



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 1HGG / pdb_00001hgg
Title : BINDING OF INFLUENZA VIRUS HEMAGGLUTININ TO ANALOGS OF ITS CELL-SURFACE RECEPTOR, SIALIC ACID: ANALYSIS BY PROTON NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY AND X-RAY CRYSTALLOGRAPHY
Authors : Sauter, N.K.; Hanson, J.E.; Glick, G.D.; Brown, J.H.; Crowther, R.L.; Park, S.-J.; Skehel, J.J.; Wiley, D.C.
Deposited on : 1991-11-01
Resolution : 2.90 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)

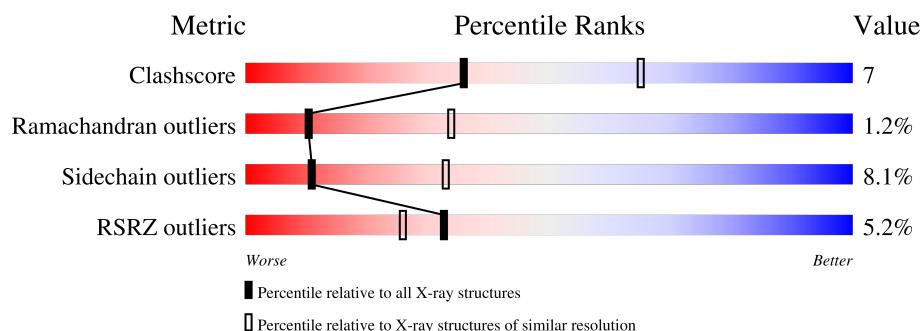
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



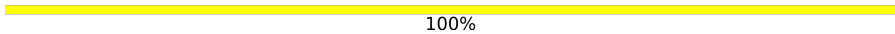
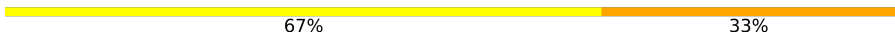
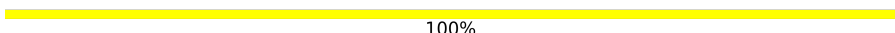
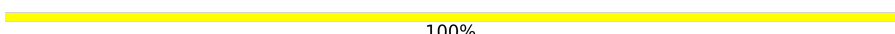
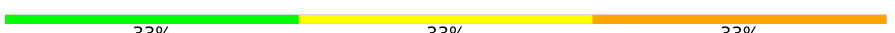
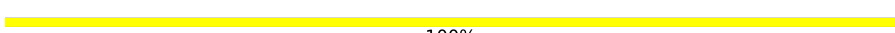
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	328	5% 72% 20% 6% .
1	C	328	7% 71% 22% 5% .
1	E	328	6% 71% 23% . .
2	B	175	3% 69% 26% . .
2	D	175	5% 64% 31% . .

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Mol	Chain	Length	Quality of chain
2	F	175	 3% 69% 26% . .
3	G	3	 100%
3	J	3	 67% 33%
3	M	3	 100%
4	H	3	 100%
4	I	3	 33% 33% 33%
4	K	3	 100%
4	L	3	 33% 33% 33%
4	N	3	 100%
4	O	3	 33% 33% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15882 atoms, of which 3408 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.

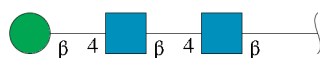
- Molecule 1 is a protein called HEMAGGLUTININ, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			
1	E	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			

- Molecule 2 is a protein called HEMAGGLUTININ, CHAIN HA2.

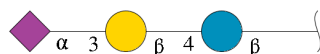
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	D	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	F	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			

- Molecule 3 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.



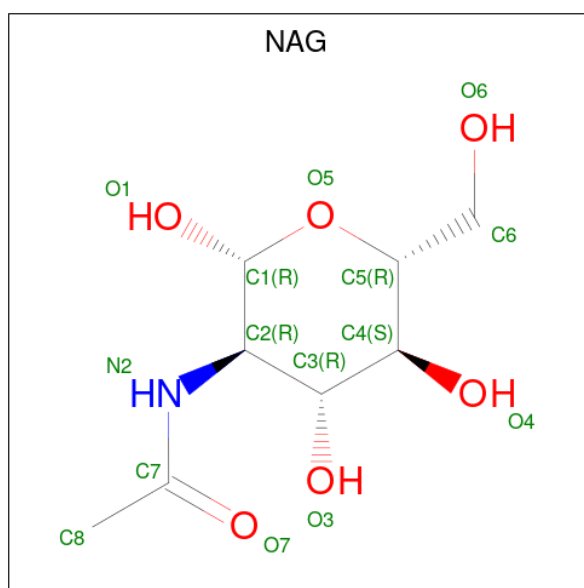
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	H	N	O	0	0	0
			76	22	37	2	15			
3	J	3	Total	C	H	N	O	0	0	0
			76	22	37	2	15			
3	M	3	Total	C	H	N	O	0	0	0
			76	22	37	2	15			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	3	Total 81	C 23	H 38	N 1	O 19	0	0	0
4	I	3	Total 81	C 23	H 38	N 1	O 19	0	0	0
4	K	3	Total 81	C 23	H 38	N 1	O 19	0	0	0
4	L	3	Total 81	C 23	H 38	N 1	O 19	0	0	0
4	N	3	Total 81	C 23	H 38	N 1	O 19	0	0	0
4	O	3	Total 81	C 23	H 38	N 1	O 19	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	C	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	C	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	C	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	D	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	F	1	Total 28	C 8	H 14	N 1	O 5	0	0

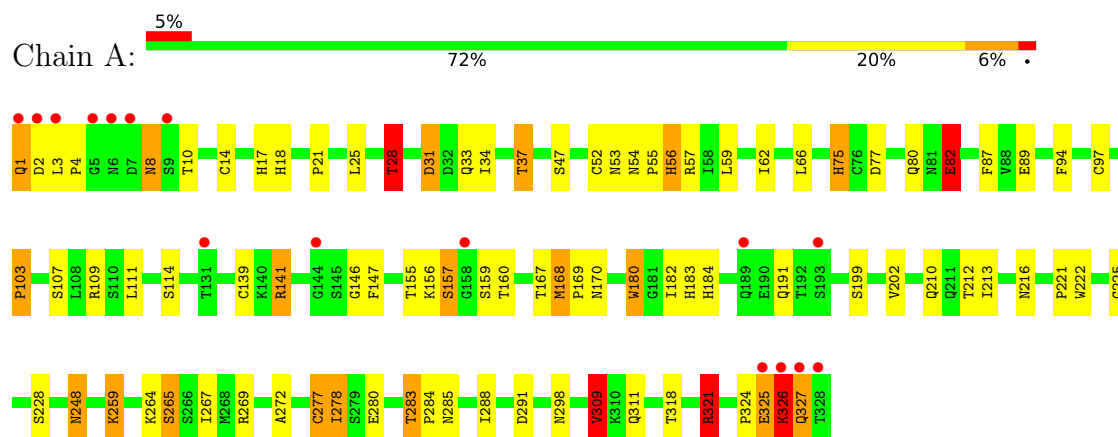
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	13	Total	H	O	0	0
			39	26	13		
6	B	11	Total	H	O	0	0
			33	22	11		
6	C	11	Total	H	O	0	0
			33	22	11		
6	D	13	Total	H	O	0	0
			39	26	13		
6	E	12	Total	H	O	0	0
			36	24	12		
6	F	12	Total	H	O	0	0
			36	24	12		

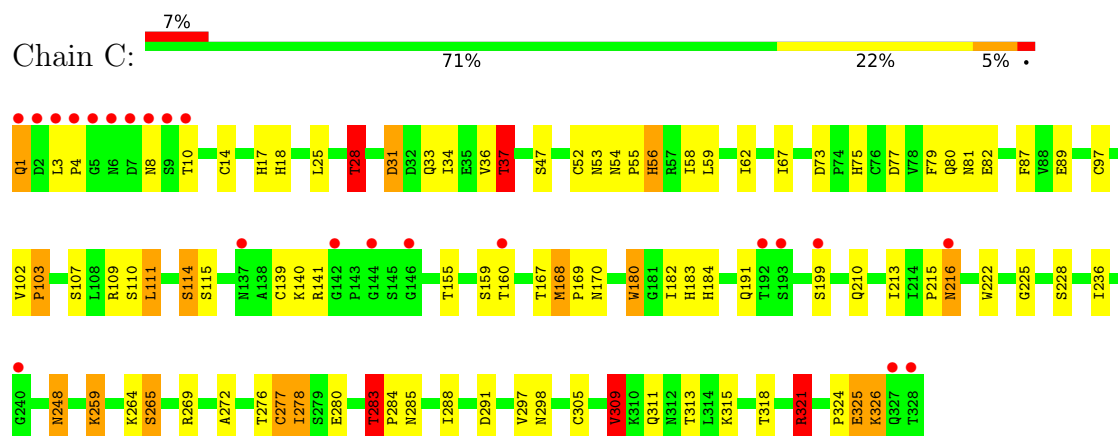
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

