
1:B:98:HIS:NE2	9:B:520:PEG:C3	2.73	0.51
1:C:250[A]:ARG:NE	11:C:601:HOH:O	2.23	0.51
1:A:111[A]:ASP:CG	1:A:111[A]:ASP:O	2.51	0.51
1:B:121:TYR:CG	1:B:229:SER:HA	2.46	0.50
9:B:526:PEG:C2	11:B:936:HOH:O	2.60	0.50
6:B:512:GOL:H12	6:B:513:GOL:O1	2.12	0.50
1:A:454[A]:ARG:HH12	4:I:2:NAG:H2	1.76	0.50
6:C:516[A]:GOL:H11	6:C:517:GOL:O1	2.11	0.50
1:A:247:ALA:CB	6:A:515[A]:GOL:H32	2.41	0.50
1:D:275:HIS:CD2	1:D:295:ASN:H	2.29	0.50
1:B:275:HIS:CD2	1:B:295:ASN:H	2.29	0.49
9:A:522:PEG:H31	1:B:170:TYR:O	2.12	0.49
1:C:365:ARG:HH21	6:C:516[B]:GOL:H32	1.77	0.49
1:A:144:HIS:CE1	1:C:465[A]:GLU:H	2.16	0.49
1:B:465[A]:GLU:H	1:D:144:HIS:CE1	2.18	0.49
1:C:421:ASN:HD22	9:C:520:PEG:C2	2.26	0.49
1:D:465[B]:GLU:CD	1:D:467[B]:ILE:HG22	2.37	0.49
9:D:517:PEG:H32	11:D:657:HOH:O	2.12	0.49
9:A:522:PEG:C1	11:B:880:HOH:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LYS:HE3	11:B:854:HOH:O	2.12	0.48
1:B:417[B]:LYS:HE2	11:D:720:HOH:O	2.13	0.48
1:B:465[B]:GLU:H	1:D:144:HIS:CE1	2.24	0.48
1:C:465[B]:GLU:CG	1:C:467[B]:ILE:CG1	2.92	0.48
1:A:87:LEU:N	1:A:234:HIS:HD2	2.06	0.48
11:A:884:HOH:O	1:B:113:HIS:CE1	2.67	0.48
1:C:418:GLU:HB3	9:C:522:PEG:H32	1.95	0.48
6:C:517:GOL:C3	11:C:693:HOH:O	2.62	0.47
1:D:225:ARG:HD2	6:D:512:GOL:H12	1.95	0.47
6:D:512:GOL:C3	11:D:910:HOH:O	2.61	0.47
1:C:465[B]:GLU:HG3	1:C:467[B]:ILE:CG1	2.45	0.47
1:A:454[B]:ARG:NE	11:A:604:HOH:O	2.34	0.47
1:A:118:ARG:HA	1:A:443:ASN:ND2	2.30	0.46
1:A:467[B]:ILE:HG13	11:A:829:HOH:O	2.15	0.46
1:C:179:TRP:O	6:C:514:GOL:H11	2.14	0.46
1:A:454[B]:ARG:NH2	11:A:604:HOH:O	2.44	0.46
1:D:318[B]:LEU:HD12	1:D:384:GLU:HA	1.97	0.46
1:C:275:HIS:CD2	1:C:295:ASN:H	2.33	0.46
1:C:461:HIS:CD2	1:C:461:HIS:H	2.33	0.46
1:B:461:HIS:H	1:B:461:HIS:CD2	2.32	0.46
1:A:461:HIS:HE1	6:A:517:GOL:C1	2.29	0.46
1:B:150[B]:HIS:CD2	1:B:152:ARG:O	2.69	0.46
9:C:521:PEG:H41	1:D:465[B]:GLU:HG2	1.97	0.46
1:B:153:SER:HB2	9:B:522:PEG:H32	1.96	0.45
1:A:247:ALA:HB1	6:A:515[A]:GOL:H32	1.98	0.45
1:C:328:ARG:HH21	6:C:517:GOL:C1	2.28	0.45
1:D:411:ILE:HB	1:D:413:TYR:CZ	2.52	0.45
1:D:130:ARG:HG3	6:D:514:GOL:H31	1.98	0.45
1:D:336:ASN:HD22	1:D:336:ASN:C	2.25	0.45
1:A:144:HIS:HD2	11:C:698:HOH:O	1.99	0.45
1:B:150[B]:HIS:CD2	9:B:522:PEG:O4	2.69	0.45
1:C:98:HIS:NE2	9:C:520:PEG:H31	2.32	0.45
9:A:522:PEG:C4	11:A:627:HOH:O	2.59	0.44
1:C:255[B]:ILE:HD12	1:C:313:HIS:CG	2.52	0.44
1:C:449:CYS:CB	9:C:520:PEG:H22	2.48	0.44
1:A:121:TYR:CG	1:A:229:SER:HA	2.53	0.44
1:D:125:ASP:HB2	1:D:126:PRO:CD	2.46	0.44
1:A:279:CYS:HB3	1:A:290:CYS:HB3	1.99	0.44
9:A:522:PEG:C3	11:A:627:HOH:O	2.25	0.44
1:B:336:ASN:HD22	1:B:336:ASN:C	2.25	0.44
1:C:319:CYS:SG	1:C:337[B]:CYS:HB2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASN:HD22	1:A:336:ASN:C	2.26	0.43
9:B:524:PEG:H31	9:B:524:PEG:H11	1.85	0.43
1:A:255[A]:ILE:HD12	1:A:255[A]:ILE:N	2.32	0.43
9:C:521:PEG:H42	1:D:465[B]:GLU:HG2	2.00	0.43
1:C:342[A]:THR:CG2	1:C:343:GLY:N	2.80	0.43
1:A:262[A]:LYS:HE3	11:C:885:HOH:O	2.19	0.43
1:B:411:ILE:HG21	1:B:420:PHE:HB3	1.99	0.43
1:B:449[A]:CYS:SG	9:B:520:PEG:H22	2.59	0.43
6:A:517:GOL:H11	1:B:155:PHE:CZ	2.54	0.42
1:B:262:LYS:CE	11:B:854:HOH:O	2.67	0.42
1:C:421:ASN:HD22	9:C:520:PEG:H21	1.83	0.42
1:B:461:HIS:CE1	6:B:515:GOL:H12	2.55	0.42
1:B:465[C]:GLU:H	1:D:144:HIS:CE1	2.20	0.42
1:A:307:ASP:OD2	1:A:310[A]:MET:HE2	2.20	0.42
1:B:316:LYS:HB2	1:B:337[B]:CYS:O	2.19	0.42
1:C:151:ASP:HB3	6:C:514:GOL:H12	2.02	0.41
1:C:348:PRO:HA	9:C:523:PEG:H42	2.02	0.41
1:D:369[B]:LYS:HB3	1:D:369[B]:LYS:HE3	1.76	0.41
1:D:412:ASP:HB2	9:D:517:PEG:C1	2.47	0.41
1:A:291:ILE:N	1:A:291:ILE:HD12	2.36	0.41
1:D:121:TYR:CG	1:D:229:SER:HA	2.56	0.41
1:D:412:ASP:CB	9:D:517:PEG:H11	2.47	0.41
1:A:180[B]:SER:OG	1:A:195:MET:HB2	2.20	0.41
1:C:411:ILE:HB	1:C:413:TYR:CZ	2.55	0.41
9:B:526:PEG:H22	11:B:936:HOH:O	2.19	0.41
1:B:162[A]:GLU:CG	11:B:692:HOH:O	2.68	0.41
1:B:449[B]:CYS:CB	9:B:520:PEG:H22	2.51	0.41
11:B:711:HOH:O	1:D:144:HIS:HD2	2.01	0.41
1:A:219[B]:TRP:CD1	1:A:254[B]:LYS:HE3	2.56	0.41
1:C:279:CYS:HB3	1:C:290:CYS:HB3	2.02	0.40
1:C:345[A]:SER:HA	1:C:346:PRO:HA	1.85	0.40
1:C:359[A]:GLU:O	1:C:359[A]:GLU:HG3	2.20	0.40
1:B:369[B]:LYS:HE3	1:B:369[B]:LYS:HB3	1.60	0.40

There are no symmetry-related clashes.

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	417/389 (107%)	400 (96%)	17 (4%)	0	100	100
1	B	414/389 (106%)	401 (97%)	13 (3%)	0	100	100
1	C	414/389 (106%)	399 (96%)	15 (4%)	0	100	100
1	D	416/389 (107%)	405 (97%)	11 (3%)	0	100	100
All	All	1661/1556 (107%)	1605 (97%)	56 (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	361/331 (109%)	359 (99%)	2 (1%)	78	62
1	B	358/331 (108%)	351 (98%)	7 (2%)	48	20
1	C	358/331 (108%)	349 (98%)	9 (2%)	42	14
1	D	360/331 (109%)	359 (100%)	1 (0%)	86	75
All	All	1437/1324 (108%)	1418 (99%)	19 (1%)	68	35

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	ASN
1	A	452	LYS

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Mol	Chain	Res	Type
1	B	82	ARG
1	B	136	GLN
1	B	162[A]	GLU
1	B	162[B]	GLU
1	B	336	ASN
1	B	417[A]	LYS
1	B	417[B]	LYS
1	C	194[A]	CYS
1	C	194[B]	CYS
1	C	345[A]	SER
1	C	345[B]	SER
1	C	346	PRO
1	C	359[A]	GLU
1	C	359[B]	GLU
1	C	458[A]	TRP
1	C	458[B]	TRP
1	D	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	144	HIS
1	A	150	HIS
1	A	227	GLN
1	A	234	HIS
1	A	275	HIS
1	A	336	ASN
1	A	394	ASN
1	A	400	ASN
1	A	421	ASN
1	A	443	ASN
1	A	461	HIS
1	B	227	GLN
1	B	234	HIS
1	B	264	GLN
1	B	275	HIS
1	B	336	ASN
1	B	382	ASN
1	B	394	ASN
1	B	416	ASN
1	B	421	ASN

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Mol	Chain	Res	Type
1	B	443	ASN
1	B	461	HIS
1	C	227	GLN
1	C	234	HIS
1	C	275	HIS
1	C	334	ASN
1	C	400	ASN
1	C	416	ASN
1	C	421	ASN
1	C	443	ASN
1	C	461	HIS
1	D	127	GLN
1	D	136	GLN
1	D	144	HIS
1	D	227	GLN
1	D	234	HIS
1	D	275	HIS
1	D	336	ASN
1	D	382	ASN
1	D	400	ASN
1	D	443	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](#)

39 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	2,1	14,14,15	0.81	0	17,19,21	1.39	2 (11%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	1.28	3 (17%)
2	NAG	F	1	2,1	14,14,15	1.09	2 (14%)	17,19,21	1.34	2 (11%)
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	1.70	5 (29%)
3	NAG	G	1	1,3	14,14,15	0.92	0	17,19,21	2.25	4 (23%)
3	NAG	G	2	3	14,14,15	0.60	0	17,19,21	1.41	4 (23%)
3	BMA	G	3	3	11,11,12	0.66	0	15,15,17	1.27	2 (13%)
3	MAN	G	4	3	11,11,12	0.59	0	15,15,17	1.21	2 (13%)
3	MAN	G	5	3	11,11,12	0.67	0	15,15,17	1.87	4 (26%)
3	MAN	G	6	3	11,11,12	1.01	1 (9%)	15,15,17	0.98	0
3	MAN	G	7	3	11,11,12	0.73	0	15,15,17	1.46	2 (13%)
3	MAN	G	8	3	11,11,12	0.84	0	15,15,17	1.18	2 (13%)
2	NAG	H	1	2,1	14,14,15	1.02	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	H	2	2	14,14,15	0.59	0	17,19,21	1.73	4 (23%)
4	NAG	I	1	1,4	14,14,15	0.81	0	17,19,21	1.80	6 (35%)
4	NAG	I	2	4	14,14,15	0.89	0	17,19,21	1.61	5 (29%)
4	BMA	I	3	4	11,11,12	0.56	0	15,15,17	1.13	1 (6%)
4	MAN	I	4	4	11,11,12	1.15	2 (18%)	15,15,17	1.27	2 (13%)
4	MAN	I	5	4	11,11,12	0.80	0	15,15,17	1.04	2 (13%)
4	MAN	I	6	4	11,11,12	0.55	0	15,15,17	1.70	4 (26%)
4	MAN	I	7	4	11,11,12	0.71	0	15,15,17	1.67	3 (20%)
2	NAG	J	1	2,1	14,14,15	1.07	1 (7%)	17,19,21	2.08	5 (29%)
2	NAG	J	2	2	14,14,15	1.15	1 (7%)	17,19,21	2.88	5 (29%)
2	NAG	K	1	2,1	14,14,15	1.23	1 (7%)	17,19,21	1.38	2 (11%)
2	NAG	K	2	2	14,14,15	0.65	0	17,19,21	1.38	2 (11%)
5	NAG	L	1	1,5	14,14,15	0.70	0	17,19,21	1.96	3 (17%)
5	NAG	L	2	5	14,14,15	0.87	0	17,19,21	1.64	5 (29%)
5	BMA	L	3	5	11,11,12	0.62	0	15,15,17	1.05	1 (6%)
5	MAN	L	4	5	11,11,12	0.81	1 (9%)	15,15,17	1.18	1 (6%)
5	MAN	L	5	5	11,11,12	0.66	0	15,15,17	1.34	2 (13%)
5	MAN	L	6	5	11,11,12	0.86	0	15,15,17	1.78	3 (20%)
5	NAG	M	1	1,5	14,14,15	0.90	0	17,19,21	1.91	2 (11%)
5	NAG	M	2	5	14,14,15	0.75	0	17,19,21	1.50	3 (17%)
5	BMA	M	3	5	11,11,12	0.90	0	15,15,17	1.28	1 (6%)
5	MAN	M	4	5	11,11,12	0.80	0	15,15,17	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	M	5	5	11,11,12	0.74	0	15,15,17	1.37	2 (13%)
5	MAN	M	6	5	11,11,12	0.51	0	15,15,17	1.51	2 (13%)
2	NAG	N	1	2,1	14,14,15	0.95	0	17,19,21	0.84	1 (5%)
2	NAG	N	2	2	14,14,15	0.63	0	17,19,21	1.62	3 (17%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
3	MAN	G	6	3	-	0/2/19/22	0/1/1/1
3	MAN	G	7	3	-	1/2/19/22	0/1/1/1
3	MAN	G	8	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	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	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
4	MAN	I	6	4	-	0/2/19/22	0/1/1/1
4	MAN	I	7	4	-	2/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
5	MAN	L	5	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	L	6	5	-	0/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
5	MAN	M	6	5	-	2/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	NAG	C1-C2	3.16	1.56	1.52
4	I	4	MAN	O5-C1	-2.62	1.39	1.43
2	F	1	NAG	O5-C1	-2.62	1.39	1.43
3	G	6	MAN	C2-C3	2.61	1.56	1.52
2	J	1	NAG	O4-C4	2.54	1.49	1.43
2	K	1	NAG	O5-C1	-2.43	1.39	1.43
4	I	4	MAN	O5-C5	2.27	1.47	1.43
2	F	1	NAG	C2-N2	-2.13	1.42	1.46
5	L	4	MAN	C2-C3	2.12	1.55	1.52
2	H	1	NAG	O5-C1	-2.10	1.40	1.43

