



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:06 PM UTC

PDB ID : 1LRH / pdb_00001lrh
Title : Crystal structure of auxin-binding protein 1 in complex with 1-naphthalene acetic acid
Authors : Woo, E.J.; Marshall, J.; Bauly, J.; Chen, J.-G.; Venis, M.; Napier, R.M.; Pickersgill, R.W.
Deposited on : 2002-05-15
Resolution : 1.90 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)
Validation Pipeline (wwPDB-VP) : 2.49

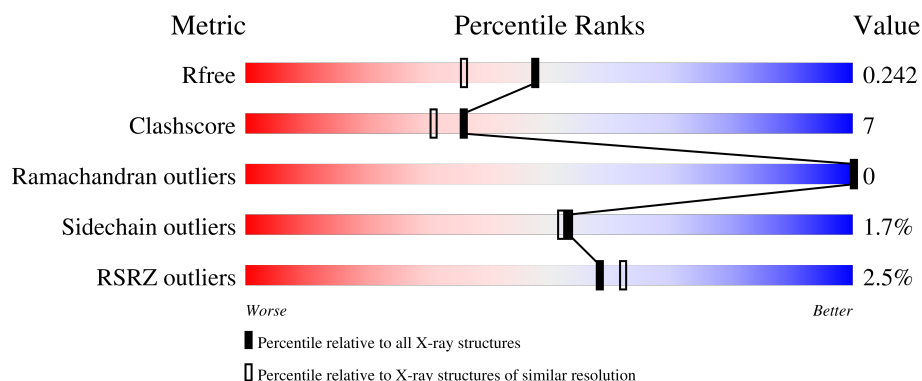
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	163	2% 85% 13% .
1	B	163	3% 72% 25% ..
1	C	163	3% 75% 20% ..
1	D	163	2% 67% 26% ...
2	E	6	100%

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Mol	Chain	Length	Quality of chain
2	F	6	 100%
2	G	6	 83% 17%
2	H	6	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	H	5	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5799 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.

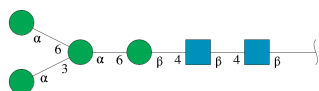
- Molecule 1 is a protein called auxin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1269	810	214	238	7			
1	B	160	Total	C	N	O	S	0	0	0
			1269	810	214	238	7			
1	C	160	Total	C	N	O	S	0	0	0
			1269	810	214	238	7			
1	D	160	Total	C	N	O	S	0	0	0
			1269	810	214	238	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	GLU	ASP	engineered mutation	UNP P13689
A	162	GLN	GLU	engineered mutation	UNP P13689
B	161	GLU	ASP	engineered mutation	UNP P13689
B	162	GLN	GLU	engineered mutation	UNP P13689
C	161	GLU	ASP	engineered mutation	UNP P13689
C	162	GLN	GLU	engineered mutation	UNP P13689
D	161	GLU	ASP	engineered mutation	UNP P13689
D	162	GLN	GLU	engineered mutation	UNP P13689

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

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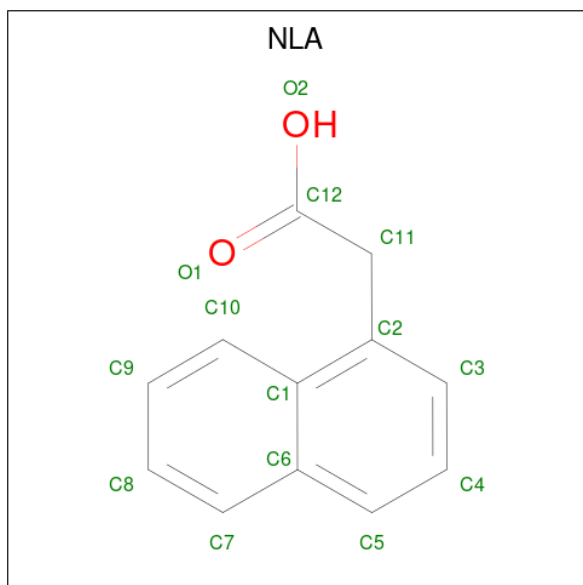
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	G	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	H	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is NAPHTHALEN-1-YL-ACETIC ACID (CCD ID: NLA) (formula: C₁₂H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	12	2		
4	B	1	Total	C	O	0	0
			14	12	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			14	12	2		
4	D	1	Total	C	O	0	0
			14	12	2		