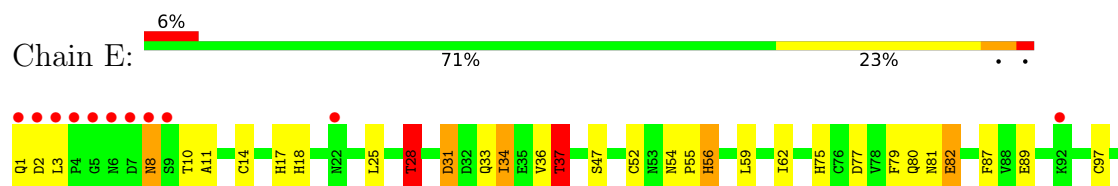
• Molecule 1: HEMAGGLUTININ, CHAIN HA1

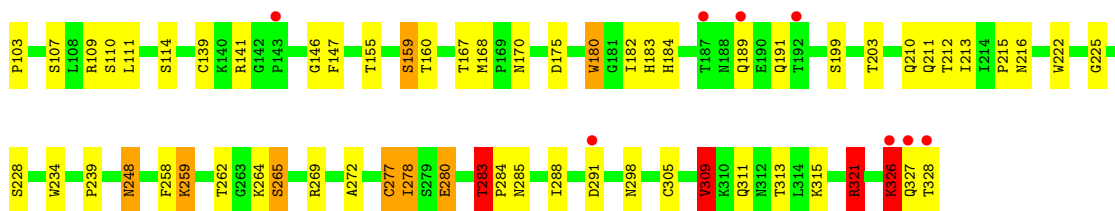


• Molecule 1: HEMAGGLUTININ, CHAIN HA1

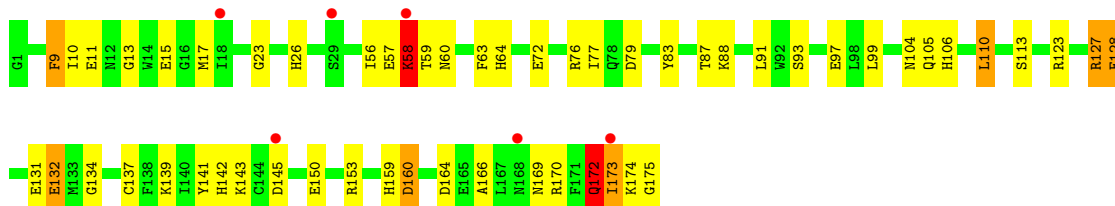


• Molecule 1: HEMAGGLUTININ, CHAIN HA1

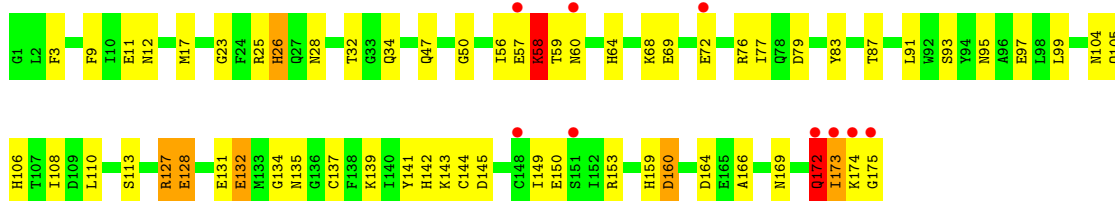




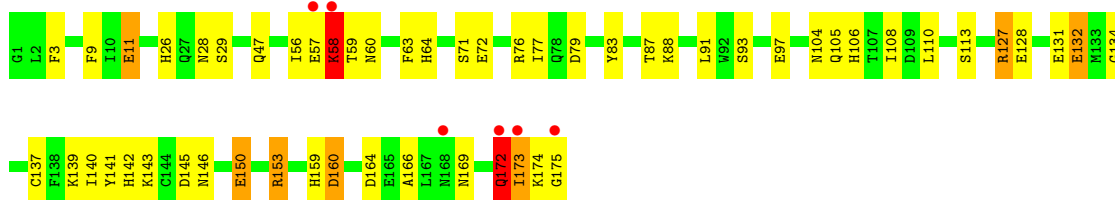
• Molecule 2: HEMAGGLUTININ, CHAIN HA2



• Molecule 2: HEMAGGLUTININ, CHAIN HA2



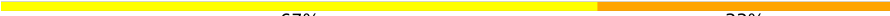
• Molecule 2: HEMAGGLUTININ, CHAIN HA2



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

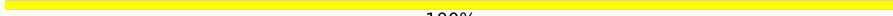


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%

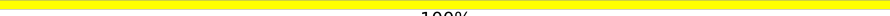
BAG1
BAG2
BAG3

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

Chain M:  100%

BAG1
BAG2
BAG3

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%

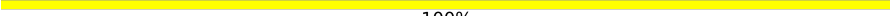
BGC1
GAL2
STAG

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain I:  33% 33% 33%

BGC1
GAL2
STAG

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:  100%

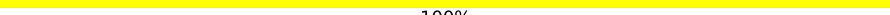
BGC1
GAL2
STAG

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:  33% 33% 33%

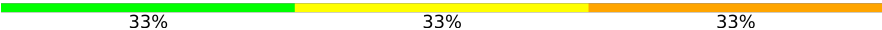
BGC1
GAL2
STAG

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain N:  100%

BGC1
GAL2
STAG

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain O:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	162.70Å 162.70Å 177.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90 7.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.90) 63.6 (7.00-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.93Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.229 , (Not available) 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15882	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: SIA, GAL, BGC, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	12/2589 (0.5%)	1.74	42/3527 (1.2%)
1	C	1.13	11/2589 (0.4%)	1.71	44/3527 (1.2%)
1	E	1.17	13/2589 (0.5%)	1.74	48/3527 (1.4%)
2	B	1.12	8/1445 (0.6%)	1.75	21/1939 (1.1%)
2	D	1.17	10/1445 (0.7%)	1.78	28/1939 (1.4%)
2	F	1.14	9/1445 (0.6%)	1.76	28/1939 (1.4%)
All	All	1.14	63/12102 (0.5%)	1.74	211/16398 (1.3%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	HIS	CD2-NE2	-7.37	1.29	1.37
2	B	64	HIS	CG-ND1	-7.37	1.30	1.38
2	F	159	HIS	CD2-NE2	-7.31	1.29	1.37
1	E	184	HIS	CD2-NE2	-7.25	1.29	1.37
1	E	56	HIS	CD2-NE2	-7.21	1.29	1.37
1	E	18	HIS	CG-ND1	-7.16	1.30	1.38
1	C	184	HIS	CD2-NE2	-7.00	1.30	1.37
2	D	26	HIS	CD2-NE2	-6.90	1.30	1.37
2	F	159	HIS	CG-ND1	-6.89	1.30	1.38
1	A	75	HIS	CD2-NE2	-6.79	1.30	1.37
2	F	26	HIS	CD2-NE2	-6.77	1.30	1.37
1	C	75	HIS	CD2-NE2	-6.74	1.30	1.37
1	C	56	HIS	CD2-NE2	-6.73	1.30	1.37
1	E	184	HIS	CG-ND1	-6.72	1.30	1.38
1	E	18	HIS	CD2-NE2	-6.68	1.30	1.37
2	D	64	HIS	CG-ND1	-6.67	1.30	1.38
2	D	106	HIS	CD2-NE2	-6.42	1.30	1.37
2	B	159	HIS	CG-ND1	-6.41	1.31	1.38
2	F	142	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	18	HIS	CG-ND1	-6.32	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	106	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	184	HIS	CD2-NE2	-6.25	1.30	1.37
2	B	26	HIS	CD2-NE2	-6.24	1.30	1.37
1	C	17	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	17	HIS	CD2-NE2	-6.20	1.31	1.37
2	B	159	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	56	HIS	CG-ND1	-6.18	1.31	1.38
1	A	18	HIS	CD2-NE2	-6.16	1.31	1.37
2	B	64	HIS	CD2-NE2	-6.04	1.31	1.37
1	C	184	HIS	CG-ND1	-6.03	1.31	1.38
1	E	183	HIS	CG-ND1	-6.01	1.31	1.38
2	D	159	HIS	CD2-NE2	-6.00	1.31	1.37
1	C	67	ILE	CA-CB	5.99	1.61	1.54
2	D	64	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	18	HIS	CD2-NE2	-5.98	1.31	1.37
2	D	159	HIS	CG-ND1	-5.96	1.31	1.38
2	B	142	HIS	CG-ND1	-5.91	1.31	1.38
1	A	183	HIS	CD2-NE2	-5.91	1.31	1.37
2	F	26	HIS	CG-ND1	-5.90	1.31	1.38
2	D	106	HIS	CG-ND1	-5.89	1.31	1.38
1	C	18	HIS	CG-ND1	-5.87	1.31	1.38
2	F	64	HIS	CG-ND1	-5.81	1.31	1.38
2	B	142	HIS	CD2-NE2	-5.77	1.31	1.37
1	E	56	HIS	CG-ND1	-5.77	1.31	1.38
1	A	184	HIS	CG-ND1	-5.75	1.31	1.38
1	E	75	HIS	CD2-NE2	-5.75	1.31	1.37
1	E	305	CYS	CA-CB	-5.73	1.46	1.54
1	E	234	TRP	CG-CD2	-5.70	1.33	1.43
1	C	183	HIS	CD2-NE2	-5.66	1.31	1.37
1	E	17	HIS	CD2-NE2	-5.62	1.31	1.37
2	F	64	HIS	CD2-NE2	-5.62	1.31	1.37
1	E	183	HIS	CD2-NE2	-5.58	1.31	1.37
2	F	106	HIS	CD2-NE2	-5.56	1.31	1.37
1	E	17	HIS	CG-ND1	-5.55	1.32	1.38
1	C	17	HIS	CG-ND1	-5.52	1.32	1.38
2	D	142	HIS	CD2-NE2	-5.49	1.31	1.37
2	F	142	HIS	CG-ND1	-5.40	1.32	1.38
1	A	75	HIS	CG-ND1	-5.40	1.32	1.38
2	D	26	HIS	CG-ND1	-5.39	1.32	1.38
2	D	142	HIS	CG-ND1	-5.37	1.32	1.38
1	A	17	HIS	CG-ND1	-5.33	1.32	1.38
1	C	305	CYS	CA-CB	-5.28	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	HIS	CG-ND1	-5.06	1.32	1.38

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	PHE	CA-CB-CG	10.16	123.97	113.80
2	B	9	PHE	CA-CB-CG	9.93	123.73	113.80
2	F	9	PHE	CA-CB-CG	9.91	123.71	113.80
2	D	160	ASP	CA-CB-CG	-9.15	103.45	112.60
2	F	160	ASP	CA-CB-CG	-8.91	103.69	112.60
1	E	56	HIS	ND1-CG-CD2	8.78	114.88	106.10
2	B	160	ASP	CA-CB-CG	-8.76	103.84	112.60
2	F	79	ASP	CA-CB-CG	8.71	121.31	112.60
1	A	56	HIS	ND1-CG-CD2	8.63	114.73	106.10
2	D	79	ASP	CA-CB-CG	8.63	121.23	112.60
1	C	56	HIS	ND1-CG-CD2	8.42	114.52	106.10
2	B	169	ASN	CA-CB-CG	8.33	120.93	112.60
2	D	169	ASN	CA-CB-CG	8.31	120.92	112.60
1	A	8	ASN	CA-CB-CG	8.20	120.80	112.60
1	E	326	LYS	CA-CB-CG	8.14	130.38	114.10
2	B	79	ASP	CA-CB-CG	8.09	120.69	112.60
2	B	159	HIS	ND1-CG-CD2	8.08	114.18	106.10
2	D	135	ASN	OD1-CG-ND2	-8.05	114.55	122.60
2	F	169	ASN	CA-CB-CG	7.97	120.57	112.60
1	A	272	ALA	CA-C-N	7.96	127.96	119.76
1	A	272	ALA	C-N-CA	7.96	127.96	119.76
1	C	272	ALA	CA-C-N	7.88	127.88	119.76
1	C	272	ALA	C-N-CA	7.88	127.88	119.76
2	B	57	GLU	CA-CB-CG	7.88	129.87	114.10
2	F	57	GLU	CA-CB-CG	7.85	129.81	114.10
1	E	272	ALA	CA-C-N	7.85	127.84	119.76
1	E	272	ALA	C-N-CA	7.85	127.84	119.76
2	D	57	GLU	CA-CB-CG	7.80	129.71	114.10
2	D	159	HIS	ND1-CG-CD2	7.76	113.86	106.10
2	D	26	HIS	ND1-CG-CD2	7.72	113.82	106.10
2	D	64	HIS	ND1-CG-CD2	7.71	113.81	106.10
1	E	8	ASN	OD1-CG-ND2	-7.67	114.93	122.60
1	A	75	HIS	CA-CB-CG	7.60	121.40	113.80
2	F	106	HIS	ND1-CG-CD2	7.58	113.68	106.10
1	A	324	PRO	O-C-N	7.56	132.39	123.01
2	B	150	GLU	CB-CG-CD	7.56	125.46	112.60
2	F	172	GLN	OE1-CD-NE2	-7.49	115.11	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	64	HIS	ND1-CG-CD2	7.47	113.57	106.10
1	E	75	HIS	CA-CB-CG	7.44	121.24	113.80
2	B	106	HIS	ND1-CG-CD2	7.39	113.49	106.10
2	B	64	HIS	ND1-CG-CD2	7.33	113.43	106.10
1	C	248	ASN	N-CA-CB	-7.30	99.38	111.49
2	F	159	HIS	ND1-CG-CD2	7.28	113.38	106.10
2	D	106	HIS	ND1-CG-CD2	7.21	113.31	106.10
2	B	172	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	E	28	THR	CA-CB-OG1	-7.16	98.87	109.60
1	A	248	ASN	N-CA-CB	-7.12	99.67	111.49
2	D	172	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	1	GLN	N-CA-C	-7.03	91.32	111.00
1	A	184	HIS	ND1-CG-CD2	7.01	113.11	106.10
2	F	26	HIS	ND1-CG-CD2	6.97	113.07	106.10
1	C	184	HIS	ND1-CG-CD2	6.95	113.05	106.10
1	C	191	GLN	OE1-CD-NE2	-6.95	115.66	122.60
1	C	75	HIS	CA-CB-CG	6.87	120.67	113.80
1	A	168	MET	CA-C-N	6.82	126.58	119.76
1	A	168	MET	C-N-CA	6.82	126.58	119.76
1	C	168	MET	CA-C-N	6.80	126.56	119.76
1	C	168	MET	C-N-CA	6.80	126.56	119.76
2	F	28	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	E	28	THR	CA-CB-CG2	6.78	122.02	110.50
1	E	184	HIS	ND1-CG-CD2	6.76	112.86	106.10
1	A	28	THR	CA-CB-OG1	-6.75	99.47	109.60
2	D	11	GLU	CA-CB-CG	-6.74	100.61	114.10
1	E	248	ASN	N-CA-CB	-6.73	100.10	111.27
2	B	26	HIS	ND1-CG-CD2	6.67	112.77	106.10
1	C	28	THR	CA-CB-OG1	-6.65	99.63	109.60
1	E	168	MET	CA-C-N	6.64	126.40	119.76
1	E	168	MET	C-N-CA	6.64	126.40	119.76
1	E	321	ARG	NE-CZ-NH2	-6.57	113.29	119.20
1	E	37	THR	CA-CB-OG1	-6.53	99.81	109.60
1	C	28	THR	CA-CB-CG2	6.49	121.54	110.50
1	A	324	PRO	CA-C-N	6.49	133.42	122.65
1	A	324	PRO	C-N-CA	6.49	133.42	122.65
1	A	326	LYS	N-CA-C	-6.41	97.15	110.80
1	A	28	THR	CA-CB-CG2	6.39	121.37	110.50
1	E	309	VAL	N-CA-CB	-6.37	100.58	112.36
1	E	248	ASN	CA-CB-CG	6.34	118.94	112.60
1	E	8	ASN	CB-CG-ND2	6.31	125.87	116.40
1	A	248	ASN	CA-CB-CG	6.28	118.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	HIS	ND1-CG-CD2	6.27	112.37	106.10
1	A	82	GLU	CB-CG-CD	6.21	123.16	112.60
1	A	321	ARG	CB-CG-CD	-6.21	97.03	111.30
1	A	159	SER	N-CA-CB	-6.17	101.25	111.49
2	B	11	GLU	N-CA-C	6.13	117.96	111.28
1	C	321	ARG	CB-CG-CD	-6.13	97.20	111.30
1	A	183	HIS	ND1-CG-CD2	6.12	112.22	106.10
1	C	324	PRO	O-C-N	-6.12	115.50	122.91
1	E	183	HIS	ND1-CG-CD2	6.07	112.17	106.10
2	B	76	ARG	N-CA-C	6.05	118.41	111.02
1	C	18	HIS	ND1-CG-CD2	6.03	112.13	106.10
1	C	56	HIS	CB-CG-CD2	-6.01	123.39	131.20
2	D	108	ILE	CA-C-O	-5.97	114.75	120.95
1	E	216	ASN	CA-CB-CG	5.97	118.57	112.60
1	E	321	ARG	CB-CG-CD	-5.95	97.61	111.30
1	E	56	HIS	CG-CD2-NE2	-5.94	101.26	107.20
1	A	325	GLU	CA-CB-CG	5.93	125.97	114.10
1	E	180	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	E	56	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	C	248	ASN	CA-CB-CG	5.92	118.52	112.60
1	C	326	LYS	O-C-N	-5.91	114.73	122.59
2	D	11	GLU	N-CA-C	5.91	118.50	111.71
1	A	18	HIS	ND1-CG-CD2	5.89	112.00	106.10
1	C	102	VAL	CA-C-O	-5.88	116.88	119.94
1	C	216	ASN	CA-CB-CG	5.87	118.47	112.60
2	B	60	ASN	CA-CB-CG	5.86	118.46	112.60
2	F	58	LYS	N-CA-C	5.86	123.28	110.80
1	A	56	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	E	1	GLN	N-CA-C	-5.81	94.73	111.00
1	C	1	GLN	N-CA-C	-5.80	94.76	111.00
2	B	99	LEU	CA-C-O	-5.78	114.93	121.00
1	A	325	GLU	CA-C-N	5.75	132.52	121.54
1	A	325	GLU	C-N-CA	5.75	132.52	121.54
2	F	64	HIS	CG-CD2-NE2	-5.74	101.46	107.20
2	D	58	LYS	N-CA-C	5.74	123.02	110.80
2	B	58	LYS	N-CA-C	5.71	122.95	110.80
1	C	107	SER	CA-CB-OG	-5.68	99.73	111.10
2	D	3	PHE	CA-CB-CG	-5.67	108.13	113.80
2	D	60	ASN	CA-CB-CG	5.66	118.26	112.60
1	E	107	SER	CA-CB-OG	-5.65	99.81	111.10
2	B	159	HIS	CG-CD2-NE2	-5.63	101.57	107.20
1	E	191	GLN	OE1-CD-NE2	-5.63	116.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	VAL	N-CA-CB	-5.60	102.00	112.36
2	F	108	ILE	CA-C-O	-5.60	115.13	120.95
1	C	183	HIS	ND1-CG-CD2	5.57	111.67	106.10
2	D	76	ARG	N-CA-C	5.57	117.81	111.02
1	A	191	GLN	OE1-CD-NE2	-5.55	117.05	122.60
2	F	71	SER	CA-CB-OG	-5.55	100.00	111.10
2	F	159	HIS	CG-CD2-NE2	-5.55	101.65	107.20
1	A	309	VAL	N-CA-CB	-5.54	102.11	112.36
1	C	37	THR	CA-CB-OG1	-5.54	101.30	109.60
2	D	99	LEU	CA-C-O	-5.54	115.01	120.82
1	E	37	THR	CA-CB-CG2	5.53	119.90	110.50
2	F	60	ASN	CA-CB-CG	5.52	118.12	112.60
1	C	170	ASN	OD1-CG-ND2	-5.51	117.08	122.60
1	A	157	SER	CA-CB-OG	-5.51	100.08	111.10
2	F	76	ARG	N-CA-C	5.49	117.72	111.02
1	C	103	PRO	CA-C-N	-5.47	115.46	122.79
1	C	103	PRO	C-N-CA	-5.47	115.46	122.79
1	A	107	SER	CA-CB-OG	-5.47	100.16	111.10
1	C	283	THR	O-C-N	-5.47	117.10	121.80
2	D	26	HIS	CG-CD2-NE2	-5.47	101.73	107.20
1	E	81	ASN	CA-CB-CG	5.46	118.06	112.60
1	C	73	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	291	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	104	ASN	OD1-CG-ND2	-5.37	117.23	122.60
2	B	56	ILE	N-CA-CB	-5.37	103.06	112.08
1	C	56	HIS	CG-CD2-NE2	-5.36	101.84	107.20
1	A	180	TRP	CG-CD2-CE3	5.34	139.24	133.90
1	A	321	ARG	NE-CZ-NH2	-5.34	114.39	119.20
2	D	159	HIS	CG-CD2-NE2	-5.34	101.86	107.20
1	C	321	ARG	NE-CZ-NH2	-5.33	114.40	119.20
2	D	64	HIS	CG-CD2-NE2	-5.33	101.87	107.20
2	D	56	ILE	N-CA-CB	-5.32	103.14	112.08
1	C	291	ASP	CA-CB-CG	5.32	117.92	112.60
2	F	132	GLU	CA-CB-CG	-5.31	103.47	114.10
1	A	4	PRO	CA-N-CD	-5.31	104.57	112.00
1	C	36	VAL	CA-C-N	5.31	127.65	120.38
1	C	36	VAL	C-N-CA	5.31	127.65	120.38
2	F	11	GLU	N-CA-C	5.30	117.81	111.71
2	D	104	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	53	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	28	THR	N-CA-CB	-5.28	102.50	111.31
1	E	283	THR	O-C-N	-5.27	117.27	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	309	VAL	CB-CA-C	5.27	119.21	110.30
1	E	8	ASN	CA-CB-CG	5.27	117.87	112.60
2	F	56	ILE	N-CA-CB	-5.26	103.23	112.08
2	F	63	PHE	CA-CB-CG	-5.26	108.53	113.80
1	E	159	SER	CA-CB-OG	-5.26	100.58	111.10
1	C	180	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	C	81	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	56	HIS	CG-CD2-NE2	-5.20	102.00	107.20
1	E	110	SER	CA-C-N	5.20	127.55	120.54
1	E	110	SER	C-N-CA	5.20	127.55	120.54
1	E	291	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	170	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	E	170	ASN	OD1-CG-ND2	-5.18	117.42	122.60
2	F	146	ASN	OD1-CG-ND2	-5.17	117.43	122.60
2	D	95	ASN	OD1-CG-ND2	-5.17	117.44	122.60
2	F	3	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	216	ASN	CA-CB-CG	5.16	117.76	112.60
1	E	280	GLU	N-CA-C	5.16	117.80	111.82
1	C	18	HIS	CA-CB-CG	5.15	118.95	113.80
2	F	60	ASN	OD1-CG-ND2	-5.15	117.45	122.60
2	B	63	PHE	CA-CB-CG	-5.14	108.66	113.80
2	D	32	THR	CA-C-O	-5.13	115.43	121.44
1	E	75	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	141	ARG	CA-CB-CG	-5.12	103.85	114.10
1	E	258	PHE	CA-C-N	-5.12	115.02	122.65
1	E	258	PHE	C-N-CA	-5.12	115.02	122.65
1	E	28	THR	N-CA-CB	-5.12	102.77	111.31
2	F	28	ASN	CA-CB-CG	5.11	117.71	112.60
1	C	325	GLU	CB-CG-CD	5.11	121.29	112.60
2	D	132	GLU	CA-CB-CG	-5.11	103.89	114.10
2	B	132	GLU	CA-CB-CG	-5.08	103.94	114.10
2	D	50	GLY	N-CA-C	-5.06	106.37	112.49
2	F	26	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	C	110	SER	CA-C-N	5.05	127.36	120.54
1	C	110	SER	C-N-CA	5.05	127.36	120.54
1	C	180	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	E	34	ILE	N-CA-C	-5.04	101.22	108.48
2	F	104	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	103	PRO	CA-C-N	-5.03	116.05	122.79
1	A	103	PRO	C-N-CA	-5.03	116.05	122.79
1	C	140	LYS	CA-C-N	-5.02	115.98	123.11
1	C	140	LYS	C-N-CA	-5.02	115.98	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	262	THR	CA-CB-OG1	-5.02	102.07	109.60
1	C	115	SER	N-CA-C	-5.01	105.82	111.28
1	E	36	VAL	CA-C-N	5.01	127.24	120.38
1	E	36	VAL	C-N-CA	5.01	127.24	120.38
1	E	3	LEU	CA-C-N	5.00	125.27	119.47
1	E	3	LEU	C-N-CA	5.00	125.27	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2532	588	2473	41	0
1	C	2532	588	2473	42	0
1	E	2532	588	2473	42	0
2	B	1421	331	1345	28	0
2	D	1421	331	1345	31	0
2	F	1421	331	1345	28	0
3	G	39	37	34	1	0
3	J	39	37	34	2	0
3	M	39	37	34	1	0
4	H	43	38	37	0	0
4	I	43	38	37	2	0
4	K	43	38	37	0	0
4	L	43	38	37	2	0
4	N	43	38	37	0	0
4	O	43	38	37	2	0
5	A	42	42	39	0	0
5	B	14	14	13	0	0
5	C	42	42	39	0	0
5	D	14	14	13	0	0
5	E	42	42	39	0	0
5	F	14	14	13	0	0
6	A	13	26	0	1	0
6	B	11	22	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	11	22	0	1	0
6	D	13	26	0	1	0
6	E	12	24	0	1	0
6	F	12	24	0	1	0
All	All	12474	3408	11934	178	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 7.