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	NAG	C1-C2-N2	8.99	124.60	110.43
3	G	1	NAG	O5-C1-C2	-7.19	100.17	111.29
5	M	1	NAG	O5-C1-C2	-6.62	101.06	111.29
5	L	1	NAG	O5-C1-C2	-6.25	101.62	111.29
2	J	1	NAG	O5-C5-C6	-5.63	96.72	107.66
2	J	2	NAG	O5-C1-C2	-5.21	103.24	111.29
5	L	6	MAN	C1-O5-C5	5.09	119.00	112.19
3	G	5	MAN	C1-O5-C5	4.52	118.24	112.19
4	I	6	MAN	C1-O5-C5	4.35	118.01	112.19
2	H	2	NAG	C3-C4-C5	-4.24	102.55	110.23
4	I	1	NAG	C1-C2-N2	-4.00	104.13	110.43
2	J	1	NAG	O4-C4-C5	3.87	118.85	109.32
5	M	5	MAN	C1-O5-C5	3.69	117.13	112.19
2	J	2	NAG	C3-C4-C5	3.65	116.85	110.23
3	G	5	MAN	O2-C2-C3	3.54	117.48	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	2	NAG	O5-C1-C2	-3.44	105.96	111.29
4	I	7	MAN	C2-C3-C4	3.39	116.83	110.86
4	I	2	NAG	C1-C2-N2	3.39	115.78	110.43
5	M	6	MAN	C3-C4-C5	3.37	116.34	110.23
5	M	3	BMA	C2-C3-C4	-3.36	104.96	110.86
2	E	2	NAG	O5-C1-C2	-3.27	106.23	111.29
5	L	5	MAN	C1-O5-C5	3.25	116.54	112.19
2	F	2	NAG	C4-C3-C2	3.18	115.68	111.02
3	G	7	MAN	O2-C2-C1	-3.18	101.94	109.22
4	I	1	NAG	O5-C1-C2	-3.09	106.50	111.29
4	I	2	NAG	O6-C6-C5	-3.09	100.80	111.33
5	M	6	MAN	C2-C3-C4	-3.09	105.43	110.86
5	L	2	NAG	O6-C6-C5	-3.06	100.92	111.33
2	H	2	NAG	O5-C5-C6	3.04	113.59	107.66
4	I	4	MAN	C1-C2-C3	3.00	114.01	109.64
4	I	1	NAG	C1-O5-C5	3.00	116.20	112.19
2	E	1	NAG	O4-C4-C5	-2.99	101.95	109.32
2	K	1	NAG	C6-C5-C4	2.96	120.29	113.02
2	E	1	NAG	C1-C2-N2	2.86	114.94	110.43
2	N	2	NAG	O5-C5-C6	2.85	113.21	107.66
5	M	2	NAG	O6-C6-C5	-2.85	101.63	111.33
3	G	1	NAG	C8-C7-N2	-2.80	111.48	116.12
2	F	1	NAG	O3-C3-C2	-2.79	103.60	109.40
3	G	5	MAN	C1-C2-C3	-2.79	105.58	109.64
5	M	2	NAG	C2-N2-C7	2.75	126.59	122.90
2	K	1	NAG	O5-C5-C6	-2.75	102.31	107.66
4	I	1	NAG	O4-C4-C5	-2.75	102.56	109.32
2	K	2	NAG	O7-C7-C8	2.71	126.88	122.05
5	L	5	MAN	O5-C5-C6	2.70	112.92	107.66
2	F	2	NAG	C1-O5-C5	-2.70	108.57	112.19
4	I	6	MAN	C1-C2-C3	-2.65	105.79	109.64
2	N	2	NAG	C1-C2-N2	-2.65	106.26	110.43
5	L	2	NAG	O5-C5-C4	-2.63	104.42	110.83
4	I	7	MAN	O4-C4-C3	-2.63	104.18	110.38
3	G	1	NAG	C3-C4-C5	2.62	114.98	110.23
3	G	3	BMA	O6-C6-C5	-2.62	102.42	111.33
3	G	4	MAN	C1-O5-C5	2.62	115.69	112.19
3	G	5	MAN	C2-C3-C4	2.62	115.46	110.86
2	F	2	NAG	C1-C2-N2	-2.61	106.32	110.43
3	G	7	MAN	C1-O5-C5	2.56	115.62	112.19
2	H	2	NAG	C4-C3-C2	-2.53	107.31	111.02
3	G	1	NAG	C6-C5-C4	2.51	119.18	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C2-N2-C7	-2.48	119.58	122.90
2	H	2	NAG	O4-C4-C5	2.47	115.41	109.32
3	G	8	MAN	O6-C6-C5	-2.45	102.97	111.33
4	I	5	MAN	C1-O5-C5	2.45	115.47	112.19
2	K	2	NAG	O3-C3-C2	-2.43	104.35	109.40
4	I	6	MAN	O2-C2-C3	2.38	115.08	110.15
2	H	1	NAG	O4-C4-C3	-2.36	104.81	110.38
3	G	2	NAG	O5-C1-C2	-2.36	107.64	111.29
5	M	2	NAG	O5-C5-C4	-2.35	105.11	110.83
5	L	2	NAG	C4-C3-C2	-2.34	107.59	111.02
4	I	3	BMA	C1-O5-C5	2.34	115.32	112.19
2	H	1	NAG	O6-C6-C5	-2.30	103.51	111.33
3	G	2	NAG	C2-N2-C7	2.27	125.94	122.90
2	J	2	NAG	C1-O5-C5	-2.26	109.16	112.19
3	G	2	NAG	O4-C4-C5	-2.26	103.76	109.32
4	I	1	NAG	O5-C5-C4	-2.25	105.34	110.83
2	N	2	NAG	O7-C7-C8	2.24	126.05	122.05
2	E	2	NAG	C1-C2-N2	2.22	113.94	110.43
4	I	2	NAG	C1-O5-C5	2.22	115.16	112.19
5	L	3	BMA	C1-O5-C5	2.21	115.15	112.19
5	M	1	NAG	C8-C7-N2	-2.21	112.45	116.12
2	J	1	NAG	O7-C7-C8	-2.21	118.12	122.05
4	I	4	MAN	C1-O5-C5	2.20	115.14	112.19
4	I	7	MAN	O5-C5-C4	-2.20	105.47	110.83
3	G	3	BMA	O2-C2-C3	-2.19	105.61	110.15
4	I	2	NAG	C8-C7-N2	-2.16	112.53	116.12
5	L	2	NAG	C3-C4-C5	-2.14	106.36	110.23
5	L	6	MAN	C3-C4-C5	2.13	114.10	110.23
2	F	2	NAG	O5-C5-C6	2.13	111.81	107.66
4	I	2	NAG	O7-C7-C8	2.13	125.85	122.05
2	J	1	NAG	C1-O5-C5	2.13	115.03	112.19
4	I	1	NAG	O4-C4-C3	2.12	115.37	110.38
4	I	6	MAN	O3-C3-C4	-2.11	105.41	110.38
5	M	5	MAN	O5-C5-C6	2.10	111.75	107.66
5	L	4	MAN	C6-C5-C4	-2.09	107.89	113.02
5	L	6	MAN	C6-C5-C4	-2.07	107.95	113.02
2	N	1	NAG	O4-C4-C3	-2.06	105.52	110.38
5	L	1	NAG	C6-C5-C4	2.06	118.08	113.02
3	G	2	NAG	C1-O5-C5	2.05	114.94	112.19
5	L	1	NAG	O4-C4-C3	-2.05	105.54	110.38
3	G	8	MAN	O4-C4-C3	-2.05	105.54	110.38
2	E	2	NAG	C4-C3-C2	-2.04	108.03	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	NAG	O7-C7-C8	2.04	125.68	122.05
3	G	4	MAN	C6-C5-C4	-2.03	108.02	113.02
2	F	1	NAG	O5-C1-C2	-2.03	108.16	111.29
4	I	5	MAN	O2-C2-C1	-2.02	104.59	109.22
2	J	1	NAG	O6-C6-C5	-2.01	104.50	111.33

There are no chirality outliers.

All (10) torsion outliers are listed below:

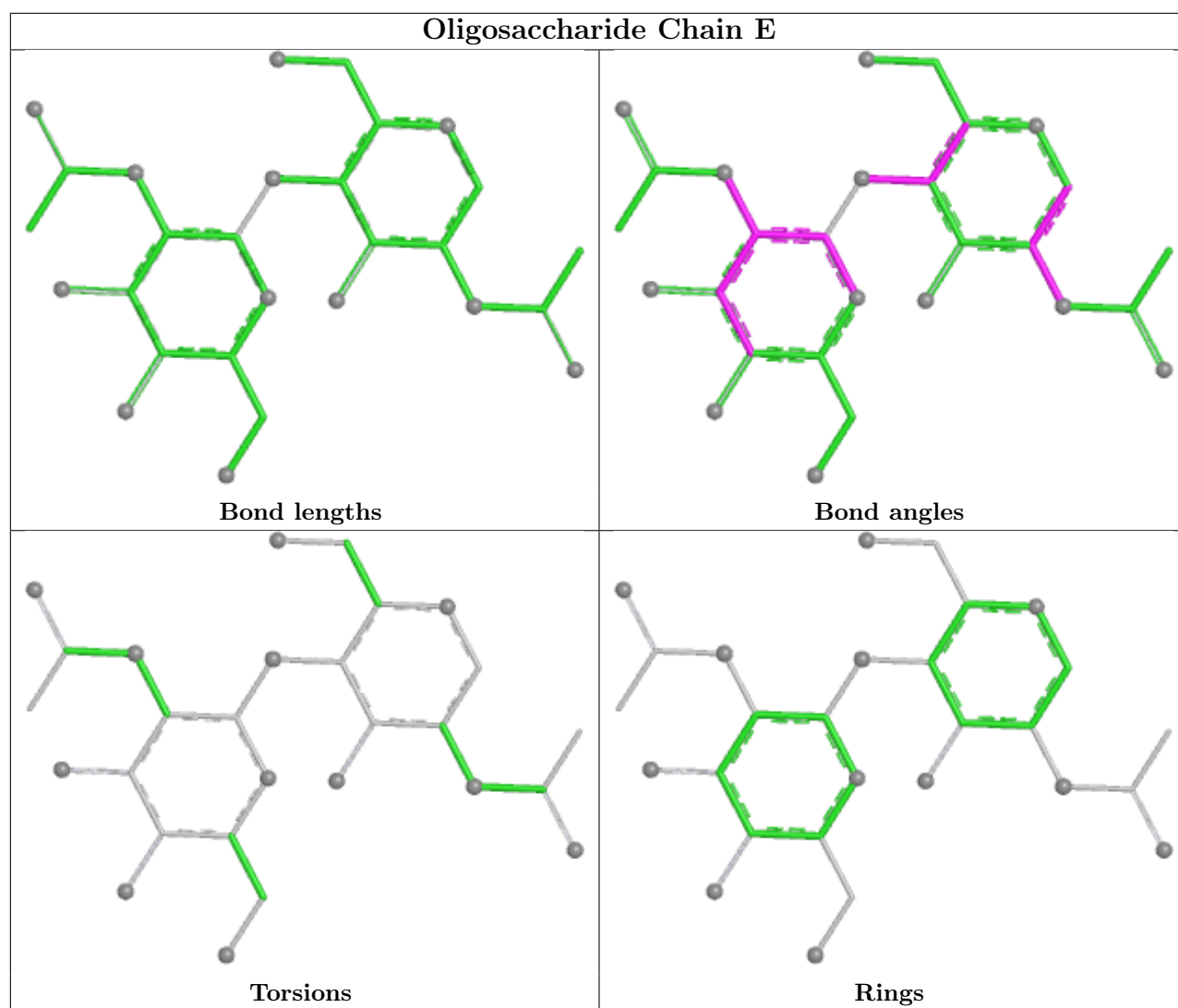
Mol	Chain	Res	Type	Atoms
4	I	7	MAN	O5-C5-C6-O6
4	I	7	MAN	C4-C5-C6-O6
5	M	6	MAN	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
5	M	6	MAN	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	G	7	MAN	C4-C5-C6-O6

