



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:47 AM UTC

PDB ID : 1G7Y / pdb_00001g7y
Title : THE CRYSTAL STRUCTURE OF THE 58KD VEGETATIVE LECTIN
FROM THE TROPICAL LEGUME DOLICHOS BIFLORUS
Authors : Buts, L.; Hamelryck, T.W.; Loris, R.; Dao-Thi, M.-H.; Wyns, L.; Etzler, M.E.
Deposited on : 2000-11-15
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

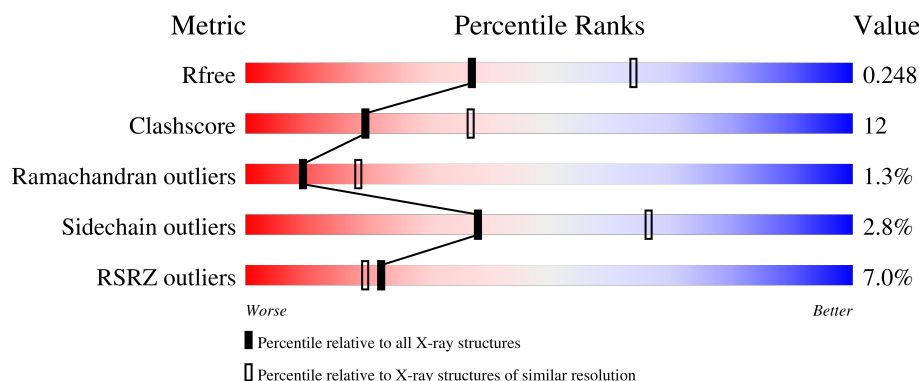
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	8% 72% 24% ..
1	B	253	9% 77% 19% ..
1	C	253	6% 73% 23% ..
1	D	253	7% 76% 21% .
1	E	253	6% 70% 24% ..

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Mol	Chain	Length	Quality of chain
1	F	253	5% 74% 21% ...
2	G	3	100%
2	I	3	100%
3	H	3	33% 67%

2 Entry composition [i](#)

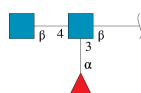
There are 6 unique types of molecules in this entry. The entry contains 11211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STEM/LEAF LECTIN DB58.

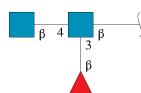
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	0	0	0
			1847	1168	299	380			
1	B	246	Total	C	N	O	0	0	0
			1823	1155	293	375			
1	C	251	Total	C	N	O	0	0	0
			1851	1169	298	384			
1	D	253	Total	C	N	O	0	0	0
			1866	1179	300	387			
1	E	249	Total	C	N	O	0	0	0
			1833	1159	297	377			
1	F	246	Total	C	N	O	0	0	0
			1824	1155	294	375			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	B	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	E	1	Total	Mn	0	0
			1	1		
5	F	1	Total	Mn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	6	Total	O	0	0
			6	6		

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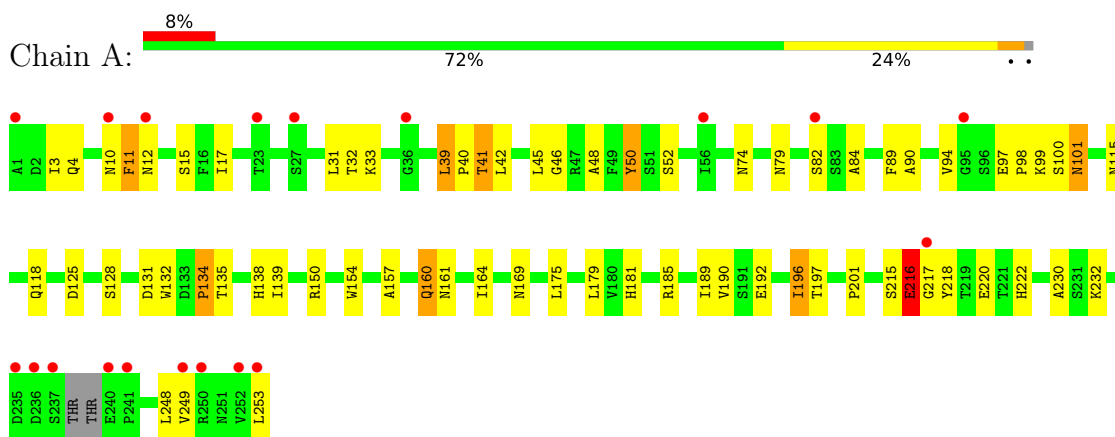
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	7	Total 7	O 7	0	0
6	D	5	Total 5	O 5	0	0
6	E	8	Total 8	O 8	0	0
6	F	8	Total 8	O 8	0	0

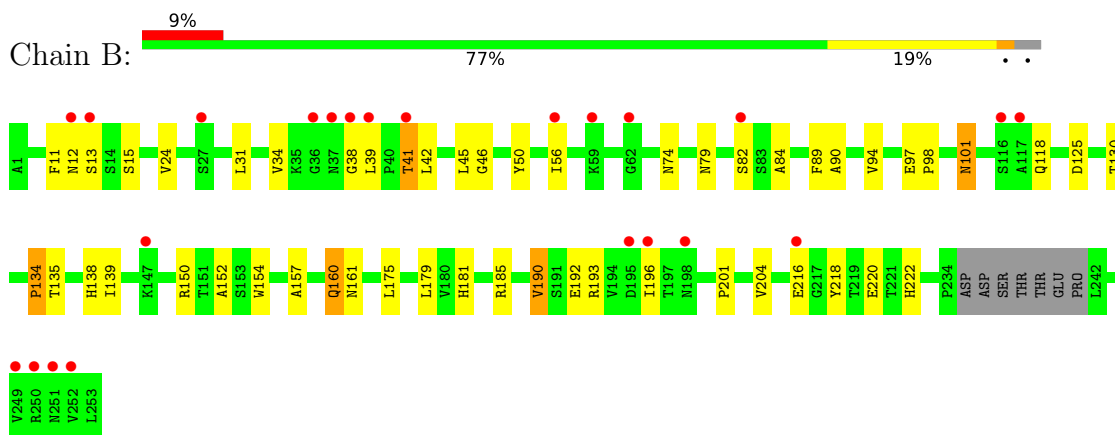
3 Residue-property plots [i](#)

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.

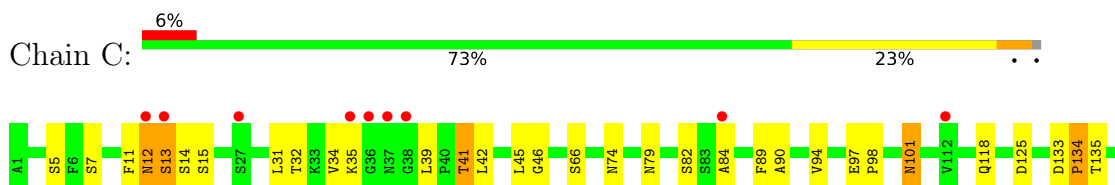
• Molecule 1: STEM/LEAF LECTIN DB58

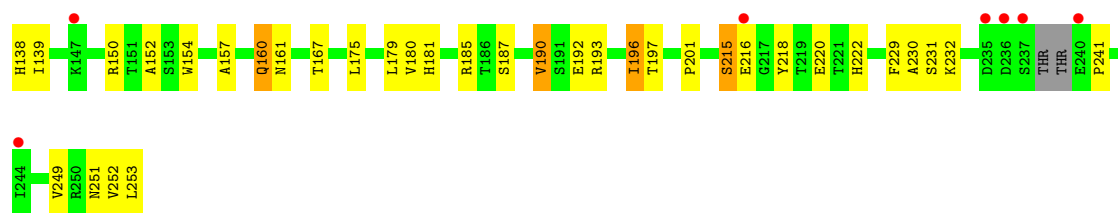


• Molecule 1: STEM/LEAF LECTIN DB58

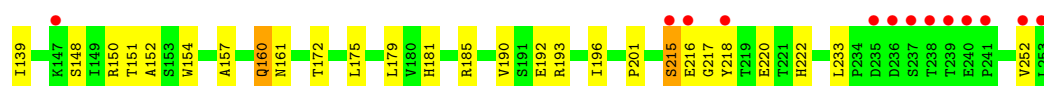
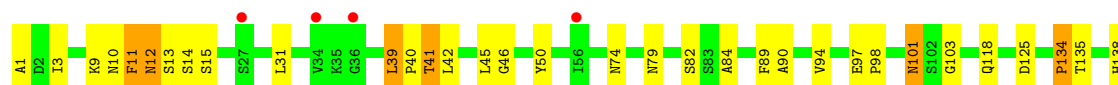
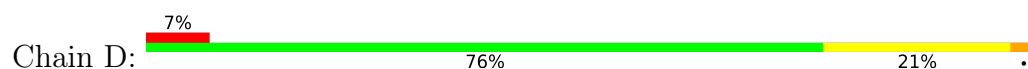