All (178) 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:321:ARG:HG2	1:A:321:ARG:HH11	1.45	0.81
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.43	0.81
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.46	0.79
2:B:83:TYR:O	2:B:87:THR:HG23	1.93	0.68
2:D:83:TYR:O	2:D:87:THR:HG23	1.95	0.67
2:F:83:TYR:O	2:F:87:THR:HG23	1.95	0.66
2:D:28:ASN:HB2	2:D:144:CYS:O	1.97	0.64
1:E:321:ARG:HG2	1:E:321:ARG:NH1	2.16	0.61
1:E:52:CYS:HB3	1:E:277:CYS:O	2.02	0.60
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.17	0.60
2:F:87:THR:HG22	6:F:405:HOH:O	2.02	0.60
2:B:164:ASP:HB3	2:F:175:GLY:HA3	1.84	0.59
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.83	0.59
2:D:87:THR:HG22	6:D:404:HOH:O	2.02	0.59
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.83	0.59
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.83	0.59
1:A:52:CYS:HB3	1:A:277:CYS:O	2.03	0.58
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.19	0.58
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.69	0.58
1:E:55:PRO:HD3	1:E:278:ILE:HD12	1.86	0.58
1:C:52:CYS:HB3	1:C:277:CYS:O	2.03	0.58
2:B:141:TYR:O	2:B:166:ALA:HA	2.04	0.58
2:B:175:GLY:HA3	2:D:164:ASP:HB3	1.86	0.57
2:B:132:GLU:HG2	2:B:134:GLY:H	1.68	0.57
2:D:132:GLU:HG2	2:D:134:GLY:H	1.69	0.57
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.70	0.57
1:C:180:TRP:HH2	1:C:213:ILE:HD13	1.69	0.56
1:C:283:THR:HG22	1:C:285:ASN:H	1.70	0.56
2:F:132:GLU:HG2	2:F:134:GLY:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HD3	1:A:278:ILE:HD12	1.87	0.56
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.19	0.56
1:C:55:PRO:HD3	1:C:278:ILE:HD12	1.87	0.55
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.22	0.55
1:E:283:THR:HG22	1:E:285:ASN:H	1.71	0.55
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.90	0.54
2:B:87:THR:HG22	6:B:404:HOH:O	2.08	0.53
2:D:141:TYR:O	2:D:166:ALA:HA	2.08	0.53
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.91	0.52
1:C:321:ARG:HG2	1:C:321:ARG:NH1	2.19	0.52
1:A:283:THR:HG22	1:A:285:ASN:H	1.74	0.52
2:F:141:TYR:O	2:F:166:ALA:HA	2.10	0.52
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.46	0.51
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.46	0.51
1:A:25:LEU:HD13	1:A:33:GLN:HB3	1.93	0.51
2:D:87:THR:HG21	2:F:88:LYS:HD2	1.93	0.50
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.46	0.50
1:E:25:LEU:HD13	1:E:33:GLN:HB3	1.94	0.49
1:A:309:VAL:HG22	2:B:93:SER:HA	1.94	0.49
1:C:309:VAL:HG22	2:D:93:SER:HA	1.94	0.49
1:A:77:ASP:O	1:A:80:GLN:HG3	2.13	0.49
1:A:167:THR:HB	3:G:1:NAG:H62	1.95	0.49
1:E:167:THR:HB	3:M:1:NAG:H62	1.95	0.49
1:A:326:LYS:HZ3	2:B:15:GLU:CD	2.21	0.48
1:C:25:LEU:HD13	1:C:33:GLN:HB3	1.95	0.48
1:E:182:ILE:HD13	1:E:213:ILE:HG22	1.96	0.48
1:C:325:GLU:HG2	1:C:325:GLU:O	2.14	0.48
1:E:309:VAL:HG22	2:F:93:SER:HA	1.96	0.48
1:A:182:ILE:HD13	1:A:213:ILE:HG22	1.94	0.48
1:C:167:THR:HB	3:J:1:NAG:H62	1.95	0.48
1:C:77:ASP:O	1:C:80:GLN:HG3	2.13	0.48
1:C:114:SER:HA	1:C:265:SER:O	2.13	0.47
1:C:182:ILE:HD13	1:C:213:ILE:HG22	1.95	0.47
2:D:25:ARG:HG3	2:D:34:GLN:HG3	1.96	0.47
1:E:77:ASP:O	1:E:80:GLN:HG3	2.14	0.47
2:D:91:LEU:HD13	2:F:91:LEU:HD13	1.96	0.47
2:F:143:LYS:NZ	2:F:145:ASP:HB3	2.29	0.47
1:A:21:PRO:O	1:A:327:GLN:HG2	2.14	0.47
2:B:131:GLU:OE1	2:D:127:ARG:NH1	2.48	0.47
1:C:10:THR:HG21	2:D:139:LYS:HE2	1.97	0.47
2:D:143:LYS:NZ	2:D:145:ASP:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:THR:HG23	2:D:105:GLN:OE1	2.13	0.47
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.47	0.46
2:D:175:GLY:HA3	2:F:164:ASP:HB3	1.97	0.46
1:C:53:ASN:OD1	1:C:276:THR:HA	2.14	0.46
1:C:79:PHE:O	1:C:82:GLU:HB2	2.16	0.46
1:E:47:SER:HA	1:E:288:ILE:HG22	1.96	0.46
1:A:28:THR:HG22	1:A:31:ASP:H	1.80	0.46
1:A:269:ARG:NH1	4:I:3:SIA:H112	2.31	0.46
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.49	0.46
1:E:10:THR:HG21	2:F:139:LYS:HE2	1.97	0.46
1:A:47:SER:HA	1:A:288:ILE:HG22	1.96	0.46
1:A:59:LEU:HD23	1:A:87:PHE:CD2	2.51	0.45
1:A:284:PRO:HG2	1:A:298:ASN:ND2	2.30	0.45
1:C:284:PRO:HG2	1:C:298:ASN:ND2	2.31	0.45
1:C:28:THR:HG22	1:C:31:ASP:H	1.81	0.45
1:C:47:SER:HA	1:C:288:ILE:HG22	1.98	0.45
2:F:72:GLU:HG2	4:O:3:SIA:H32	1.98	0.45
1:A:10:THR:HG21	2:B:139:LYS:HE2	1.98	0.45
1:C:59:LEU:HD23	1:C:87:PHE:CD2	2.51	0.45
1:C:269:ARG:NH1	4:L:3:SIA:H112	2.32	0.45
2:D:72:GLU:HG2	4:L:3:SIA:H32	1.99	0.45
1:A:97:CYS:HA	1:A:139:CYS:HA	1.98	0.45
1:C:97:CYS:HA	1:C:139:CYS:HA	1.98	0.45
2:B:58:LYS:HE2	2:B:59:THR:O	2.17	0.45
1:E:28:THR:HG22	1:E:31:ASP:H	1.81	0.45
2:B:72:GLU:HG2	4:I:3:SIA:H32	1.99	0.45
1:E:284:PRO:HG2	1:E:298:ASN:ND2	2.32	0.45
1:E:114:SER:HA	1:E:265:SER:O	2.17	0.44
2:D:127:ARG:HB3	2:D:128:GLU:H	1.69	0.44
1:E:28:THR:HG23	2:F:105:GLN:OE1	2.17	0.44
1:E:326:LYS:HD2	1:E:327:GLN:H	1.82	0.44
1:E:259:LYS:HB2	1:E:259:LYS:NZ	2.33	0.44
2:F:110:LEU:O	2:F:113:SER:HB3	2.17	0.44
1:A:114:SER:HA	1:A:265:SER:O	2.18	0.44
1:C:37:THR:HG21	6:C:357:HOH:O	2.18	0.44
1:E:269:ARG:NH1	4:O:3:SIA:H112	2.32	0.44
2:D:47:GLN:HB3	2:D:110:LEU:HD11	2.00	0.44
1:E:79:PHE:O	1:E:82:GLU:HB2	2.17	0.44
1:E:180:TRP:CH2	1:E:213:ILE:HD13	2.52	0.44
2:D:58:LYS:HE2	2:D:59:THR:O	2.18	0.44
1:C:56:HIS:ND1	1:C:264:LYS:NZ	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:THR:HG23	2:B:105:GLN:OE1	2.18	0.43
2:B:143:LYS:NZ	2:B:145:ASP:HB3	2.33	0.43
2:F:58:LYS:HE2	2:F:59:THR:O	2.17	0.43
1:A:14:CYS:HA	2:B:137:CYS:HA	2.00	0.43
1:C:14:CYS:HA	2:D:137:CYS:HA	2.00	0.43
2:B:88:LYS:HD2	2:F:87:THR:HG21	1.99	0.43
2:B:110:LEU:O	2:B:113:SER:HB3	2.19	0.43
2:B:58:LYS:HG3	2:B:59:THR:O	2.18	0.43
1:C:89:GLU:OE1	1:C:109:ARG:NH1	2.51	0.43
1:E:59:LEU:HD23	1:E:87:PHE:CD2	2.53	0.43
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.52	0.43
1:A:57:ARG:NH2	1:A:82:GLU:OE1	2.52	0.43
1:C:180:TRP:CH2	1:C:213:ILE:HD13	2.51	0.43
1:E:97:CYS:HA	1:E:139:CYS:HA	1.99	0.43
1:A:56:HIS:ND1	1:A:264:LYS:NZ	2.66	0.43
2:B:128:GLU:HG3	2:B:170:ARG:HH21	1.84	0.43
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.66	0.42
1:C:313:THR:OG1	1:C:315:LYS:NZ	2.52	0.42
1:A:259:LYS:HB2	1:A:259:LYS:NZ	2.34	0.42
1:A:221:PRO:HA	3:J:2:NAG:O7	2.18	0.42
2:B:17:MET:HE1	2:B:23:GLY:HA3	2.01	0.42
1:C:311:GLN:HE22	2:D:97:GLU:HB2	1.84	0.42
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.55	0.42
1:E:313:THR:OG1	1:E:315:LYS:NZ	2.53	0.42
1:A:77:ASP:CG	1:A:141:ARG:HH21	2.28	0.42
2:F:47:GLN:HB3	2:F:110:LEU:HD11	2.01	0.42
1:C:1:GLN:OE1	1:C:1:GLN:HA	2.18	0.42
1:C:77:ASP:CG	1:C:141:ARG:HH21	2.27	0.42
2:D:58:LYS:HG3	2:D:59:THR:O	2.20	0.42
1:E:37:THR:HG21	6:E:357:HOH:O	2.18	0.42
1:A:37:THR:HG21	6:A:357:HOH:O	2.19	0.42
2:D:131:GLU:OE1	2:F:127:ARG:NH1	2.52	0.42
2:D:17:MET:HE1	2:D:23:GLY:HA3	2.02	0.41
2:D:68:LYS:O	2:D:69:GLU:HG3	2.20	0.41
1:E:141:ARG:NH1	1:E:147:PHE:O	2.48	0.41
2:D:26:HIS:CD2	2:D:149:ILE:HG13	2.55	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.02	0.41
1:A:75:HIS:HE1	1:A:94:PHE:O	2.04	0.41
1:A:141:ARG:NH1	1:A:147:PHE:O	2.49	0.41
2:F:58:LYS:HG3	2:F:59:THR:O	2.20	0.41
2:F:150:GLU:OE2	2:F:153:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD22	1:A:267:ILE:HD12	2.03	0.41
1:C:53:ASN:HD21	1:C:276:THR:HG23	1.85	0.41
1:A:10:THR:HG22	2:B:141:TYR:HA	2.03	0.41
1:C:182:ILE:HD11	1:C:215:PRO:HD3	2.03	0.41
1:C:325:GLU:HB2	2:D:12:ASN:ND2	2.35	0.41
1:E:10:THR:HG22	2:F:141:TYR:HA	2.02	0.41
1:E:182:ILE:HD11	1:E:215:PRO:HD3	2.02	0.41
2:D:26:HIS:CE1	2:D:149:ILE:HG21	2.55	0.41
1:A:75:HIS:CE1	1:A:94:PHE:O	2.74	0.41
1:C:259:LYS:NZ	1:C:259:LYS:HB2	2.35	0.41
1:A:139:CYS:HB3	1:A:146:GLY:O	2.21	0.41
1:A:325:GLU:HB2	2:B:13:GLY:O	2.21	0.41
1:E:139:CYS:HB3	1:E:146:GLY:O	2.21	0.41
1:E:283:THR:HG22	1:E:285:ASN:N	2.36	0.41
1:A:202:VAL:O	1:A:212:THR:HA	2.22	0.40
1:C:168:MET:HA	1:C:169:PRO:HD3	1.88	0.40
1:E:11:ALA:HB3	2:F:140:ILE:HB	2.03	0.40
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.22	0.40
1:A:168:MET:HA	1:A:169:PRO:HD3	1.87	0.40
2:B:123:ARG:HH11	2:B:123:ARG:HD3	1.72	0.40
1:C:111:LEU:HD21	1:C:236:ILE:HD11	2.03	0.40
1:C:288:ILE:HG21	1:C:297:VAL:HG21	2.03	0.40
1:E:77:ASP:CG	1:E:141:ARG:HH21	2.29	0.40
2:D:110:LEU:O	2:D:113:SER:HB3	2.22	0.40
1:E:203:THR:HA	1:E:211:GLN:O	2.21	0.40
1:E:311:GLN:HE22	2:F:97:GLU:HB2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	326/328 (99%)	304 (93%)	17 (5%)	5 (2%)	8	28
1	C	326/328 (99%)	307 (94%)	16 (5%)	3 (1%)	14	41
1	E	326/328 (99%)	309 (95%)	16 (5%)	1 (0%)	36	65
2	B	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	7	26
2	D	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	7	26
2	F	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	7	26
All	All	1497/1509 (99%)	1400 (94%)	79 (5%)	18 (1%)	10	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	326	LYS
2	B	58	LYS
2	B	173	ILE
2	D	58	LYS
2	D	173	ILE
2	F	58	LYS
2	F	173	ILE
1	A	327	GLN
1	C	326	LYS
2	B	172	GLN
2	D	172	GLN
2	F	172	GLN
1	A	2	ASP
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
1	C	4	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/289 (100%)	261 (90%)	28 (10%)	8	25
1	C	289/289 (100%)	262 (91%)	27 (9%)	8	27
1	E	289/289 (100%)	261 (90%)	28 (10%)	8	25
2	B	149/149 (100%)	142 (95%)	7 (5%)	23	56
2	D	149/149 (100%)	142 (95%)	7 (5%)	23	56
2	F	149/149 (100%)	140 (94%)	9 (6%)	17	47
All	All	1314/1314 (100%)	1208 (92%)	106 (8%)	11	33