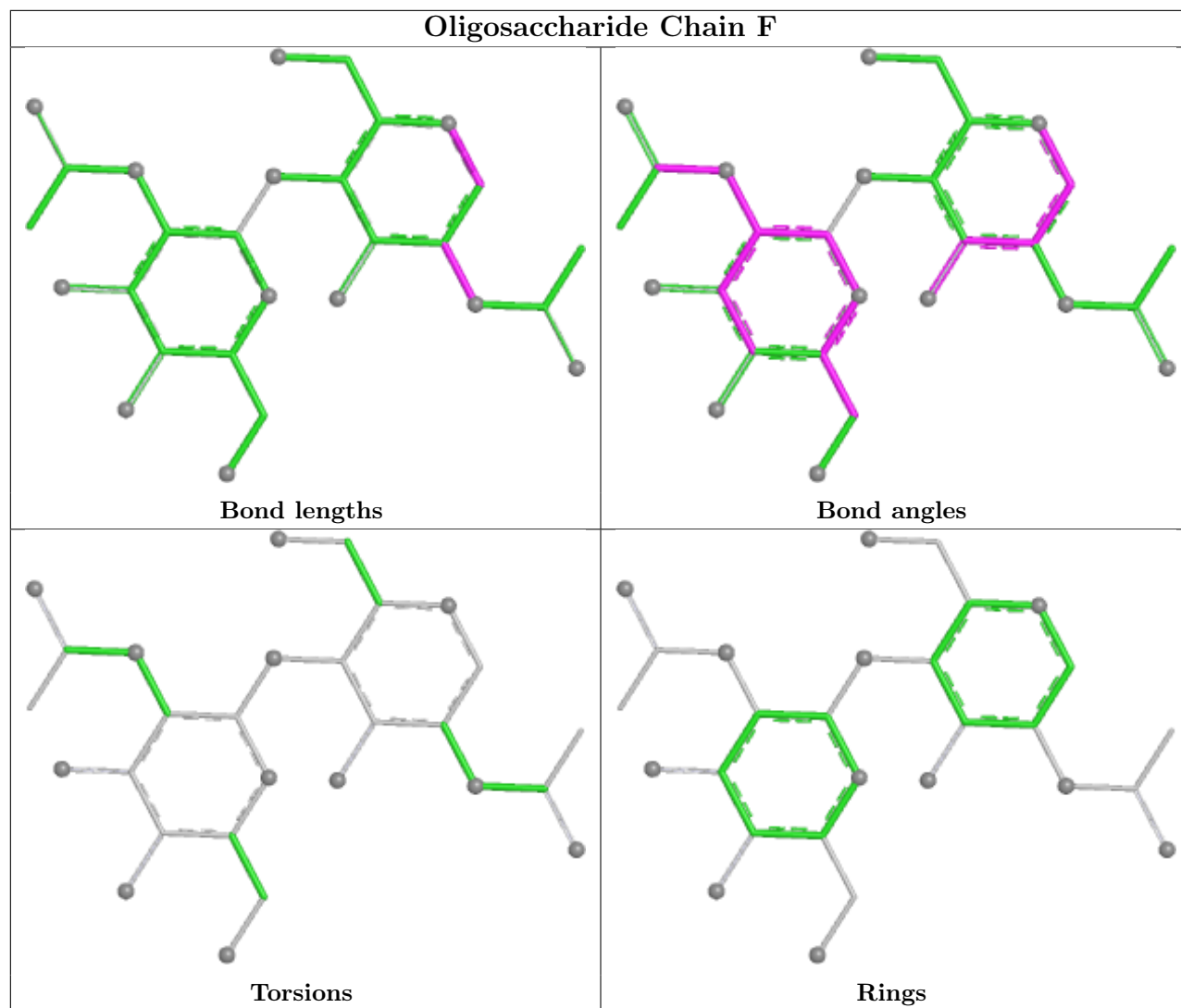
There are no ring outliers.

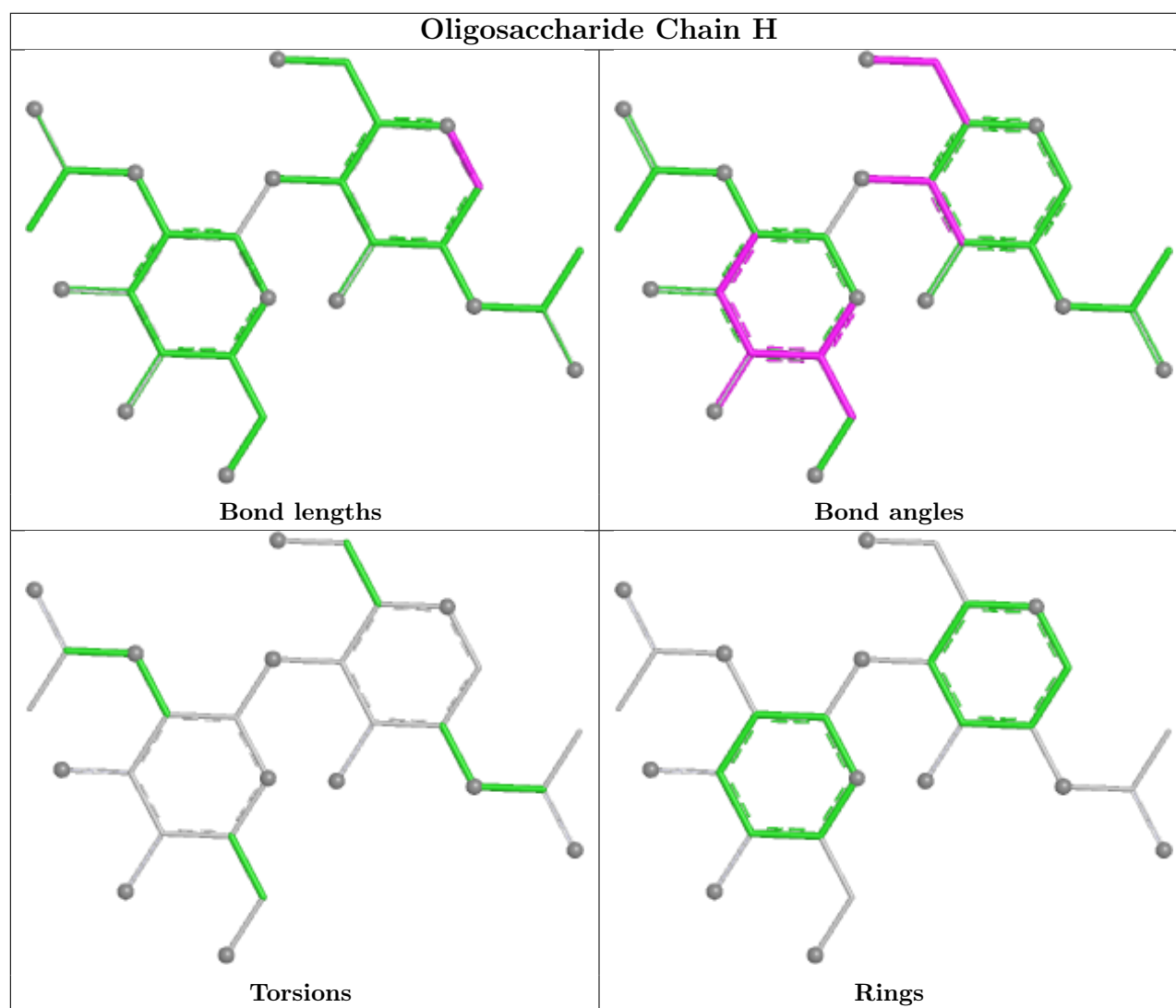
3 monomers are involved in 6 short contacts:

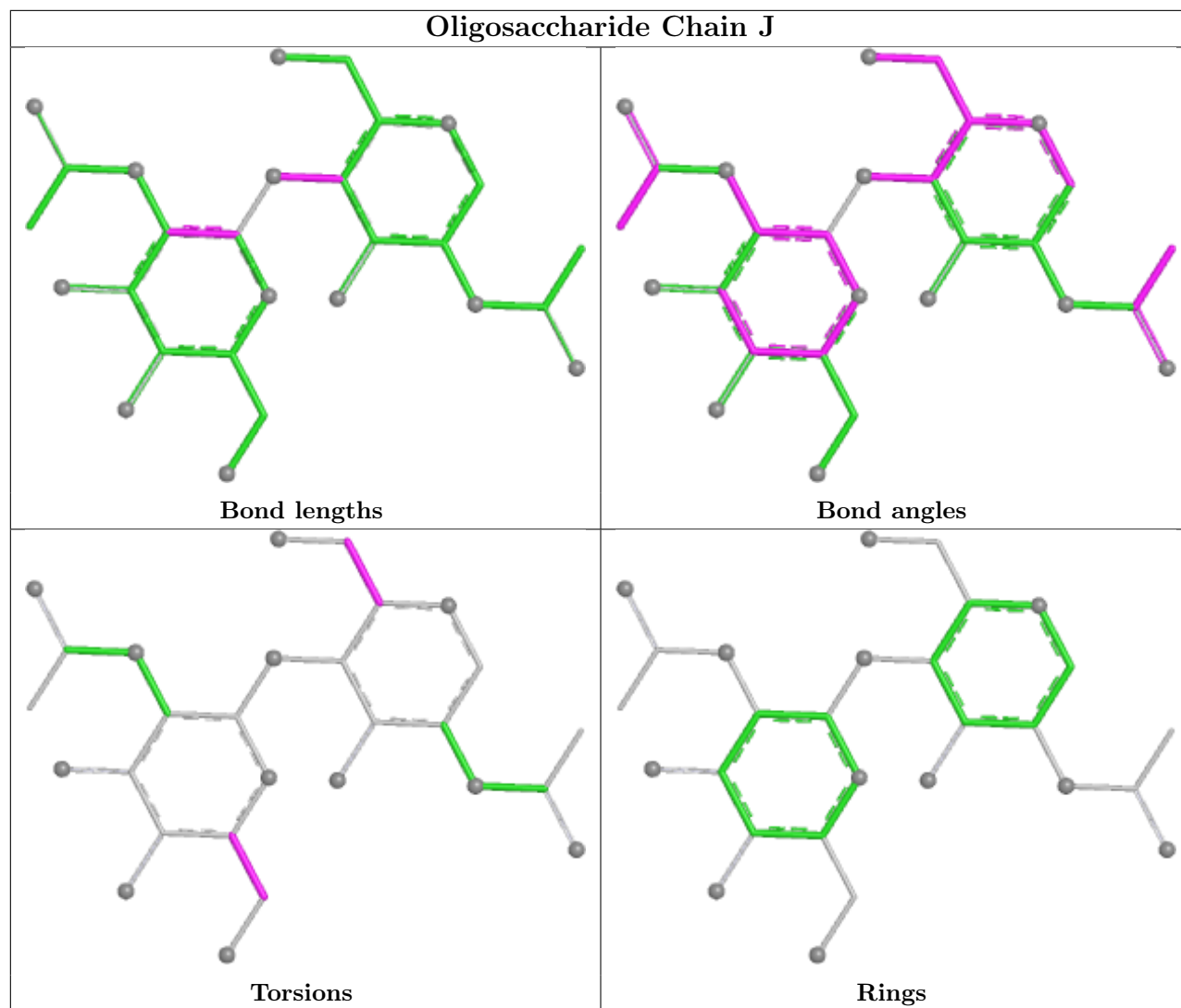
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	2	0
4	I	1	NAG	1	0
2	J	1	NAG	3	0