• Molecule 1: STEM/LEAF LECTIN DB58

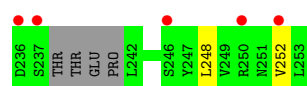
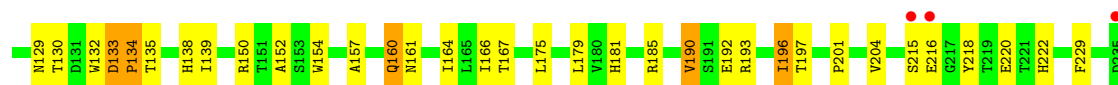
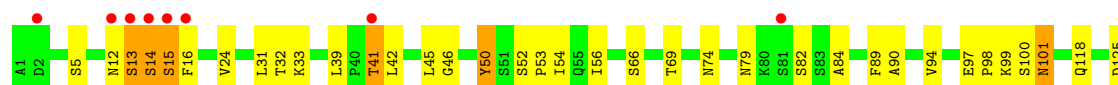




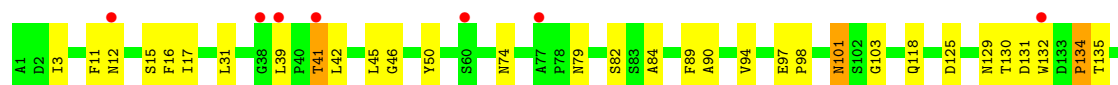
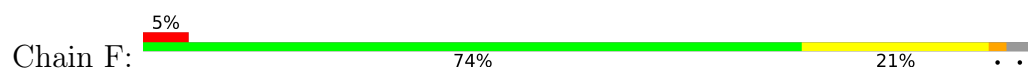
• Molecule 1: STEM/LEAF LECTIN DB58



• Molecule 1: STEM/LEAF LECTIN DB58



• Molecule 1: STEM/LEAF LECTIN DB58



• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
FUC2
MAG3

- Molecule 2: α -L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
FUC2
MAG3

- Molecule 3: β -L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33%  67%

MAG1
FUC2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.94Å 130.27Å 137.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.00-2.50) 93.4 (20.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.247 0.222 , 0.248	Depositor DCC
R_{free} test set	5994 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11211	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: FUC, FUL, NAG, MN, CA

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	0.48	0/1887	0.98	16/2579 (0.6%)
1	B	0.45	0/1862	0.99	13/2548 (0.5%)
1	C	0.52	0/1890	1.02	16/2585 (0.6%)
1	D	0.46	0/1907	0.98	15/2612 (0.6%)
1	E	0.48	0/1873	1.00	16/2561 (0.6%)
1	F	0.45	0/1864	1.00	15/2550 (0.6%)
All	All	0.47	0/11283	1.00	91/15435 (0.6%)

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ALA	CA-C-N	7.85	135.83	121.70
1	C	84	ALA	C-N-CA	7.85	135.83	121.70
1	E	130	THR	N-CA-C	7.35	120.16	111.71
1	B	196	ILE	N-CA-C	7.12	117.83	110.36
1	E	196	ILE	N-CA-C	7.04	117.75	110.36
1	C	196	ILE	N-CA-C	7.03	117.74	110.36
1	F	17	ILE	N-CA-C	-7.01	97.06	107.51
1	D	196	ILE	N-CA-C	7.00	117.71	110.36
1	F	196	ILE	N-CA-C	6.97	117.67	110.36
1	A	196	ILE	N-CA-C	6.86	117.57	110.36
1	F	12	ASN	N-CA-C	-6.39	105.34	113.01
1	F	190	VAL	CB-CA-C	-5.90	101.25	110.69
1	C	12	ASN	N-CA-C	-5.87	98.31	110.80
1	F	90	ALA	N-CA-C	5.84	118.28	109.23
1	A	135	THR	N-CA-C	5.79	117.59	111.28
1	B	84	ALA	CA-C-N	5.75	132.05	121.70
1	B	84	ALA	C-N-CA	5.75	132.05	121.70
1	A	90	ALA	N-CA-C	5.70	118.06	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	ILE	N-CA-C	-5.69	100.28	108.53
1	B	39	LEU	CA-C-N	5.66	125.61	119.78
1	B	39	LEU	C-N-CA	5.66	125.61	119.78
1	D	84	ALA	CA-C-N	5.66	131.89	121.70
1	D	84	ALA	C-N-CA	5.66	131.89	121.70
1	A	84	ALA	CA-C-N	5.65	131.88	121.70
1	A	84	ALA	C-N-CA	5.65	131.88	121.70
1	E	84	ALA	CA-C-N	5.64	131.85	121.70
1	E	84	ALA	C-N-CA	5.64	131.85	121.70
1	B	90	ALA	N-CA-C	5.62	117.94	109.23
1	C	90	ALA	N-CA-C	5.61	117.93	109.23
1	B	130	THR	N-CA-C	5.57	118.11	111.71
1	E	90	ALA	N-CA-C	5.57	117.86	109.23
1	F	84	ALA	CA-C-N	5.57	131.72	121.70
1	F	84	ALA	C-N-CA	5.57	131.72	121.70
1	F	50	TYR	N-CA-C	-5.56	102.05	110.28
1	E	39	LEU	CA-C-N	5.56	125.51	119.78
1	E	39	LEU	C-N-CA	5.56	125.51	119.78
1	F	139	ILE	N-CA-C	-5.56	100.47	108.53
1	B	50	TYR	N-CA-C	-5.55	102.07	110.28
1	E	135	THR	N-CA-C	5.55	117.33	111.28
1	D	90	ALA	N-CA-C	5.53	117.81	109.23
1	A	139	ILE	N-CA-C	-5.50	100.55	108.53
1	A	89	PHE	N-CA-C	-5.49	100.34	109.46
1	C	39	LEU	CA-C-N	5.49	125.43	119.78
1	C	39	LEU	C-N-CA	5.49	125.43	119.78
1	D	14	SER	N-CA-C	-5.47	106.58	113.20
1	E	134	PRO	N-CA-C	-5.46	102.99	111.13
1	B	135	THR	N-CA-C	5.46	117.23	111.28
1	C	135	THR	N-CA-C	5.46	117.23	111.28
1	A	134	PRO	N-CA-C	-5.45	103.01	111.13
1	E	50	TYR	N-CA-C	-5.44	101.80	109.96
1	D	139	ILE	N-CA-C	-5.44	100.65	108.53
1	C	134	PRO	N-CA-C	-5.43	103.03	111.13
1	F	134	PRO	N-CA-C	-5.43	103.04	111.13
1	D	134	PRO	N-CA-C	-5.43	103.05	111.13
1	E	89	PHE	N-CA-C	-5.43	100.45	109.46
1	D	135	THR	N-CA-C	5.42	117.19	111.28
1	F	39	LEU	CA-C-N	5.42	125.36	119.78
1	F	39	LEU	C-N-CA	5.42	125.36	119.78
1	B	134	PRO	N-CA-C	-5.39	103.10	111.13
1	C	89	PHE	N-CA-C	-5.38	100.53	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	LEU	CA-C-N	5.37	125.31	119.78
1	D	39	LEU	C-N-CA	5.37	125.31	119.78
1	A	39	LEU	CA-C-N	5.36	125.30	119.78
1	A	39	LEU	C-N-CA	5.36	125.30	119.78
1	F	135	THR	N-CA-C	5.35	117.11	111.28
1	E	139	ILE	N-CA-C	-5.34	100.79	108.53
1	F	89	PHE	N-CA-C	-5.33	100.61	109.46
1	D	11	PHE	N-CA-C	5.33	117.57	109.63
1	B	139	ILE	N-CA-C	-5.32	100.81	108.53
1	C	251	ASN	N-CA-C	5.31	120.12	113.43
1	B	89	PHE	N-CA-C	-5.30	100.66	109.46
1	C	84	ALA	O-C-N	-5.27	117.58	123.48
1	A	33	LYS	N-CA-C	5.23	117.81	110.23
1	E	94	VAL	N-CA-C	5.21	120.19	109.34
1	A	15	SER	N-CA-C	-5.20	106.79	112.72
1	D	89	PHE	N-CA-C	-5.19	100.84	109.46
1	C	11	PHE	N-CA-C	5.19	118.19	110.14
1	C	133	ASP	N-CA-C	5.19	117.20	110.40
1	B	94	VAL	N-CA-C	5.17	120.09	109.34
1	D	50	TYR	N-CA-C	-5.15	102.65	110.28
1	E	33	LYS	N-CA-C	5.14	117.89	110.28
1	A	50	TYR	N-CA-C	-5.14	102.67	110.28
1	A	164	ILE	N-CA-C	5.13	115.97	108.53
1	D	94	VAL	N-CA-C	5.12	119.99	109.34
1	C	94	VAL	N-CA-C	5.11	119.97	109.34
1	A	94	VAL	N-CA-C	5.09	119.93	109.34
1	D	9	LYS	N-CA-C	-5.08	106.86	113.16
1	E	164	ILE	N-CA-C	5.05	115.86	108.53
1	F	94	VAL	N-CA-C	5.05	119.84	109.34
1	A	128	SER	N-CA-C	5.03	116.46	108.67
1	E	133	ASP	N-CA-C	5.00	116.96	110.40

