



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:59 PM UTC

PDB ID : 5L5C / pdb_00005l5c
Title : Plexin A1 full extracellular region, domains 1 to 10, to 6 angstrom, spacegroup P4(3)2(1)2
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Deposited on : 2016-05-28
Resolution : 6.00 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

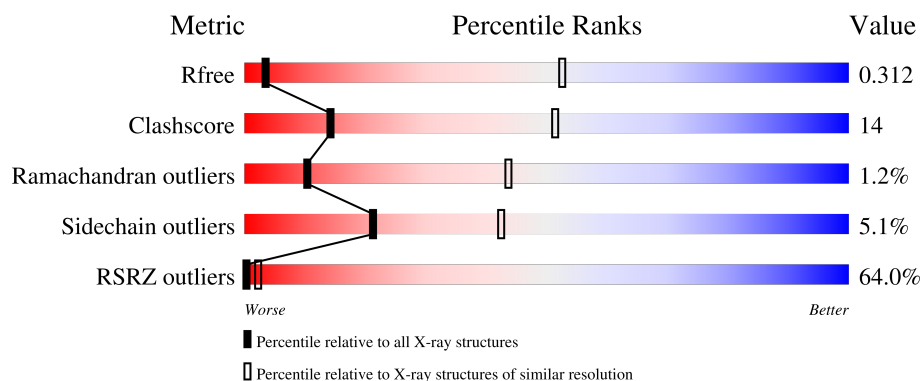
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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.



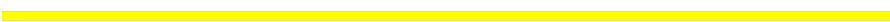
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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	1212	62% 68% 25% . .
2	B	4	25% 50% 25%
2	D	4	100%
3	C	5	20% 80%

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Mol	Chain	Length	Quality of chain
3	G	5	 100%
4	E	6	 67% 33%
4	I	6	 17% 83%
5	F	2	 100%
6	H	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	1	-	-	X	-
4	NAG	I	1	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9546 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.

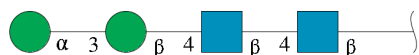
- Molecule 1 is a protein called Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1171	9085	5719	1593	1715	58	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

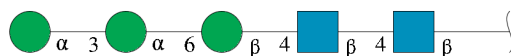
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLU	-	expression tag	UNP P70206
A	35	THR	-	expression tag	UNP P70206
A	36	GLY	-	expression tag	UNP P70206
A	1237	ARG	-	expression tag	UNP P70206
A	1238	THR	-	expression tag	UNP P70206
A	1239	LYS	-	expression tag	UNP P70206
A	1240	HIS	-	expression tag	UNP P70206
A	1241	HIS	-	expression tag	UNP P70206
A	1242	HIS	-	expression tag	UNP P70206
A	1243	HIS	-	expression tag	UNP P70206
A	1244	HIS	-	expression tag	UNP P70206
A	1245	HIS	-	expression tag	UNP P70206

- Molecule 2 is an oligosaccharide called 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.



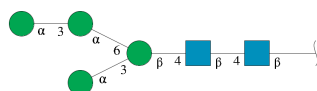
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0
2	D	4	50	28	2	20	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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	E	6	Total	C	N	O	0	0	0
			72	40	2	30			
4	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



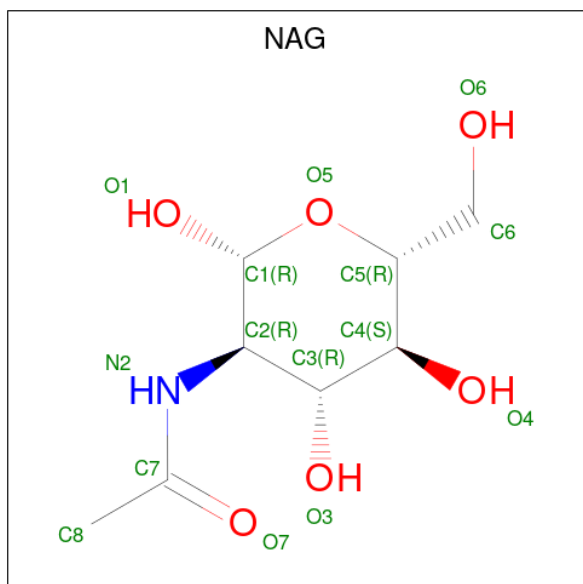
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

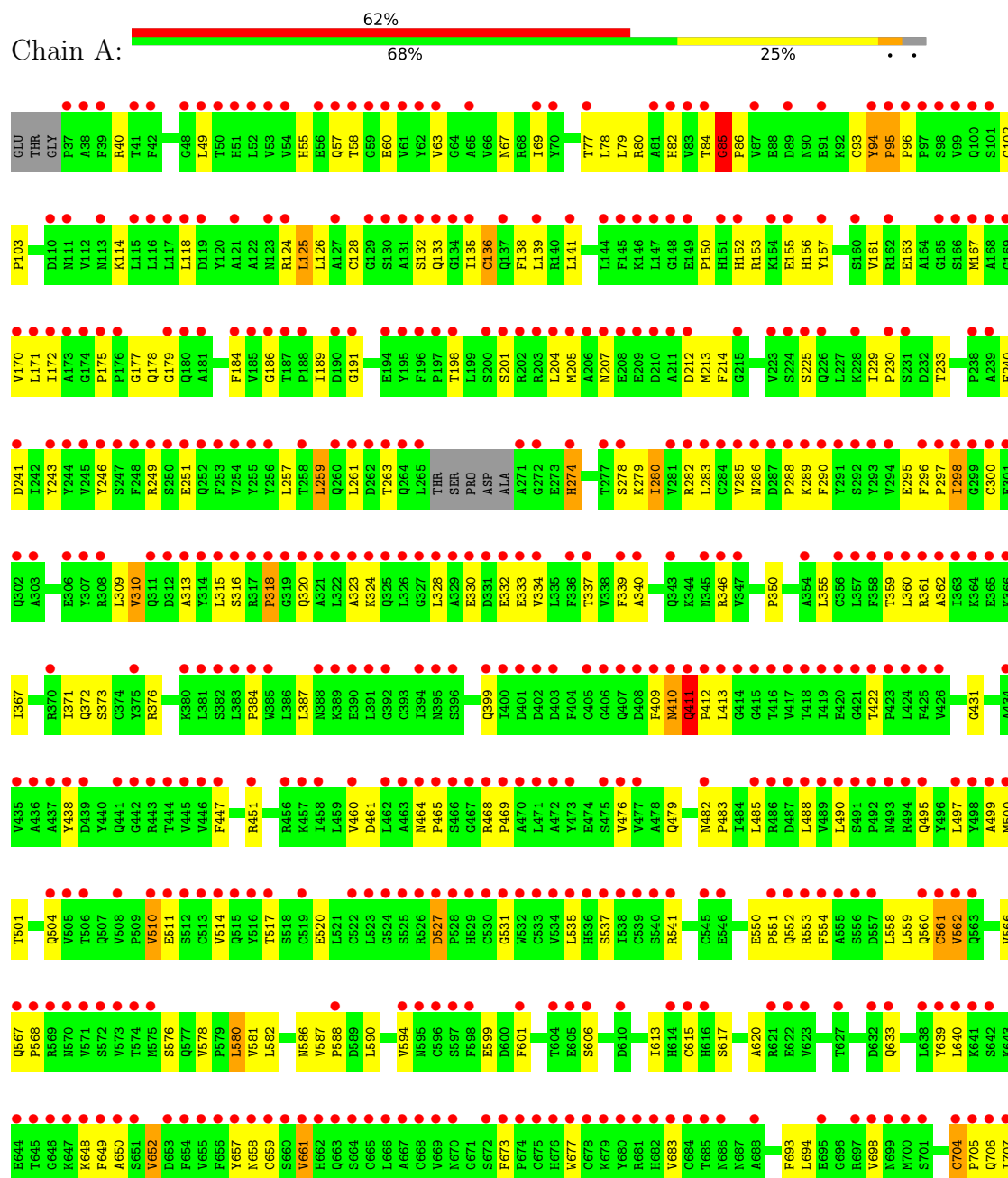


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

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: Plexin-A1





- Molecule 3: 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 G:  100%



- Molecule 4: alpha-D-mannopyranose-(1-3)-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

Chain E:  67%  33%



- Molecule 4: alpha-D-mannopyranose-(1-3)-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

Chain I:  17%  83%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	198.15Å 198.15Å 228.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.50 – 6.00 119.50 – 6.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (119.50-6.00) 97.7 (119.50-6.00)	Depositor EDS
R_{merge}	0.71	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 6.19Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.305 , 0.316 0.310 , 0.312	Depositor DCC
R_{free} test set	589 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	326.8	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 777.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9546	wwPDB-VP
Average B, all atoms (Å ²)	283.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: BMA, NAG, 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	0.86	5/9294 (0.1%)	1.12	34/12632 (0.3%)

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	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	VAL	C-N	50.02	1.99	1.33
1	A	561	CYS	C-N	40.77	1.83	1.33
1	A	1043	THR	C-N	22.89	1.66	1.33
1	A	704	CYS	C-N	14.62	1.68	1.33
1	A	859	CYS	C-N	-11.57	1.18	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	THR	CA-C-N	-45.03	55.44	122.09
1	A	1043	THR	C-N-CA	-45.03	55.44	122.09
1	A	1043	THR	O-C-N	17.25	145.87	122.59
1	A	859	CYS	O-C-N	-17.05	100.62	123.12
1	A	561	CYS	O-C-N	14.40	140.53	122.81
1	A	859	CYS	CA-C-N	14.28	145.00	120.87
1	A	859	CYS	C-N-CA	14.28	145.00	120.87
1	A	561	CYS	CA-C-N	-12.83	102.04	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	CYS	C-N-CA	-12.83	102.04	120.77
1	A	704	CYS	CA-C-N	9.45	131.65	119.84
1	A	704	CYS	C-N-CA	9.45	131.65	119.84
1	A	510	VAL	O-C-N	8.39	130.13	121.91
1	A	704	CYS	O-C-N	-8.34	111.73	121.32
1	A	527	ASP	CA-C-N	8.18	127.83	119.82
1	A	527	ASP	C-N-CA	8.18	127.83	119.82
1	A	1052	ASP	N-CA-C	7.62	123.59	110.02
1	A	868	SER	CA-C-N	7.44	129.13	119.84
1	A	868	SER	C-N-CA	7.44	129.13	119.84
1	A	809	ALA	N-CA-C	-5.92	105.71	113.17
1	A	510	VAL	CA-C-N	-5.89	114.87	123.00
1	A	510	VAL	C-N-CA	-5.89	114.87	123.00
1	A	841	CYS	CA-C-N	5.77	125.71	119.76
1	A	841	CYS	C-N-CA	5.77	125.71	119.76
1	A	85	GLY	CA-C-N	5.76	127.04	119.84
1	A	85	GLY	C-N-CA	5.76	127.04	119.84
1	A	965	SER	CA-C-N	-5.75	112.65	119.84
1	A	965	SER	C-N-CA	-5.75	112.65	119.84
1	A	712	HIS	N-CA-C	5.73	118.38	110.35
1	A	854	HIS	N-CA-C	-5.68	105.75	114.16
1	A	965	SER	N-CA-C	5.49	121.95	109.81
1	A	1053	PRO	N-CA-C	-5.11	101.94	112.47
1	A	295	GLU	N-CA-C	5.08	115.84	107.20
1	A	316	SER	N-CA-C	5.06	114.82	108.45
1	A	915	ALA	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	ASP	Peptide
1	A	410	ASN	Peptide
1	A	527	ASP	Peptide
1	A	807	CYS	Peptide
1	A	85	GLY	Peptide
1	A	859	CYS	Mainchain
1	A	868	SER	Peptide
1	A	94	TYR	Peptide
1	A	965	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	9085	0	8873	266	38
2	B	50	0	43	1	0
2	D	50	0	43	0	0
3	C	61	0	51	0	0
3	G	61	0	52	0	0
4	E	72	0	61	22	0
4	I	72	0	61	0	0
5	F	28	0	25	0	0
6	H	39	0	34	0	0
7	A	28	0	26	0	0
All	All	9546	0	9269	267	38

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 14.