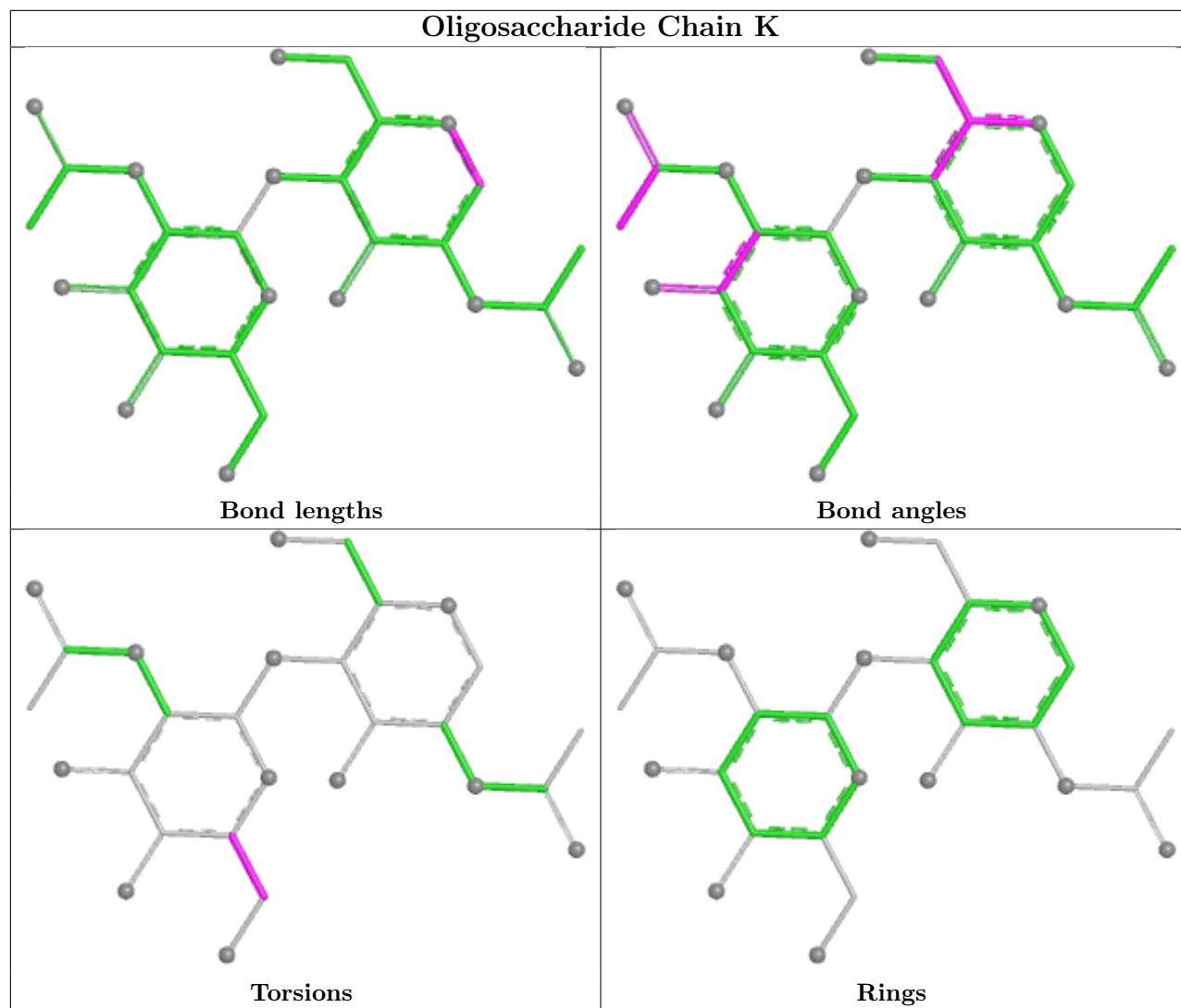
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