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	1847	0	1714	50	0
1	B	1823	0	1699	33	0
1	C	1851	0	1708	50	0
1	D	1866	0	1733	39	0
1	E	1833	0	1706	51	0
1	F	1824	0	1707	45	0
2	G	38	0	34	1	0
2	I	38	0	34	0	0
3	H	38	0	34	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	7	0	0	0	0
6	B	6	0	0	0	0
6	C	7	0	0	0	0
6	D	5	0	0	1	0
6	E	8	0	0	1	0
6	F	8	0	0	0	0
All	All	11211	0	10369	248	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 12.

All (248) 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:E:193:ARG:HB2	1:E:193:ARG:NH1	1.97	0.80
1:E:185:ARG:HD2	1:F:192:GLU:OE2	1.87	0.73
1:B:152:ALA:HB2	1:B:190:VAL:HG13	1.70	0.72
1:D:152:ALA:HB3	1:D:190:VAL:HG22	1.71	0.72
1:C:152:ALA:HB2	1:C:190:VAL:HG13	1.71	0.72
1:E:152:ALA:HB2	1:E:190:VAL:HG13	1.72	0.71
1:E:193:ARG:HB2	1:E:193:ARG:HH11	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:HD13	1:C:215:SER:O	1.94	0.68
1:A:185:ARG:HD2	1:C:192:GLU:OE2	1.96	0.66
1:C:152:ALA:CB	1:C:190:VAL:HG13	2.26	0.65
1:F:129:ASN:HD22	1:F:132:TRP:HZ2	1.41	0.65
1:B:185:ARG:HD2	1:D:192:GLU:OE2	1.98	0.64
1:A:189:ILE:HD13	1:C:187:SER:HB2	1.81	0.63
1:C:150:ARG:NH1	1:C:192:GLU:OE1	2.33	0.62
1:D:152:ALA:CB	1:D:190:VAL:HG22	2.29	0.61
1:F:3:ILE:HD12	1:F:3:ILE:N	2.16	0.61
1:B:13:SER:C	1:B:15:SER:H	2.09	0.60
1:D:42:LEU:HD13	1:D:215:SER:O	2.02	0.60
1:C:97:GLU:HG3	1:C:98:PRO:HD2	1.85	0.59
1:D:42:LEU:HD11	1:D:216:GLU:HA	1.83	0.59
1:C:180:VAL:HG22	1:C:187:SER:HB3	1.85	0.59
1:E:97:GLU:HG3	1:E:98:PRO:HD2	1.85	0.59
1:F:97:GLU:HG3	1:F:98:PRO:HD2	1.86	0.58
1:A:97:GLU:HG3	1:A:98:PRO:HD2	1.86	0.57
1:A:192:GLU:OE2	1:C:185:ARG:HD2	2.04	0.57
1:B:97:GLU:HG3	1:B:98:PRO:HD2	1.86	0.57
1:A:216:GLU:HA	1:A:216:GLU:OE1	2.04	0.57
1:D:97:GLU:HG3	1:D:98:PRO:HD2	1.87	0.56
1:E:152:ALA:CB	1:E:190:VAL:HG13	2.35	0.55
1:E:13:SER:HA	1:E:24:VAL:HG21	1.90	0.54
1:E:192:GLU:OE2	1:F:185:ARG:HD2	2.08	0.54
1:A:253:LEU:HB3	1:C:66:SER:HB3	1.89	0.54
1:D:103:GLY:HA2	6:D:4255:HOH:O	2.08	0.54
1:C:13:SER:O	1:C:14:SER:HB2	2.08	0.54
1:A:45:LEU:C	1:A:45:LEU:HD23	2.33	0.54
1:F:45:LEU:C	1:F:45:LEU:HD23	2.33	0.54
1:A:249:VAL:HG13	1:C:232:LYS:HB2	1.90	0.53
1:E:45:LEU:HD23	1:E:45:LEU:C	2.34	0.53
1:B:45:LEU:C	1:B:45:LEU:HD23	2.34	0.53
1:D:45:LEU:C	1:D:45:LEU:HD23	2.34	0.53
1:F:129:ASN:ND2	1:F:132:TRP:CZ2	2.71	0.53
1:A:11:PHE:N	1:A:11:PHE:CD1	2.77	0.53
1:A:74:ASN:HD22	1:A:161:ASN:HD22	1.57	0.52
1:B:101:ASN:C	1:B:101:ASN:HD22	2.18	0.52
1:F:150:ARG:NH1	1:F:192:GLU:OE1	2.43	0.52
1:C:74:ASN:HD22	1:C:161:ASN:HD22	1.57	0.52
1:C:45:LEU:C	1:C:45:LEU:HD23	2.35	0.52
1:C:152:ALA:HB2	1:C:190:VAL:CG1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:ASN:O	1:E:14:SER:N	2.43	0.51
1:E:150:ARG:NH1	1:E:192:GLU:OE1	2.44	0.51
1:F:74:ASN:HD22	1:F:161:ASN:HD22	1.58	0.51
1:A:101:ASN:C	1:A:101:ASN:HD22	2.19	0.51
1:B:179:LEU:C	1:B:179:LEU:HD23	2.36	0.51
1:D:74:ASN:HD22	1:D:161:ASN:HD22	1.58	0.51
1:F:15:SER:C	1:F:16:PHE:HD2	2.19	0.51
1:B:118:GLN:HB3	1:B:201:PRO:HD3	1.93	0.50
1:C:179:LEU:C	1:C:179:LEU:HD23	2.37	0.50
1:A:216:GLU:O	1:A:218:TYR:N	2.42	0.50
1:E:13:SER:O	1:E:15:SER:N	2.44	0.50
1:E:74:ASN:HD22	1:E:161:ASN:HD22	1.58	0.50
1:A:179:LEU:C	1:A:179:LEU:HD23	2.37	0.50
1:B:192:GLU:HG3	1:B:193:ARG:N	2.27	0.50
1:F:101:ASN:C	1:F:101:ASN:HD22	2.19	0.50
1:E:179:LEU:HD23	1:E:179:LEU:C	2.37	0.50
1:A:118:GLN:HB3	1:A:201:PRO:HD3	1.94	0.50
1:D:179:LEU:C	1:D:179:LEU:HD23	2.37	0.50
1:B:74:ASN:HD22	1:B:161:ASN:HD22	1.57	0.49
1:A:248:LEU:HD13	1:C:167:THR:HG21	1.93	0.49
1:E:101:ASN:C	1:E:101:ASN:HD22	2.20	0.49
1:F:11:PHE:CE2	1:F:16:PHE:HZ	2.30	0.49
1:E:118:GLN:HB3	1:E:201:PRO:HD3	1.94	0.49
1:A:50:TYR:CE2	1:A:52:SER:HB3	2.47	0.49
1:D:118:GLN:HB3	1:D:201:PRO:HD3	1.94	0.49
1:E:167:THR:HG21	1:F:248:LEU:HD13	1.93	0.49
1:C:34:VAL:HG12	1:C:35:LYS:O	2.13	0.49
1:C:118:GLN:HB3	1:C:201:PRO:HD3	1.93	0.49
1:D:172:THR:O	1:D:193:ARG:NH1	2.46	0.49
1:A:216:GLU:C	1:A:218:TYR:H	2.20	0.48
1:F:41:THR:CG2	1:F:42:LEU:N	2.76	0.48
1:F:179:LEU:C	1:F:179:LEU:HD23	2.37	0.48
1:C:101:ASN:C	1:C:101:ASN:HD22	2.21	0.48
1:F:74:ASN:HD22	1:F:161:ASN:ND2	2.11	0.48
1:E:41:THR:CG2	1:E:42:LEU:N	2.77	0.48
2:G:2:FUC:H5	2:G:3:NAG:O5	2.13	0.48
1:A:41:THR:CG2	1:A:42:LEU:N	2.76	0.48
1:A:74:ASN:HD22	1:A:161:ASN:ND2	2.11	0.48
1:E:74:ASN:HD22	1:E:161:ASN:ND2	2.11	0.48
1:D:82:SER:O	1:D:218:TYR:HA	2.14	0.48
1:F:16:PHE:N	1:F:16:PHE:CD2	2.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:SER:O	1:F:218:TYR:HA	2.13	0.48
1:F:118:GLN:HB3	1:F:201:PRO:HD3	1.95	0.48
1:B:74:ASN:HD22	1:B:161:ASN:ND2	2.12	0.48
1:D:101:ASN:C	1:D:101:ASN:HD22	2.19	0.48
1:D:185:ARG:HB2	1:D:185:ARG:NH2	2.29	0.48
1:E:53:PRO:C	1:E:54:ILE:HD12	2.39	0.47
1:D:13:SER:C	1:D:15:SER:H	2.22	0.47
1:C:32:THR:OG1	1:C:222:HIS:HD2	1.98	0.47
1:D:41:THR:CG2	1:D:42:LEU:N	2.77	0.47
1:E:66:SER:HB3	1:F:253:LEU:HB3	1.96	0.47
1:E:13:SER:H	1:E:24:VAL:HG11	1.80	0.47
1:B:82:SER:O	1:B:218:TYR:HA	2.15	0.47
1:D:74:ASN:HD22	1:D:161:ASN:ND2	2.11	0.47
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.79	0.47
1:E:82:SER:O	1:E:218:TYR:HA	2.14	0.47
1:B:160:GLN:HE21	1:B:160:GLN:HA	1.80	0.47
1:C:160:GLN:HE21	1:C:160:GLN:HA	1.79	0.47
1:B:41:THR:CG2	1:B:42:LEU:N	2.77	0.47
1:C:74:ASN:HD22	1:C:161:ASN:ND2	2.12	0.47
1:F:215:SER:HB3	1:F:218:TYR:CD1	2.50	0.47
1:C:157:ALA:H	1:C:181:HIS:CE1	2.33	0.46
1:A:115:ASN:ND2	1:F:203:TYR:OH	2.48	0.46
1:D:160:GLN:HE21	1:D:160:GLN:HA	1.80	0.46
1:C:41:THR:CG2	1:C:42:LEU:N	2.77	0.46
1:A:82:SER:O	1:A:218:TYR:HA	2.13	0.46
1:C:97:GLU:HG3	1:C:98:PRO:CD	2.46	0.46
1:F:160:GLN:HE21	1:F:160:GLN:HA	1.80	0.46
1:E:97:GLU:HG3	1:E:98:PRO:CD	2.45	0.46
1:F:42:LEU:HD13	1:F:215:SER:O	2.16	0.46
1:B:97:GLU:HG3	1:B:98:PRO:CD	2.46	0.46
1:C:82:SER:O	1:C:218:TYR:HA	2.15	0.46
1:D:11:PHE:O	1:D:12:ASN:CB	2.64	0.46
1:E:5:SER:HA	1:E:229:PHE:O	2.16	0.46
1:E:160:GLN:HA	1:E:160:GLN:HE21	1.81	0.46
1:B:152:ALA:CB	1:B:190:VAL:HG13	2.44	0.45
1:F:16:PHE:HD2	1:F:16:PHE:N	2.13	0.45
1:D:157:ALA:H	1:D:181:HIS:CE1	2.34	0.45
1:E:129:ASN:O	1:E:133:ASP:HB2	2.16	0.45
1:D:10:ASN:OD1	1:D:10:ASN:C	2.59	0.45
1:D:97:GLU:HG3	1:D:98:PRO:CD	2.46	0.45
1:E:16:PHE:N	1:E:16:PHE:CD2	2.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:PHE:N	1:E:16:PHE:HD2	2.14	0.45
1:E:79:ASN:HB3	1:E:82:SER:HB3	1.98	0.45