All (267) 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:704:CYS:C	1:A:705:PRO:N	1.68	1.44
1:A:661:VAL:HG13	4:E:1:NAG:C6	1.47	1.44
1:A:561:CYS:C	1:A:562:VAL:N	1.83	1.33
1:A:661:VAL:CG1	4:E:1:NAG:O6	1.88	1.20
1:A:510:VAL:C	1:A:511:GLU:N	1.99	1.20
1:A:553:ARG:HD2	1:A:588:PRO:CB	1.78	1.13
1:A:661:VAL:CG1	4:E:1:NAG:C6	2.27	1.13
1:A:633:GLN:OE1	1:A:673:PHE:CE1	2.03	1.11
1:A:553:ARG:HD2	1:A:588:PRO:CG	1.81	1.09
1:A:411:GLN:HG2	1:A:412:PRO:HD2	1.35	1.06
1:A:1055:TRP:HH2	1:A:1184:LEU:HD21	1.17	1.06
1:A:860:THR:HA	1:A:946:TYR:CE1	1.93	1.03
1:A:661:VAL:HG13	4:E:1:NAG:H62	1.06	1.02
1:A:1055:TRP:CH2	1:A:1184:LEU:HD21	1.93	1.02
1:A:661:VAL:HG11	4:E:1:NAG:O6	1.56	1.00
1:A:661:VAL:HG13	4:E:1:NAG:O6	1.53	0.99
1:A:661:VAL:CG1	4:E:1:NAG:H62	1.88	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:VAL:CG2	4:E:1:NAG:O5	2.12	0.97
1:A:553:ARG:HG2	1:A:588:PRO:HB3	1.47	0.95
1:A:633:GLN:OE1	1:A:673:PHE:HE1	1.48	0.94
1:A:806:LYS:C	1:A:807:CYS:N	2.25	0.94
1:A:553:ARG:HD2	1:A:588:PRO:HG3	1.50	0.93
1:A:553:ARG:CD	1:A:588:PRO:CB	2.46	0.92
1:A:661:VAL:HG21	4:E:1:NAG:O5	1.67	0.92
1:A:468:ARG:HG2	1:A:469:PRO:HD2	1.51	0.91
1:A:560:GLN:C	1:A:586:ASN:HD22	1.79	0.90
1:A:860:THR:HA	1:A:946:TYR:HE1	1.28	0.89
1:A:189:ILE:HD12	1:A:198:THR:HG23	1.52	0.88
1:A:94:TYR:CD2	1:A:95:PRO:HD3	2.08	0.88
1:A:661:VAL:HG22	4:E:1:NAG:C5	2.04	0.87
1:A:808:PRO:HD2	1:A:835:CYS:O	1.76	0.85
1:A:633:GLN:OE1	1:A:673:PHE:CZ	2.29	0.84
1:A:567:GLN:HB3	1:A:568:PRO:HD3	1.61	0.81
1:A:553:ARG:CG	1:A:588:PRO:HB3	2.09	0.81
1:A:552:GLN:O	1:A:588:PRO:HD3	1.79	0.81
1:A:658:ASN:C	1:A:659:CYS:N	2.39	0.80
1:A:818:LEU:HB3	1:A:852:ALA:HB2	1.62	0.80
1:A:153:ARG:H	1:A:156:HIS:HD2	1.30	0.78
1:A:789:ASN:HD22	1:A:792:PHE:HE2	1.31	0.78
1:A:560:GLN:O	1:A:586:ASN:HB3	1.82	0.78
1:A:280:ILE:HB	1:A:298:ILE:HD12	1.64	0.78
1:A:553:ARG:CD	1:A:588:PRO:HB2	2.14	0.78
1:A:553:ARG:HD2	1:A:588:PRO:HB2	1.67	0.77
1:A:561:CYS:C	1:A:562:VAL:CA	2.57	0.77
1:A:259:LEU:HD23	1:A:346:ARG:HG3	1.66	0.76
1:A:230:PRO:O	1:A:233:THR:HG22	1.86	0.76
1:A:535:LEU:HD21	1:A:590:LEU:HD21	1.67	0.75
1:A:923:GLY:HA2	1:A:1030:ARG:HH22	1.52	0.74
1:A:877:GLY:HA3	1:A:1030:ARG:HG3	1.68	0.74
1:A:895:ARG:O	1:A:896:LEU:HB2	1.85	0.74
1:A:411:GLN:CG	1:A:412:PRO:HD2	2.14	0.74
1:A:658:ASN:OD1	1:A:661:VAL:HG23	1.88	0.74
1:A:661:VAL:HG22	4:E:1:NAG:O5	1.84	0.72
1:A:743:LEU:HD22	1:A:752:ARG:HG2	1.70	0.72
1:A:860:THR:CA	1:A:946:TYR:HE1	2.03	0.72
1:A:561:CYS:CA	1:A:562:VAL:N	2.53	0.71
1:A:852:ALA:HA	1:A:857:SER:OG	1.91	0.71
1:A:1079:ILE:HD11	1:A:1102:CYS:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:SER:HB3	1:A:615:CYS:HB3	1.74	0.70
1:A:171:LEU:HD22	1:A:204:LEU:HD11	1.72	0.70
1:A:55:HIS:HE2	1:A:141:LEU:HD21	1.57	0.69
1:A:82:HIS:HD2	1:A:84:THR:HG22	1.55	0.69
1:A:310:VAL:HG22	1:A:339:PHE:CE1	2.28	0.69
1:A:138:PHE:CZ	1:A:213:MET:HE2	2.28	0.69
1:A:560:GLN:HA	1:A:586:ASN:ND2	2.08	0.68
1:A:566:VAL:HG22	1:A:582:LEU:HD23	1.76	0.68
1:A:1055:TRP:CH2	1:A:1176:PRO:HG3	2.28	0.68
1:A:661:VAL:CG2	4:E:1:NAG:C1	2.72	0.67
1:A:746:ILE:HB	1:A:749:SER:O	1.95	0.67
1:A:175:PRO:HG2	1:A:178:GLN:HG3	1.76	0.67
1:A:114:LYS:HE2	1:A:167:MET:HE3	1.75	0.67
1:A:704:CYS:C	1:A:705:PRO:CD	2.66	0.67
1:A:1055:TRP:CH2	1:A:1184:LEU:CD2	2.76	0.66
1:A:895:ARG:HA	1:A:907:PRO:HG2	1.76	0.66
1:A:468:ARG:CG	1:A:469:PRO:HD2	2.24	0.65
1:A:315:LEU:HD11	1:A:333:GLU:HB3	1.78	0.64
1:A:560:GLN:O	1:A:586:ASN:CB	2.44	0.64
1:A:553:ARG:CD	1:A:588:PRO:HB3	2.28	0.64
1:A:887:LEU:HB2	1:A:915:ALA:HA	1.80	0.64
1:A:1057:ILE:HD12	1:A:1147:ASP:OD1	1.97	0.64
1:A:550:GLU:HB3	1:A:551:PRO:HD2	1.80	0.63
1:A:58:THR:OG1	1:A:60:GLU:HG2	1.99	0.63
1:A:1055:TRP:CZ2	1:A:1176:PRO:HG3	2.34	0.63
1:A:69:ILE:HD12	1:A:84:THR:HG21	1.79	0.63
1:A:939:VAL:HG22	1:A:946:TYR:HB3	1.82	0.62
1:A:740:TYR:CD1	1:A:788:TRP:HB3	2.36	0.61
1:A:732:GLN:HG2	1:A:757:ARG:HH22	1.66	0.61
1:A:560:GLN:C	1:A:586:ASN:ND2	2.57	0.60
1:A:639:TYR:CD2	1:A:648:LYS:HD2	2.36	0.60
1:A:259:LEU:HD23	1:A:346:ARG:CG	2.31	0.60
1:A:878:THR:HB	1:A:922:ILE:HD12	1.84	0.59
1:A:658:ASN:CG	1:A:661:VAL:HG23	2.27	0.59
1:A:153:ARG:N	1:A:156:HIS:HD2	1.99	0.59
1:A:661:VAL:HG21	4:E:1:NAG:C1	2.33	0.59
1:A:578:VAL:H	1:A:617:SER:HB3	1.66	0.59
1:A:447:PHE:HZ	1:A:510:VAL:HG23	1.69	0.58
1:A:559:LEU:O	1:A:586:ASN:ND2	2.37	0.58
1:A:55:HIS:NE2	1:A:141:LEU:HD21	2.17	0.58
1:A:560:GLN:CA	1:A:586:ASN:ND2	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:H	1:A:156:HIS:CD2	2.18	0.57
1:A:337:THR:O	1:A:355:LEU:HD12	2.05	0.57
1:A:531:GLY:HA3	1:A:554:PHE:CZ	2.40	0.57
1:A:246:TYR:CD2	1:A:313:ALA:HB3	2.39	0.57
1:A:279:LYS:HG2	1:A:297:PRO:HA	1.87	0.56
1:A:172:ILE:HG22	1:A:249:ARG:HD2	1.87	0.56
1:A:661:VAL:HG22	4:E:1:NAG:C6	2.34	0.56
1:A:732:GLN:HG2	1:A:757:ARG:NH2	2.20	0.56
1:A:485:LEU:HD12	1:A:500:MET:HG2	1.86	0.56
1:A:789:ASN:HB3	1:A:792:PHE:CD2	2.41	0.56
1:A:808:PRO:HG3	1:A:835:CYS:HB3	1.87	0.56
1:A:537:SER:HB2	1:A:649:PHE:HA	1.88	0.56
1:A:296:PHE:CE1	1:A:367:ILE:HG12	2.41	0.55
1:A:132:SER:HB2	1:A:135:ILE:HG12	1.87	0.55
1:A:488:LEU:HD12	1:A:499:ALA:HA	1.89	0.55
1:A:567:GLN:HB2	1:A:581:VAL:HG22	1.87	0.55
1:A:93:CYS:O	1:A:133:GLN:NE2	2.40	0.55
1:A:737:GLN:HG2	1:A:789:ASN:ND2	2.22	0.55
1:A:318:PRO:HG2	1:A:323:ALA:HB2	1.89	0.55
1:A:693:PHE:HZ	1:A:734:GLN:OE1	1.90	0.55
1:A:552:GLN:HB2	1:A:587:VAL:C	2.32	0.55
1:A:464:ASN:CG	1:A:465:PRO:HD2	2.32	0.54
1:A:566:VAL:HG22	1:A:582:LEU:CD2	2.37	0.54
1:A:661:VAL:CG2	4:E:1:NAG:C5	2.76	0.54
1:A:738:ARG:HB2	1:A:789:ASN:HA	1.89	0.54
1:A:789:ASN:HB3	1:A:792:PHE:HD2	1.73	0.54
1:A:661:VAL:CB	4:E:1:NAG:H62	2.37	0.54
1:A:278:SER:HB3	1:A:310:VAL:HG23	1.91	0.53
1:A:282:ARG:HG3	1:A:283:LEU:N	2.22	0.53
1:A:205:MET:HG3	1:A:212:ASP:HB3	1.90	0.53
1:A:640:LEU:HD12	1:A:650:ALA:HB3	1.91	0.53
1:A:658:ASN:CG	1:A:661:VAL:CG2	2.82	0.53
1:A:332:GLU:OE2	1:A:361:ARG:NH2	2.41	0.52
1:A:58:THR:CB	1:A:60:GLU:HG2	2.39	0.52
1:A:821:ASP:HB2	1:A:824:PHE:CD2	2.44	0.52
1:A:126:LEU:HD11	1:A:136:CYS:SG	2.49	0.52
1:A:677:TRP:HB3	1:A:698:VAL:HB	1.92	0.52
1:A:124:ARG:HD2	1:A:138:PHE:HD2	1.74	0.52
1:A:818:LEU:HB2	1:A:889:LEU:HD11	1.92	0.52
1:A:438:TYR:CE1	1:A:510:VAL:HG21	2.46	0.51
1:A:461:ASP:HA	1:A:464:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLN:HB2	1:A:1031:ALA:HB2	1.92	0.51
1:A:1061:GLY:O	1:A:1223:GLY:HA3	2.11	0.51
1:A:170:VAL:HG11	1:A:249:ARG:HB2	1.91	0.51
1:A:560:GLN:CA	1:A:586:ASN:HD22	2.24	0.51
1:A:310:VAL:HG22	1:A:339:PHE:HE1	1.72	0.51
1:A:447:PHE:CZ	1:A:510:VAL:HG23	2.45	0.51
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.77	0.50
1:A:55:HIS:CE1	1:A:57:GLN:HB2	2.46	0.50
1:A:153:ARG:NH2	1:A:212:ASP:HA	2.26	0.50
1:A:229:ILE:HD12	1:A:240:PHE:HE2	1.76	0.50
1:A:939:VAL:CG2	1:A:946:TYR:HB3	2.42	0.50
1:A:658:ASN:ND2	1:A:661:VAL:HG21	2.27	0.50
1:A:186:GLY:HA2	1:A:198:THR:O	2.12	0.49
1:A:553:ARG:HA	1:A:588:PRO:HG3	1.93	0.49
1:A:323:ALA:HA	1:A:328:LEU:HD12	1.94	0.49
1:A:708:LEU:H	1:A:727:ALA:HA	1.77	0.49
1:A:431:GLY:HA3	1:A:451:ARG:HD2	1.93	0.49
1:A:153:ARG:HB2	1:A:156:HIS:CD2	2.48	0.49
1:A:495:GLN:O	1:A:510:VAL:HG12	2.13	0.49
1:A:1055:TRP:CZ2	1:A:1184:LEU:CD2	2.96	0.48
1:A:96:PRO:HD2	1:A:157:TYR:CZ	2.48	0.48
1:A:172:ILE:HD11	1:A:184:PHE:HE2	1.77	0.48
1:A:468:ARG:HG2	1:A:469:PRO:CD	2.36	0.48
1:A:661:VAL:CG2	4:E:1:NAG:C6	2.91	0.48
1:A:661:VAL:HG22	4:E:1:NAG:H62	1.96	0.48
1:A:1055:TRP:CH2	1:A:1184:LEU:HD11	2.49	0.47
1:A:460:VAL:HA	1:A:469:PRO:HB3	1.96	0.47
1:A:1027:ASN:HB3	1:A:1032:GLN:HG3	1.95	0.47
1:A:501:THR:OG1	1:A:504:GLN:N	2.44	0.47
1:A:821:ASP:HB2	1:A:824:PHE:CE2	2.49	0.47
1:A:40:ARG:NH2	2:B:1:NAG:O3	2.47	0.47
1:A:172:ILE:HD13	1:A:285:VAL:HG13	1.97	0.47
1:A:567:GLN:CB	1:A:581:VAL:HG22	2.44	0.47
1:A:907:PRO:HA	1:A:920:CYS:HA	1.96	0.47
1:A:461:ASP:CA	1:A:464:ASN:HB3	2.45	0.47
1:A:818:LEU:HD22	1:A:852:ALA:H	1.80	0.47
1:A:372:GLN:O	1:A:376:ARG:HD3	2.15	0.47
1:A:447:PHE:CD2	1:A:497:LEU:HD22	2.49	0.47
1:A:566:VAL:CG2	1:A:652:VAL:HG21	2.45	0.46
1:A:63:VAL:HG13	1:A:500:MET:HE1	1.96	0.46
1:A:806:LYS:CA	1:A:807:CYS:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:THR:HG22	1:A:946:TYR:OH	2.16	0.46
1:A:558:LEU:HD12	1:A:561:CYS:SG	2.56	0.46
1:A:934:LEU:HD23	1:A:953:ARG:HB3	1.97	0.46
1:A:887:LEU:HD23	1:A:918:ILE:HD11	1.98	0.46
1:A:661:VAL:HG22	4:E:1:NAG:H5	1.92	0.45
1:A:201:SER:HB2	1:A:290:PHE:HE1	1.81	0.45
1:A:553:ARG:HD3	1:A:588:PRO:HB2	1.97	0.45
1:A:932:ASP:OD1	1:A:932:ASP:N	2.50	0.45
1:A:79:LEU:O	1:A:80:ARG:HG3	2.16	0.45
1:A:125:LEU:HD23	1:A:139:LEU:HB2	1.99	0.45
1:A:818:LEU:HB3	1:A:852:ALA:CB	2.41	0.45
1:A:132:SER:CB	1:A:135:ILE:HG12	2.47	0.45
1:A:566:VAL:HG23	1:A:652:VAL:HG21	1.98	0.44
1:A:1078:ARG:HG3	1:A:1127:ILE:HB	1.99	0.44
1:A:815:GLY:O	1:A:819:LYS:HB2	2.17	0.44
1:A:894:VAL:HG11	1:A:918:ILE:HD13	1.99	0.44
1:A:576:SER:OG	1:A:620:ALA:N	2.51	0.44
1:A:937:VAL:HG23	1:A:948:ALA:HB3	1.98	0.44
1:A:67:ASN:CB	1:A:85:GLY:HA3	2.48	0.44
1:A:1088:ARG:HD2	1:A:1106:SER:O	2.18	0.44
1:A:261:LEU:HD11	1:A:274:HIS:CB	2.48	0.43
1:A:551:PRO:O	1:A:588:PRO:HA	2.18	0.43
1:A:657:TYR:HB3	1:A:673:PHE:CE2	2.52	0.43
1:A:155:GLU:N	1:A:155:GLU:OE1	2.51	0.43
1:A:1055:TRP:CZ2	1:A:1184:LEU:HD21	2.50	0.43
1:A:1071:LEU:HD13	1:A:1100:MET:HE3	2.01	0.43
1:A:150:PRO:HB2	1:A:156:HIS:ND1	2.34	0.43
1:A:952:LYS:HD2	1:A:952:LYS:HA	1.70	0.43
1:A:1104:ALA:HA	1:A:1105:PRO:HD3	1.89	0.43
1:A:58:THR:HB	1:A:60:GLU:HG2	2.01	0.43
1:A:102:CYS:HA	1:A:103:PRO:HD3	1.87	0.43
1:A:808:PRO:HB2	1:A:811:ARG:H	1.83	0.43
1:A:359:THR:HG23	1:A:362:ALA:CB	2.48	0.43
1:A:476:VAL:HB	1:A:479:GLN:HG2	2.01	0.43
1:A:568:PRO:HG2	1:A:580:LEU:HD23	2.01	0.43
1:A:740:TYR:HE1	1:A:794:ILE:HD11	1.83	0.43
1:A:838:ARG:NH1	1:A:841:CYS:O	2.51	0.43
1:A:959:PRO:HA	1:A:983:HIS:HB2	2.01	0.42
1:A:49:LEU:HD13	1:A:500:MET:HE2	2.02	0.42
1:A:69:ILE:CD1	1:A:84:THR:HG21	2.48	0.42
1:A:550:GLU:HB2	1:A:553:ARG:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLN:C	1:A:588:PRO:HD3	2.43	0.42
1:A:818:LEU:HD22	1:A:852:ALA:N	2.34	0.42
1:A:488:LEU:HG	1:A:497:LEU:HD11	2.02	0.42
1:A:599:GLU:C	1:A:601:PHE:H	2.28	0.42
1:A:658:ASN:ND2	1:A:661:VAL:CG2	2.82	0.42
1:A:661:VAL:CG2	4:E:1:NAG:H62	2.49	0.42
1:A:582:LEU:HB2	1:A:613:ILE:HB	2.02	0.42
1:A:161:VAL:HG12	1:A:163:GLU:H	1.83	0.42
1:A:944:LEU:HD12	1:A:944:LEU:H	1.85	0.42
1:A:309:LEU:O	1:A:339:PHE:HA	2.19	0.42
1:A:371:ILE:C	1:A:373:SER:H	2.28	0.42
1:A:410:ASN:O	1:A:411:GLN:O	2.37	0.42
1:A:606:SER:CB	1:A:615:CYS:HB3	2.48	0.42
1:A:706:GLN:O	1:A:727:ALA:HB1	2.19	0.42
1:A:263:THR:HB	1:A:384:PRO:HB2	2.02	0.41
1:A:661:VAL:HG22	4:E:1:NAG:C1	2.47	0.41
1:A:871:THR:HG22	1:A:955:THR:HB	2.02	0.41
1:A:1176:PRO:HA	1:A:1177:PRO:HD3	1.92	0.41
1:A:225:SER:HB3	1:A:288:PRO:O	2.20	0.41
1:A:789:ASN:ND2	1:A:792:PHE:HE2	2.09	0.41
1:A:340:ALA:HB1	1:A:350:PRO:HG2	2.02	0.41
1:A:877:GLY:CA	1:A:1030:ARG:HG3	2.45	0.41
1:A:150:PRO:O	1:A:156:HIS:HB3	2.21	0.41
1:A:261:LEU:HD11	1:A:274:HIS:HB3	2.03	0.41
1:A:541:ARG:H	1:A:541:ARG:HG2	1.74	0.41
1:A:553:ARG:HG2	1:A:588:PRO:CB	2.33	0.41
1:A:824:PHE:C	1:A:826:CYS:H	2.27	0.41
1:A:1169:LEU:HB2	1:A:1204:LEU:HB2	2.02	0.41
1:A:241:ASP:HB3	1:A:243:TYR:CZ	2.56	0.41
1:A:409:PHE:C	1:A:411:GLN:H	2.29	0.41
1:A:438:TYR:HB3	1:A:490:LEU:HD11	2.03	0.41
1:A:490:LEU:HD23	1:A:497:LEU:HB2	2.03	0.41
1:A:787:VAL:HG22	1:A:793:VAL:HG22	2.01	0.41
1:A:189:ILE:HG22	1:A:191:GLY:H	1.86	0.40
1:A:734:GLN:O	1:A:737:GLN:HB2	2.21	0.40
1:A:836:SER:O	1:A:849:TRP:NE1	2.54	0.40
1:A:1001:PHE:HZ	1:A:1004:ARG:HB2	1.85	0.40
1:A:136:CYS:HB3	1:A:214:PHE:CZ	2.56	0.40
1:A:461:ASP:CB	1:A:464:ASN:HB3	2.50	0.40
1:A:778:SER:HB3	1:A:810:LEU:HD22	2.02	0.40
1:A:289:LYS:O	1:A:290:PHE:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:GLN:H	1:A:798:GLN:HG2	1.72	0.40
1:A:482:ASN:HA	1:A:483:PRO:HD3	1.98	0.40
1:A:510:VAL:HG13	1:A:511:GLU:N	2.37	0.40
1:A:520:GLU:HA	1:A:558:LEU:HD11	2.04	0.40