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	8	ASN
1	A	28	THR
1	A	31	ASP
1	A	34	ILE
1	A	37	THR
1	A	54	ASN
1	A	82	GLU
1	A	103	PRO
1	A	111	LEU
1	A	155	THR
1	A	156	LYS
1	A	157	SER
1	A	160	THR
1	A	199	SER
1	A	210	GLN
1	A	228	SER
1	A	248	ASN
1	A	259	LYS
1	A	265	SER
1	A	277	CYS
1	A	278	ILE
1	A	280	GLU
1	A	283	THR
1	A	309	VAL
1	A	318	THR
1	A	321	ARG

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Mol	Chain	Res	Type
1	A	326	LYS
2	B	77	ILE
2	B	110	LEU
2	B	127	ARG
2	B	128	GLU
2	B	153	ARG
2	B	160	ASP
2	B	172	GLN
1	C	3	LEU
1	C	8	ASN
1	C	28	THR
1	C	31	ASP
1	C	34	ILE
1	C	37	THR
1	C	54	ASN
1	C	58	ILE
1	C	103	PRO
1	C	111	LEU
1	C	114	SER
1	C	155	THR
1	C	159	SER
1	C	160	THR
1	C	199	SER
1	C	210	GLN
1	C	228	SER
1	C	248	ASN
1	C	259	LYS
1	C	265	SER
1	C	277	CYS
1	C	278	ILE
1	C	280	GLU
1	C	283	THR
1	C	309	VAL
1	C	318	THR
1	C	321	ARG
2	D	77	ILE
2	D	127	ARG
2	D	128	GLU
2	D	150	GLU
2	D	153	ARG
2	D	160	ASP
2	D	172	GLN

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Mol	Chain	Res	Type
1	E	2	ASP
1	E	8	ASN
1	E	28	THR
1	E	31	ASP
1	E	34	ILE
1	E	37	THR
1	E	54	ASN
1	E	82	GLU
1	E	103	PRO
1	E	111	LEU
1	E	155	THR
1	E	159	SER
1	E	160	THR
1	E	189	GLN
1	E	199	SER
1	E	210	GLN
1	E	228	SER
1	E	248	ASN
1	E	259	LYS
1	E	265	SER
1	E	277	CYS
1	E	278	ILE
1	E	280	GLU
1	E	283	THR
1	E	309	VAL
1	E	321	ARG
1	E	326	LYS
1	E	328	THR
2	F	11	GLU
2	F	29	SER
2	F	77	ILE
2	F	127	ARG
2	F	128	GLU
2	F	150	GLU
2	F	153	ARG
2	F	160	ASP
2	F	172	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN

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Mol	Chain	Res	Type
1	A	171	ASN
2	B	27	GLN
2	B	49	ASN
2	B	172	GLN
1	C	132	GLN
1	C	171	ASN
2	D	12	ASN
2	D	49	ASN
2	D	172	GLN
1	E	8	ASN
1	E	132	GLN
1	E	171	ASN
2	F	26	HIS
2	F	42	GLN
2	F	49	ASN
2	F	172	GLN

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 ⓘ

27 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.65	0	17,19,21	0.72	0
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	G	3	3	11,11,12	0.35	0	15,15,17	1.03	2 (13%)
4	BGC	H	1	4	12,12,12	1.33	1 (8%)	17,17,17	1.01	1 (5%)
4	GAL	H	2	4	11,11,12	0.53	0	15,15,17	1.20	1 (6%)
4	SIA	H	3	4	20,20,21	0.93	2 (10%)	21,28,31	1.66	7 (33%)
4	BGC	I	1	4	12,12,12	0.52	0	17,17,17	0.81	0
4	GAL	I	2	4	11,11,12	0.59	0	15,15,17	1.18	2 (13%)
4	SIA	I	3	4	20,20,21	1.03	2 (10%)	21,28,31	1.63	7 (33%)
3	NAG	J	1	1,3	14,14,15	0.77	0	17,19,21	0.85	0
3	NAG	J	2	3	14,14,15	0.50	0	17,19,21	0.90	1 (5%)
3	BMA	J	3	3	11,11,12	0.81	0	15,15,17	1.47	2 (13%)
4	BGC	K	1	4	12,12,12	1.33	1 (8%)	17,17,17	0.94	1 (5%)
4	GAL	K	2	4	11,11,12	0.66	0	15,15,17	1.21	2 (13%)
4	SIA	K	3	4	20,20,21	0.88	1 (5%)	21,28,31	1.55	5 (23%)
4	BGC	L	1	4	12,12,12	0.56	0	17,17,17	0.73	0
4	GAL	L	2	4	11,11,12	0.64	0	15,15,17	1.20	2 (13%)
4	SIA	L	3	4	20,20,21	1.01	2 (10%)	21,28,31	1.60	6 (28%)
3	NAG	M	1	1,3	14,14,15	0.70	0	17,19,21	0.83	0
3	NAG	M	2	3	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
3	BMA	M	3	3	11,11,12	0.91	0	15,15,17	1.07	1 (6%)
4	BGC	N	1	4	12,12,12	1.20	1 (8%)	17,17,17	0.99	1 (5%)
4	GAL	N	2	4	11,11,12	0.62	0	15,15,17	1.23	1 (6%)
4	SIA	N	3	4	20,20,21	0.93	1 (5%)	21,28,31	1.64	7 (33%)
4	BGC	O	1	4	12,12,12	0.48	0	17,17,17	0.69	0
4	GAL	O	2	4	11,11,12	0.67	0	15,15,17	1.20	2 (13%)
4	SIA	O	3	4	20,20,21	1.01	2 (10%)	21,28,31	1.67	7 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	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
4	BGC	H	1	4	-	2/2/22/22	0/1/1/1
4	GAL	H	2	4	-	1/2/19/22	0/1/1/1
4	SIA	H	3	4	-	1/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	I	1	4	-	0/2/22/22	0/1/1/1
4	GAL	I	2	4	-	1/2/19/22	0/1/1/1
4	SIA	I	3	4	-	0/18/34/38	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
4	BGC	K	1	4	-	2/2/22/22	0/1/1/1
4	GAL	K	2	4	-	1/2/19/22	0/1/1/1
4	SIA	K	3	4	-	1/18/34/38	0/1/1/1
4	BGC	L	1	4	-	0/2/22/22	0/1/1/1
4	GAL	L	2	4	-	1/2/19/22	0/1/1/1
4	SIA	L	3	4	-	0/18/34/38	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
4	BGC	N	1	4	-	2/2/22/22	0/1/1/1
4	GAL	N	2	4	-	1/2/19/22	0/1/1/1
4	SIA	N	3	4	-	1/18/34/38	0/1/1/1
4	BGC	O	1	4	-	0/2/22/22	0/1/1/1
4	GAL	O	2	4	-	1/2/19/22	0/1/1/1
4	SIA	O	3	4	-	0/18/34/38	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	SIA	C2-C1	3.13	1.56	1.52
4	H	1	BGC	C4-C5	3.06	1.59	1.53
4	K	1	BGC	C4-C5	2.95	1.59	1.53
4	O	3	SIA	C2-C1	2.92	1.55	1.52
4	N	1	BGC	C4-C5	2.80	1.59	1.53
4	L	3	SIA	C2-C1	2.74	1.55	1.52
4	K	3	SIA	O1B-C1	-2.48	1.22	1.30
4	N	3	SIA	O1B-C1	-2.43	1.22	1.30
4	H	3	SIA	O1B-C1	-2.42	1.22	1.30
4	I	3	SIA	O1B-C1	-2.09	1.24	1.30
4	O	3	SIA	O1B-C1	-2.07	1.24	1.30
4	L	3	SIA	O1B-C1	-2.07	1.24	1.30
4	H	3	SIA	C2-C1	2.06	1.54	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	3	BMA	C1-O5-C5	4.17	117.78	112.19
4	L	2	GAL	C1-O5-C5	3.75	117.21	112.19
4	O	2	GAL	C1-O5-C5	3.75	117.21	112.19
4	I	2	GAL	C1-O5-C5	3.62	117.03	112.19
4	H	2	GAL	C1-O5-C5	3.09	116.33	112.19
4	K	3	SIA	C4-C5-N5	-3.07	104.39	110.44
4	H	3	SIA	O1B-C1-C2	2.98	120.45	112.71
4	N	2	GAL	C1-O5-C5	2.96	116.15	112.19
4	I	3	SIA	O1B-C1-C2	2.96	120.40	112.71
4	O	3	SIA	O1B-C1-C2	2.95	120.39	112.71
4	L	3	SIA	O1B-C1-C2	2.92	120.31	112.71
4	K	2	GAL	C1-O5-C5	2.92	116.10	112.19
4	O	3	SIA	O9-C9-C8	-2.90	105.07	111.16
4	I	3	SIA	O6-C2-C3	-2.89	106.67	110.56
4	O	3	SIA	C11-C10-N5	2.87	120.88	116.12
4	N	3	SIA	O1B-C1-C2	2.84	120.10	112.71
4	K	3	SIA	O1B-C1-C2	2.83	120.08	112.71
4	I	3	SIA	C11-C10-N5	2.78	120.73	116.12
4	I	3	SIA	O9-C9-C8	-2.75	105.39	111.16
4	N	3	SIA	O6-C2-C1	2.71	112.84	107.72
4	L	3	SIA	O6-C2-C3	-2.70	106.92	110.56
4	K	3	SIA	C6-C5-N5	2.68	115.18	110.91
4	H	3	SIA	C11-C10-N5	2.67	120.55	116.12
4	L	3	SIA	C11-C10-N5	2.60	120.43	116.12
3	J	3	BMA	C6-C5-C4	-2.58	106.69	113.02
4	N	3	SIA	C4-C5-N5	-2.56	105.39	110.44
4	L	3	SIA	O9-C9-C8	-2.55	105.80	111.16
4	H	3	SIA	C4-C5-N5	-2.52	105.47	110.44
4	H	3	SIA	O6-C2-C1	2.48	112.40	107.72
4	H	1	BGC	C4-C3-C2	-2.47	106.49	110.83
4	N	3	SIA	C6-C5-N5	2.46	114.82	110.91
4	N	3	SIA	C11-C10-N5	2.44	120.17	116.12
4	N	1	BGC	C4-C3-C2	-2.39	106.63	110.83
3	G	3	BMA	C1-O5-C5	2.38	115.38	112.19
4	N	3	SIA	O9-C9-C8	-2.38	106.16	111.16
4	H	3	SIA	C6-C5-N5	2.37	114.69	110.91
4	O	3	SIA	O6-C2-C3	-2.37	107.37	110.56
3	G	2	NAG	C4-C3-C2	-2.35	107.57	111.02
3	M	2	NAG	C4-C3-C2	-2.33	107.61	111.02
4	O	2	GAL	C2-C3-C4	-2.30	106.82	110.86
3	M	3	BMA	O5-C5-C6	2.28	112.10	107.66
4	H	3	SIA	O9-C9-C8	-2.25	106.43	111.16
4	O	3	SIA	O10-C10-C11	-2.23	118.09	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	SIA	O10-C10-C11	-2.22	118.09	122.05
4	O	3	SIA	C6-C5-N5	2.21	114.43	110.91
4	I	2	GAL	C2-C3-C4	-2.20	106.99	110.86
4	L	3	SIA	C8-C7-C6	-2.20	108.93	113.05
4	L	3	SIA	O10-C10-C11	-2.16	118.21	122.05
4	K	1	BGC	C4-C3-C2	-2.15	107.05	110.83
3	J	2	NAG	C4-C3-C2	-2.15	107.87	111.02
4	O	3	SIA	C8-C7-C6	-2.11	109.08	113.05
4	L	2	GAL	C2-C3-C4	-2.10	107.18	110.86
4	K	2	GAL	O2-C2-C1	2.06	113.94	109.22
4	N	3	SIA	O1B-C1-O1A	-2.06	119.42	124.08
3	G	3	BMA	C1-C2-C3	-2.05	106.65	109.64
4	K	3	SIA	C11-C10-N5	2.03	119.49	116.12
4	K	3	SIA	O6-C2-C1	2.03	111.55	107.72
4	H	3	SIA	O1B-C1-O1A	-2.02	119.50	124.08
4	I	3	SIA	O1B-C1-O1A	-2.01	119.52	124.08
4	I	3	SIA	C8-C7-C6	-2.00	109.30	113.05

There are no chirality outliers.