1:F:154:TRP:HE1	1:F:181:HIS:CE1	2.35	0.45
1:D:82:SER:HG	1:D:217:GLY:C	2.23	0.45
1:C:7:SER:HB3	1:D:3:ILE:HB	1.99	0.45
1:A:154:TRP:HE1	1:A:181:HIS:CE1	2.35	0.45
1:A:32:THR:OG1	1:A:222:HIS:HD2	2.00	0.45
1:C:79:ASN:HB3	1:C:82:SER:HB3	1.99	0.45
1:F:97:GLU:HG3	1:F:98:PRO:CD	2.45	0.45
1:B:157:ALA:H	1:B:181:HIS:CE1	2.35	0.45
1:C:193:ARG:HH11	1:C:193:ARG:HG3	1.80	0.45
1:E:157:ALA:H	1:E:181:HIS:CE1	2.35	0.45
1:E:248:LEU:HD13	1:F:167:THR:HG21	1.99	0.45
1:A:79:ASN:HB3	1:A:82:SER:HB3	1.98	0.44
1:F:154:TRP:HE1	1:F:181:HIS:HE1	1.65	0.44
1:A:10:ASN:OD1	1:A:10:ASN:C	2.60	0.44
1:A:17:ILE:O	1:A:48:ALA:HA	2.18	0.44
1:A:31:LEU:O	1:A:46:GLY:HA3	2.18	0.44
1:A:157:ALA:H	1:A:181:HIS:CE1	2.35	0.44
1:D:79:ASN:HB3	1:D:82:SER:HB3	1.98	0.44
1:F:31:LEU:O	1:F:46:GLY:HA3	2.17	0.44
1:E:31:LEU:O	1:E:46:GLY:HA3	2.18	0.44
1:C:5:SER:HA	1:C:229:PHE:O	2.18	0.44
1:C:31:LEU:O	1:C:46:GLY:HA3	2.16	0.44
1:E:154:TRP:HE1	1:E:181:HIS:CE1	2.35	0.44
1:F:125:ASP:HB3	1:F:138:HIS:CE1	2.52	0.44
1:A:97:GLU:HG3	1:A:98:PRO:CD	2.46	0.44
1:A:115:ASN:CG	1:F:203:TYR:CZ	2.96	0.44
1:B:79:ASN:HB3	1:B:82:SER:HB3	1.99	0.44
1:D:154:TRP:HE1	1:D:181:HIS:CE1	2.36	0.44
1:B:12:ASN:HA	1:B:24:VAL:HG11	2.00	0.44
1:D:101:ASN:C	1:D:101:ASN:ND2	2.76	0.44
1:C:12:ASN:O	1:C:13:SER:O	2.35	0.44
1:D:148:SER:HB2	1:D:151:THR:CG2	2.48	0.44
1:E:101:ASN:C	1:E:101:ASN:ND2	2.76	0.44
1:E:125:ASP:HB3	1:E:138:HIS:CE1	2.53	0.43
1:F:157:ALA:H	1:F:181:HIS:CE1	2.36	0.43
1:A:101:ASN:C	1:A:101:ASN:ND2	2.76	0.43
1:A:169:ASN:HA	1:C:253:LEU:HD22	1.99	0.43
1:F:79:ASN:HB3	1:F:82:SER:HB3	1.99	0.43
1:A:115:ASN:CB	1:F:203:TYR:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:O	1:B:46:GLY:HA3	2.18	0.43
1:B:161:ASN:O	1:B:181:HIS:HD2	2.01	0.43
1:D:125:ASP:HB3	1:D:138:HIS:CE1	2.53	0.43
1:E:56:ILE:HG23	6:E:5260:HOH:O	2.19	0.43
1:C:154:TRP:HE1	1:C:181:HIS:CE1	2.36	0.43
1:D:31:LEU:O	1:D:46:GLY:HA3	2.17	0.43
1:A:134:PRO:HD2	1:A:138:HIS:CE1	2.53	0.43
1:E:154:TRP:HE1	1:E:181:HIS:HE1	1.67	0.43
1:A:161:ASN:O	1:A:181:HIS:HD2	2.01	0.43
1:C:42:LEU:HD21	1:C:216:GLU:O	2.19	0.43
1:A:154:TRP:HE1	1:A:181:HIS:HE1	1.67	0.43
1:D:1:ALA:HA	1:D:233:LEU:O	2.19	0.43
1:A:3:ILE:HG22	1:A:4:GLN:N	2.34	0.43
1:B:150:ARG:NH1	1:B:192:GLU:OE1	2.52	0.43
1:B:154:TRP:HE1	1:B:181:HIS:CE1	2.36	0.43
1:E:50:TYR:CE2	1:E:52:SER:HB3	2.54	0.43
1:E:161:ASN:O	1:E:181:HIS:HD2	2.02	0.43
1:B:11:PHE:O	1:B:12:ASN:CB	2.67	0.42
1:B:101:ASN:C	1:B:101:ASN:ND2	2.75	0.42
1:E:99:LYS:HB3	1:E:100:SER:H	1.71	0.42
1:C:134:PRO:HD2	1:C:138:HIS:CE1	2.54	0.42
1:B:220:GLU:OE2	1:B:222:HIS:HE1	2.02	0.42
1:F:220:GLU:OE2	1:F:222:HIS:HE1	2.02	0.42
1:A:150:ARG:NH1	1:A:192:GLU:OE1	2.53	0.42
1:F:42:LEU:HD21	1:F:216:GLU:O	2.19	0.42
1:C:125:ASP:HB3	1:C:138:HIS:CE1	2.54	0.42
1:F:103:GLY:HA3	1:F:129:ASN:HD21	1.83	0.42
1:F:161:ASN:O	1:F:181:HIS:HD2	2.02	0.42
1:A:99:LYS:HB3	1:A:100:SER:H	1.73	0.42
1:C:220:GLU:OE2	1:C:222:HIS:HE1	2.02	0.42
1:F:175:LEU:C	1:F:175:LEU:HD23	2.45	0.42
1:A:232:LYS:HB2	1:C:249:VAL:CG1	2.50	0.42
1:B:125:ASP:HB3	1:B:138:HIS:CE1	2.54	0.42
1:F:3:ILE:HD12	1:F:3:ILE:H	1.84	0.42
1:B:157:ALA:HB1	1:B:160:GLN:HG3	2.02	0.42
1:C:161:ASN:O	1:C:181:HIS:HD2	2.03	0.42
1:C:175:LEU:C	1:C:175:LEU:HD23	2.45	0.42
1:D:175:LEU:C	1:D:175:LEU:HD23	2.44	0.42
1:A:157:ALA:HB1	1:A:160:GLN:HG3	2.02	0.41
1:B:134:PRO:HD2	1:B:138:HIS:CE1	2.54	0.41
1:E:15:SER:C	1:E:16:PHE:HD2	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:TRP:HE1	1:D:181:HIS:HE1	1.67	0.41
1:A:220:GLU:OE2	1:A:222:HIS:HE1	2.03	0.41
1:B:12:ASN:CA	1:B:24:VAL:HG11	2.50	0.41
1:C:101:ASN:C	1:C:101:ASN:ND2	2.78	0.41
1:D:220:GLU:OE2	1:D:222:HIS:HE1	2.04	0.41
1:F:196:ILE:CG2	1:F:197:THR:N	2.83	0.41
1:C:154:TRP:HE1	1:C:181:HIS:HE1	1.67	0.41
1:E:132:TRP:CD1	1:E:132:TRP:C	2.98	0.41
1:F:101:ASN:C	1:F:101:ASN:ND2	2.76	0.41
1:B:34:VAL:HG12	1:B:38:GLY:HA2	2.03	0.41
1:B:175:LEU:HD23	1:B:175:LEU:C	2.45	0.41
1:E:220:GLU:OE2	1:E:222:HIS:HE1	2.03	0.41
1:A:249:VAL:CG1	1:C:232:LYS:HB2	2.48	0.41
1:D:134:PRO:HD2	1:D:138:HIS:CE1	2.55	0.41
1:D:150:ARG:NH1	1:D:192:GLU:OE1	2.54	0.41
1:B:56:ILE:HG12	1:B:204:VAL:HG22	2.03	0.41
1:E:134:PRO:HD2	1:E:138:HIS:CE1	2.55	0.41
1:A:175:LEU:C	1:A:175:LEU:HD23	2.46	0.41
1:C:157:ALA:HB1	1:C:160:GLN:HG3	2.02	0.41
1:C:196:ILE:CG2	1:C:197:THR:N	2.84	0.41
1:D:82:SER:OG	1:D:217:GLY:O	2.35	0.41
1:A:196:ILE:CG2	1:A:197:THR:N	2.84	0.41
1:A:125:ASP:HB3	1:A:138:HIS:CE1	2.55	0.40
1:E:32:THR:OG1	1:E:222:HIS:HD2	2.03	0.40
1:F:134:PRO:HD2	1:F:138:HIS:CE1	2.56	0.40
1:A:39:LEU:HA	1:A:40:PRO:HD3	1.84	0.40
1:D:39:LEU:HA	1:D:40:PRO:HD3	1.84	0.40
1:E:53:PRO:O	1:E:54:ILE:HD12	2.21	0.40
1:E:69:THR:HG22	1:E:166:ILE:HB	2.03	0.40
1:E:196:ILE:CG2	1:E:197:THR:N	2.85	0.40
1:E:175:LEU:HD23	1:E:175:LEU:C	2.45	0.40
1:F:157:ALA:HB1	1:F:160:GLN:HG3	2.02	0.40
1:A:230:ALA:HB3	1:C:249:VAL:HG21	2.03	0.40
1:A:249:VAL:HG21	1:C:230:ALA:C	2.47	0.40
1:C:229:PHE:CE1	1:C:231:SER:HB2	2.56	0.40
1:E:56:ILE:HG12	1:E:204:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/253 (98%)	225 (91%)	17 (7%)	5 (2%)	6	10
1	B	242/253 (96%)	224 (93%)	17 (7%)	1 (0%)	30	49
1	C	247/253 (98%)	229 (93%)	15 (6%)	3 (1%)	10	20
1	D	251/253 (99%)	234 (93%)	14 (6%)	3 (1%)	10	20
1	E	245/253 (97%)	224 (91%)	17 (7%)	4 (2%)	7	14
1	F	242/253 (96%)	224 (93%)	15 (6%)	3 (1%)	10	20
All	All	1474/1518 (97%)	1360 (92%)	95 (6%)	19 (1%)	9	18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLU
1	C	13	SER
1	E	14	SER
1	A	12	ASN
1	A	215	SER
1	A	217	GLY
1	B	216	GLU
1	C	215	SER
1	D	215	SER
1	E	13	SER
1	E	15	SER
1	F	130	THR
1	A	132	TRP
1	D	12	ASN
1	E	215	SER
1	F	216	GLU
1	F	252	VAL
1	D	252	VAL
1	C	241	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/216 (92%)	191 (96%)	7 (4%)	32	58
1	B	197/216 (91%)	193 (98%)	4 (2%)	48	75
1	C	199/216 (92%)	193 (97%)	6 (3%)	36	64
1	D	202/216 (94%)	199 (98%)	3 (2%)	57	80
1	E	197/216 (91%)	191 (97%)	6 (3%)	36	64
1	F	198/216 (92%)	191 (96%)	7 (4%)	32	58
All	All	1191/1296 (92%)	1158 (97%)	33 (3%)	38	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	41	THR
1	A	101	ASN
1	A	131	ASP
1	A	160	GLN
1	A	190	VAL
1	A	216	GLU
1	B	41	THR
1	B	101	ASN
1	B	160	GLN
1	B	190	VAL
1	C	15	SER
1	C	41	THR
1	C	101	ASN
1	C	160	GLN
1	C	190	VAL
1	C	252	VAL
1	D	41	THR
1	D	101	ASN
1	D	160	GLN
1	E	41	THR
1	E	101	ASN