All (38) 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)
1:A:178:GLN:NE2	1:A:921:GLU:N[5_454]	0.50	1.70
1:A:178:GLN:OE1	1:A:921:GLU:O[5_454]	0.98	1.22
1:A:178:GLN:NE2	1:A:921:GLU:CA[5_454]	0.98	1.22
1:A:931:HIS:CD2	1:A:982:SER:OG[8_444]	1.18	1.02
1:A:399:GLN:CB	1:A:963:ARG:NH1[4_545]	1.21	0.99
1:A:175:PRO:CG	1:A:921:GLU:CD[5_454]	1.28	0.92
1:A:179:GLY:N	1:A:906:SER:CB[5_454]	1.38	0.82
1:A:175:PRO:CG	1:A:921:GLU:OE1[5_454]	1.40	0.80
1:A:399:GLN:CG	1:A:963:ARG:NH1[4_545]	1.43	0.77
1:A:178:GLN:CD	1:A:921:GLU:CA[5_454]	1.46	0.74
1:A:175:PRO:CG	1:A:921:GLU:OE2[5_454]	1.50	0.70
1:A:178:GLN:CG	1:A:921:GLU:CB[5_454]	1.53	0.67
1:A:177:GLY:O	1:A:907:PRO:O[5_454]	1.54	0.66
1:A:932:ASP:O	1:A:1007:ARG:NH2[8_444]	1.55	0.65
1:A:175:PRO:CB	1:A:921:GLU:OE2[5_454]	1.61	0.59
1:A:178:GLN:CD	1:A:921:GLU:N[5_454]	1.61	0.59
1:A:931:HIS:CD2	1:A:982:SER:CB[8_444]	1.62	0.58
1:A:178:GLN:NE2	1:A:920:CYS:C[5_454]	1.70	0.50
1:A:178:GLN:OE1	1:A:921:GLU:C[5_454]	1.72	0.48
1:A:178:GLN:CD	1:A:921:GLU:CB[5_454]	1.75	0.45
1:A:178:GLN:CB	1:A:906:SER:OG[5_454]	1.80	0.40
1:A:931:HIS:NE2	1:A:982:SER:OG[8_444]	1.84	0.36
1:A:399:GLN:CG	1:A:963:ARG:CZ[4_545]	1.87	0.33
1:A:178:GLN:CD	1:A:921:GLU:C[5_454]	1.91	0.29
1:A:399:GLN:CG	1:A:963:ARG:NH2[4_545]	1.92	0.28
1:A:178:GLN:CD	1:A:921:GLU:O[5_454]	1.94	0.26
1:A:175:PRO:CB	1:A:921:GLU:OE1[5_454]	2.03	0.17
1:A:178:GLN:NE2	1:A:921:GLU:C[5_454]	2.04	0.16
1:A:399:GLN:CD	1:A:963:ARG:NH1[4_545]	2.04	0.16
1:A:175:PRO:CB	1:A:921:GLU:CD[5_454]	2.05	0.15
1:A:177:GLY:O	1:A:907:PRO:C[5_454]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLY:O	1:A:908:VAL:CA[5_454]	2.10	0.10
1:A:178:GLN:NE2	1:A:921:GLU:CB[5_454]	2.10	0.10
1:A:399:GLN:OE1	1:A:963:ARG:NH1[4_545]	2.14	0.06
1:A:286:ASN:OD1	1:A:904:LEU:CD1[5_454]	2.16	0.04
1:A:178:GLN:CA	1:A:906:SER:O[5_454]	2.18	0.02
1:A:178:GLN:CD	1:A:906:SER:O[5_454]	2.19	0.01
1:A:320:GLN:OE1	1:A:324:LYS:CE[7_555]	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	1157/1212 (96%)	1049 (91%)	94 (8%)	14 (1%)	10 44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	95	PRO
1	A	411	GLN
1	A	869	PRO
1	A	915	ALA
1	A	1192	SER
1	A	251	GLU
1	A	1053	PRO
1	A	1182	SER
1	A	694	LEU
1	A	966	PRO
1	A	318	PRO
1	A	1108	ASP
1	A	774	GLY

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	1015/1051 (97%)	963 (95%)	52 (5%)	21	42

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	78	LEU
1	A	118	LEU
1	A	125	LEU
1	A	128	CYS
1	A	136	CYS
1	A	152	HIS
1	A	207	ASN
1	A	257	LEU
1	A	259	LEU
1	A	274	HIS
1	A	280	ILE
1	A	298	ILE
1	A	300	CYS
1	A	310	VAL
1	A	330	GLU
1	A	334	VAL
1	A	360	LEU
1	A	387	LEU
1	A	411	GLN
1	A	413	LEU
1	A	422	THR
1	A	514	VAL
1	A	517	THR
1	A	562	VAL
1	A	580	LEU
1	A	594	VAL
1	A	652	VAL
1	A	661	VAL
1	A	683	VAL

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Mol	Chain	Res	Type
1	A	707	ILE
1	A	765	CYS
1	A	812	GLN
1	A	814	CYS
1	A	821	ASP
1	A	837	LEU
1	A	854	HIS
1	A	860	THR
1	A	867	LEU
1	A	882	ILE
1	A	890	ARG
1	A	929	ARG
1	A	934	LEU
1	A	937	VAL
1	A	949	LEU
1	A	977	ILE
1	A	982	SER
1	A	1018	THR
1	A	1030	ARG
1	A	1033	LEU
1	A	1048	ILE
1	A	1079	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	156	HIS
1	A	260	GLN
1	A	563	GLN
1	A	586	ASN
1	A	616	HIS
1	A	706	GLN
1	A	729	ASN
1	A	764	GLN
1	A	766	GLN
1	A	840	HIS
1	A	899	HIS
1	A	931	HIS
1	A	983	HIS
1	A	1027	ASN
1	A	1035	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 ⓘ

35 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	B	1	1,2	14,14,15	0.81	0	17,19,21	1.74	3 (17%)
2	NAG	B	2	2	14,14,15	0.58	0	17,19,21	1.54	2 (11%)
2	BMA	B	3	2	11,11,12	0.63	0	15,15,17	0.72	0
2	MAN	B	4	2	11,11,12	0.64	0	15,15,17	0.94	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.62	0	17,19,21	1.21	1 (5%)
3	NAG	C	2	3	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
3	BMA	C	3	3	11,11,12	0.53	0	15,15,17	0.58	0
3	MAN	C	4	3	11,11,12	0.66	0	15,15,17	0.88	1 (6%)
3	MAN	C	5	3	11,11,12	0.58	0	15,15,17	1.19	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.67	0	17,19,21	1.27	1 (5%)
2	NAG	D	2	2	14,14,15	0.56	0	17,19,21	1.22	2 (11%)
2	BMA	D	3	2	11,11,12	0.81	1 (9%)	15,15,17	1.92	3 (20%)
2	MAN	D	4	2	11,11,12	0.57	0	15,15,17	0.99	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.68	0	17,19,21	1.19	1 (5%)
4	NAG	E	2	4	14,14,15	0.53	0	17,19,21	1.16	2 (11%)
4	BMA	E	3	4	11,11,12	0.60	0	15,15,17	1.54	3 (20%)
4	MAN	E	4	4	11,11,12	0.62	0	15,15,17	0.87	1 (6%)
4	MAN	E	5	4	11,11,12	0.53	0	15,15,17	1.22	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	E	6	4	11,11,12	0.59	0	15,15,17	0.84	1 (6%)
5	NAG	F	1	1,5	14,14,15	0.62	0	17,19,21	1.25	1 (5%)
5	NAG	F	2	5	14,14,15	0.53	0	17,19,21	1.08	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.62	0	17,19,21	1.05	1 (5%)
3	NAG	G	2	3	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
3	BMA	G	3	3	11,11,12	0.42	0	15,15,17	1.63	2 (13%)
3	MAN	G	4	3	11,11,12	0.55	0	15,15,17	0.87	1 (6%)
3	MAN	G	5	3	11,11,12	0.52	0	15,15,17	1.43	2 (13%)
6	NAG	H	1	1,6	14,14,15	0.59	0	17,19,21	1.10	1 (5%)
6	NAG	H	2	6	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
6	BMA	H	3	6	11,11,12	0.47	0	15,15,17	1.13	2 (13%)
4	NAG	I	1	1,4	14,14,15	0.69	0	17,19,21	1.29	3 (17%)
4	NAG	I	2	4	14,14,15	0.53	0	17,19,21	1.46	3 (17%)
4	BMA	I	3	4	11,11,12	0.39	0	15,15,17	0.75	1 (6%)
4	MAN	I	4	4	11,11,12	0.61	0	15,15,17	0.89	0
4	MAN	I	5	4	11,11,12	0.62	0	15,15,17	1.13	1 (6%)
4	MAN	I	6	4	11,11,12	0.60	0	15,15,17	1.03	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C2-C3	2.12	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C1-C2-C3	6.15	118.60	109.64
2	B	1	NAG	C4-C3-C2	5.16	118.58	111.02
2	B	2	NAG	C4-C3-C2	4.90	118.20	111.02
3	G	3	BMA	C1-O5-C5	4.61	118.36	112.19
3	G	5	MAN	C1-O5-C5	4.53	118.25	112.19
4	E	5	MAN	C1-O5-C5	4.22	117.84	112.19
2	D	1	NAG	C4-C3-C2	4.08	117.00	111.02
3	C	2	NAG	C1-O5-C5	4.07	117.64	112.19
4	E	1	NAG	C4-C3-C2	4.00	116.88	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2	NAG	C1-O5-C5	3.71	117.16	112.19
4	E	3	BMA	C3-C4-C5	3.67	116.88	110.23
3	C	5	MAN	C1-O5-C5	3.49	116.86	112.19
6	H	1	NAG	C4-C3-C2	3.29	115.84	111.02
5	F	1	NAG	C4-C3-C2	3.27	115.82	111.02
6	H	3	BMA	C1-O5-C5	3.24	116.52	112.19
3	G	3	BMA	C1-C2-C3	3.21	114.33	109.64
3	G	2	NAG	C4-C3-C2	3.07	115.52	111.02
4	I	2	NAG	C4-C3-C2	3.05	115.48	111.02
2	B	1	NAG	C3-C4-C5	3.00	115.68	110.23
6	H	2	NAG	C4-C3-C2	2.99	115.41	111.02
3	G	1	NAG	C4-C3-C2	2.99	115.40	111.02
2	D	2	NAG	C1-O5-C5	2.98	116.18	112.19
4	E	3	BMA	C2-C3-C4	2.97	116.08	110.86
4	I	5	MAN	C1-C2-C3	2.92	113.90	109.64
4	I	2	NAG	C3-C4-C5	2.89	115.48	110.23
3	C	1	NAG	C4-C3-C2	2.85	115.19	111.02
4	E	3	BMA	C1-C2-C3	2.68	113.55	109.64
2	D	2	NAG	C4-C3-C2	2.67	114.93	111.02
3	G	4	MAN	C1-O5-C5	2.60	115.67	112.19
4	I	2	NAG	O5-C1-C2	-2.52	107.39	111.29
3	C	5	MAN	C1-C2-C3	2.46	113.23	109.64
4	I	6	MAN	C1-C2-C3	2.45	113.21	109.64
2	B	1	NAG	C2-N2-C7	2.34	126.03	122.90
4	I	1	NAG	C4-C3-C2	2.33	114.43	111.02
6	H	2	NAG	O5-C1-C2	-2.31	107.71	111.29
2	D	3	BMA	C2-C3-C4	2.31	114.92	110.86
2	D	4	MAN	C1-O5-C5	2.29	115.25	112.19
4	I	6	MAN	C1-O5-C5	2.28	115.24	112.19
4	E	6	MAN	C1-O5-C5	2.23	115.18	112.19
6	H	3	BMA	C1-C2-C3	2.21	112.86	109.64
4	E	2	NAG	C3-C4-C5	2.20	114.22	110.23
2	B	4	MAN	C1-C2-C3	2.19	112.83	109.64
3	C	4	MAN	C1-C2-C3	2.18	112.81	109.64
2	D	3	BMA	C1-O5-C5	2.16	115.08	112.19
4	I	3	BMA	C1-O5-C5	2.10	115.00	112.19
3	G	5	MAN	C1-C2-C3	2.10	112.70	109.64
4	E	2	NAG	O5-C1-C2	-2.09	108.05	111.29
4	I	1	NAG	C2-N2-C7	2.06	125.66	122.90
4	I	1	NAG	O5-C5-C6	2.05	111.65	107.66
2	B	2	NAG	C1-C2-N2	-2.03	107.24	110.43
4	E	4	MAN	O5-C5-C6	2.02	111.59	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	1	NAG	C1