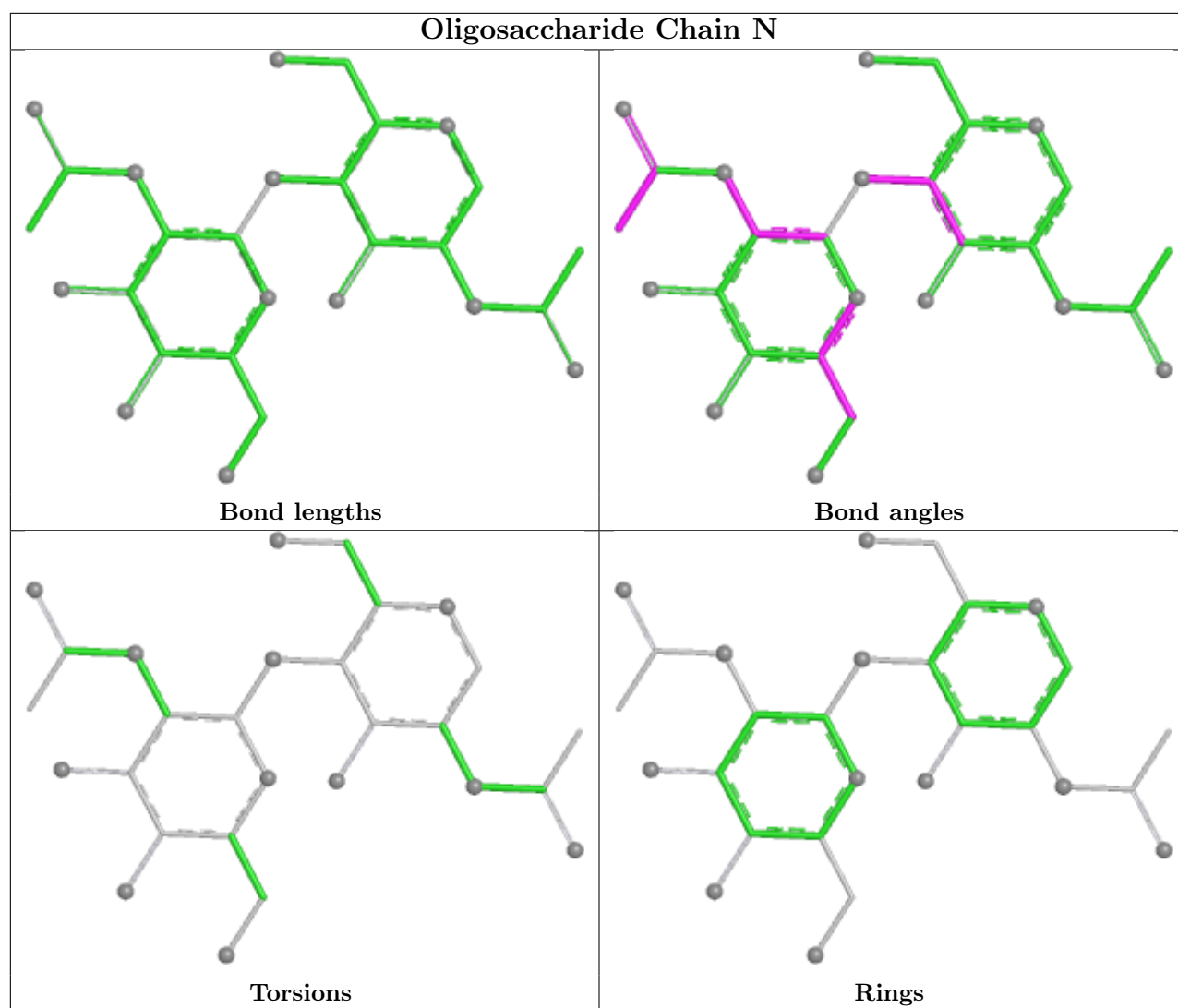


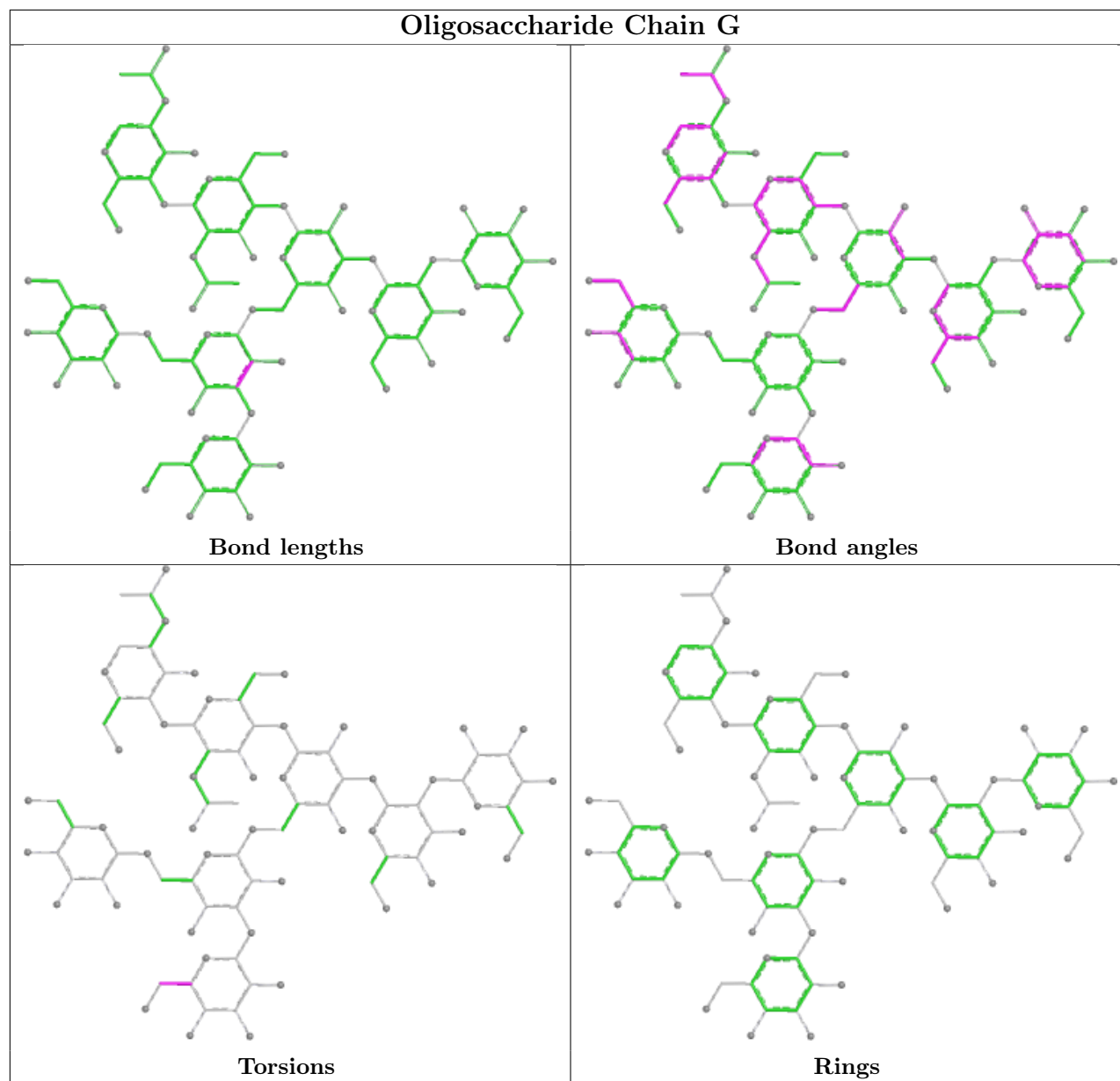


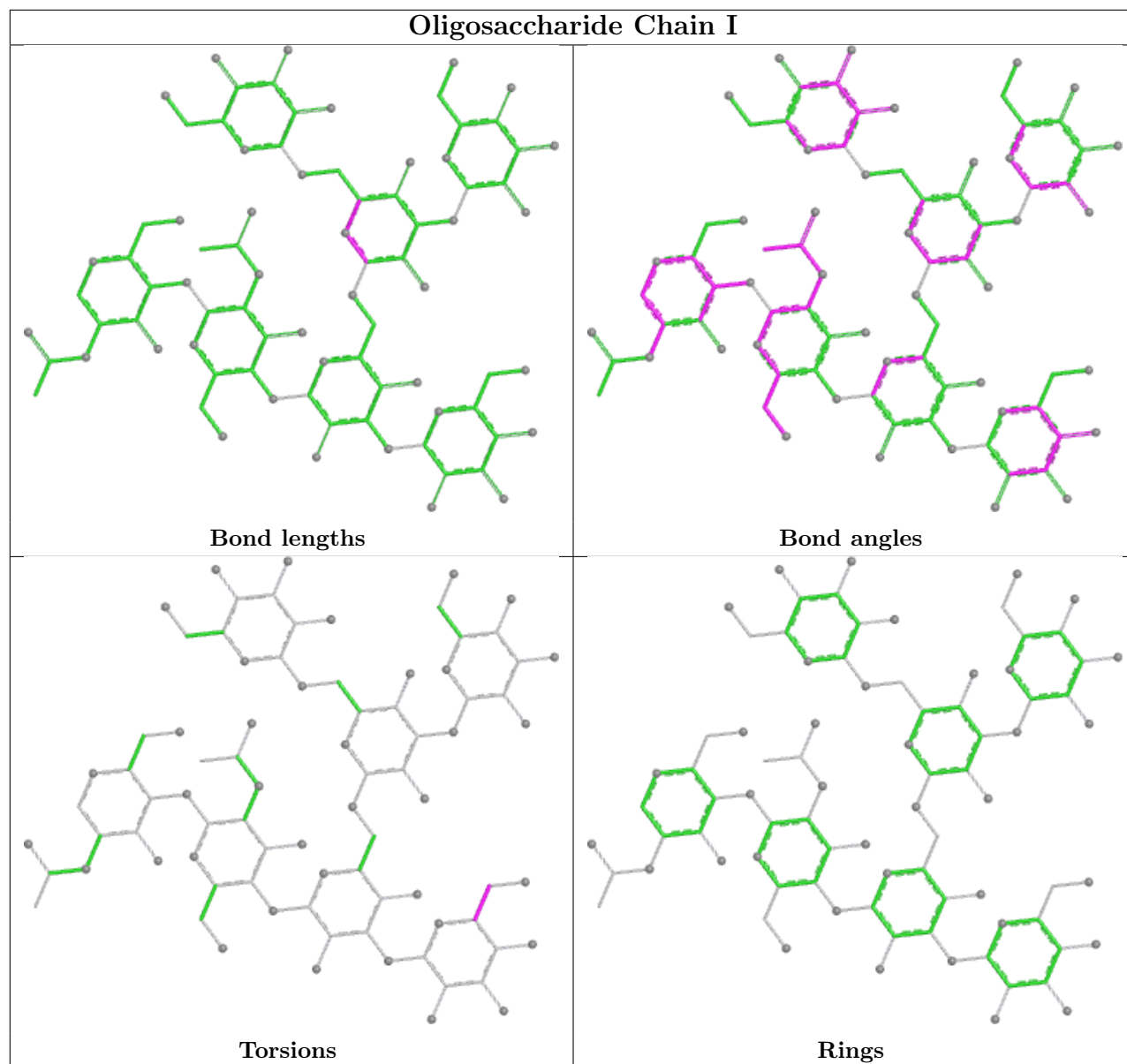


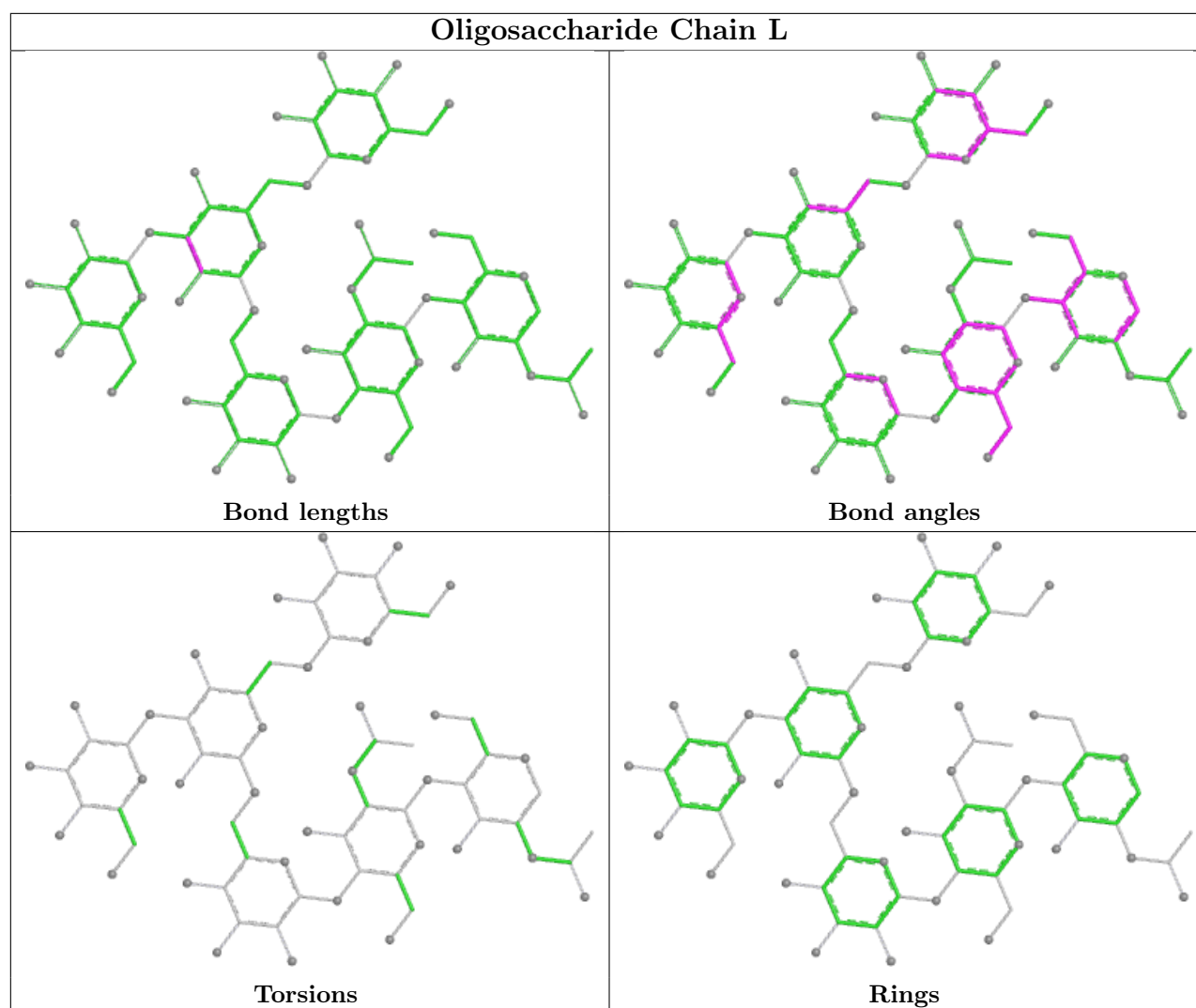


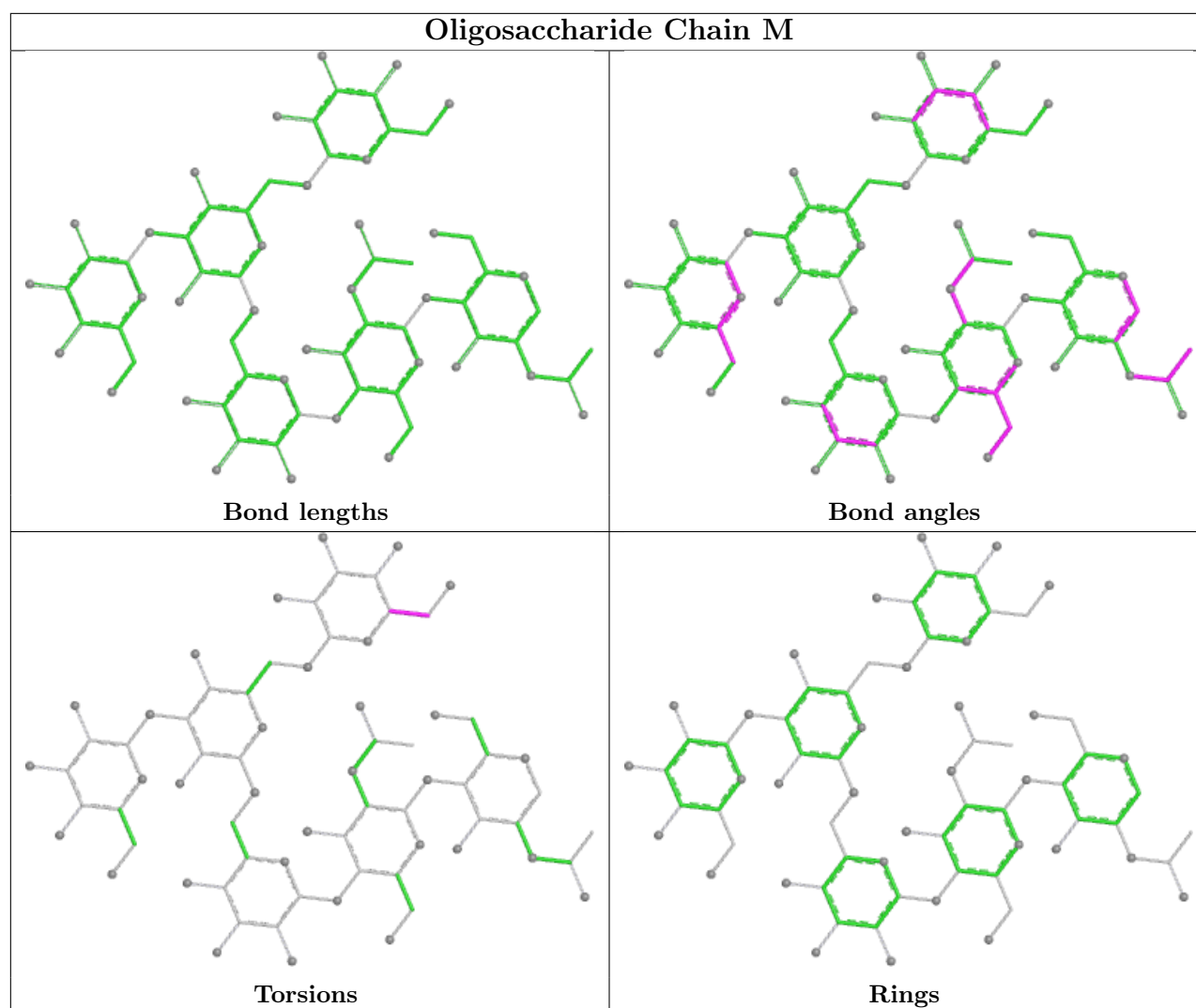












5.6 Ligand geometry [i](#)

Of 59 ligands modelled in this entry, 4 are monoatomic - leaving 55 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	GOL	C	511	-	5,5,5	0.60	0	5,5,5	1.04	1 (20%)
6	GOL	C	512	-	5,5,5	1.11	0	5,5,5	2.51	2 (40%)
6	GOL	D	511	-	5,5,5	0.56	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PO4	A	520	-	4,4,4	0.94	0	6,6,6	0.75	0
6	GOL	D	514	-	5,5,5	0.55	0	5,5,5	0.77	0
9	PEG	C	522	-	6,6,6	0.31	0	5,5,5	0.21	0
6	GOL	A	516[B]	-	5,5,5	0.47	0	5,5,5	0.58	0
6	GOL	A	517	-	5,5,5	0.75	0	5,5,5	1.31	0
8	PO4	B	518	-	4,4,4	1.07	0	6,6,6	0.84	0
9	PEG	B	520	-	6,6,6	0.45	0	5,5,5	0.25	0
6	GOL	C	515[A]	-	5,5,5	0.60	0	5,5,5	1.11	0
9	PEG	B	522	-	6,6,6	0.21	0	5,5,5	0.29	0
9	PEG	D	516	-	6,6,6	0.37	0	5,5,5	0.33	0
9	PEG	B	525	-	6,6,6	0.18	0	5,5,5	0.07	0
9	PEG	C	523	-	6,6,6	0.39	0	5,5,5	0.35	0
10	NAG	D	501	1	14,14,15	0.68	0	17,19,21	0.80	0
6	GOL	C	514	-	5,5,5	0.97	0	5,5,5	1.80	2 (40%)
9	PEG	B	523[A]	-	6,6,6	0.41	0	5,5,5	0.38	0
9	PEG	B	524	-	6,6,6	0.34	0	5,5,5	0.47	0
6	GOL	C	516[A]	-	5,5,5	0.60	0	5,5,5	0.96	0
9	PEG	D	518	-	6,6,6	0.26	0	5,5,5	0.20	0
6	GOL	A	513[B]	-	5,5,5	0.46	0	5,5,5	0.68	0
6	GOL	A	515[A]	-	5,5,5	0.24	0	5,5,5	1.13	0
6	GOL	D	510	-	5,5,5	0.62	0	5,5,5	0.98	0
6	GOL	B	513	-	5,5,5	0.65	0	5,5,5	0.91	0
9	PEG	D	519	-	6,6,6	0.19	0	5,5,5	0.13	0
6	GOL	A	514	-	5,5,5	0.70	0	5,5,5	1.22	0
6	GOL	A	516[A]	-	5,5,5	0.34	0	5,5,5	0.42	0
6	GOL	C	518	-	5,5,5	0.61	0	5,5,5	0.77	0
6	GOL	B	511	-	5,5,5	0.48	0	5,5,5	1.50	1 (20%)
9	PEG	D	517	-	6,6,6	0.73	0	5,5,5	0.99	0
9	PEG	D	521	-	6,6,6	0.53	0	5,5,5	0.49	0
9	PEG	B	523[B]	-	6,6,6	0.20	0	5,5,5	0.19	0
8	PO4	A	521	-	4,4,4	0.90	0	6,6,6	1.71	2 (33%)
9	PEG	C	520	-	6,6,6	0.60	0	5,5,5	0.25	0
9	PEG	D	520	-	6,6,6	0.48	0	5,5,5	0.13	0
9	PEG	A	522	-	6,6,6	0.36	0	5,5,5	0.17	0
9	PEG	C	521	-	6,6,6	0.29	0	5,5,5	0.35	0
6	GOL	A	518	-	5,5,5	0.28	0	5,5,5	0.91	0
9	PEG	B	521	-	6,6,6	0.37	0	5,5,5	0.32	0
6	GOL	D	513	-	5,5,5	1.22	1 (20%)	5,5,5	1.09	1 (20%)
6	GOL	C	515[B]	-	5,5,5	0.52	0	5,5,5	0.57	0
9	PEG	B	526	-	6,6,6	0.23	0	5,5,5	0.22	0
6	GOL	A	513[A]	-	5,5,5	0.25	0	5,5,5	0.85	0
6	GOL	B	514	-	5,5,5	0.33	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	B	501	1	14,14,15	0.57	0	17,19,21	1.81	5 (29%)
6	GOL	B	515	-	5,5,5	0.59	0	5,5,5	0.72	0
6	GOL	B	512	-	5,5,5	0.62	0	5,5,5	1.57	1 (20%)
6	GOL	D	512	-	5,5,5	0.28	0	5,5,5	0.98	1 (20%)
6	GOL	C	513	-	5,5,5	1.92	1 (20%)	5,5,5	1.00	0
6	GOL	C	516[B]	-	5,5,5	0.35	0	5,5,5	0.46	0
6	GOL	C	517	-	5,5,5	0.80	0	5,5,5	1.13	0
9	PEG	B	519	-	6,6,6	0.16	0	5,5,5	0.16	0
6	GOL	B	516	-	5,5,5	0.63	0	5,5,5	0.91	0
6	GOL	A	515[B]	-	5,5,5	0.27	0	5,5,5	0.88	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
6	GOL	C	511	-	-	2/4/4/4	-
6	GOL	C	512	-	-	2/4/4/4	-
6	GOL	D	511	-	-	2/4/4/4	-
9	PEG	C	522	-	-	1/4/4/4	-
6	GOL	D	514	-	-	2/4/4/4	-
6	GOL	A	516[B]	-	-	4/4/4/4	-
6	GOL	A	517	-	-	4/4/4/4	-
9	PEG	B	520	-	-	3/4/4/4	-
6	GOL	C	515[A]	-	-	1/4/4/4	-
9	PEG	B	522	-	-	3/4/4/4	-
9	PEG	D	516	-	-	1/4/4/4	-
9	PEG	B	525	-	-	2/4/4/4	-
9	PEG	C	523	-	-	3/4/4/4	-
10	NAG	D	501	1	-	0/6/23/26	0/1/1/1
6	GOL	C	514	-	-	2/4/4/4	-
9	PEG	B	523[A]	-	-	3/4/4/4	-
9	PEG	B	524	-	-	4/4/4/4	-
6	GOL	C	516[A]	-	-	0/4/4/4	-
9	PEG	D	518	-	-	2/4/4/4	-
6	GOL	A	513[B]	-	-	3/4/4/4	-
6	GOL	A	515[A]	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	510	-	-	0/4/4/4	-
6	GOL	B	513	-	-	2/4/4/4	-
9	PEG	D	519	-	-	1/4/4/4	-
6	GOL	A	514	-	-	0/4/4/4	-
6	GOL	A	516[A]	-	-	0/4/4/4	-
6	GOL	C	518	-	-	2/4/4/4	-
6	GOL	B	511	-	-	0/4/4/4	-
9	PEG	D	517	-	-	3/4/4/4	-
9	PEG	D	521	-	-	2/4/4/4	-
9	PEG	B	523[B]	-	-	4/4/4/4	-
9	PEG	C	520	-	-	3/4/4/4	-
9	PEG	D	520	-	-	1/4/4/4	-
9	PEG	A	522	-	-	3/4/4/4	-
9	PEG	C	521	-	-	0/4/4/4	-
6	GOL	A	518	-	-	2/4/4/4	-
9	PEG	B	521	-	-	1/4/4/4	-
6	GOL	D	513	-	-	2/4/4/4	-
6	GOL	C	515[B]	-	-	4/4/4/4	-
9	PEG	B	526	-	-	4/4/4/4	-
6	GOL	A	513[A]	-	-	0/4/4/4	-
6	GOL	B	514	-	-	0/4/4/4	-
10	NAG	B	501	1	-	1/6/23/26	0/1/1/1
6	GOL	B	515	-	-	3/4/4/4	-
6	GOL	B	512	-	-	3/4/4/4	-
6	GOL	D	512	-	-	2/4/4/4	-
6	GOL	C	513	-	-	2/4/4/4	-
6	GOL	C	516[B]	-	-	2/4/4/4	-
6	GOL	C	517	-	-	2/4/4/4	-
9	PEG	B	519	-	-	1/4/4/4	-
6	GOL	B	516	-	-	2/4/4/4	-
6	GOL	A	515[B]	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	513	GOL	O1-C1	3.91	1.58	1.42
6	D	513	GOL	O1-C1	2.69	1.53	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	501	NAG	C1-C2-N2	-4.43	103.46	110.43
6	C	512	GOL	C3-C2-C1	-4.13	96.66	111.80
6	C	514	GOL	O2-C2-C1	-2.92	97.10	109.18
10	B	501	NAG	C4-C3-C2	2.81	115.13	111.02
6	B	511	GOL	O2-C2-C1	-2.80	97.58	109.18
10	B	501	NAG	O5-C1-C2	2.77	115.58	111.29
10	B	501	NAG	C1-O5-C5	2.52	115.57	112.19
8	A	521	PO4	O4-P-O3	2.52	115.75	107.91
6	B	512	GOL	C3-C2-C1	-2.33	103.24	111.80
6	C	511	GOL	C3-C2-C1	-2.26	103.51	111.80
6	C	512	GOL	O3-C3-C2	-2.25	100.25	110.38
6	C	514	GOL	C3-C2-C1	2.18	119.78	111.80
10	B	501	NAG	O3-C3-C4	-2.16	105.28	110.38
6	D	513	GOL	O1-C1-C2	2.14	120.02	110.38
6	D	512	GOL	C3-C2-C1	-2.02	104.38	111.80
8	A	521	PO4	O2-P-O1	-2.01	103.84	110.95