All (15) torsion outliers are listed below:

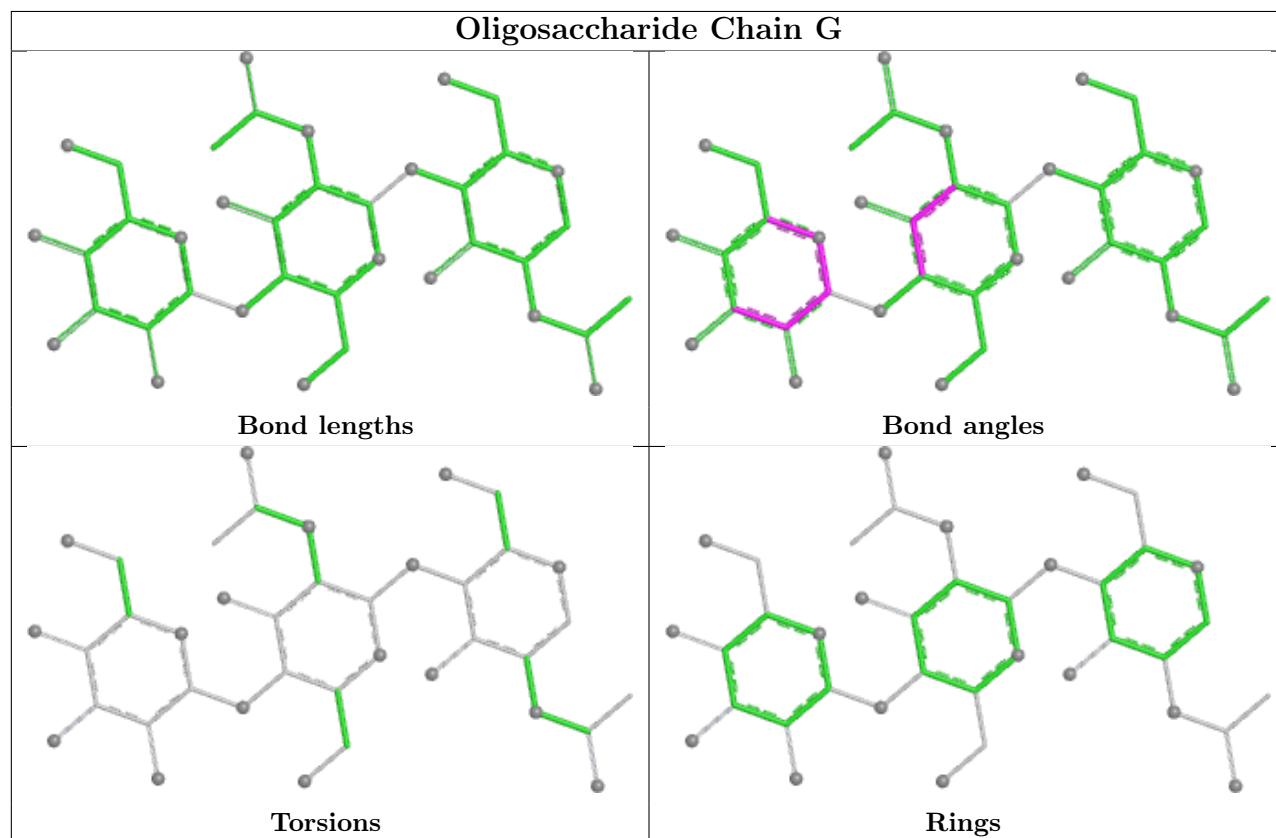
Mol	Chain	Res	Type	Atoms
4	N	1	BGC	O5-C5-C6-O6
4	H	1	BGC	O5-C5-C6-O6
4	K	1	BGC	O5-C5-C6-O6
4	L	2	GAL	O5-C5-C6-O6
4	I	2	GAL	O5-C5-C6-O6
4	O	2	GAL	O5-C5-C6-O6
4	H	1	BGC	C4-C5-C6-O6
4	N	1	BGC	C4-C5-C6-O6
4	N	2	GAL	O5-C5-C6-O6
4	K	1	BGC	C4-C5-C6-O6
4	H	2	GAL	O5-C5-C6-O6
4	H	3	SIA	O8-C8-C9-O9
4	K	2	GAL	O5-C5-C6-O6
4	N	3	SIA	O8-C8-C9-O9
4	K	3	SIA	O8-C8-C9-O9

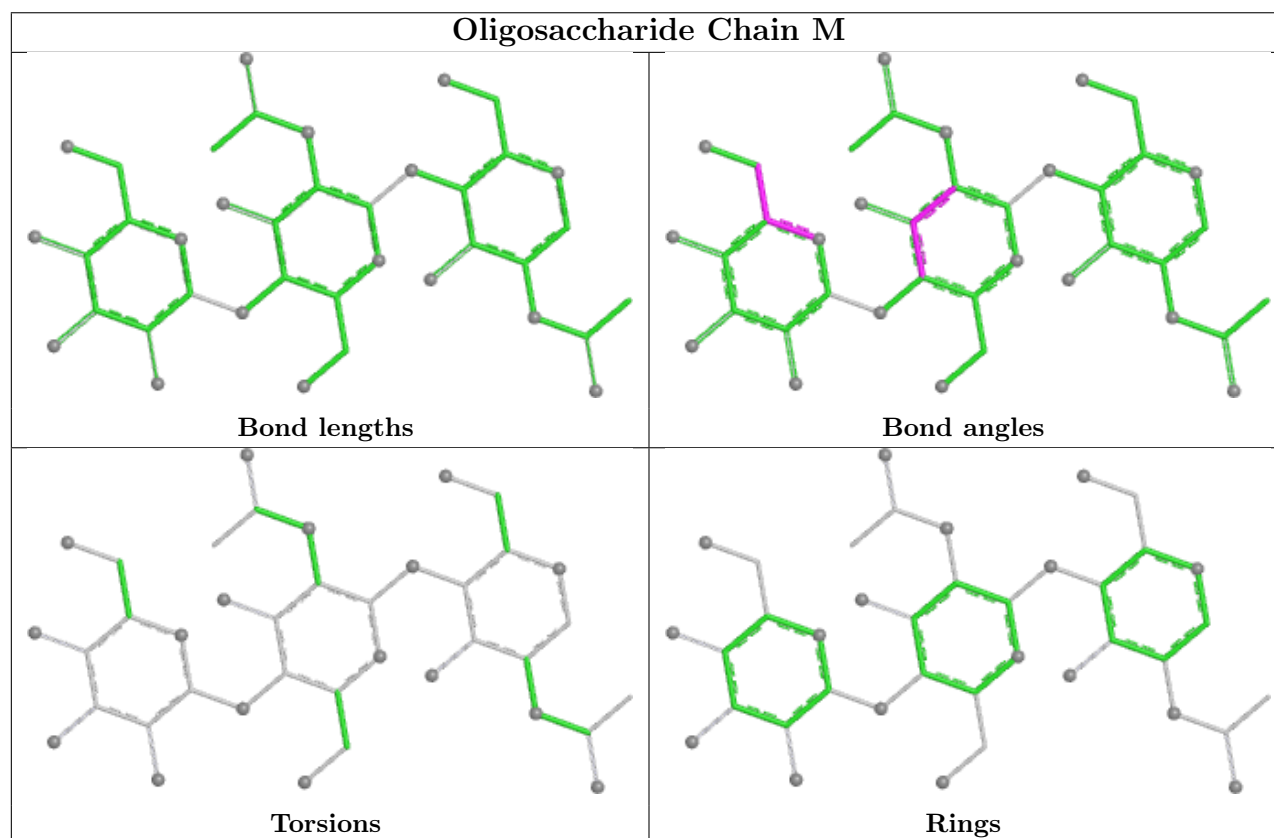
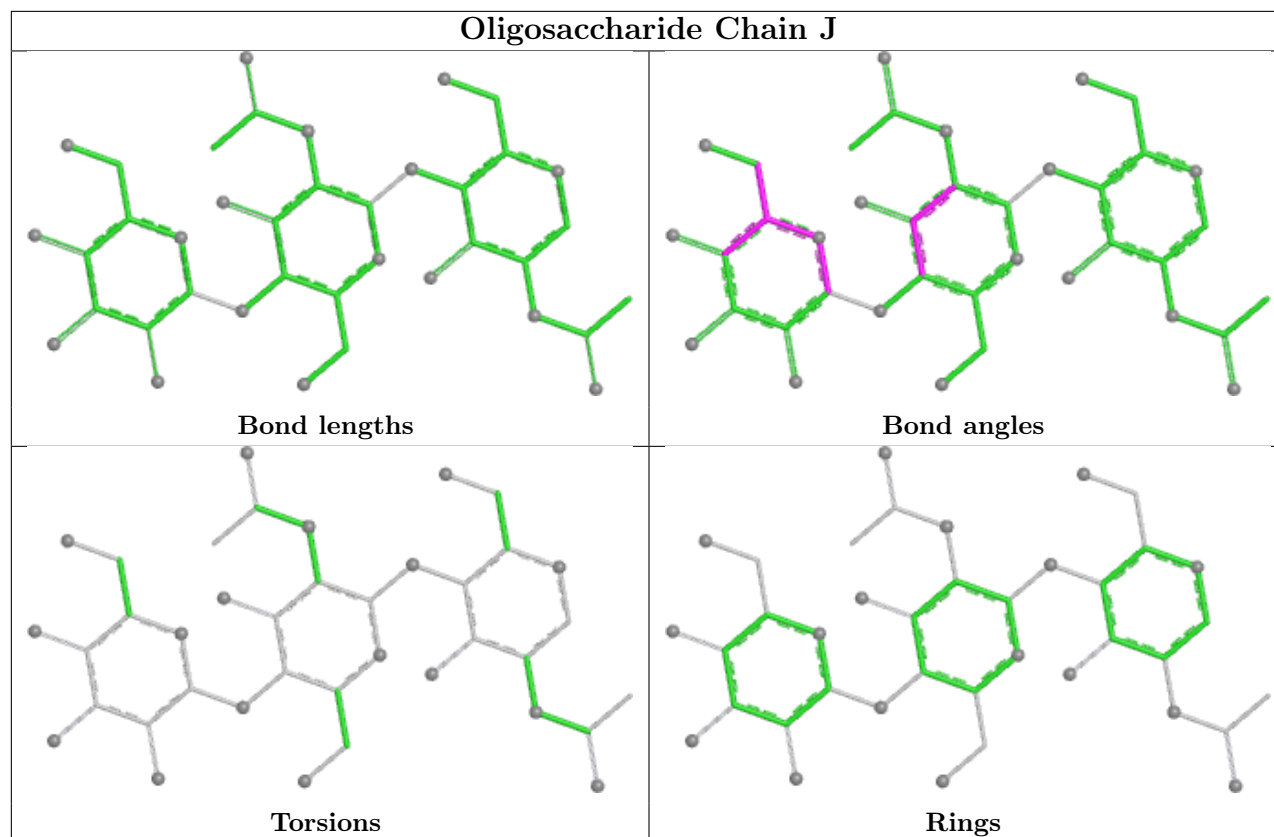
There are no ring outliers.

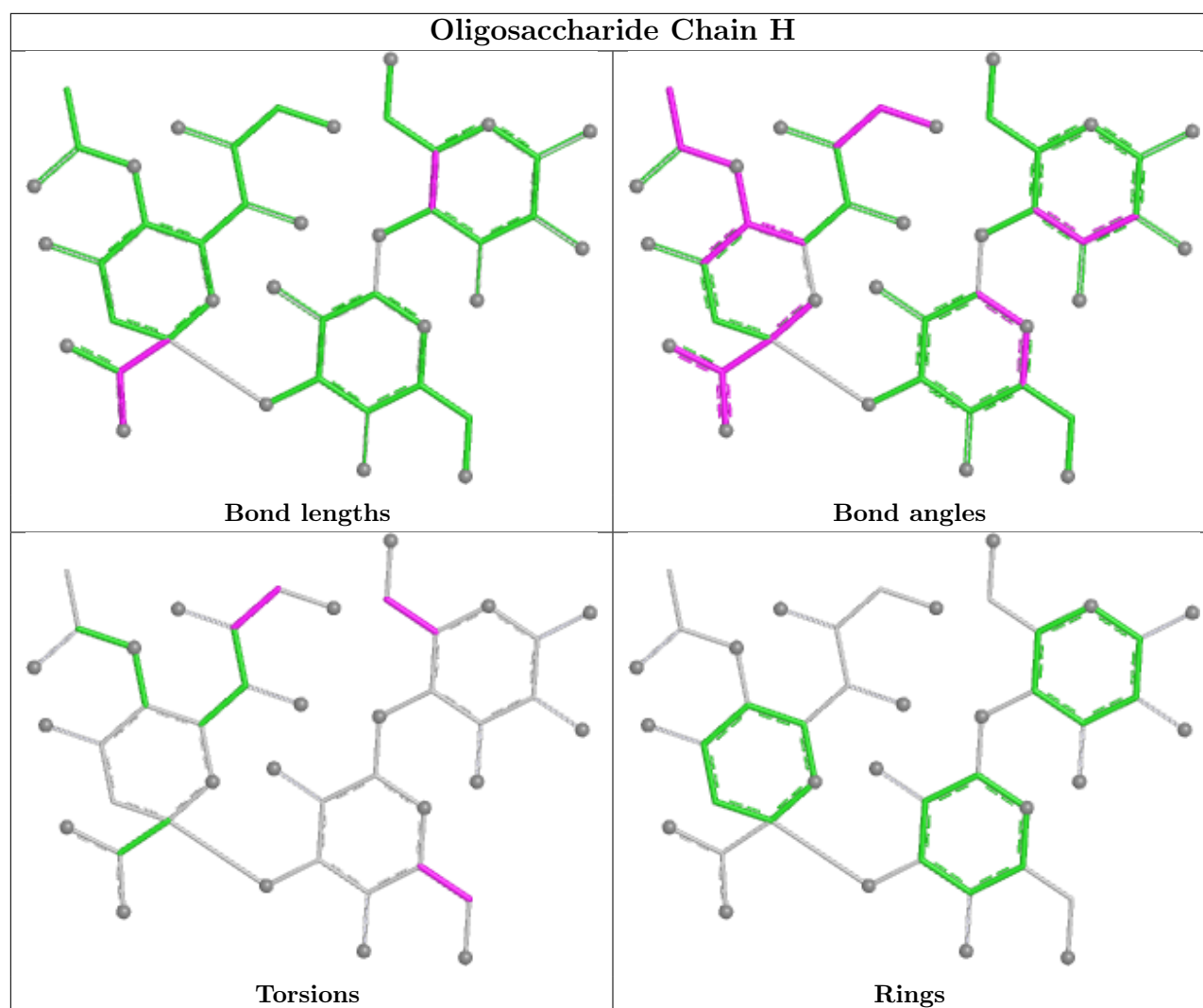
7 monomers are involved in 10 short contacts:

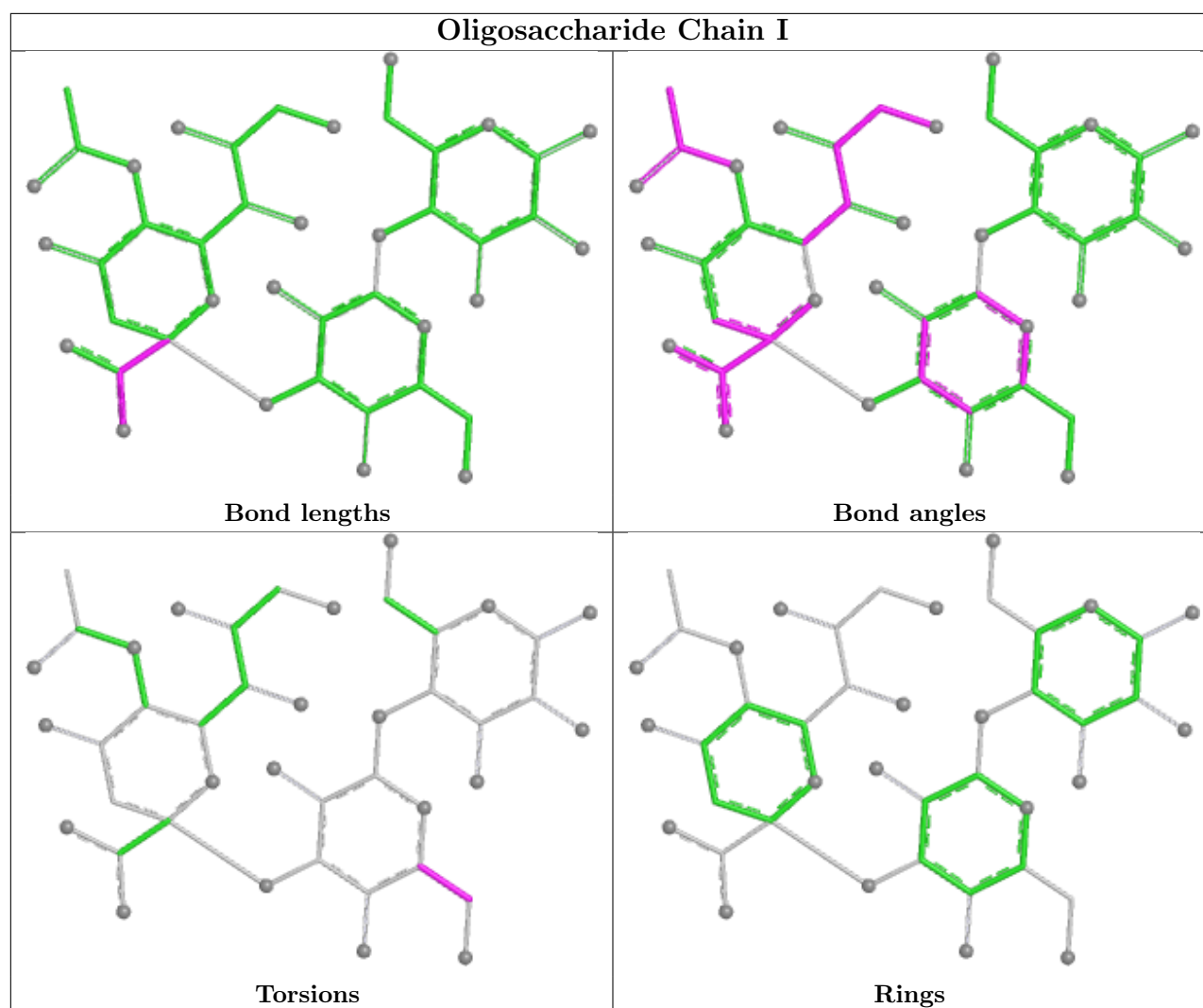
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
4	L	3	SIA	2	0
3	M	1	NAG	1	0
4	O	3	SIA	2	0
3	J	1	NAG	1	0
3	J	2	NAG	1	0
4	I	3	SIA	2	0

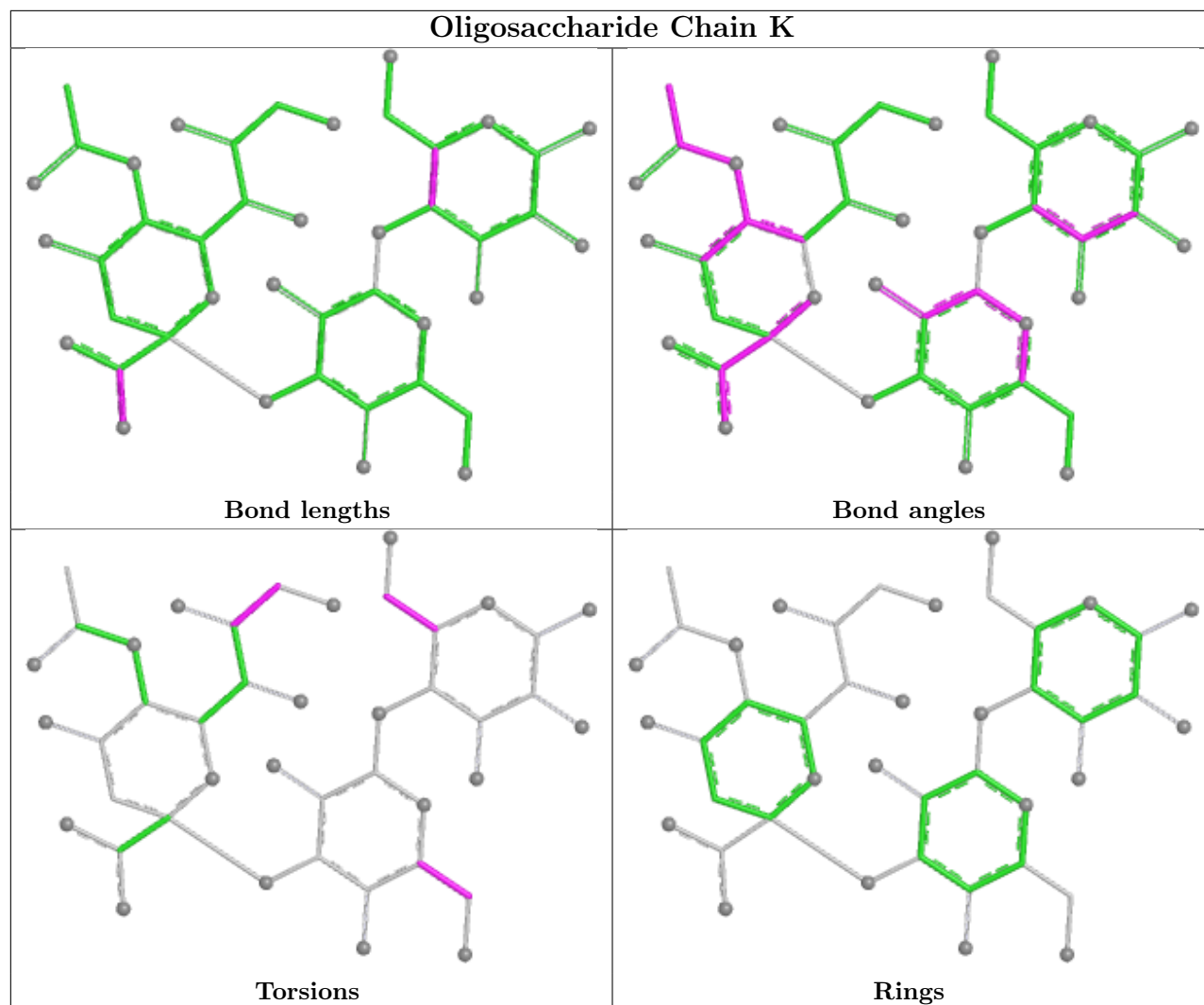
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