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	I	6	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
6	H	3	BMA	C4-C5-C6-O6
4	E	6	MAN	C4-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
4	I	6	MAN	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
3	G	5	MAN	C4-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6

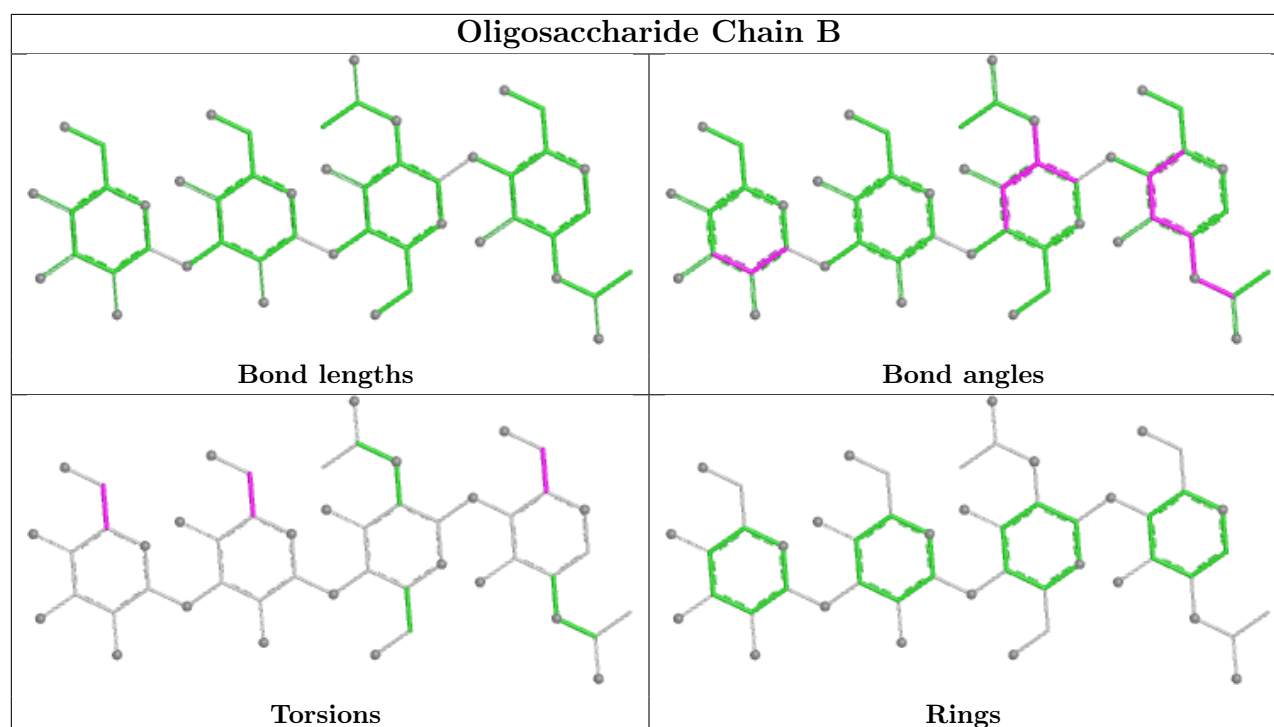
All (1) ring outliers are listed below:

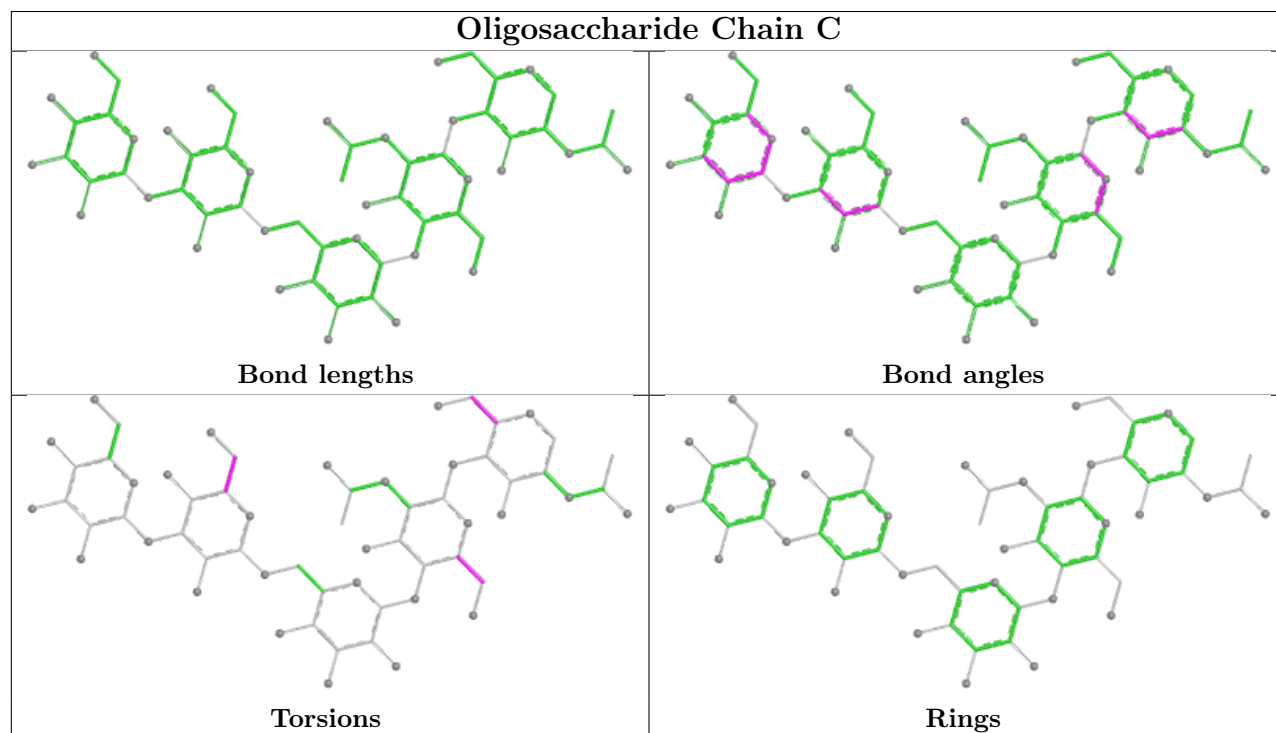
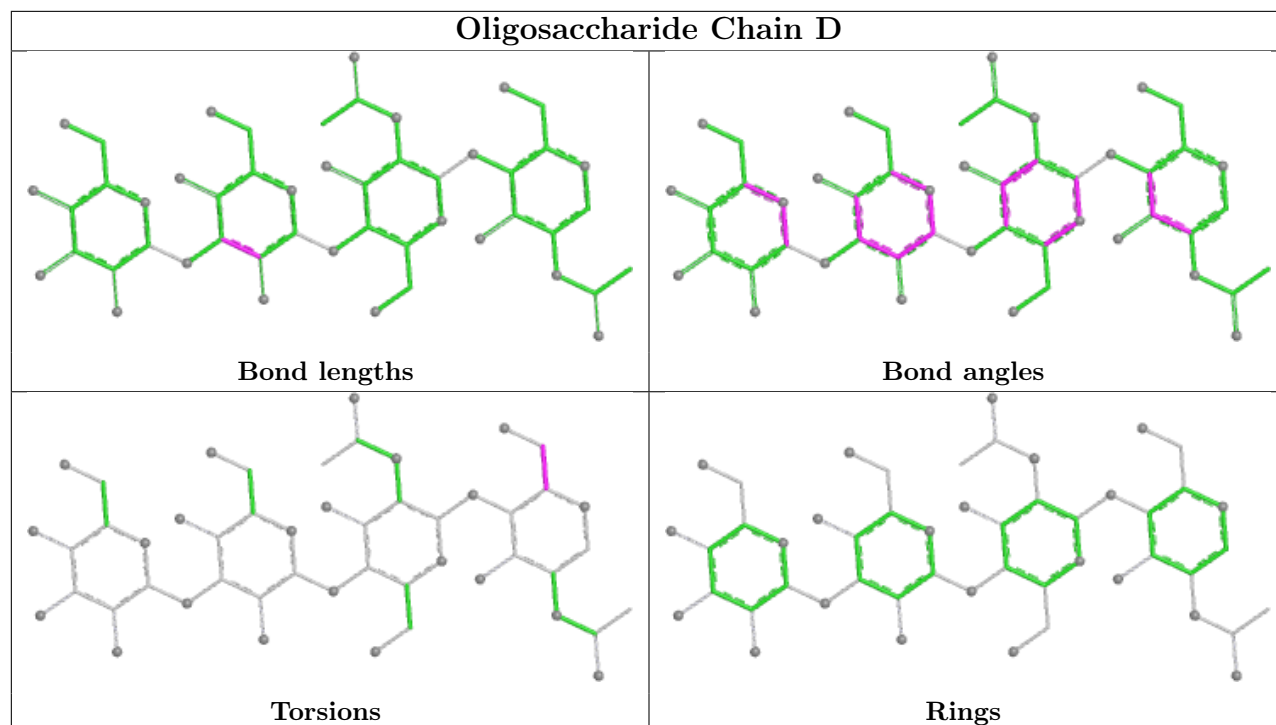
Mol	Chain	Res	Type	Atoms
3	G	5	MAN	C1-C2-C3-C4-C5-O5

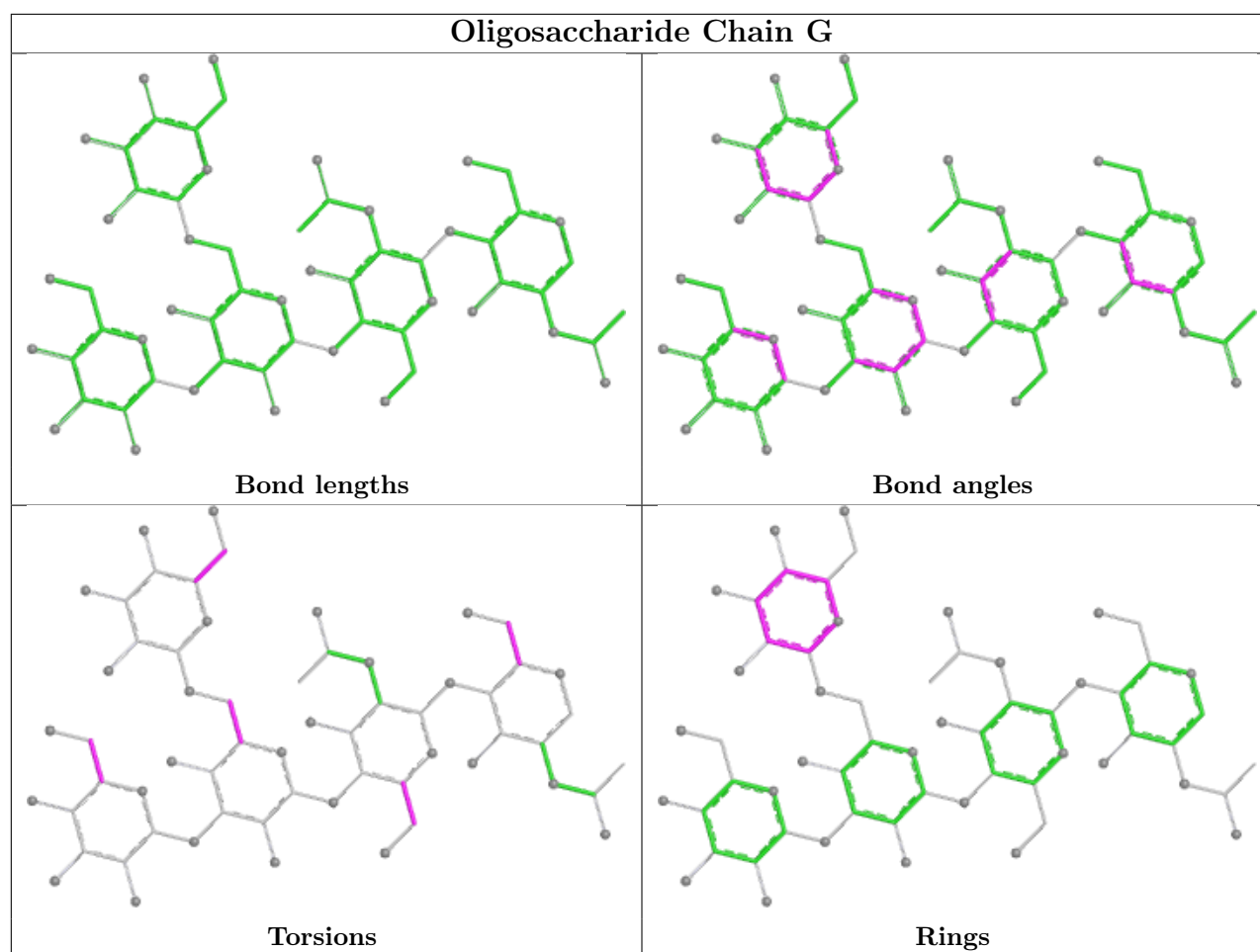
3 monomers are involved in 23 short contacts:

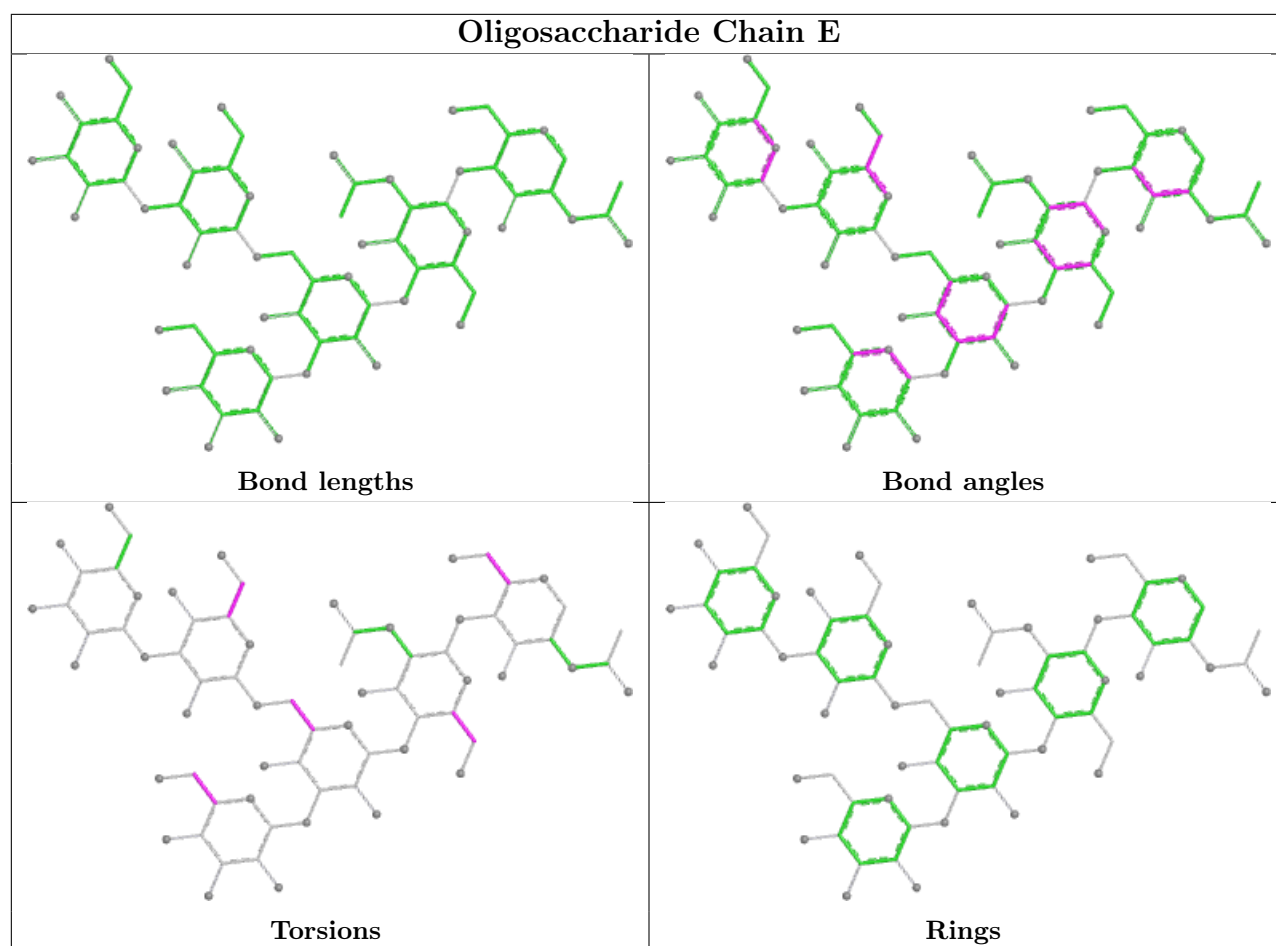
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
2	B	1	NAG	1	0
4	E	1	NAG	22	0

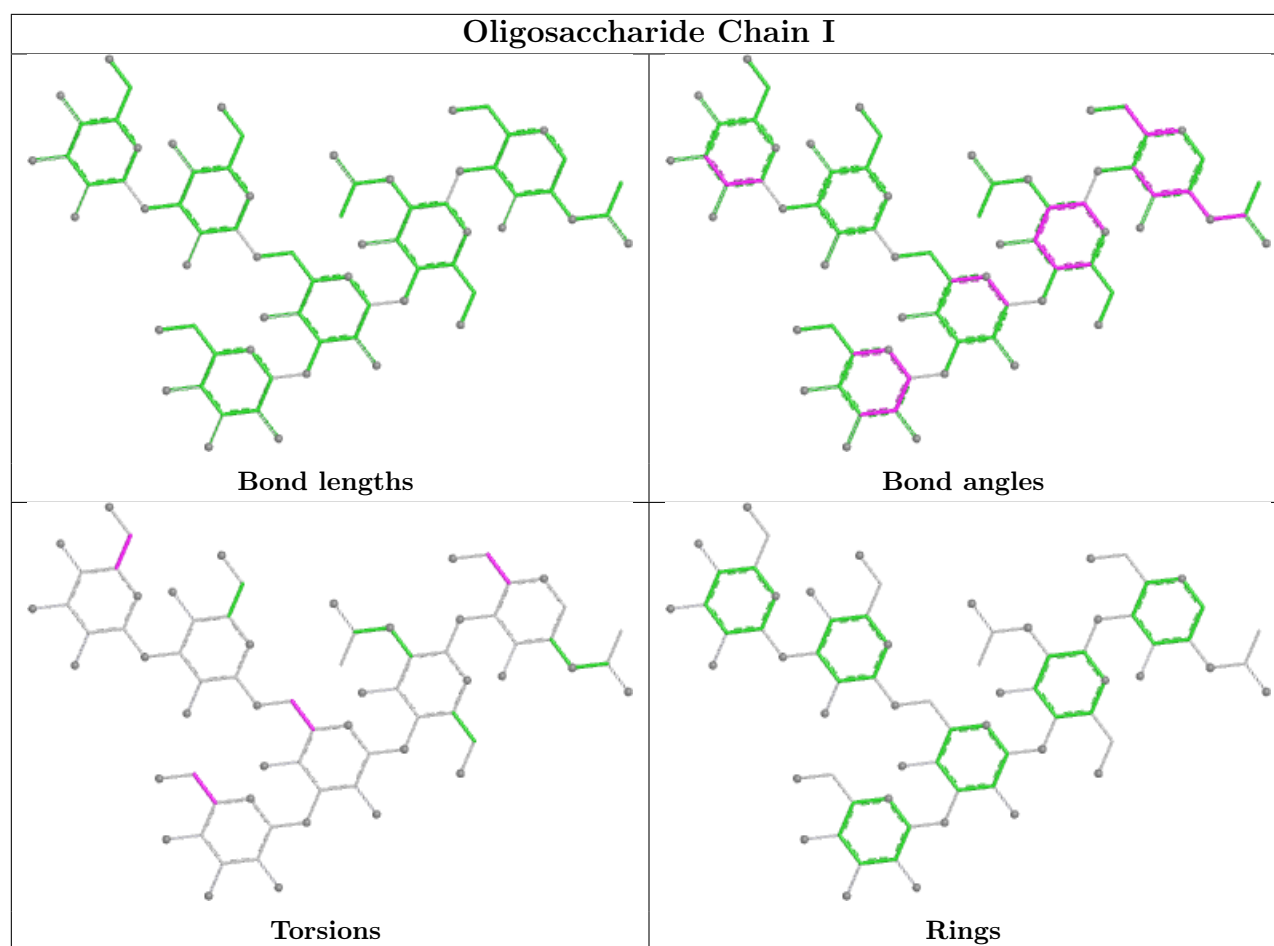
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

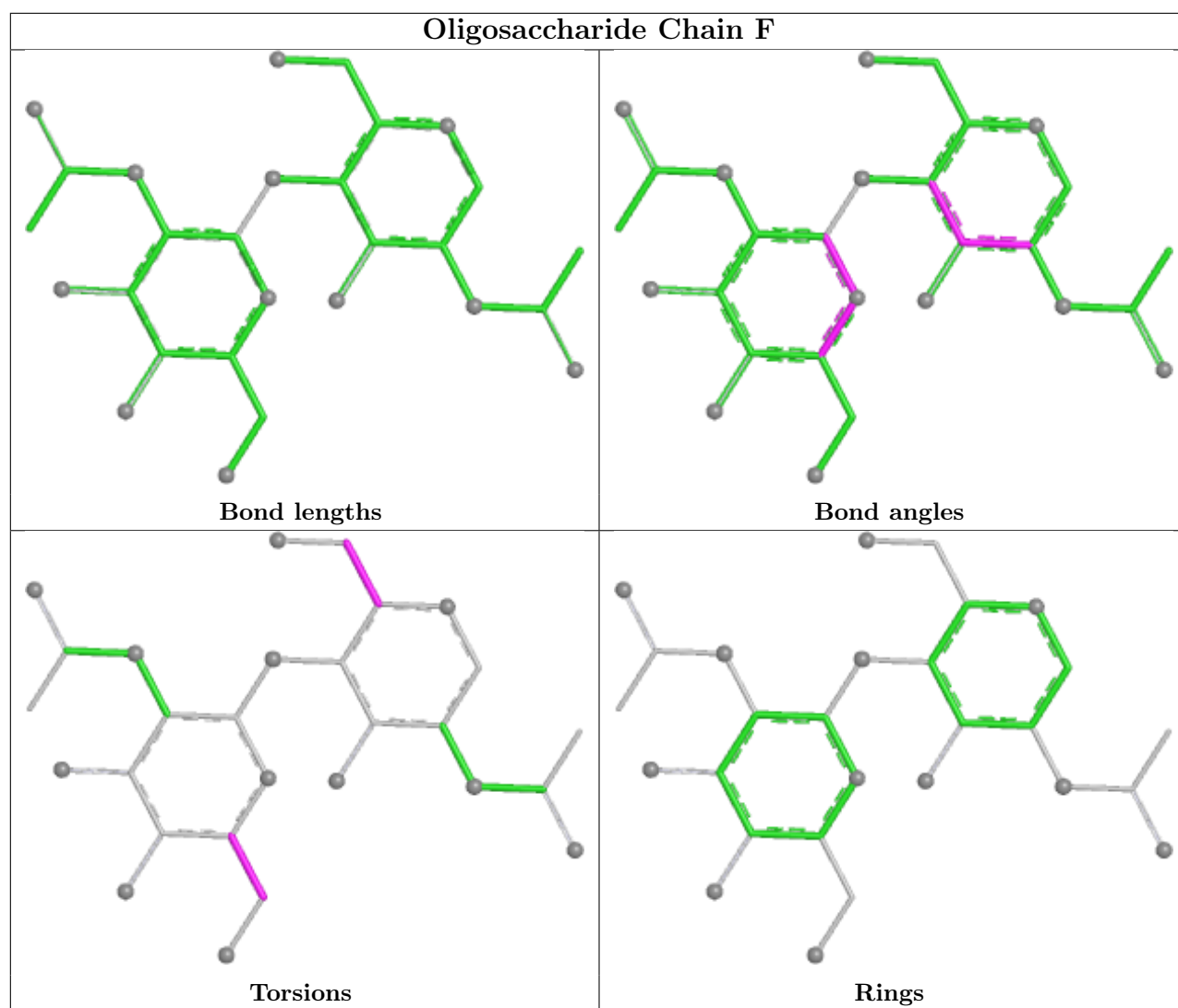


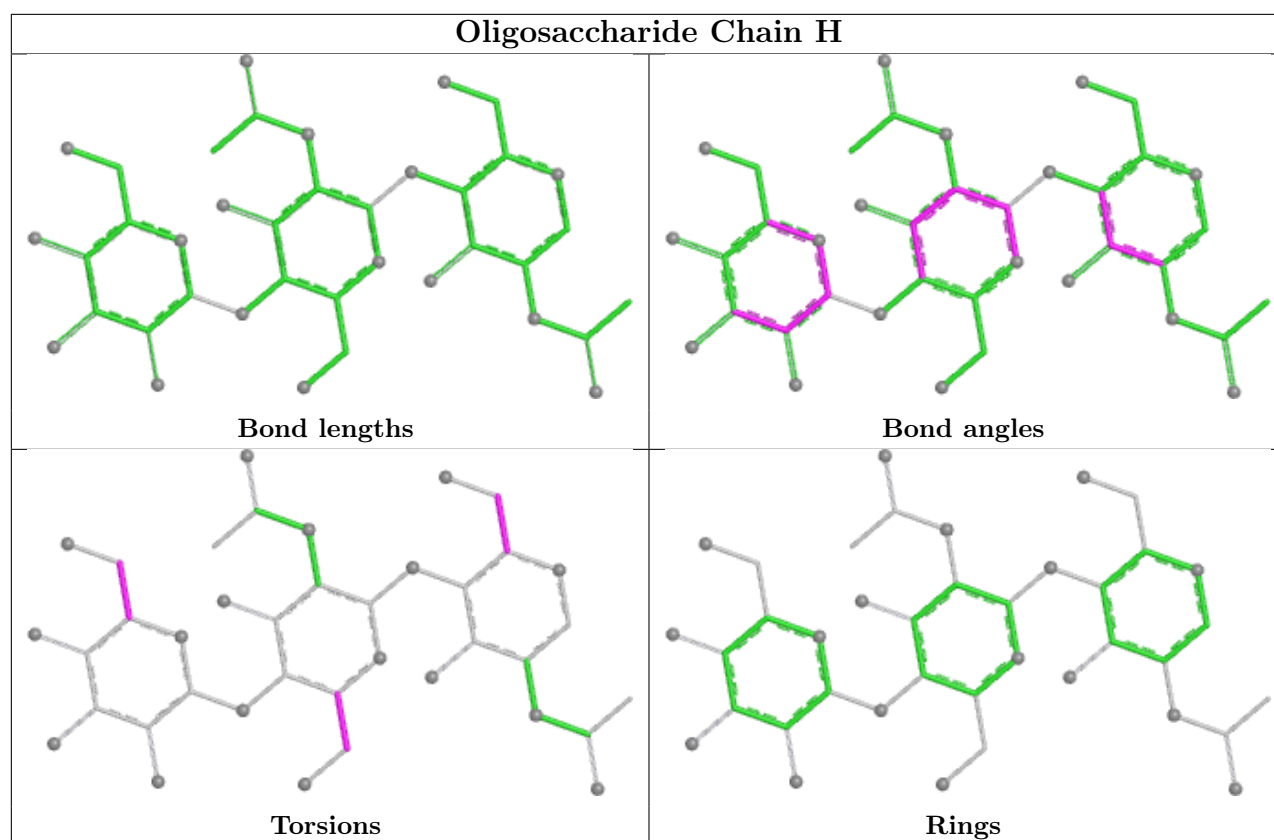












5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1327	1	14,14,15	0.52	0	17,19,21	0.98	1 (5%)
7	NAG	A	1331	1	14,14,15	0.61	0	17,19,21	1.08	1 (5%)