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Mol	Chain	Res	Type
1	E	160	GLN
1	E	190	VAL
1	E	216	GLU
1	E	252	VAL
1	F	41	THR
1	F	101	ASN
1	F	131	ASP
1	F	160	GLN
1	F	190	VAL
1	F	193	ARG
1	F	216	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	115	ASN
1	A	160	GLN
1	A	161	ASN
1	A	181	HIS
1	A	198	ASN
1	A	222	HIS
1	B	101	ASN
1	B	115	ASN
1	B	160	GLN
1	B	161	ASN
1	B	181	HIS
1	B	198	ASN
1	B	222	HIS
1	C	55	GLN
1	C	101	ASN
1	C	115	ASN
1	C	160	GLN
1	C	161	ASN
1	C	181	HIS
1	C	198	ASN
1	C	222	HIS
1	D	101	ASN
1	D	115	ASN
1	D	160	GLN
1	D	161	ASN
1	D	181	HIS

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Mol	Chain	Res	Type
1	D	198	ASN
1	D	222	HIS
1	D	251	ASN
1	E	4	GLN
1	E	101	ASN
1	E	115	ASN
1	E	160	GLN
1	E	161	ASN
1	E	181	HIS
1	E	198	ASN
1	E	222	HIS
1	E	251	ASN
1	F	101	ASN
1	F	160	GLN
1	F	161	ASN
1	F	181	HIS
1	F	198	ASN
1	F	222	HIS