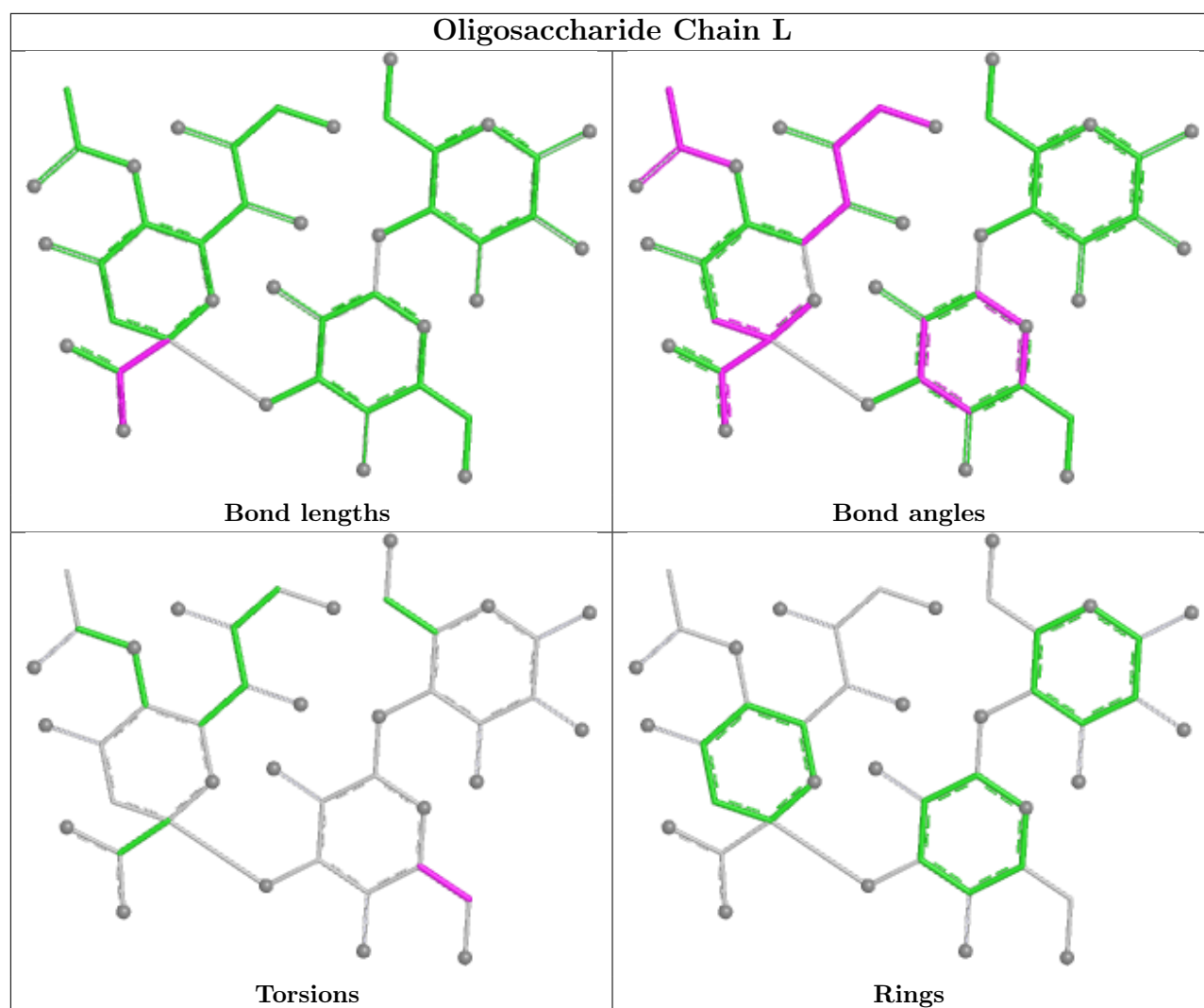


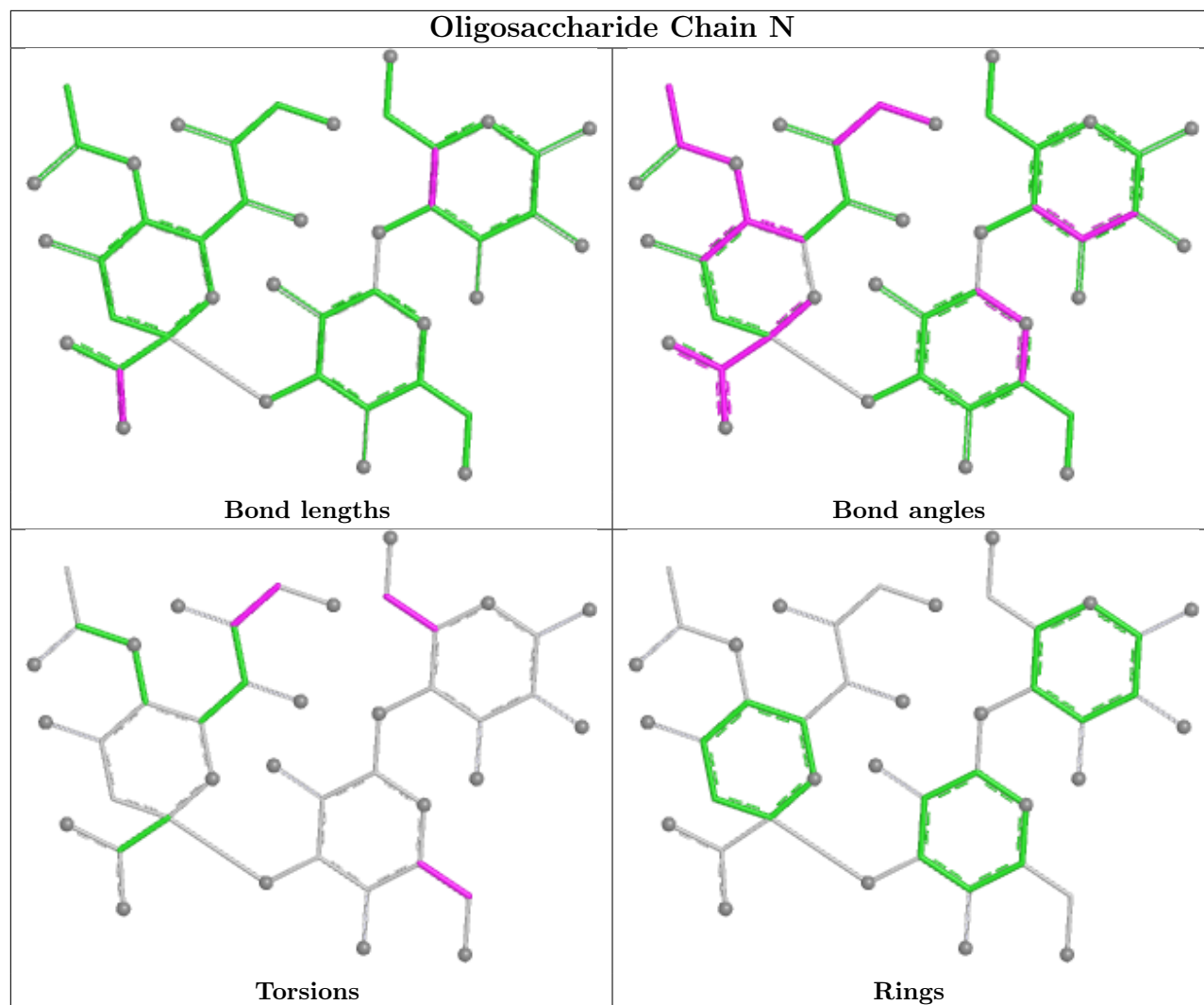


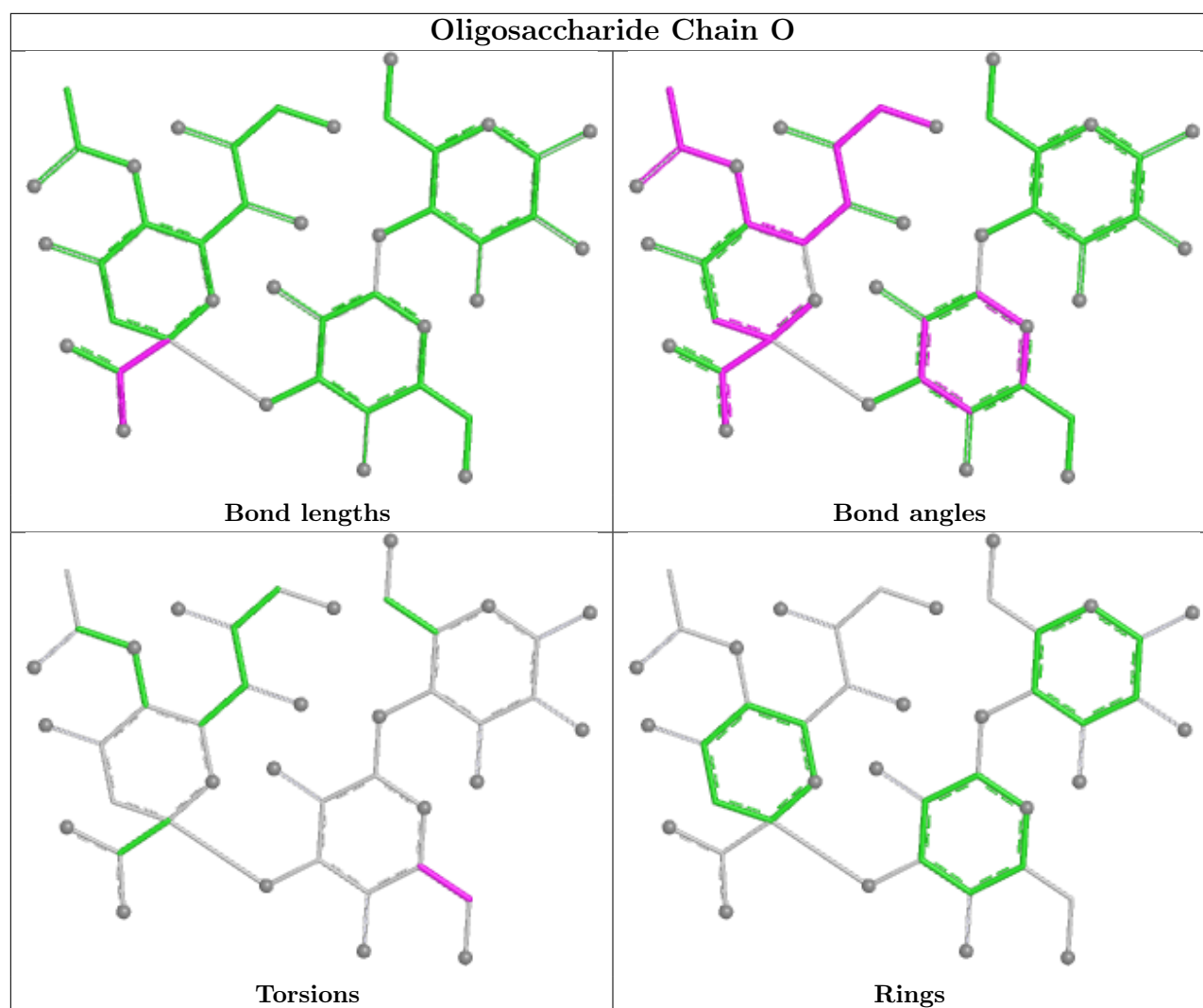












5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	F	401	2	14,14,15	0.91	1 (7%)	17,19,21	1.33	1 (5%)
5	NAG	C	334	1	14,14,15	0.82	0	17,19,21	1.42	1 (5%)
5	NAG	D	401	2	14,14,15	0.87	0	17,19,21	1.34	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	348	1	14,14,15	0.92	1 (7%)	17,19,21	1.45	4 (23%)
5	NAG	C	348	1	14,14,15	0.69	0	17,19,21	1.58	4 (23%)
5	NAG	A	334	1	14,14,15	0.71	0	17,19,21	1.36	2 (11%)
5	NAG	B	401	2	14,14,15	0.86	0	17,19,21	1.28	1 (5%)
5	NAG	E	329	1	14,14,15	0.85	0	17,19,21	1.07	1 (5%)
5	NAG	A	329	1	14,14,15	0.87	1 (7%)	17,19,21	1.11	1 (5%)
5	NAG	C	329	1	14,14,15	0.70	0	17,19,21	1.11	1 (5%)
5	NAG	E	334	1	14,14,15	0.79	0	17,19,21	1.38	2 (11%)
5	NAG	E	348	1	14,14,15	0.80	0	17,19,21	1.53	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	401	2	-	0/6/23/26	0/1/1/1
5	NAG	C	334	1	-	0/6/23/26	0/1/1/1
5	NAG	D	401	2	-	0/6/23/26	0/1/1/1
5	NAG	A	348	1	-	2/6/23/26	0/1/1/1
5	NAG	C	348	1	-	2/6/23/26	0/1/1/1
5	NAG	A	334	1	-	0/6/23/26	0/1/1/1
5	NAG	B	401	2	-	0/6/23/26	0/1/1/1
5	NAG	E	329	1	-	0/6/23/26	0/1/1/1
5	NAG	A	329	1	-	0/6/23/26	0/1/1/1
5	NAG	C	329	1	-	0/6/23/26	0/1/1/1
5	NAG	E	334	1	-	0/6/23/26	0/1/1/1
5	NAG	E	348	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	348	NAG	C1-C2	2.24	1.55	1.52
5	F	401	NAG	C4-C5	2.12	1.57	1.53
5	A	329	NAG	C4-C5	2.08	1.57	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	401	NAG	C1-O5-C5	3.77	117.23	112.19
5	D	401	NAG	C1-O5-C5	3.60	117.01	112.19
5	C	348	NAG	C1-O5-C5	3.48	116.85	112.19
5	B	401	NAG	C1-O5-C5	3.41	116.75	112.19
5	A	348	NAG	C1-O5-C5	3.21	116.49	112.19
5	E	348	NAG	C1-O5-C5	2.94	116.12	112.19
5	E	348	NAG	C8-C7-N2	2.71	120.62	116.12
5	A	334	NAG	C1-O5-C5	2.65	115.73	112.19
5	E	334	NAG	C1-O5-C5	2.59	115.66	112.19
5	C	348	NAG	C8-C7-N2	2.58	120.39	116.12
5	C	334	NAG	C1-O5-C5	2.50	115.53	112.19
5	E	348	NAG	C3-C4-C5	-2.48	105.73	110.23
5	A	348	NAG	C3-C4-C5	-2.24	106.17	110.23
5	E	348	NAG	O4-C4-C5	2.18	114.70	109.32
5	A	334	NAG	C1-C2-N2	2.18	113.87	110.43
5	C	348	NAG	C3-C4-C5	-2.18	106.28	110.23
5	E	334	NAG	C1-C2-N2	2.18	113.86	110.43
5	C	329	NAG	C1-O5-C5	2.13	115.05	112.19
5	A	348	NAG	C8-C7-N2	2.13	119.64	116.12
5	C	348	NAG	O4-C4-C5	2.11	114.51	109.32
5	A	348	NAG	O4-C4-C5	2.10	114.49	109.32
5	E	329	NAG	C1-O5-C5	2.07	114.97	112.19
5	A	329	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	348	NAG	O5-C5-C6-O6
5	C	348	NAG	O5-C5-C6-O6
5	E	348	NAG	O5-C5-C6-O6
5	A	348	NAG	C4-C5-C6-O6
5	C	348	NAG	C4-C5-C6-O6
5	E	348	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/328 (100%)	-0.07	16 (4%) 35 27	5, 21, 42, 135	0
1	C	328/328 (100%)	-0.01	22 (6%) 24 19	5, 21, 41, 141	0
1	E	328/328 (100%)	-0.12	19 (5%) 29 22	5, 21, 41, 138	0
2	B	175/175 (100%)	-0.17	6 (3%) 48 39	2, 16, 39, 88	0
2	D	175/175 (100%)	-0.14	9 (5%) 33 26	2, 16, 38, 88	0
2	F	175/175 (100%)	-0.30	6 (3%) 48 39	2, 16, 38, 88	0
All	All	1509/1509 (100%)	-0.11	78 (5%) 33 26	2, 20, 41, 141	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	8	ASN	7.6
1	C	7	ASP	6.1
1	C	5	GLY	5.9
1	A	328	THR	5.5
1	E	4	PRO	5.3
1	E	6	ASN	5.2
2	F	172	GLN	5.1
1	E	327	GLN	4.8
1	E	3	LEU	4.7
2	D	173	ILE	4.6
1	A	326	LYS	4.5
2	B	173	ILE	4.4
1	A	6	ASN	4.4
2	F	173	ILE	4.4
1	E	2	ASP	4.3
1	E	7	ASP	4.0
2	F	175	GLY	4.0
1	C	8	ASN	4.0
2	D	174	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	58	LYS	3.8
1	C	4	PRO	3.7
2	D	57	GLU	3.7
1	C	3	LEU	3.7
1	E	1	GLN	3.7
1	C	6	ASN	3.7
1	A	5	GLY	3.6
1	E	328	THR	3.6
1	E	9	SER	3.5
2	B	58	LYS	3.4
1	A	1	GLN	3.3
2	D	172	GLN	3.2
1	A	7	ASP	3.1
2	F	57	GLU	3.1
1	A	2	ASP	3.1
1	C	146	GLY	3.1
1	C	192	THR	3.1
2	D	175	GLY	3.0
1	C	327	GLN	3.0
1	E	291	ASP	2.9
1	A	131	THR	2.8
1	E	187	THR	2.8
1	A	144	GLY	2.8
1	C	240	GLY	2.8
1	A	327	GLN	2.7
1	C	216	ASN	2.7
1	C	137	ASN	2.6
1	A	193	SER	2.6
1	A	9	SER	2.5
1	E	22	ASN	2.5
2	B	29	SER	2.5
1	E	92	LYS	2.5
2	B	168	ASN	2.4
2	D	60	ASN	2.4
1	C	199	SER	2.4
1	C	328	THR	2.4
1	E	189	GLN	2.3
1	C	160	THR	2.3
1	C	10	THR	2.3
2	D	151	SER	2.3
2	B	145	ASP	2.2
2	B	18	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	9	SER	2.2
1	C	193	SER	2.2
1	E	143	PRO	2.2
1	A	189	GLN	2.2
1	E	5	GLY	2.2
1	A	3	LEU	2.2
1	A	158	GLY	2.2
2	D	148	CYS	2.2
2	F	168	ASN	2.1
1	C	2	ASP	2.1
1	C	142	GLY	2.1
1	C	144	GLY	2.1
2	D	72	GLU	2.1
1	A	325	GLU	2.1
1	C	1	GLN	2.1
1	E	326	LYS	2.1
1	E	192	THR	2.1

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

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

6.3 Carbohydrates ⓘ

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

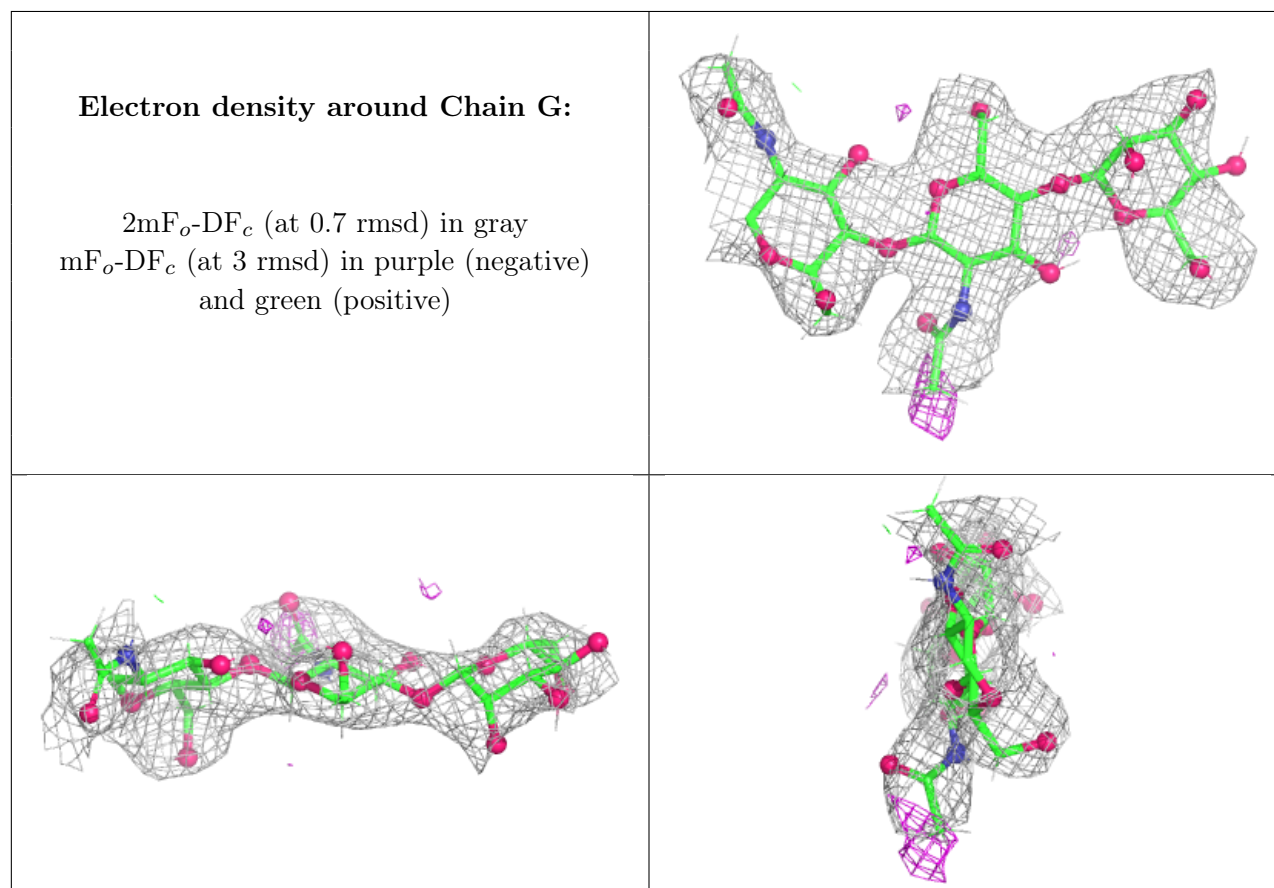
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	K	1	12/12	0.53	0.25	0,0,67,68	23
4	BGC	H	1	12/12	0.57	0.30	0,0,67,68	23
4	GAL	I	2	11/12	0.65	0.17	0,0,47,48	21
3	BMA	G	3	11/12	0.68	0.14	0,0,64,65	0
4	BGC	N	1	12/12	0.73	0.28	0,0,67,68	23
4	BGC	O	1	12/12	0.73	0.24	0,0,49,50	23
3	BMA	M	3	11/12	0.76	0.14	0,0,65,68	0
4	SIA	L	3	20/21	0.78	0.25	0,41,44,44	37
4	GAL	L	2	11/12	0.79	0.13	0,0,47,48	21
4	BGC	I	1	12/12	0.79	0.19	0,0,49,50	23
3	NAG	J	2	14/15	0.80	0.13	0,0,57,60	0