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	513[B]	GOL	O1-C1-C2-C3
6	A	517	GOL	O1-C1-C2-C3
6	A	517	GOL	C1-C2-C3-O3
6	A	518	GOL	O1-C1-C2-C3
6	B	512	GOL	C1-C2-C3-O3
6	B	515	GOL	O1-C1-C2-C3
6	C	511	GOL	O1-C1-C2-C3
6	C	512	GOL	O1-C1-C2-C3
6	C	513	GOL	O1-C1-C2-O2
6	C	513	GOL	O1-C1-C2-C3
6	C	518	GOL	O1-C1-C2-C3
6	D	513	GOL	O1-C1-C2-C3
9	B	523[B]	PEG	C1-C2-O2-C3
9	D	518	PEG	C1-C2-O2-C3
9	B	523[B]	PEG	C4-C3-O2-C2
9	B	524	PEG	C1-C2-O2-C3
9	B	519	PEG	O1-C1-C2-O2
6	A	517	GOL	O2-C2-C3-O3
9	D	517	PEG	C4-C3-O2-C2
9	C	520	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
9	C	523	PEG	O1-C1-C2-O2
9	D	519	PEG	O1-C1-C2-O2
9	D	521	PEG	O1-C1-C2-O2
9	A	522	PEG	O1-C1-C2-O2
9	B	526	PEG	O2-C3-C4-O4
9	C	523	PEG	O2-C3-C4-O4
6	A	515[A]	GOL	C1-C2-C3-O3
6	A	515[B]	GOL	O1-C1-C2-C3
6	A	516[B]	GOL	O1-C1-C2-C3
6	A	516[B]	GOL	C1-C2-C3-O3
6	B	513	GOL	C1-C2-C3-O3
6	B	515	GOL	C1-C2-C3-O3
6	B	516	GOL	O1-C1-C2-C3
6	C	514	GOL	O1-C1-C2-C3
6	C	515[B]	GOL	C1-C2-C3-O3
6	C	516[B]	GOL	O1-C1-C2-C3
6	C	517	GOL	C1-C2-C3-O3
6	D	511	GOL	O1-C1-C2-C3
6	D	512	GOL	C1-C2-C3-O3
6	D	514	GOL	C1-C2-C3-O3
9	B	520	PEG	O2-C3-C4-O4
9	B	522	PEG	O1-C1-C2-O2
9	B	523[A]	PEG	O2-C3-C4-O4
9	B	526	PEG	O1-C1-C2-O2
9	C	520	PEG	O1-C1-C2-O2
6	A	515[A]	GOL	O2-C2-C3-O3
6	A	517	GOL	O1-C1-C2-O2
6	A	518	GOL	O1-C1-C2-O2
6	B	515	GOL	O1-C1-C2-O2
6	C	512	GOL	O1-C1-C2-O2
6	C	518	GOL	O1-C1-C2-O2
6	D	513	GOL	O1-C1-C2-O2
9	B	520	PEG	O1-C1-C2-O2
9	B	523[B]	PEG	O1-C1-C2-O2
6	A	513[B]	GOL	O1-C1-C2-O2
6	B	512	GOL	O2-C2-C3-O3
6	C	514	GOL	O1-C1-C2-O2
6	C	516[B]	GOL	O1-C1-C2-O2
6	C	517	GOL	O2-C2-C3-O3
9	D	517	PEG	O2-C3-C4-O4
6	A	516[B]	GOL	O1-C1-C2-O2
6	D	511	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	B	523[B]	PEG	O2-C3-C4-O4
6	B	513	GOL	O2-C2-C3-O3
6	B	516	GOL	O1-C1-C2-O2
6	C	511	GOL	O1-C1-C2-O2
6	D	512	GOL	O2-C2-C3-O3
9	D	518	PEG	O1-C1-C2-O2
9	B	525	PEG	C4-C3-O2-C2
6	B	512	GOL	O1-C1-C2-C3
6	C	515[B]	GOL	O1-C1-C2-C3
9	B	526	PEG	C4-C3-O2-C2
9	C	522	PEG	O2-C3-C4-O4
9	B	520	PEG	C1-C2-O2-C3
9	B	522	PEG	C4-C3-O2-C2
9	B	524	PEG	O2-C3-C4-O4
9	D	521	PEG	O2-C3-C4-O4
9	B	525	PEG	O2-C3-C4-O4
9	D	516	PEG	O1-C1-C2-O2
9	C	520	PEG	C1-C2-O2-C3
9	C	523	PEG	C1-C2-O2-C3
9	B	524	PEG	O1-C1-C2-O2
9	B	522	PEG	C1-C2-O2-C3
9	A	522	PEG	O2-C3-C4-O4
6	D	514	GOL	O2-C2-C3-O3
10	B	501	NAG	C4-C5-C6-O6
9	B	521	PEG	O1-C1-C2-O2
9	D	517	PEG	O1-C1-C2-O2
9	D	520	PEG	C1-C2-O2-C3
9	B	524	PEG	C4-C3-O2-C2
6	A	513[B]	GOL	C1-C2-C3-O3
6	A	515[B]	GOL	O1-C1-C2-O2
6	C	515[B]	GOL	O2-C2-C3-O3
9	A	522	PEG	C1-C2-O2-C3
6	A	516[B]	GOL	O2-C2-C3-O3
6	C	515[A]	GOL	O1-C1-C2-O2
6	C	515[B]	GOL	O1-C1-C2-O2
9	B	526	PEG	C1-C2-O2-C3
9	B	523[A]	PEG	O1-C1-C2-O2
9	B	523[A]	PEG	C4-C3-O2-C2

There are no ring outliers.

30 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	511	GOL	1	0
6	D	514	GOL	1	0
9	C	522	PEG	3	0
6	A	517	GOL	2	0
9	B	520	PEG	10	0
9	B	522	PEG	3	0
9	C	523	PEG	1	0
6	C	514	GOL	2	0
9	B	523[A]	PEG	2	0
9	B	524	PEG	1	0
6	C	516[A]	GOL	3	0
9	D	518	PEG	3	0
6	A	515[A]	GOL	2	0
6	B	513	GOL	2	0
9	D	519	PEG	1	0
9	D	517	PEG	8	0
9	D	521	PEG	2	0
9	B	523[B]	PEG	5	0
9	C	520	PEG	11	0
9	A	522	PEG	5	0
9	C	521	PEG	4	0
6	A	518	GOL	1	0
9	B	521	PEG	2	0
6	C	515[B]	GOL	1	0
9	B	526	PEG	4	0
6	B	515	GOL	1	0
6	B	512	GOL	1	0
6	D	512	GOL	3	0
6	C	516[B]	GOL	2	0
6	C	517	GOL	17	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	389/389 (100%)	-0.45	0 100 100	4, 12, 19, 36	29 (7%)
1	B	389/389 (100%)	-0.47	2 (0%) 87 89	4, 11, 18, 45	24 (6%)
1	C	389/389 (100%)	-0.50	3 (0%) 82 86	5, 11, 19, 39	27 (6%)
1	D	389/389 (100%)	-0.52	0 100 100	5, 11, 18, 40	29 (7%)
All	All	1556/1556 (100%)	-0.48	5 (0%) 90 91	4, 11, 19, 45	109 (7%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	GLY	3.3
1	B	88[A]	THR	2.8
1	C	345[A]	SER	2.7
1	B	82	ARG	2.4
1	C	344	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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	J	2	14/15	0.43	0.22	52,77,82,84	0
2	NAG	J	1	14/15	0.62	0.19	43,51,58,63	0