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 ⓘ

9 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	G	1	1,2	14,14,15	0.83	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	G	2	2	10,10,11	0.80	0	14,14,16	0.47	0
2	NAG	G	3	2	14,14,15	0.76	0	17,19,21	0.72	0
3	NAG	H	1	1,3	14,14,15	0.68	0	17,19,21	0.97	1 (5%)
3	FUL	H	2	3	10,10,11	0.54	0	14,14,16	0.36	0
3	NAG	H	3	3	14,14,15	0.56	0	17,19,21	1.01	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.54	0	17,19,21	0.66	0
2	FUC	I	2	2	10,10,11	0.67	0	14,14,16	0.48	0
2	NAG	I	3	2	14,14,15	0.59	0	17,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	FUL	H	2	3	-	-	0/1/1/1
3	NAG	H	3	3	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1
2	NAG	I	3	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C2-N2-C7	-2.77	119.19	122.90
3	H	3	NAG	C2-N2-C7	-2.45	119.61	122.90
2	G	1	NAG	C4-C3-C2	2.07	114.06	111.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

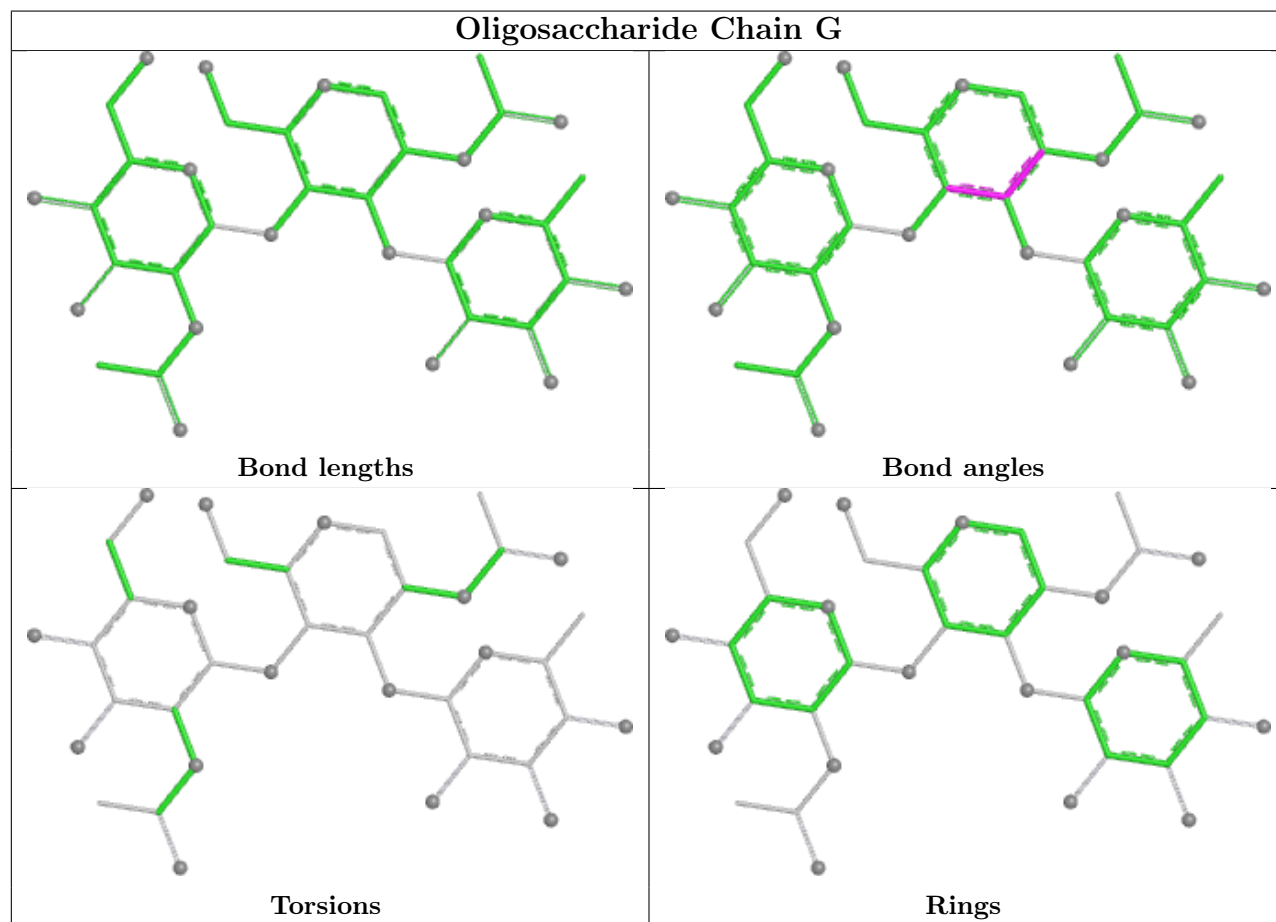
Mol	Chain	Res	Type	Atoms
2	I	3	NAG	C4-C5-C6-O6
2	I	3	NAG	O5-C5-C6-O6
2	I	1	NAG	C1-C2-N2-C7

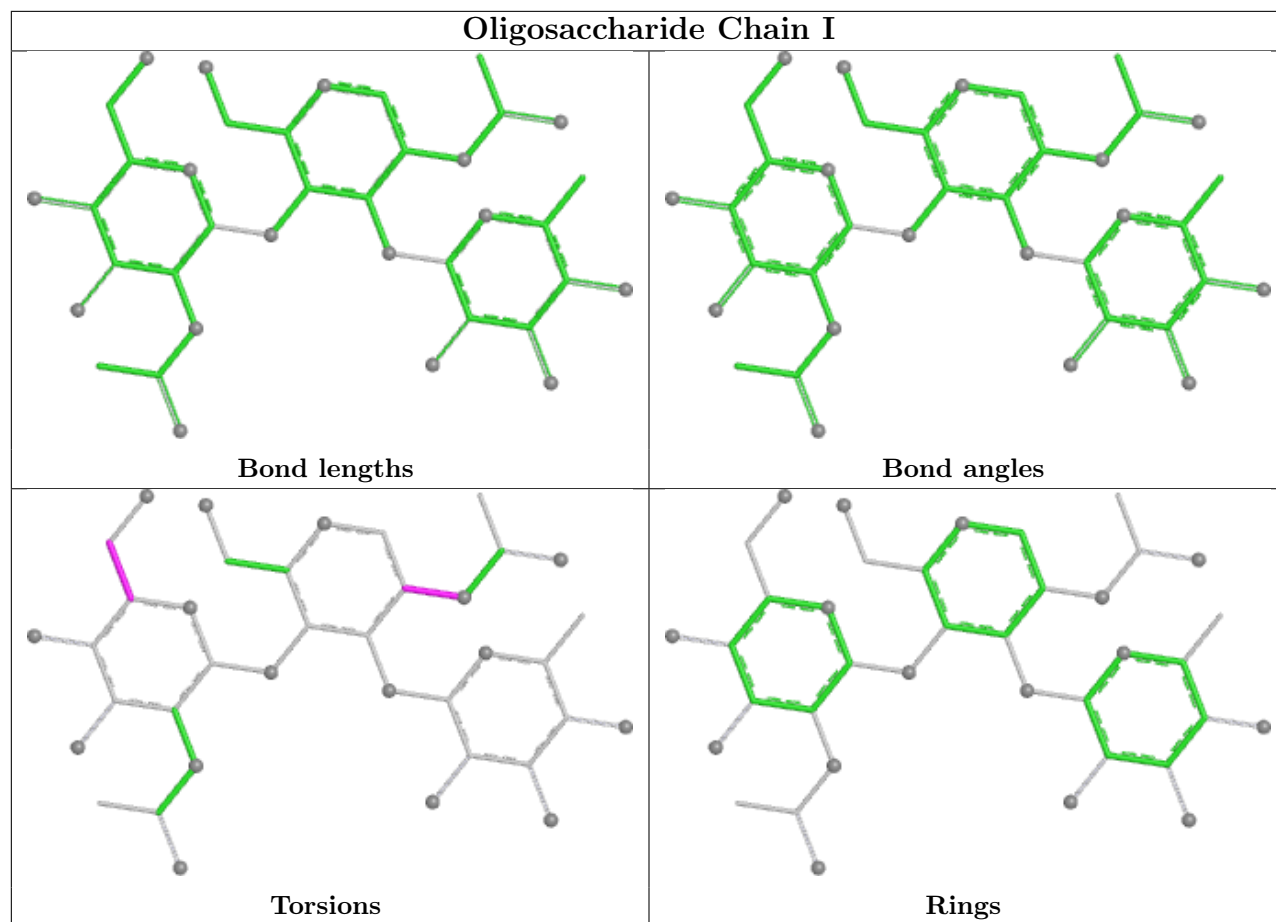
There are no ring outliers.