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
7	NAG	A	1327	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1331	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1331	NAG	C1-O5-C5	3.34	116.67	112.19
7	A	1327	NAG	C4-C3-C2	2.24	114.31	111.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1327	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1147:ASP	C	1148:PRO	N	4.89
1	A	658:ASN	C	659:CYS	N	2.39
1	A	806:LYS	C	807:CYS	N	2.25
1	A	510:VAL	C	511:GLU	N	1.99
1	A	561:CYS	C	562:VAL	N	1.83
1	A	704:CYS	C	705:PRO	N	1.68
1	A	1043:THR	C	1044:GLU	N	1.66

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	859:CYS	C	860:THR	N	1.18

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	1171/1212 (96%)	3.73	749 (63%) 0 2	235, 263, 432, 432	0

All (749) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1223	GLY	35.9
1	A	1225	GLU	26.6
1	A	1061	GLY	25.8
1	A	1218	THR	24.0
1	A	675	CYS	23.6
1	A	536	HIS	20.6
1	A	1168	ILE	18.6
1	A	1060	GLY	18.4
1	A	659	CYS	18.0
1	A	537	SER	17.5
1	A	169	GLY	17.4
1	A	839	HIS	16.8
1	A	662	HIS	16.8
1	A	533	CYS	16.5
1	A	1104	ALA	16.2
1	A	1205	LEU	16.1
1	A	1227	SER	16.1
1	A	676	HIS	15.9
1	A	663	GLN	15.8
1	A	1052	ASP	15.1
1	A	632	ASP	14.7
1	A	645	THR	14.7
1	A	648	LYS	14.7
1	A	647	LYS	14.3
1	A	1222	GLY	14.3
1	A	859	CYS	14.3
1	A	657	TYR	13.8

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Mol	Chain	Res	Type	RSRZ
1	A	674	PRO	13.7
1	A	168	ALA	13.5
1	A	1103	ARG	13.2
1	A	1102	CYS	13.2
1	A	1106	SER	13.1
1	A	698	VAL	13.0
1	A	247	SER	12.8
1	A	673	PHE	12.8
1	A	1077	PRO	12.3
1	A	1090	ASN	12.3
1	A	686	ASN	12.1
1	A	658	ASN	11.8
1	A	838	ARG	11.8
1	A	1198	THR	11.7
1	A	157	TYR	11.7
1	A	1226	PHE	11.7
1	A	1065	THR	11.5
1	A	650	ALA	11.3
1	A	359	THR	11.1
1	A	532	TRP	11.1
1	A	1105	PRO	11.1
1	A	1185	ASN	11.1
1	A	251	GLU	11.1
1	A	1149	VAL	11.0
1	A	555	ALA	10.9
1	A	173	ALA	10.8
1	A	1059	SER	10.6
1	A	1070	ASN	10.6
1	A	394	ILE	10.5
1	A	1092	CYS	10.5
1	A	181	ALA	10.4
1	A	639	TYR	10.3
1	A	677	TRP	10.2
1	A	665	CYS	10.2
1	A	444	THR	9.9
1	A	258	THR	9.9
1	A	1166	PRO	9.8
1	A	621	ARG	9.7
1	A	546	GLU	9.6
1	A	655	VAL	9.6
1	A	264	GLN	9.5
1	A	1187	THR	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	514	VAL	9.3
1	A	814	CYS	9.3
1	A	969	GLY	9.3
1	A	180	GLN	9.3
1	A	1175	LEU	9.3
1	A	246	TYR	9.3
1	A	1189	LEU	9.2
1	A	795	ASP	9.2
1	A	825	GLU	9.1
1	A	672	SER	9.1
1	A	1127	ILE	9.1
1	A	667	ALA	9.1
1	A	1134	LEU	9.0
1	A	370	ARG	9.0
1	A	1053	PRO	9.0
1	A	664	SER	9.0
1	A	535	LEU	9.0
1	A	596	CYS	8.9
1	A	1125	GLY	8.9
1	A	668	CYS	8.8
1	A	849	TRP	8.8
1	A	320	GLN	8.7
1	A	308	ARG	8.7
1	A	1195	CYS	8.6
1	A	661	VAL	8.6
1	A	649	PHE	8.6
1	A	1050	ARG	8.5
1	A	531	GLY	8.5
1	A	402	ASP	8.5
1	A	416	THR	8.5
1	A	1182	SER	8.4
1	A	423	PRO	8.4
1	A	362	ALA	8.4
1	A	958	THR	8.3
1	A	1207	GLU	8.3
1	A	569	ARG	8.3
1	A	1203	GLN	8.2
1	A	708	LEU	8.2
1	A	1224	PHE	8.1
1	A	422	THR	8.1
1	A	1074	VAL	8.1
1	A	534	VAL	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	8.1
1	A	420	GLU	8.0
1	A	851	HIS	8.0
1	A	1200	SER	8.0
1	A	545	CYS	7.9
1	A	278	SER	7.9
1	A	1216	LYS	7.9
1	A	519	CYS	7.9
1	A	1136	VAL	7.8
1	A	292	SER	7.8
1	A	605	GLU	7.8
1	A	554	PHE	7.8
1	A	117	LEU	7.7
1	A	206	ALA	7.7
1	A	669	VAL	7.7
1	A	850	MET	7.7
1	A	860	THR	7.6
1	A	858	ARG	7.6
1	A	1049	LEU	7.5
1	A	1046	PRO	7.5
1	A	970	PRO	7.5
1	A	927	THR	7.5
1	A	1170	LYS	7.5
1	A	487	ASP	7.5
1	A	354	ALA	7.4
1	A	1045	ASP	7.4
1	A	286	ASN	7.4
1	A	1043	THR	7.3
1	A	467	GLY	7.3
1	A	1091	SER	7.3
1	A	714	TYR	7.3
1	A	570	ASN	7.3
1	A	252	GLN	7.1
1	A	165	GLY	7.0
1	A	170	VAL	7.0
1	A	552	GLN	6.9
1	A	960	THR	6.9
1	A	333	GLU	6.9
1	A	314	TYR	6.9
1	A	1135	LEU	6.9
1	A	316	SER	6.9
1	A	110	ASP	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	437	ALA	6.8
1	A	1062	THR	6.8
1	A	407	GLN	6.8
1	A	408	ASP	6.8
1	A	538	ILE	6.8
1	A	318	PRO	6.8
1	A	684	CYS	6.8
1	A	390	GLU	6.7
1	A	174	GLY	6.7
1	A	319	GLY	6.7
1	A	249	ARG	6.7
1	A	411	GLN	6.6
1	A	1202	THR	6.6
1	A	330	GLU	6.6
1	A	1183	ARG	6.6
1	A	797	PRO	6.5
1	A	99	VAL	6.5
1	A	796	ASN	6.5
1	A	96	PRO	6.5
1	A	443	ARG	6.5
1	A	418	THR	6.4
1	A	256	TYR	6.4
1	A	317	ARG	6.4
1	A	100	GLN	6.3
1	A	886	ASN	6.3
1	A	924	ASP	6.3
1	A	223	VAL	6.3
1	A	493	ASN	6.3
1	A	291	TYR	6.2
1	A	771	SER	6.2
1	A	94	TYR	6.2
1	A	133	GLN	6.2
1	A	470	ALA	6.1
1	A	1201	GLU	6.1
1	A	315	LEU	6.1
1	A	439	ASP	6.1
1	A	1071	LEU	6.1
1	A	1194	PRO	6.1
1	A	425	PHE	6.1
1	A	356	CYS	6.1
1	A	1098	THR	6.1
1	A	406	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	197	PRO	6.0
1	A	829	CYS	6.0
1	A	527	ASP	6.0
1	A	260	GLN	6.0
1	A	366	LYS	6.0
1	A	1129	ASP	6.0
1	A	58	THR	6.0
1	A	1199	VAL	6.0
1	A	403	ASP	5.9
1	A	195	TYR	5.9
1	A	97	PRO	5.9
1	A	1179	PRO	5.9
1	A	284	CYS	5.8
1	A	836	SER	5.8
1	A	843	ALA	5.8
1	A	571	VAL	5.8
1	A	901	GLY	5.8
1	A	1047	THR	5.8
1	A	324	LYS	5.8
1	A	281	VAL	5.7
1	A	98	SER	5.7
1	A	818	LEU	5.7
1	A	200	SER	5.7
1	A	289	LYS	5.7
1	A	660	SER	5.6
1	A	255	TYR	5.6
1	A	248	PHE	5.6
1	A	399	GLN	5.6
1	A	53	VAL	5.6
1	A	300	CYS	5.6
1	A	489	VAL	5.6
1	A	642	SER	5.6
1	A	902	LYS	5.6
1	A	176	PRO	5.6
1	A	1054	GLU	5.6
1	A	1119	GLU	5.6
1	A	1034	SER	5.6
1	A	1073	THR	5.6
1	A	299	GLY	5.5
1	A	382	SER	5.5
1	A	1058	ASN	5.5
1	A	680	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	923	GLY	5.5
1	A	1101	VAL	5.4
1	A	1128	MET	5.4
1	A	654	PHE	5.4
1	A	798	GLN	5.4
1	A	968	ARG	5.4
1	A	1220	ARG	5.4
1	A	1196	ILE	5.4
1	A	417	VAL	5.3
1	A	361	ARG	5.3
1	A	1063	LEU	5.3
1	A	1079	ILE	5.3
1	A	492	PRO	5.3
1	A	364	LYS	5.3
1	A	515	GLN	5.3
1	A	334	VAL	5.3
1	A	857	SER	5.3
1	A	56	GLU	5.3
1	A	807	CYS	5.3
1	A	500	MET	5.2
1	A	844	ASP	5.2
1	A	116	LEU	5.2
1	A	186	GLY	5.2
1	A	881	THR	5.2
1	A	282	ARG	5.2
1	A	539	CYS	5.2
1	A	706	GLN	5.2
1	A	95	PRO	5.2
1	A	172	ILE	5.2
1	A	245	VAL	5.2
1	A	1137	LEU	5.2
1	A	793	VAL	5.2
1	A	1141	SER	5.2
1	A	699	ASN	5.1
1	A	1069	THR	5.1
1	A	287	ASP	5.1
1	A	540	SER	5.1
1	A	1188	VAL	5.1
1	A	82	HIS	5.1
1	A	196	PHE	5.1
1	A	1221	ALA	5.1
1	A	832	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	301	GLU	5.1
1	A	187	THR	5.0
1	A	1193	THR	5.0
1	A	388	ASN	5.0
1	A	1219	VAL	5.0
1	A	1147	ASP	5.0
1	A	1133	THR	5.0
1	A	1217	VAL	5.0
1	A	466	SER	5.0
1	A	414	GLY	5.0
1	A	421	GLY	5.0
1	A	49	LEU	5.0
1	A	327	GLY	5.0
1	A	358	PHE	4.9
1	A	556	SER	4.9
1	A	39	PHE	4.9
1	A	154	LYS	4.9
1	A	633	GLN	4.9
1	A	1032	GLN	4.9
1	A	966	PRO	4.9
1	A	148	GLY	4.9
1	A	1117	LEU	4.9
1	A	201	SER	4.9
1	A	244	TYR	4.9
1	A	641	LYS	4.9
1	A	1118	GLY	4.8
1	A	438	TYR	4.8
1	A	1037	GLU	4.8
1	A	568	PRO	4.8
1	A	506	THR	4.8
1	A	1131	VAL	4.8
1	A	230	PRO	4.8
1	A	653	ASP	4.8
1	A	651	SER	4.8
1	A	939	VAL	4.7
1	A	468	ARG	4.7
1	A	828	TRP	4.7
1	A	1095	TYR	4.7
1	A	203	ARG	4.7
1	A	595	ASN	4.7
1	A	644	GLU	4.7
1	A	707	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	4.6
1	A	465	PRO	4.6
1	A	573	VAL	4.6
1	A	1206	CYS	4.6
1	A	640	LEU	4.6
1	A	328	LEU	4.6
1	A	331	ASP	4.5
1	A	567	GLN	4.5
1	A	766	GLN	4.5
1	A	490	LEU	4.5
1	A	1123	GLU	4.5
1	A	751	ALA	4.5
1	A	198	THR	4.5
1	A	678	CYS	4.5
1	A	716	PRO	4.4
1	A	837	LEU	4.4
1	A	512	SER	4.4
1	A	167	MET	4.4
1	A	1067	THR	4.4
1	A	688	ALA	4.4
1	A	889	LEU	4.4
1	A	754	THR	4.4
1	A	934	LEU	4.4
1	A	1143	LEU	4.4
1	A	1171	GLY	4.4
1	A	209	GLU	4.4
1	A	419	ILE	4.4
1	A	683	VAL	4.4
1	A	409	PHE	4.4
1	A	471	LEU	4.4
1	A	290	PHE	4.3
1	A	1190	ILE	4.3
1	A	741	GLU	4.3
1	A	963	ARG	4.3
1	A	254	VAL	4.3
1	A	339	PHE	4.3
1	A	1169	LEU	4.3
1	A	597	SER	4.3
1	A	511	GLU	4.3
1	A	494	ARG	4.3
1	A	322	LEU	4.3
1	A	250	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1150	LEU	4.2
1	A	738	ARG	4.2
1	A	59	GLY	4.2
1	A	442	GLY	4.2
1	A	384	PRO	4.2
1	A	681	ARG	4.2
1	A	523	LEU	4.2
1	A	329	ALA	4.2
1	A	835	CYS	4.2
1	A	312	ASP	4.2
1	A	1151	GLU	4.1
1	A	965	SER	4.1
1	A	724	THR	4.1
1	A	756	LEU	4.1
1	A	400	ILE	4.1
1	A	1140	SER	4.1
1	A	508	VAL	4.1
1	A	1173	ASN	4.1
1	A	560	GLN	4.1
1	A	1056	SER	4.1
1	A	54	VAL	4.1
1	A	347	VAL	4.1
1	A	717	VAL	4.1
1	A	1178	ALA	4.0
1	A	1172	ARG	4.0
1	A	770	TYR	4.0
1	A	57	GLN	4.0
1	A	740	TYR	4.0
1	A	1097	ASP	4.0
1	A	283	LEU	4.0
1	A	1025	VAL	4.0
1	A	323	ALA	4.0
1	A	460	VAL	4.0
1	A	70	TYR	3.9
1	A	166	SER	3.9
1	A	972	SER	3.9
1	A	171	LEU	3.9
1	A	285	VAL	3.9
1	A	410	ASN	3.9
1	A	720	VAL	3.9
1	A	51	HIS	3.9
1	A	191	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	426	VAL	3.9
1	A	951	PRO	3.9
1	A	553	ARG	3.9
1	A	817	CYS	3.9
1	A	815	GLY	3.9
1	A	904	LEU	3.9
1	A	405	CYS	3.9
1	A	973	GLY	3.9
1	A	115	LEU	3.9
1	A	332	GLU	3.9
1	A	1113	SER	3.9
1	A	1030	ARG	3.8
1	A	562	VAL	3.8
1	A	389	LYS	3.8
1	A	271	ALA	3.8
1	A	715	VAL	3.8
1	A	190	ASP	3.8
1	A	840	HIS	3.8
1	A	1080	ARG	3.8
1	A	477	VAL	3.8
1	A	131	ALA	3.8
1	A	445	VAL	3.7
1	A	210	ASP	3.7
1	A	365	GLU	3.7
1	A	721	LYS	3.7
1	A	83	VAL	3.7
1	A	1041	ASN	3.7
1	A	846	PRO	3.7
1	A	204	LEU	3.7
1	A	253	PHE	3.7
1	A	326	LEU	3.7
1	A	160	SER	3.7
1	A	1107	ILE	3.7
1	A	929	ARG	3.7
1	A	272	GLY	3.7
1	A	499	ALA	3.7
1	A	277	THR	3.7
1	A	575	MET	3.7
1	A	826	CYS	3.7
1	A	1115	PRO	3.7
1	A	800	ILE	3.7
1	A	926	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	63	VAL	3.6
1	A	263	THR	3.6
1	A	899	HIS	3.6
1	A	572	SER	3.6
1	A	936	GLU	3.6
1	A	517	THR	3.6
1	A	852	ALA	3.6
1	A	1081	ALA	3.6
1	A	1094	VAL	3.6
1	A	903	VAL	3.6
1	A	695	GLU	3.6
1	A	360	LEU	3.6
1	A	1121	PRO	3.5
1	A	1146	PRO	3.5
1	A	396	SER	3.5
1	A	337	THR	3.5
1	A	656	PHE	3.5
1	A	726	ALA	3.5
1	A	215	GLY	3.5
1	A	1120	ARG	3.5
1	A	239	ALA	3.5
1	A	1044	GLU	3.5
1	A	638	LEU	3.5
1	A	145	PHE	3.5
1	A	226	GLN	3.5
1	A	262	ASP	3.5
1	A	615	CYS	3.5
1	A	588	PRO	3.5
1	A	152	HIS	3.5
1	A	598	PHE	3.5
1	A	491	SER	3.5
1	A	121	ALA	3.5
1	A	243	TYR	3.5
1	A	52	LEU	3.4
1	A	241	ASP	3.4
1	A	486	ARG	3.4
1	A	311	GLN	3.4
1	A	805	TYR	3.4
1	A	697	ARG	3.4
1	A	1145	TYR	3.4
1	A	380	LYS	3.4
1	A	392	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	752	ARG	3.4
1	A	274	HIS	3.4
1	A	306	GLU	3.4
1	A	412	PRO	3.4
1	A	385	TRP	3.4
1	A	185	VAL	3.4
1	A	879	ARG	3.4
1	A	967	SER	3.4
1	A	37	PRO	3.3
1	A	462	LEU	3.3
1	A	41	THR	3.3
1	A	679	LYS	3.3
1	A	293	TYR	3.3
1	A	909	GLU	3.3
1	A	1088	ARG	3.3
1	A	48	GLY	3.3
1	A	522	CYS	3.3
1	A	1126	PHE	3.3
1	A	525	SER	3.3
1	A	601	PHE	3.3
1	A	1040	TYR	3.3
1	A	1208	ALA	3.3
1	A	914	SER	3.3
1	A	528	PRO	3.3
1	A	302	GLN	3.3
1	A	1064	LEU	3.2
1	A	910	SER	3.2
1	A	436	ALA	3.2
1	A	155	GLU	3.2
1	A	381	LEU	3.2
1	A	875	GLN	3.2
1	A	906	SER	3.2
1	A	773	GLU	3.2
1	A	357	LEU	3.2
1	A	1089	GLU	3.2
1	A	297	PRO	3.1
1	A	526	ARG	3.1
1	A	928	LEU	3.1
1	A	89	ASP	3.1
1	A	949	LEU	3.1
1	A	1177	PRO	3.1
1	A	383	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	622	GLU	3.1
1	A	830	VAL	3.1
1	A	862	PRO	3.1
1	A	1176	PRO	3.1
1	A	713	ILE	3.1
1	A	758	PHE	3.1
1	A	764	GLN	3.1
1	A	1209	PRO	3.1
1	A	666	LEU	3.1
1	A	810	LEU	3.1
1	A	113	ASN	3.1
1	A	1124	ILE	3.1
1	A	224	SER	3.0
1	A	497	LEU	3.0
1	A	1066	VAL	3.0
1	A	944	LEU	3.0
1	A	132	SER	3.0
1	A	395	ASN	3.0
1	A	594	VAL	3.0
1	A	794	ILE	3.0
1	A	401	ASP	3.0
1	A	485	LEU	3.0
1	A	175	PRO	3.0
1	A	498	TYR	3.0
1	A	146	LYS	3.0
1	A	834	ARG	3.0
1	A	670	ASN	3.0
1	A	855	GLY	3.0
1	A	888	GLY	3.0
1	A	1033	LEU	3.0
1	A	179	GLY	3.0
1	A	516	TYR	3.0
1	A	336	PHE	3.0
1	A	298	ILE	3.0
1	A	1197	LEU	3.0
1	A	1036	PRO	3.0
1	A	1035	ASN	3.0
1	A	435	VAL	3.0
1	A	940	ARG	3.0
1	A	118	LEU	2.9
1	A	959	PRO	2.9
1	A	1072	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1100	MET	2.9
1	A	606	SER	2.9
1	A	60	GLU	2.9
1	A	139	LEU	2.9
1	A	424	LEU	2.9
1	A	874	ARG	2.9
1	A	646	GLY	2.9
1	A	469	PRO	2.9
1	A	463	ALA	2.9
1	A	1116	GLU	2.9
1	A	202	ARG	2.9
1	A	767	ASN	2.9
1	A	488	LEU	2.9
1	A	472	ALA	2.9
1	A	841	CYS	2.9
1	A	952	LYS	2.8
1	A	530	CYS	2.8
1	A	1139	SER	2.8
1	A	343	GLN	2.8
1	A	184	PHE	2.8
1	A	735	SER	2.8
1	A	943	SER	2.8
1	A	313	ALA	2.8
1	A	415	GLY	2.8
1	A	482	ASN	2.8
1	A	1075	ARG	2.8
1	A	700	MET	2.8
1	A	307	TYR	2.8
1	A	894	VAL	2.8
1	A	610	ASP	2.8
1	A	705	PRO	2.7
1	A	941	ASP	2.7
1	A	719	VAL	2.7
1	A	704	CYS	2.7
1	A	802	ALA	2.7
1	A	77	THR	2.7
1	A	38	ALA	2.7
1	A	1144	TYR	2.7
1	A	769	SER	2.7
1	A	42	PHE	2.7
1	A	510	VAL	2.7
1	A	147	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	682	HIS	2.7
1	A	604	THR	2.7
1	A	91	GLU	2.7
1	A	768	SER	2.7
1	A	65	ALA	2.6
1	A	205	MET	2.6
1	A	458	ILE	2.6
1	A	892	GLU	2.6
1	A	81	ALA	2.6
1	A	288	PRO	2.6
1	A	446	VAL	2.6
1	A	101	SER	2.6
1	A	1152	PRO	2.6
1	A	623	VAL	2.6
1	A	831	ALA	2.6
1	A	162	ARG	2.6
1	A	456	ARG	2.6
1	A	1042	TYR	2.6
1	A	391	LEU	2.6
1	A	62	TYR	2.6
1	A	561	CYS	2.5
1	A	718	GLY	2.5
1	A	340	ALA	2.5
1	A	557	ASP	2.5
1	A	345	ASN	2.5
1	A	1164	SER	2.5
1	A	434	ALA	2.5
1	A	413	LEU	2.5
1	A	130	SER	2.5
1	A	883	THR	2.5
1	A	228	LYS	2.5
1	A	946	TYR	2.5
1	A	775	ASN	2.5
1	A	123	ASN	2.5
1	A	231	SER	2.4
1	A	1078	ARG	2.4
1	A	878	THR	2.4
1	A	1051	ILE	2.4
1	A	1086	ILE	2.4
1	A	778	SER	2.4
1	A	529	HIS	2.4
1	A	473	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	739	GLY	2.4
1	A	755	ALA	2.4
1	A	893	ASP	2.4
1	A	50	THR	2.4
1	A	495	GLN	2.4
1	A	627	THR	2.4
1	A	701	SER	2.4
1	A	749	SER	2.4
1	A	119	ASP	2.4
1	A	1057	ILE	2.4
1	A	803	HIS	2.4
1	A	947	ARG	2.4
1	A	866	LYS	2.4
1	A	363	ILE	2.4
1	A	129	GLY	2.4
1	A	134	GLY	2.4
1	A	785	SER	2.4
1	A	1167	LEU	2.4
1	A	303	ALA	2.3
1	A	868	SER	2.3
1	A	208	GLU	2.3
1	A	685	THR	2.3
1	A	61	VAL	2.3
1	A	505	VAL	2.3
1	A	144	LEU	2.3
1	A	861	ASP	2.3
1	A	149	GLU	2.3
1	A	759	ASN	2.3
1	A	574	THR	2.3
1	A	475	SER	2.3
1	A	1165	SER	2.3
1	A	524	GLY	2.3
1	A	87	VAL	2.3
1	A	135	ILE	2.3
1	A	211	ALA	2.3
1	A	464	ASN	2.3
1	A	188	PRO	2.3
1	A	616	HIS	2.3
1	A	942	CYS	2.3
1	A	441	GLN	2.3
1	A	504	GLN	2.3
1	A	265	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	294	VAL	2.2
1	A	1096	ASN	2.2
1	A	776	ASP	2.2
1	A	207	ASN	2.2
1	A	1153	LEU	2.2
1	A	1181	ASN	2.2
1	A	124	ARG	2.2
1	A	541	ARG	2.2
1	A	551	PRO	2.2
1	A	1068	GLY	2.2
1	A	961	PHE	2.2
1	A	1048	ILE	2.2
1	A	84	THR	2.2
1	A	225	SER	2.2
1	A	296	PHE	2.2
1	A	745	HIS	2.2
1	A	346	ARG	2.2
1	A	451	ARG	2.2
1	A	513	CYS	2.2
1	A	734	GLN	2.2
1	A	801	GLN	2.2
1	A	1112	ARG	2.2
1	A	212	ASP	2.1
1	A	111	ASN	2.1
1	A	1076	GLU	2.1
1	A	261	LEU	2.1
1	A	476	VAL	2.1
1	A	69	ILE	2.1
1	A	824	PHE	2.1
1	A	614	HIS	2.1
1	A	127	ALA	2.1
1	A	194	GLU	2.1
1	A	921	GLU	2.1
1	A	1180	GLY	2.1
1	A	976	TRP	2.1
1	A	731	PRO	2.1
1	A	919	VAL	2.1
1	A	375	TYR	2.1
1	A	1083	TYR	2.1
1	A	988	SER	2.1
1	A	865	LEU	2.1
1	A	447	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	563	GLN	2.1
1	A	760	SER	2.1
1	A	457	LYS	2.1
1	A	238	PRO	2.1
1	A	141	LEU	2.0
1	A	325	GLN	2.0
1	A	763	LEU	2.0
1	A	151	HIS	2.0