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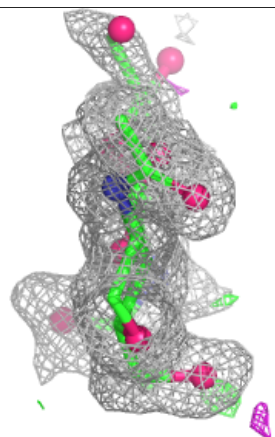
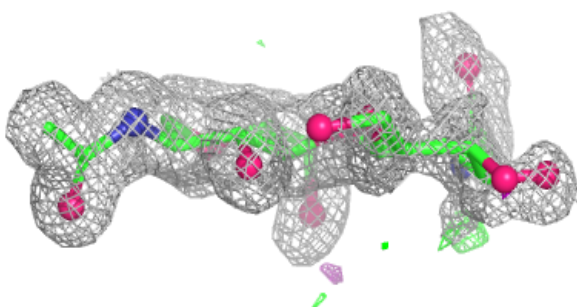
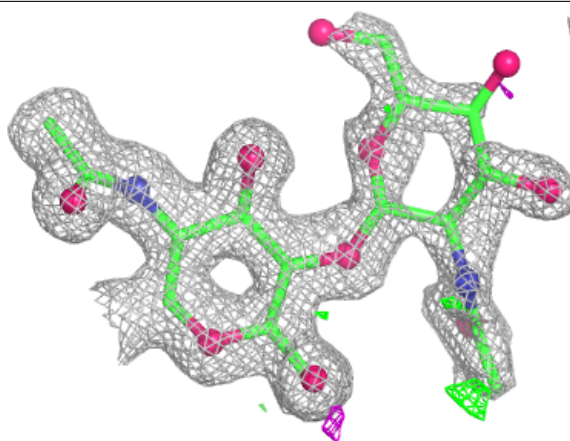
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	I	7	11/12	0.64	0.16	36,45,55,55	0
2	NAG	N	2	14/15	0.65	0.17	45,51,67,71	0
2	NAG	E	2	14/15	0.67	0.17	40,47,50,59	0
2	NAG	F	2	14/15	0.69	0.16	44,51,64,68	0
2	NAG	H	2	14/15	0.75	0.14	43,49,59,61	0
3	MAN	G	5	11/12	0.75	0.13	33,39,43,47	0
2	NAG	K	2	14/15	0.75	0.15	36,42,46,47	0
5	MAN	L	5	11/12	0.80	0.12	30,35,38,39	0
5	MAN	M	5	11/12	0.83	0.11	29,34,38,41	0
5	MAN	L	6	11/12	0.84	0.12	25,28,34,40	0
5	NAG	M	1	14/15	0.85	0.11	22,24,27,29	0
4	NAG	I	1	14/15	0.85	0.12	22,26,37,37	0
3	NAG	G	1	14/15	0.86	0.11	22,26,30,31	0
5	BMA	M	3	11/12	0.86	0.11	26,29,34,36	0
5	NAG	L	1	14/15	0.86	0.11	23,27,31,35	0
5	MAN	M	6	11/12	0.87	0.11	25,28,37,45	0
5	NAG	M	2	14/15	0.88	0.10	19,24,28,30	0
5	BMA	L	3	11/12	0.89	0.09	25,27,28,32	0
4	NAG	I	2	14/15	0.89	0.09	17,19,23,29	0
5	NAG	L	2	14/15	0.90	0.09	18,22,27,29	0
3	MAN	G	8	11/12	0.90	0.09	19,23,31,35	0
4	MAN	I	6	11/12	0.90	0.10	20,22,31,37	0
5	MAN	M	4	11/12	0.92	0.09	25,27,30,31	0
5	MAN	L	4	11/12	0.92	0.09	27,29,30,31	0
2	NAG	F	1	14/15	0.92	0.08	16,19,29,34	0
2	NAG	E	1	14/15	0.93	0.08	18,21,25,29	0
2	NAG	H	1	14/15	0.94	0.08	14,20,29,35	0
2	NAG	N	1	14/15	0.95	0.07	15,18,30,36	0
3	NAG	G	2	14/15	0.95	0.07	13,16,21,24	0
3	MAN	G	4	11/12	0.95	0.07	18,21,23,28	0
4	MAN	I	5	11/12	0.95	0.07	18,19,21,22	0
2	NAG	K	1	14/15	0.95	0.07	15,19,26,30	0
3	MAN	G	6	11/12	0.95	0.06	14,15,16,19	0
3	MAN	G	7	11/12	0.96	0.06	14,15,19,19	0
3	BMA	G	3	11/12	0.96	0.05	14,14,16,16	0
4	BMA	I	3	11/12	0.96	0.05	16,18,21,24	0
4	MAN	I	4	11/12	0.97	0.05	16,18,19,19	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.

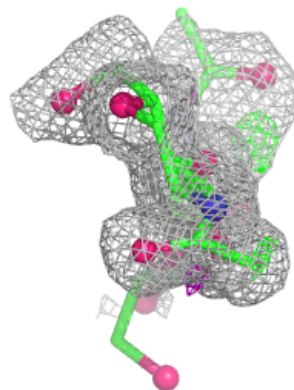
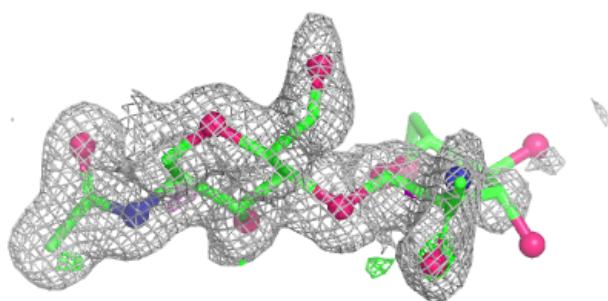
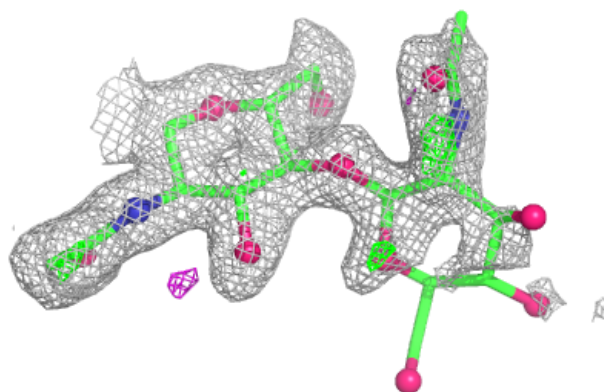
Electron density around Chain E:

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

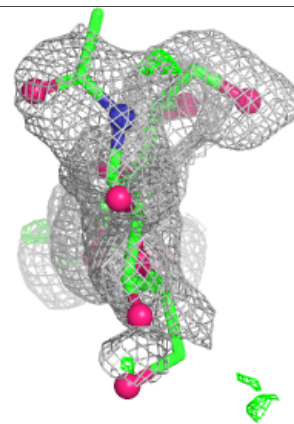
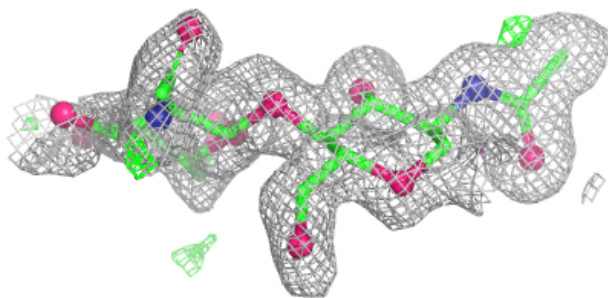
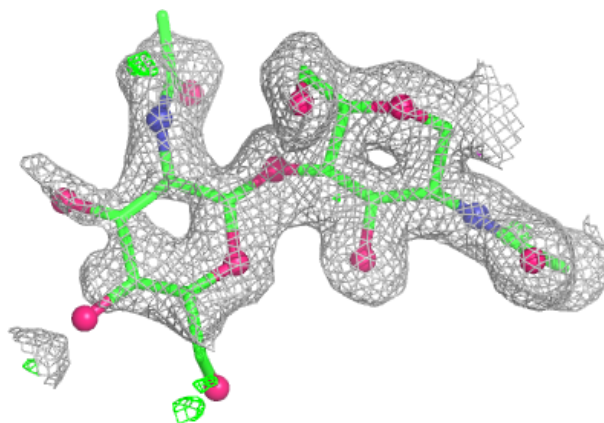


Electron density around Chain F:

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and green (positive)

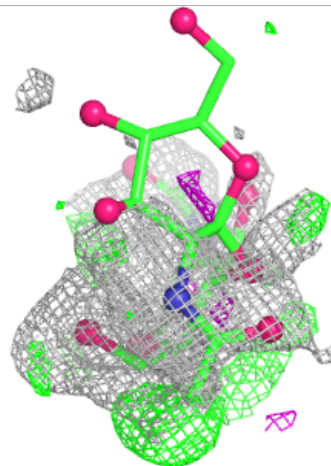
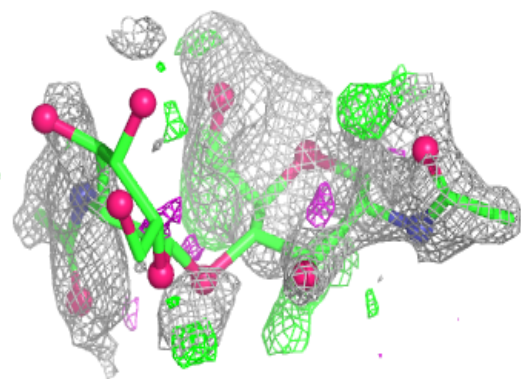
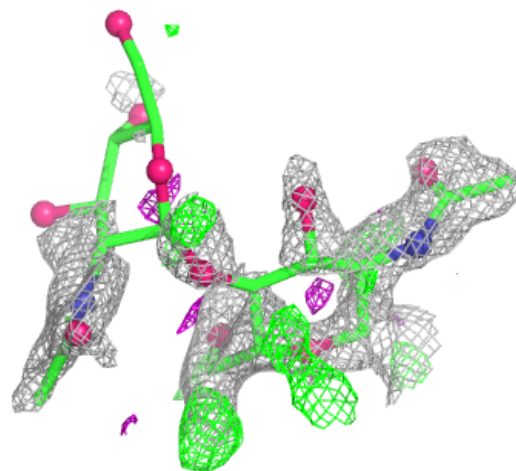
**Electron density around Chain H:**

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



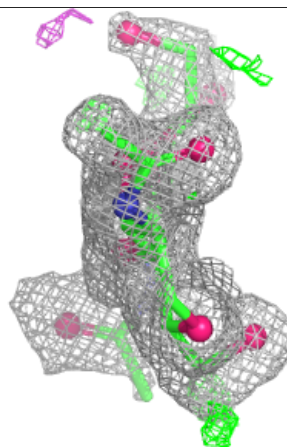
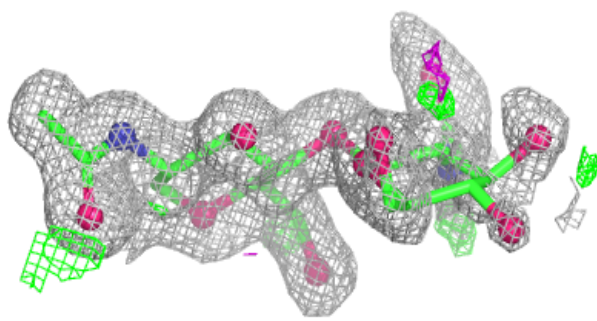
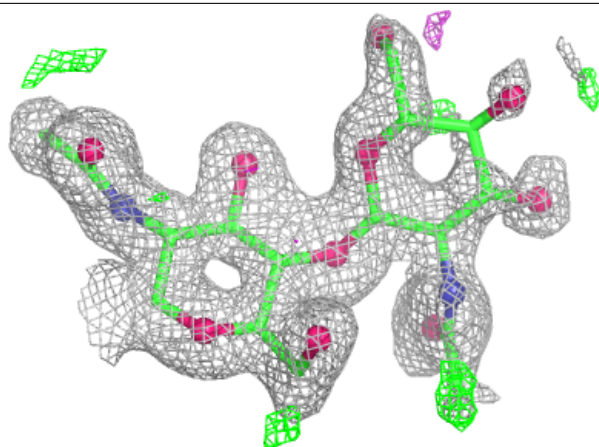
Electron density around Chain J:

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



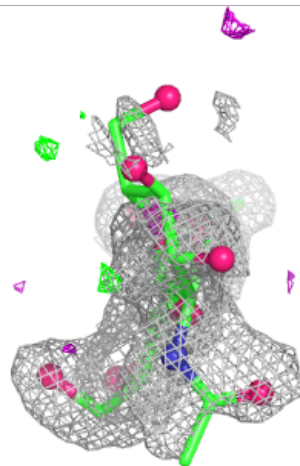
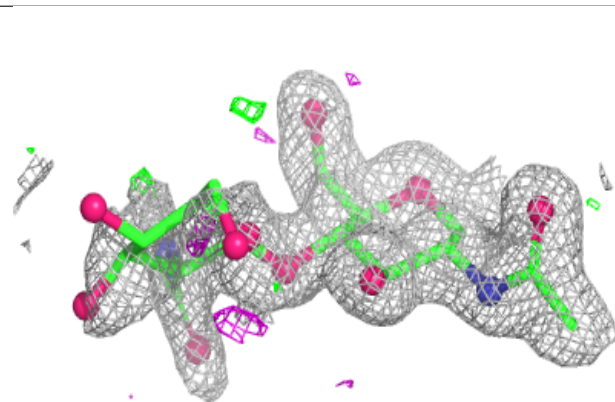
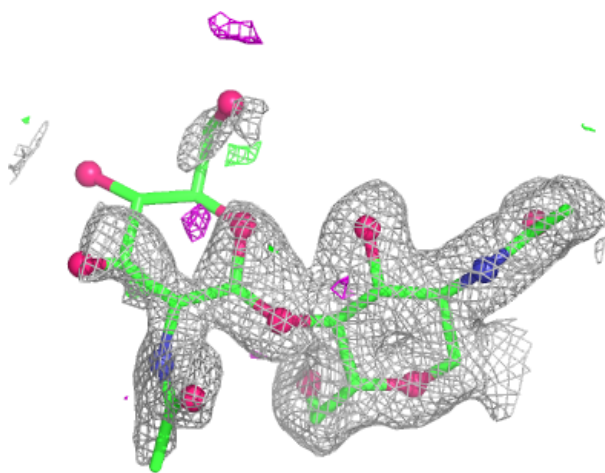
Electron density around Chain K:

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



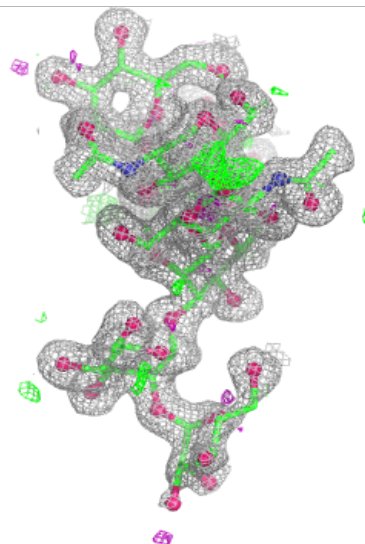
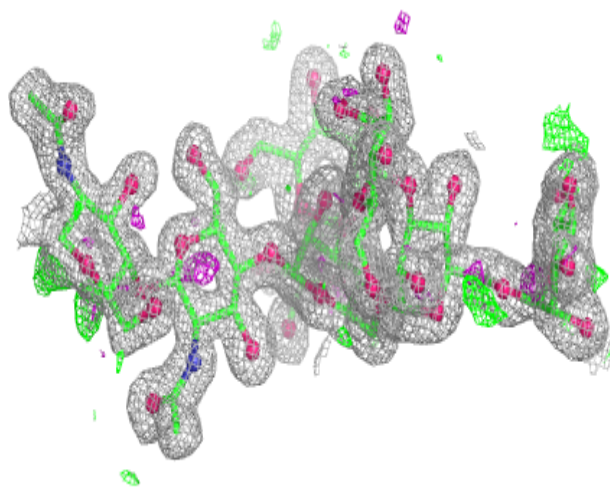
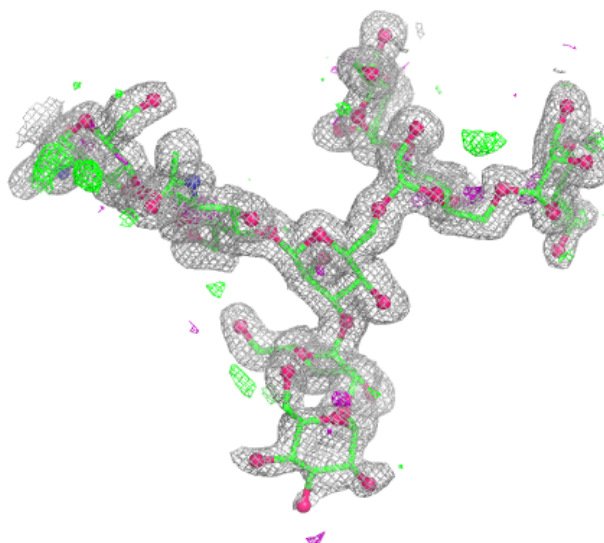
Electron density around Chain N:

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



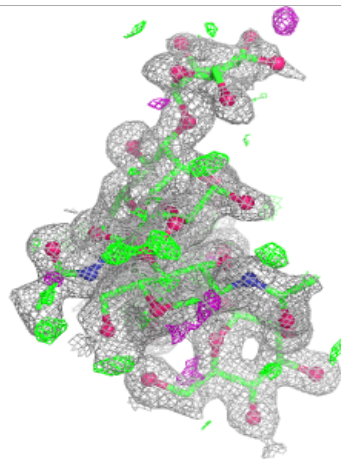
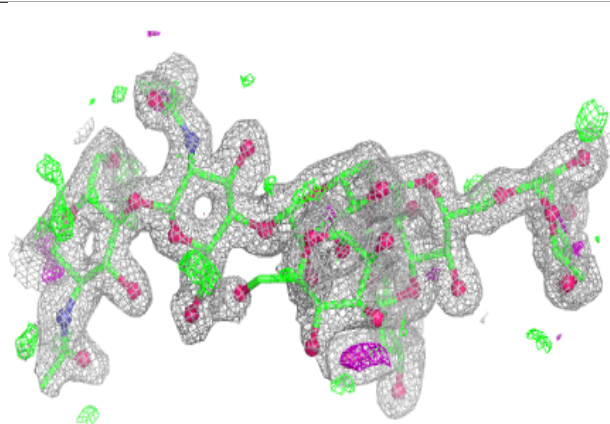
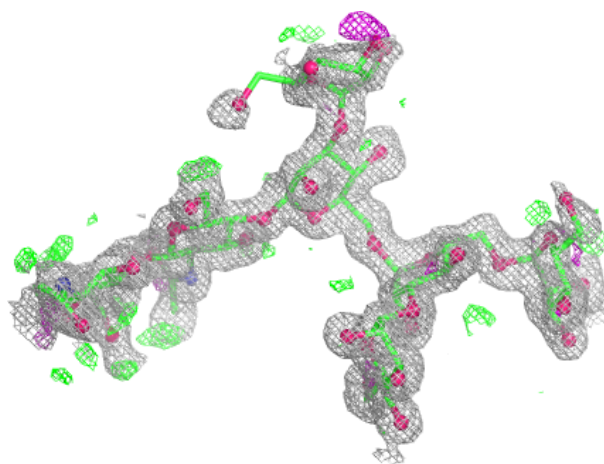
Electron density around Chain G:

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



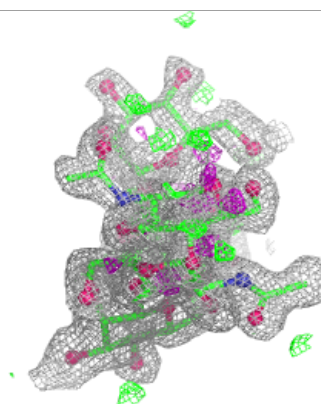
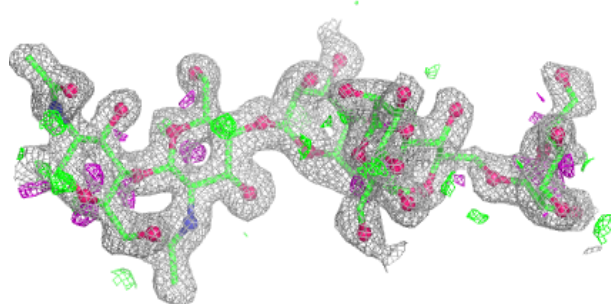
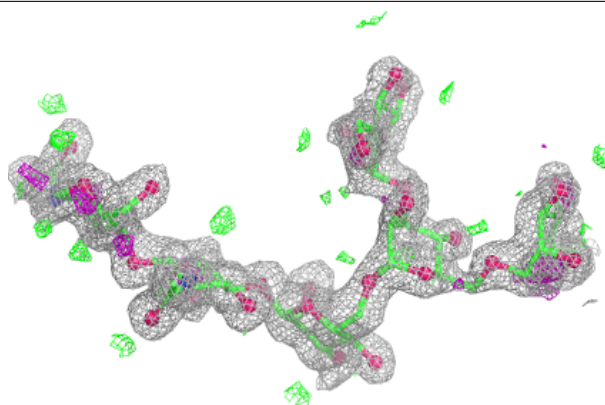
Electron density around Chain I:

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

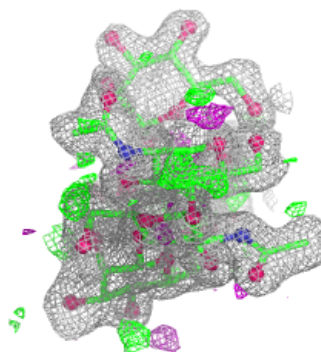
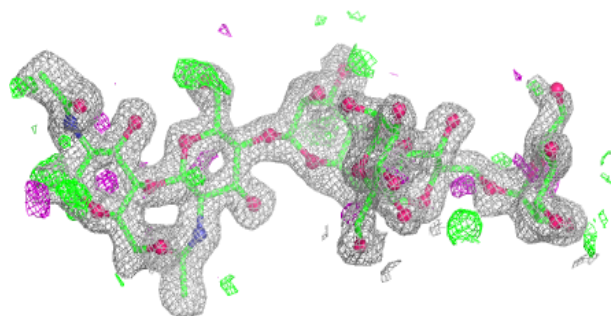
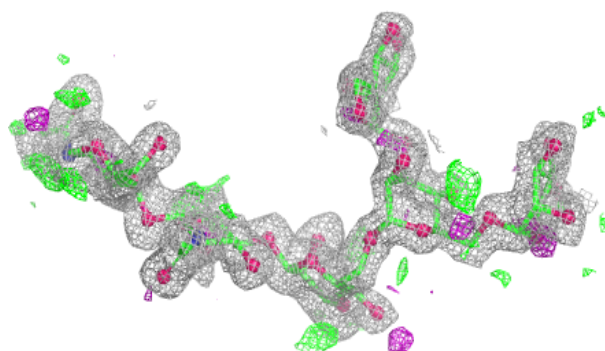


Electron density around Chain L:

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

**Electron density around Chain M:**

$2mF_o-DF_c$ (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	GOL	D	512	6/6	0.59	0.25	35,42,50,56	0
6	GOL	A	518	6/6	0.66	0.20	43,45,45,52	0
9	PEG	C	523	7/7	0.68	0.22	41,47,52,55	0
10	NAG	B	501	14/15	0.68	0.16	48,52,56,64	0
9	PEG	B	525	7/7	0.71	0.22	48,56,60,62	0
9	PEG	B	523[A]	7/7	0.71	0.22	31,33,35,36	7
9	PEG	B	523[B]	7/7	0.71	0.22	18,20,22,22	7
9	PEG	D	519	7/7	0.72	0.19	43,48,57,62	0
9	PEG	D	516	7/7	0.72	0.20	33,40,46,47	0
9	PEG	B	522	7/7	0.73	0.23	46,50,54,58	0
9	PEG	C	522	7/7	0.73	0.23	53,56,58,60	0
6	GOL	A	517	6/6	0.74	0.20	37,43,46,50	0
8	PO4	B	518	5/5	0.75	0.15	67,73,79,84	0
9	PEG	A	522	7/7	0.75	0.21	40,48,53,53	0
9	PEG	B	521	7/7	0.75	0.21	36,52,56,60	0
6	GOL	D	514	6/6	0.75	0.21	39,52,54,62	0
9	PEG	C	521	7/7	0.78	0.17	36,42,48,50	0
9	PEG	D	520	7/7	0.78	0.19	31,40,52,54	0
9	PEG	D	521	7/7	0.78	0.17	26,37,48,50	0
8	PO4	A	520	5/5	0.78	0.18	95,96,99,110	0
6	GOL	C	517	6/6	0.79	0.17	25,27,28,28	6
10	NAG	D	501	14/15	0.79	0.13	33,38,42,43	0
6	GOL	A	514	6/6	0.80	0.16	26,35,41,49	0
6	GOL	C	511	6/6	0.80	0.17	26,34,37,45	0
9	PEG	D	518	7/7	0.81	0.15	31,36,38,40	0
9	PEG	B	526	7/7	0.81	0.17	27,36,46,48	0
6	GOL	B	513	6/6	0.82	0.17	28,36,41,41	0
8	PO4	A	521	5/5	0.82	0.15	21,42,47,51	5
6	GOL	C	513	6/6	0.83	0.15	19,24,27,40	0
6	GOL	B	512	6/6	0.83	0.18	27,38,42,44	0
9	PEG	B	524	7/7	0.83	0.16	41,43,48,49	0
9	PEG	B	520	7/7	0.84	0.14	21,22,26,30	7
6	GOL	A	515[B]	6/6	0.85	0.15	8,8,9,9	6
6	GOL	C	515[A]	6/6	0.85	0.14	30,31,34,38	6
6	GOL	C	515[B]	6/6	0.85	0.14	13,13,14,15	6
6	GOL	C	516[A]	6/6	0.85	0.11	20,21,21,22	6
6	GOL	C	516[B]	6/6	0.85	0.11	22,24,25,26	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	PEG	B	519	7/7	0.85	0.17	39,47,53,53	0
6	GOL	B	516	6/6	0.85	0.16	25,40,43,48	0
6	GOL	A	515[A]	6/6	0.85	0.15	31,33,34,35	6
6	GOL	D	511	6/6	0.86	0.14	23,33,34,35	0
6	GOL	B	515	6/6	0.86	0.15	33,43,47,47	0
6	GOL	C	518	6/6	0.87	0.15	22,37,42,56	0
6	GOL	C	514	6/6	0.88	0.14	25,33,34,35	0
6	GOL	D	513	6/6	0.88	0.12	22,24,27,37	0
9	PEG	D	517	7/7	0.89	0.15	16,18,23,25	7
9	PEG	C	520	7/7	0.90	0.10	25,28,31,33	0
6	GOL	D	510	6/6	0.90	0.11	21,23,25,26	0
6	GOL	B	511	6/6	0.90	0.11	23,26,27,34	0
6	GOL	C	512	6/6	0.90	0.11	20,25,26,30	0
6	GOL	B	514	6/6	0.93	0.10	20,24,30,34	0
6	GOL	A	516[A]	6/6	0.95	0.08	18,22,28,31	6
6	GOL	A	516[B]	6/6	0.95	0.08	12,13,13,13	6
6	GOL	A	513[B]	6/6	0.96	0.06	9,10,11,11	6
6	GOL	A	513[A]	6/6	0.96	0.06	17,19,20,22	6
7	CA	A	519	1/1	0.98	0.04	15,15,15,15	1
7	CA	D	515	1/1	0.99	0.03	9,9,9,9	1
7	CA	C	519	1/1	0.99	0.12	19,19,19,19	0
7	CA	B	517	1/1	1.00	0.02	7,7,7,7	1

6.5 Other polymers

There are no such residues in this entry.