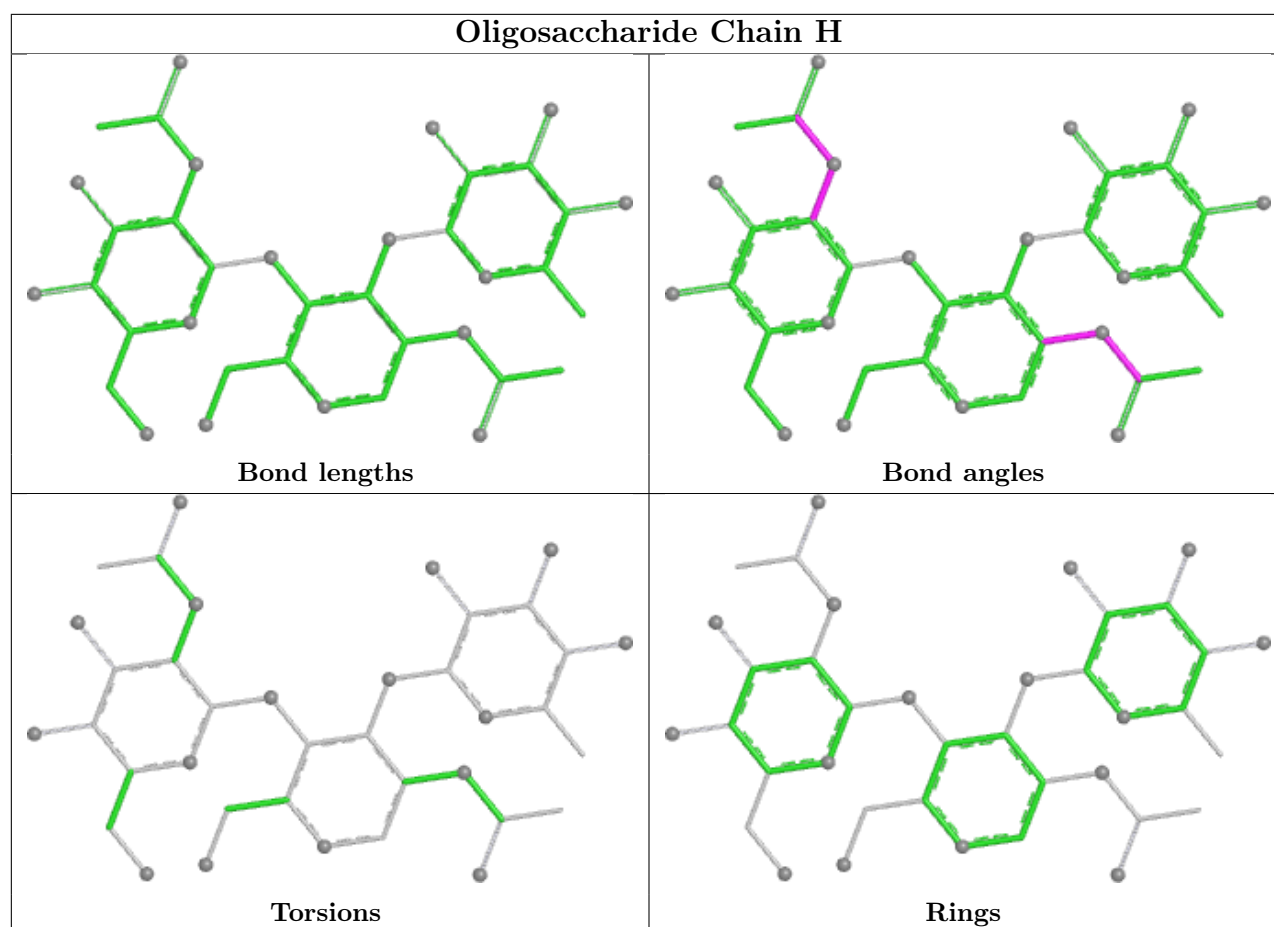
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	FUC	1	0
2	G	3	NAG	1	0

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







5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	251/253 (99%)	0.22	19 (7%)	20	17	12, 35, 62, 81	17 (6%)
1	B	246/253 (97%)	0.38	23 (9%)	14	12	19, 35, 59, 82	12 (4%)
1	C	251/253 (99%)	0.24	16 (6%)	25	22	12, 34, 60, 78	17 (6%)
1	D	253/253 (100%)	0.47	17 (6%)	24	21	11, 37, 63, 87	19 (7%)
1	E	249/253 (98%)	0.21	16 (6%)	25	22	11, 33, 62, 86	15 (6%)
1	F	246/253 (97%)	0.29	13 (5%)	32	28	9, 36, 63, 88	12 (4%)
All	All	1496/1518 (98%)	0.30	104 (6%)	22	20	9, 35, 62, 88	92 (6%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	SER	8.4
1	C	237	SER	6.9
1	D	216	GLU	6.5
1	E	235	ASP	6.5
1	C	36	GLY	6.1
1	D	236	ASP	6.0
1	E	237	SER	5.5
1	A	236	ASP	5.4
1	C	240	GLU	5.4
1	B	252	VAL	5.3
1	E	236	ASP	4.9
1	D	237	SER	4.9
1	D	235	ASP	4.8
1	A	250	ARG	4.7
1	A	252	VAL	4.6
1	A	235	ASP	4.6
1	D	27	SER	4.6
1	B	37	ASN	4.5
1	A	240	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	252	VAL	4.2
1	D	253	LEU	4.1
1	D	147	LYS	4.1
1	B	250	ARG	4.0
1	E	250	ARG	3.6
1	E	16	PHE	3.6
1	B	38	GLY	3.6
1	C	27	SER	3.5
1	E	14	SER	3.4
1	C	235	ASP	3.4
1	B	36	GLY	3.4
1	D	239	THR	3.4
1	D	240	GLU	3.4
1	F	250	ARG	3.4
1	C	12	ASN	3.3
1	F	253	LEU	3.3
1	A	27	SER	3.3
1	F	39	LEU	3.2
1	A	241	PRO	3.2
1	B	59	LYS	3.1
1	C	38	GLY	3.1
1	A	12	ASN	3.1
1	B	251	ASN	3.0
1	C	147	LYS	3.0
1	B	62	GLY	3.0
1	D	241	PRO	3.0
1	C	13	SER	3.0
1	D	215	SER	3.0
1	B	12	ASN	2.8
1	B	27	SER	2.8
1	B	198	ASN	2.8
1	A	253	LEU	2.8
1	C	37	ASN	2.7
1	F	244	ILE	2.7
1	E	12	ASN	2.7
1	E	13	SER	2.7
1	E	246	SER	2.7
1	E	216	GLU	2.7
1	F	60	SER	2.7
1	B	216	GLU	2.6
1	E	15	SER	2.6
1	B	117	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	12	ASN	2.6
1	B	249	VAL	2.6
1	E	215	SER	2.6
1	A	1	ALA	2.6
1	D	238	THR	2.6
1	C	244	ILE	2.5
1	B	147	LYS	2.5
1	B	116	SER	2.5
1	D	34	VAL	2.5
1	B	56	ILE	2.5
1	C	112	VAL	2.4
1	A	36	GLY	2.4
1	A	217	GLY	2.4
1	D	36	GLY	2.4
1	A	56	ILE	2.4
1	E	41	THR	2.3
1	F	218	TYR	2.3
1	E	81	SER	2.3
1	B	195	ASP	2.3
1	D	56	ILE	2.3
1	E	2	ASP	2.3
1	F	41	THR	2.3
1	A	82	SER	2.3
1	B	39	LEU	2.3
1	C	236	ASP	2.3
1	A	249	VAL	2.3
1	B	13	SER	2.2
1	B	196	ILE	2.2
1	C	216	GLU	2.2
1	A	10	ASN	2.2
1	F	217	GLY	2.2
1	E	252	VAL	2.2
1	B	41	THR	2.2
1	A	95	GLY	2.2
1	A	23	THR	2.2
1	B	82	SER	2.2
1	F	132	TRP	2.1
1	F	77	ALA	2.1
1	C	84	ALA	2.1
1	F	198	ASN	2.0
1	F	38	GLY	2.0
1	C	35	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	218	TYR	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](#)