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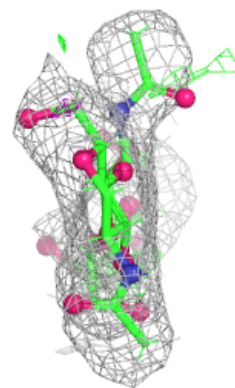
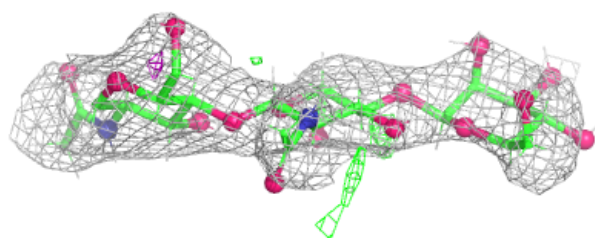
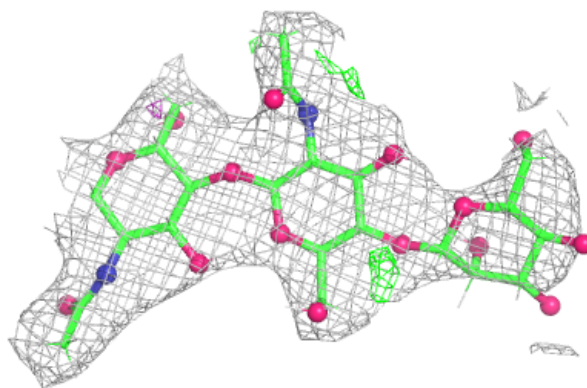
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	L	1	12/12	0.80	0.22	0,0,49,50	23
3	BMA	J	3	11/12	0.80	0.15	0,0,70,72	0
3	NAG	G	2	14/15	0.81	0.12	0,0,57,59	0
3	NAG	J	1	14/15	0.81	0.11	0,0,45,48	0
4	SIA	I	3	20/21	0.82	0.24	0,41,44,44	37
4	SIA	K	3	20/21	0.86	0.14	0,35,41,42	37
3	NAG	G	1	14/15	0.86	0.10	0,0,45,48	0
3	NAG	M	1	14/15	0.86	0.11	0,0,44,48	0
4	GAL	O	2	11/12	0.86	0.14	0,0,47,48	21
4	SIA	N	3	20/21	0.88	0.14	0,35,41,42	37
4	GAL	H	2	11/12	0.88	0.15	0,0,51,53	21
4	GAL	N	2	11/12	0.88	0.14	0,0,51,53	21
4	GAL	K	2	11/12	0.89	0.13	0,0,51,53	21
3	NAG	M	2	14/15	0.89	0.11	0,0,57,59	0
4	SIA	H	3	20/21	0.90	0.12	0,35,41,42	37
4	SIA	O	3	20/21	0.90	0.20	0,42,44,44	37

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

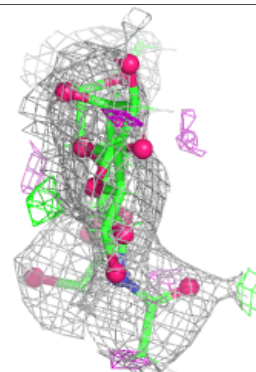
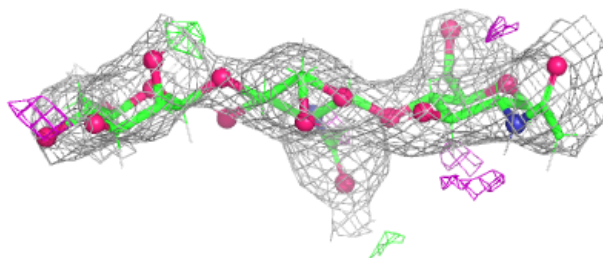
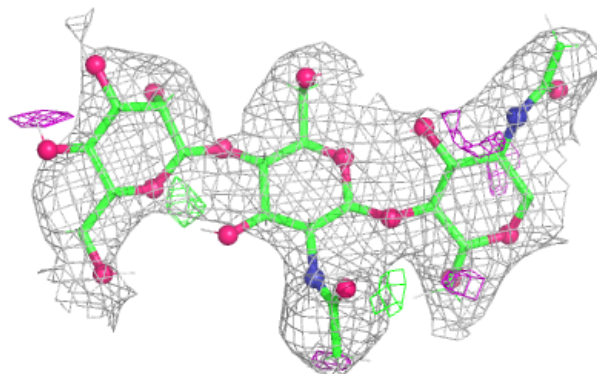


Electron density around Chain J:

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

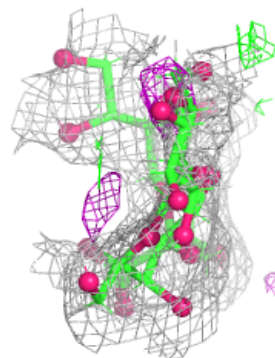
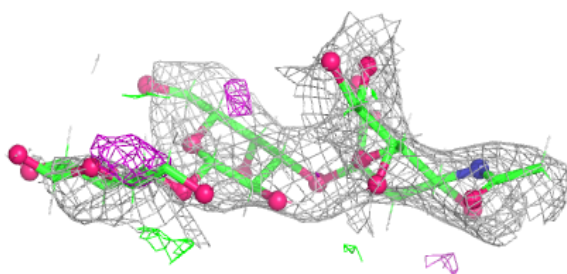
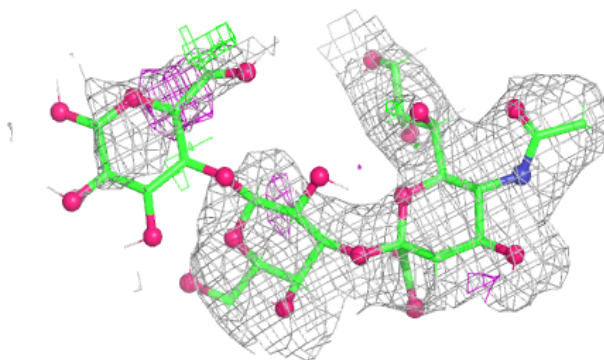
**Electron density around Chain M:**

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

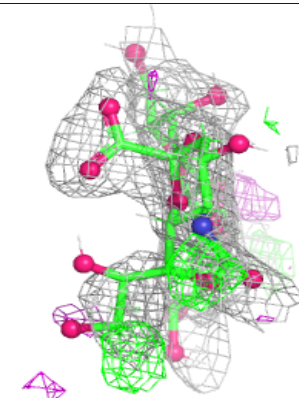
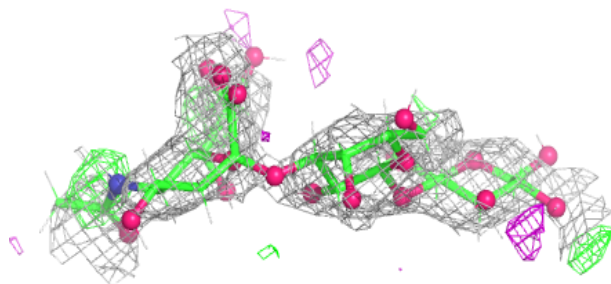
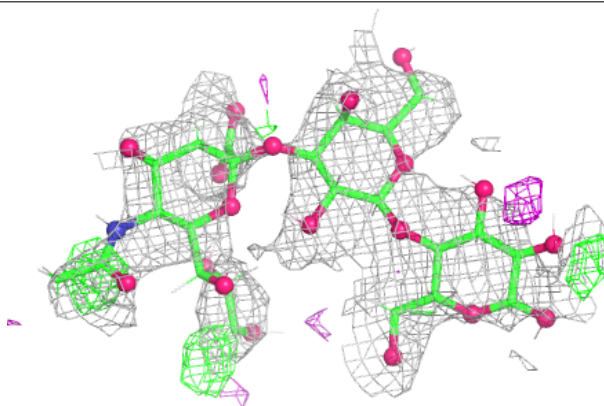


Electron density around Chain H:

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

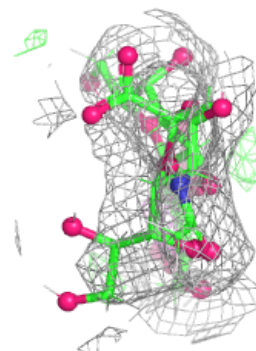
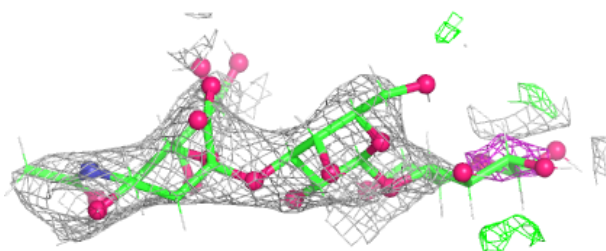
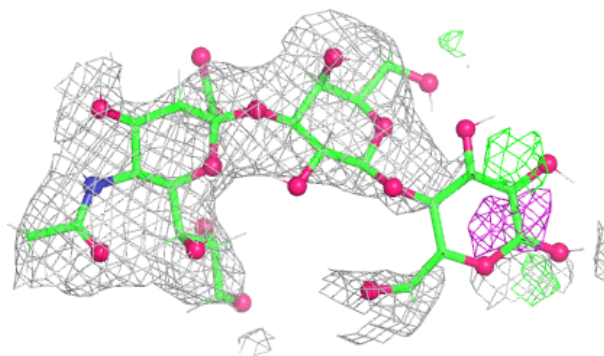
**Electron density around Chain I:**

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

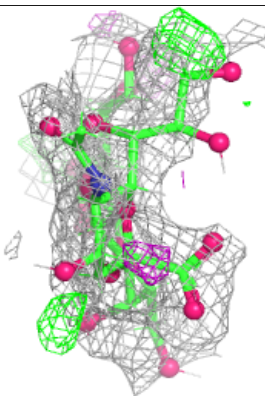
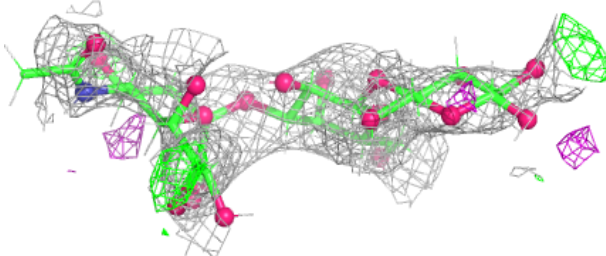
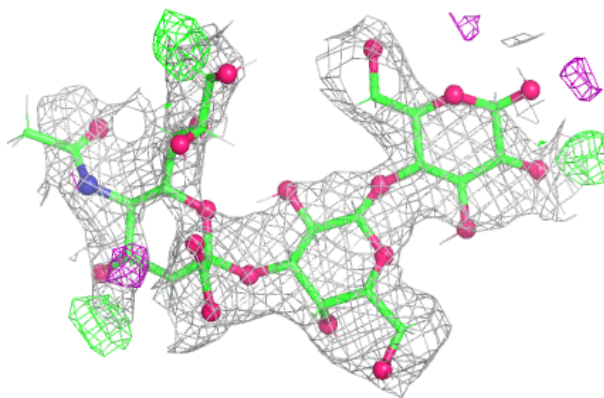


Electron density around Chain K:

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

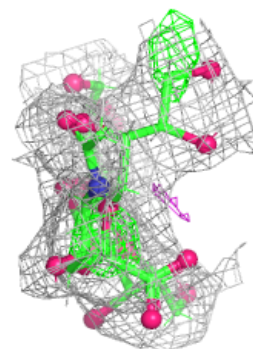
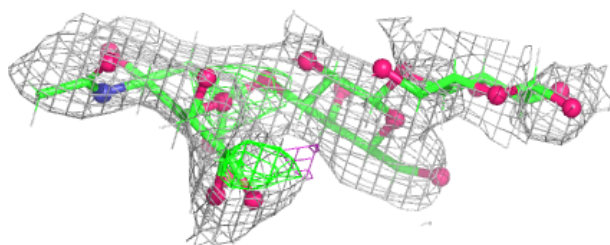
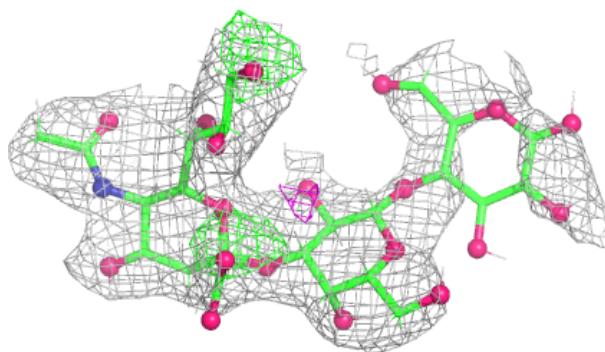
**Electron density around Chain L:**

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

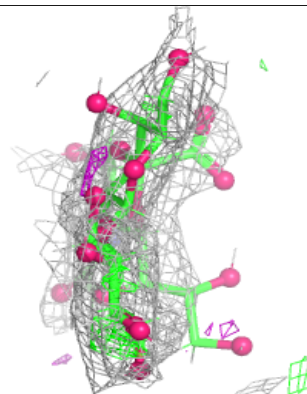
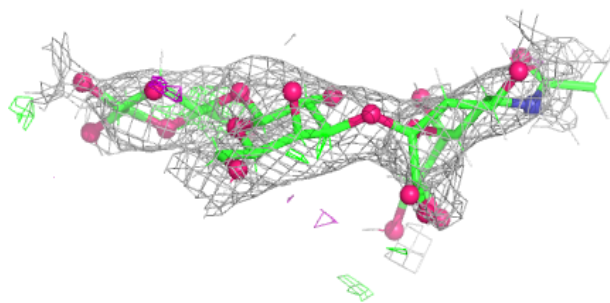
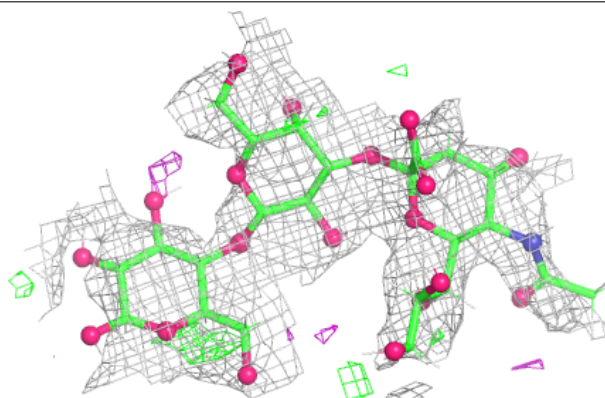


Electron density around Chain N:

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

**Electron density around Chain O:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
5	NAG	E	348	14/15	0.75	0.16	0,0,49,50	0
5	NAG	F	401	14/15	0.75	0.18	0,0,61,61	0
5	NAG	E	329	14/15	0.76	0.18	0,0,50,50	0
5	NAG	B	401	14/15	0.78	0.20	0,0,61,61	0
5	NAG	D	401	14/15	0.79	0.19	0,0,61,62	0
5	NAG	C	348	14/15	0.79	0.15	0,0,49,51	0
5	NAG	C	334	14/15	0.80	0.15	0,0,44,46	0
5	NAG	A	334	14/15	0.81	0.09	0,0,44,45	0
5	NAG	A	329	14/15	0.82	0.19	0,0,49,50	0
5	NAG	A	348	14/15	0.84	0.14	0,0,50,51	0
5	NAG	C	329	14/15	0.90	0.13	0,0,49,50	0
5	NAG	E	334	14/15	0.90	0.09	0,0,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.