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.

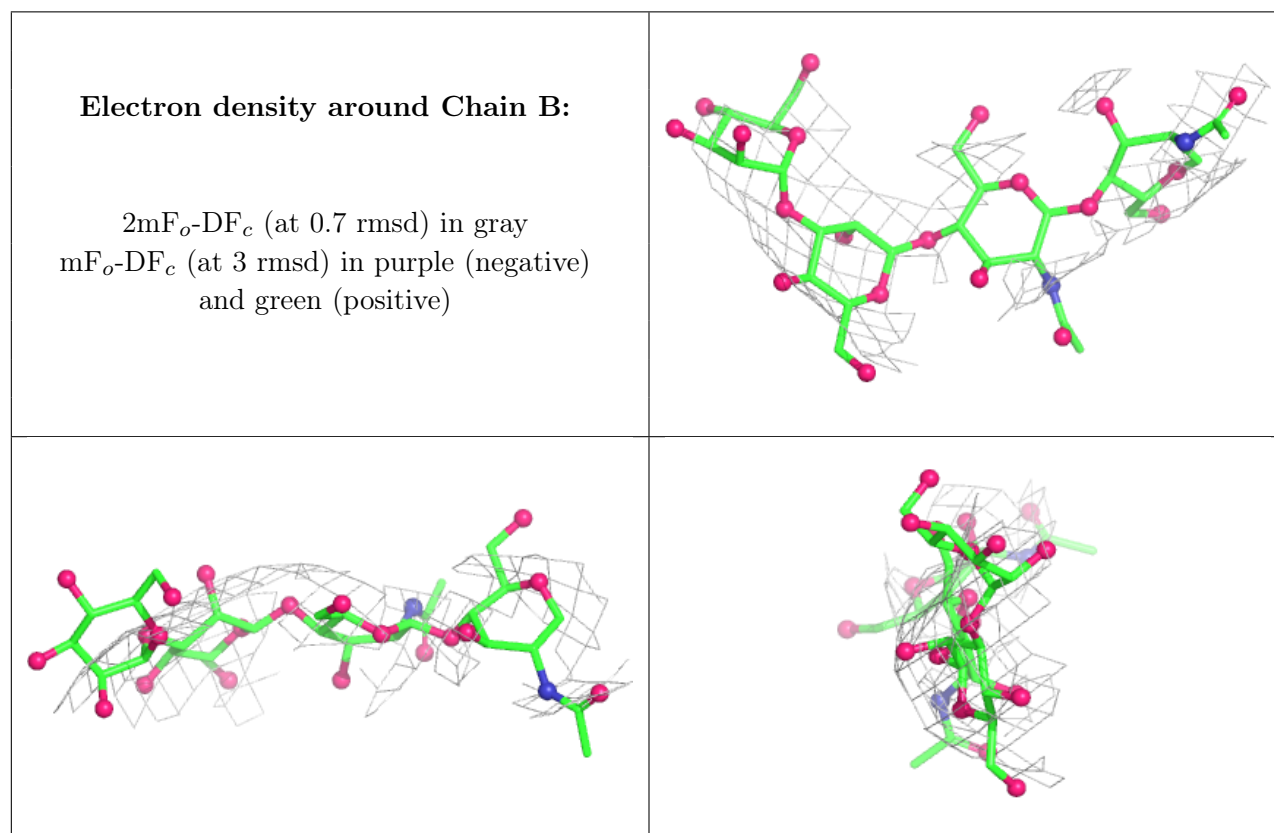
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	I	3	11/12	-0.07	0.18	431,431,431,431	0
4	BMA	E	3	11/12	-0.02	0.19	269,269,269,269	0
4	MAN	E	4	11/12	0.13	0.21	269,269,269,269	0
2	BMA	D	3	11/12	0.22	0.12	269,269,269,269	0
2	NAG	B	1	14/15	0.43	0.21	262,262,262,262	0
4	MAN	E	6	11/12	0.48	0.19	269,269,269,269	0
2	MAN	D	4	11/12	0.48	0.12	269,269,269,269	0
3	MAN	C	4	11/12	0.51	0.17	269,269,269,269	0
2	NAG	B	2	14/15	0.55	0.13	262,262,262,262	0
2	BMA	B	3	11/12	0.58	0.11	262,262,262,262	0
4	MAN	I	6	11/12	0.64	0.22	431,431,431,431	0
3	MAN	G	4	11/12	0.68	0.13	252,252,252,252	0
5	NAG	F	1	14/15	0.68	0.15	252,252,252,252	0
3	BMA	G	3	11/12	0.71	0.13	252,252,252,252	0
5	NAG	F	2	14/15	0.71	0.14	252,252,252,252	0
6	NAG	H	1	14/15	0.73	0.18	252,252,252,252	0
6	NAG	H	2	14/15	0.75	0.20	252,252,252,252	0
3	MAN	G	5	11/12	0.78	0.21	252,252,252,252	0
2	MAN	B	4	11/12	0.81	0.25	262,262,262,262	0
3	NAG	G	2	14/15	0.81	0.32	252,252,252,252	0