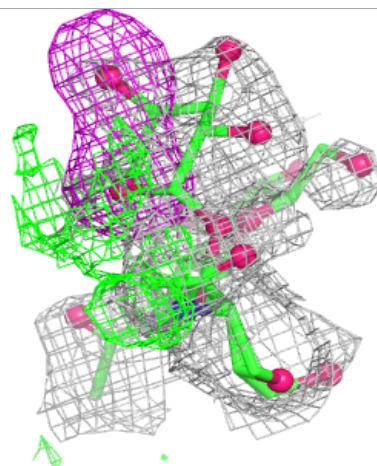
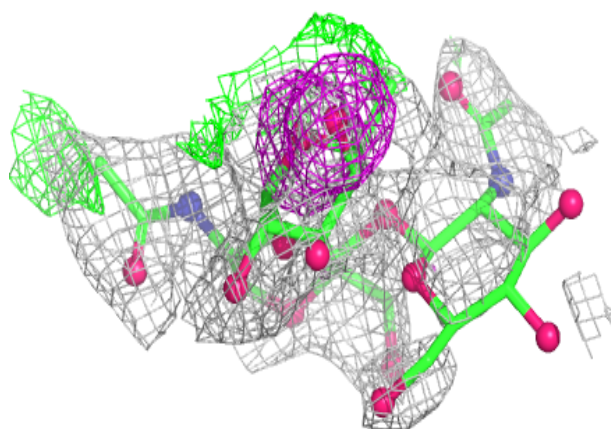
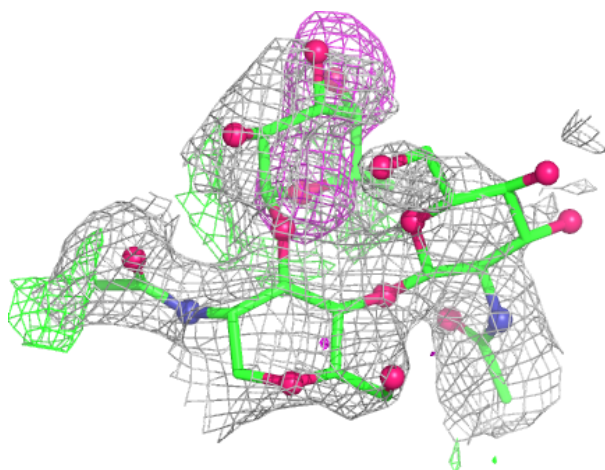
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUL	H	2	10/11	0.42	0.28	1,94,98,98	0
2	NAG	G	1	14/15	0.53	0.16	57,77,88,97	0
3	NAG	H	3	14/15	0.54	0.15	85,93,98,99	0
2	FUC	G	2	10/11	0.55	0.29	1,95,99,100	0
2	NAG	G	3	14/15	0.59	0.15	69,85,93,98	0
3	NAG	H	1	14/15	0.69	0.13	71,77,89,93	0
2	NAG	I	3	14/15	0.87	0.10	52,60,64,76	0
2	NAG	I	1	14/15	0.94	0.08	29,35,48,52	0
2	FUC	I	2	10/11	0.94	0.07	28,46,51,53	0

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

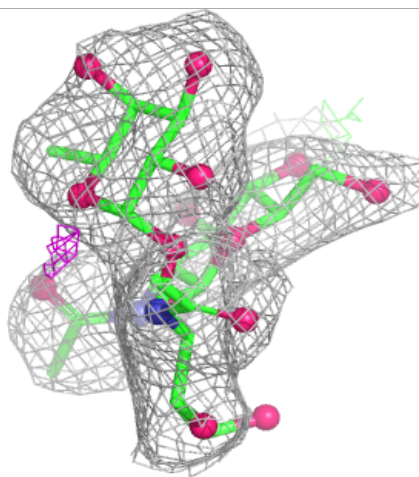
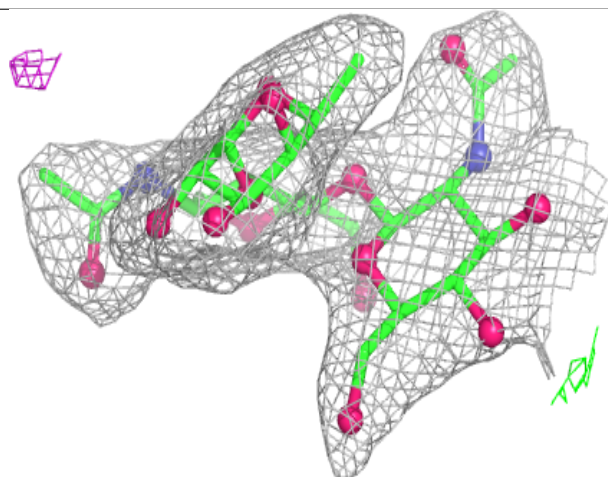
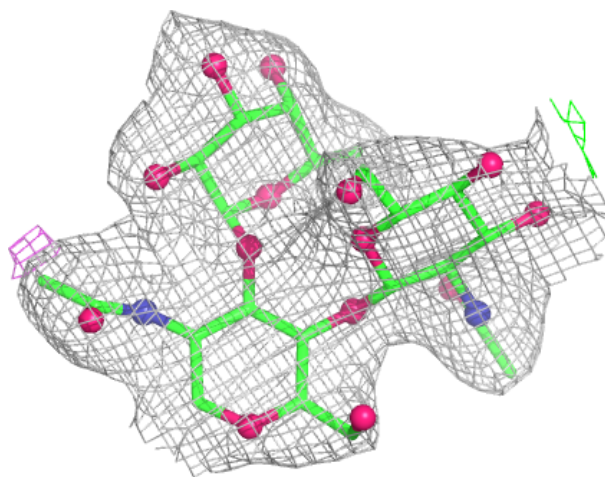
Electron density around Chain G:

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



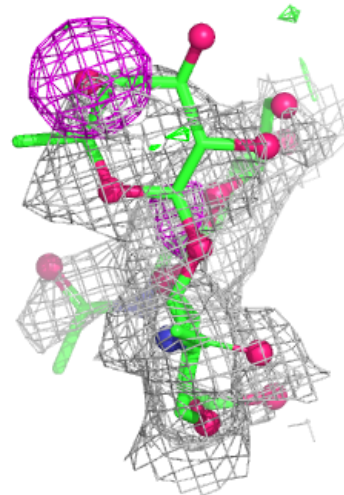
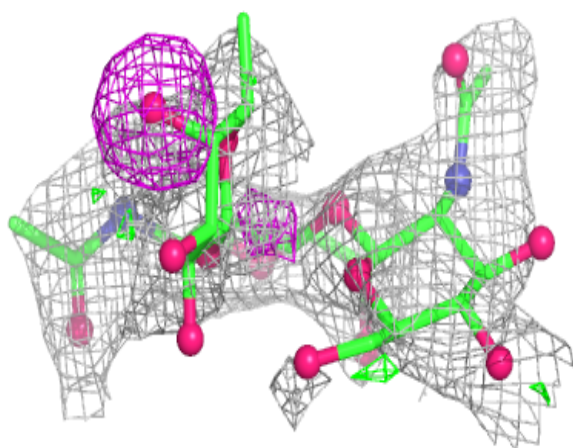
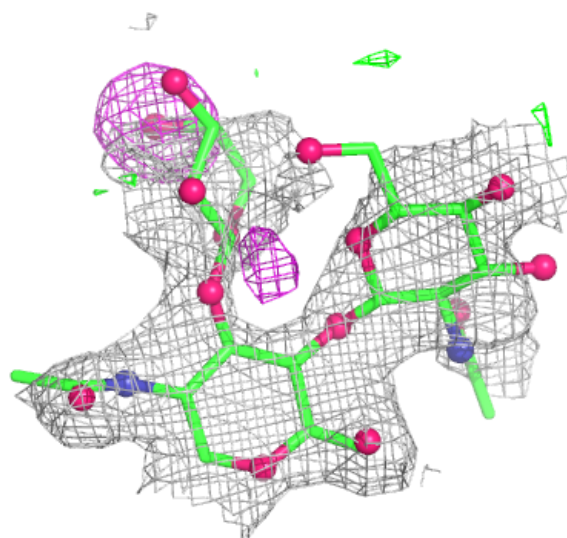
Electron density around Chain I:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
5	MN	B	257	1/1	0.96	0.04	29,29,29,29	0
4	CA	A	254	1/1	0.97	0.03	43,43,43,43	0
4	CA	E	254	1/1	0.98	0.03	30,30,30,30	0
4	CA	F	254	1/1	0.98	0.03	54,54,54,54	0
4	CA	D	254	1/1	0.98	0.04	41,41,41,41	0
4	CA	B	254	1/1	0.99	0.03	31,31,31,31	0
4	CA	C	254	1/1	0.99	0.02	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MN	D	257	1/1	0.99	0.03	35,35,35,35	0
5	MN	E	257	1/1	0.99	0.02	23,23,23,23	0
5	MN	F	257	1/1	0.99	0.04	38,38,38,38	0
5	MN	C	257	1/1	1.00	0.03	29,29,29,29	0
5	MN	A	257	1/1	1.00	0.03	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.