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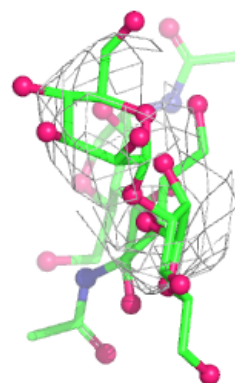
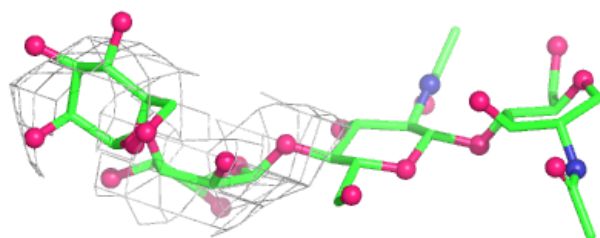
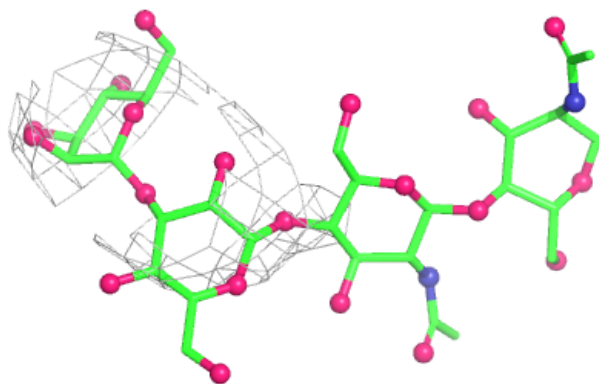
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	2	14/15	0.82	0.13	269,269,269,269	0
6	BMA	H	3	11/12	0.83	0.13	252,252,252,252	0
3	MAN	C	5	11/12	0.86	0.11	269,269,269,269	0
4	MAN	I	4	11/12	0.86	0.31	431,431,431,431	0
4	MAN	E	5	11/12	0.87	0.21	269,269,269,269	0
3	NAG	C	1	14/15	0.87	0.16	269,269,269,269	0
3	NAG	G	1	14/15	0.88	0.26	252,252,252,252	0
3	BMA	C	3	11/12	0.89	0.17	269,269,269,269	0
2	NAG	D	2	14/15	0.90	0.15	269,269,269,269	0
4	NAG	I	2	14/15	0.90	0.27	431,431,431,431	0
2	NAG	D	1	14/15	0.91	0.24	269,269,269,269	0
4	NAG	I	1	14/15	0.92	0.52	431,431,431,431	0
4	MAN	I	5	11/12	0.92	0.49	431,431,431,431	0
4	NAG	E	2	14/15	0.98	0.16	269,269,269,269	0
4	NAG	E	1	14/15	0.99	0.16	269,269,269,269	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.



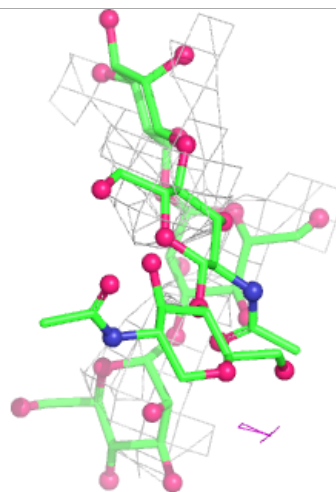
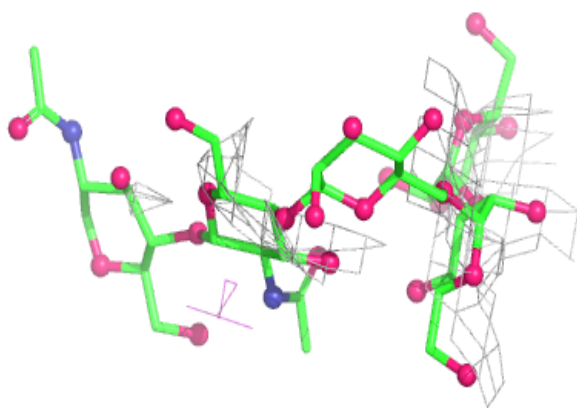
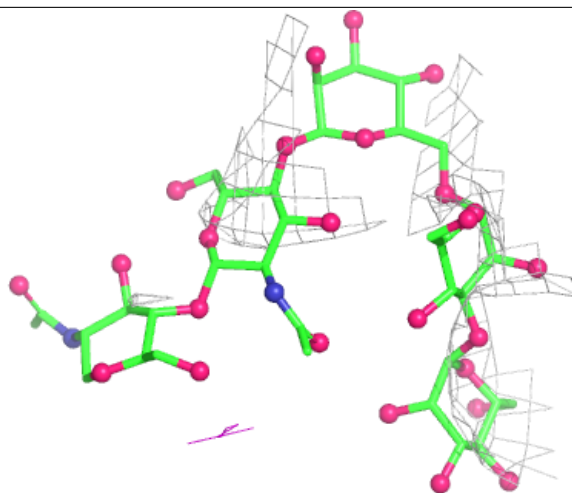
Electron density around Chain D:

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



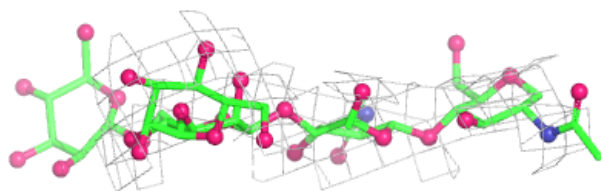
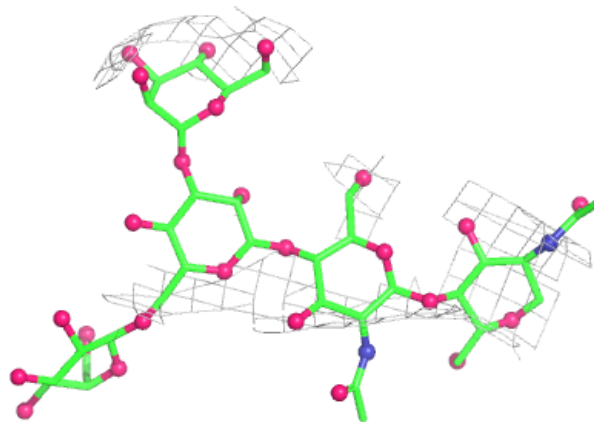
Electron density around Chain C:

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



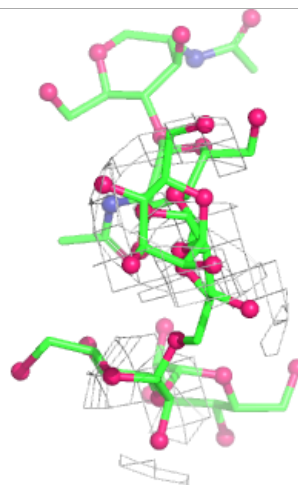
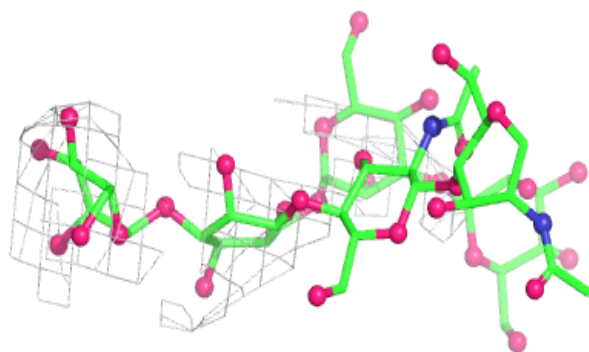
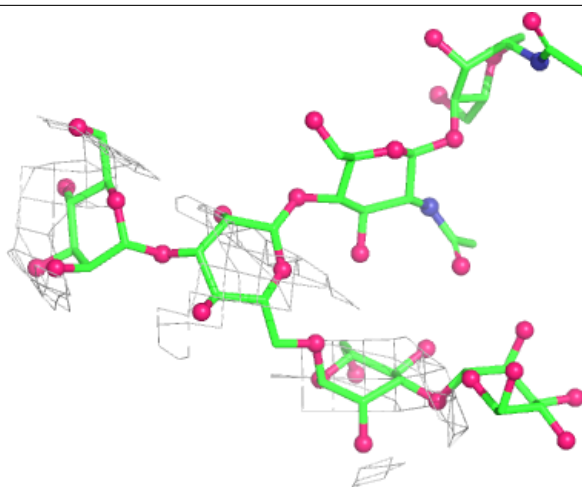
Electron density around Chain G:

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



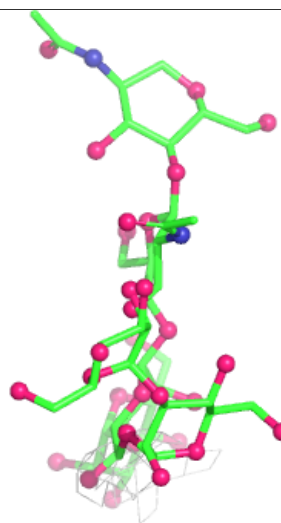
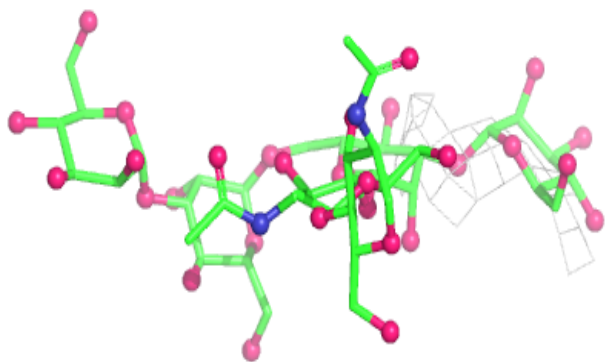
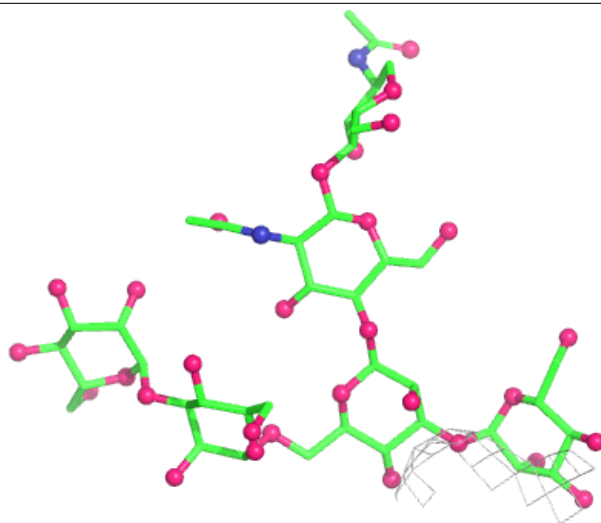
Electron density around Chain E:

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



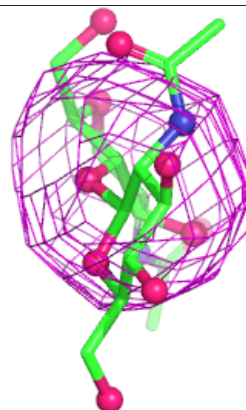
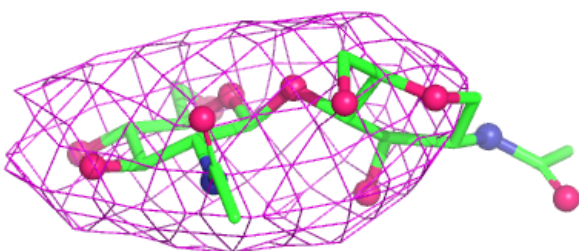
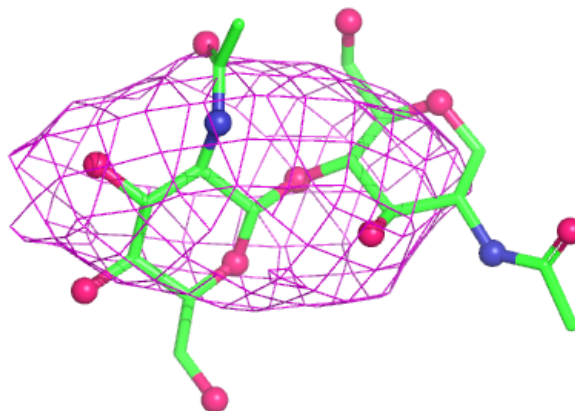
Electron density around Chain I:

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

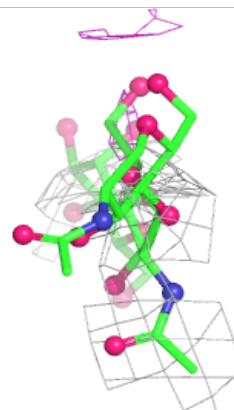
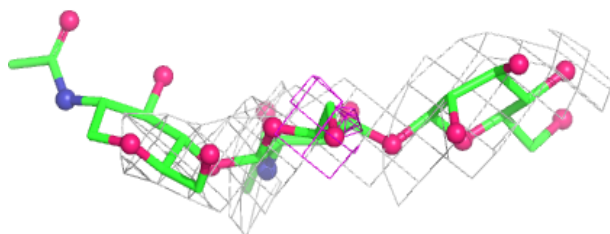
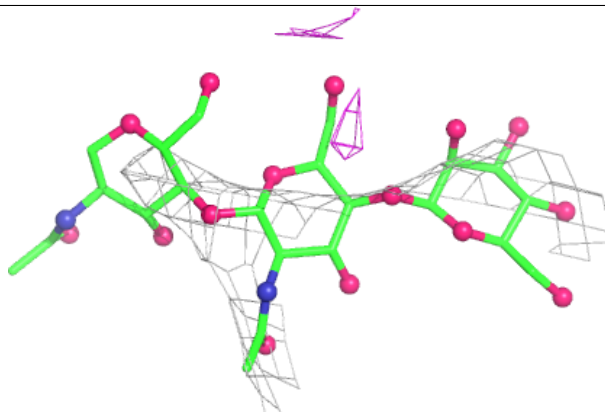


Electron density around Chain F:

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

**Electron density around Chain H:**

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



6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
7	NAG	A	1331	14/15	0.30	0.27	268,268,268,268	0
7	NAG	A	1327	14/15	0.93	0.13	252,252,252,252	0

6.5 Other polymers [i](#)

There are no such residues in this entry.