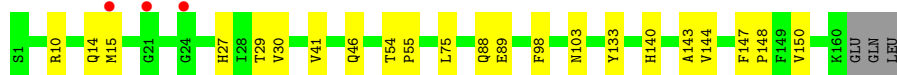
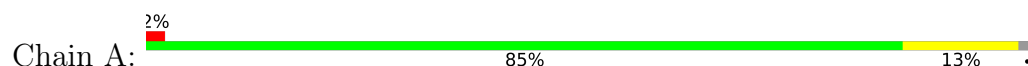
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		
5	B	96	Total	O	0	0
			96	96		
5	C	87	Total	O	0	0
			87	87		
5	D	104	Total	O	0	0
			104	104		

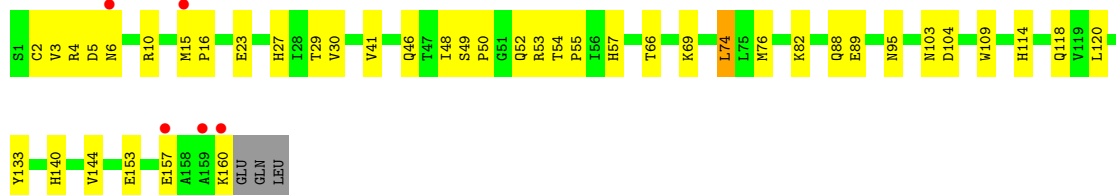
3 Residue-property plots [i](#)

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.

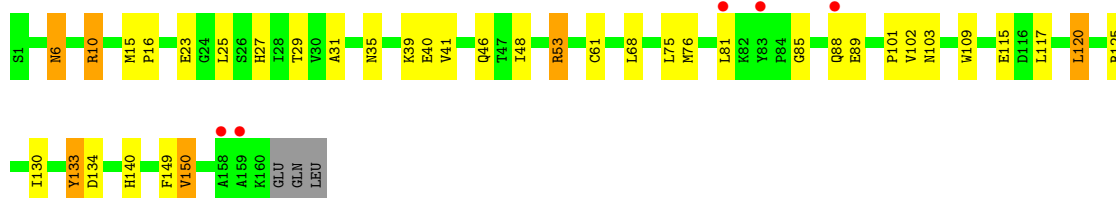
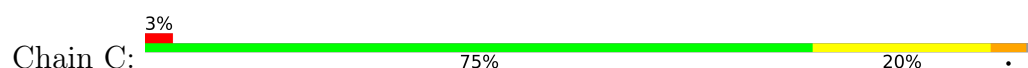
- Molecule 1: auxin-binding protein 1



- Molecule 1: auxin-binding protein 1



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- Molecule 1: auxin-binding protein 1





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

Chain E: 100%



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

Chain F: 100%



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

Chain G: 83% 17%



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

Chain H: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.58Å 82.43Å 69.96Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 15.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.90) 98.5 (15.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.31 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.240 0.193 , 0.242	Depositor DCC
R_{free} test set	2715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5799	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NLA, ZN, 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	0.90	0/1306	1.70	6/1779 (0.3%)
1	B	0.85	0/1306	1.69	17/1779 (1.0%)
1	C	0.93	1/1306 (0.1%)	1.82	26/1779 (1.5%)
1	D	0.96	1/1306 (0.1%)	1.89	30/1779 (1.7%)
All	All	0.91	2/5224 (0.0%)	1.78	79/7116 (1.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	ARG	CD-NE	5.88	1.54	1.46
1	D	100	ILE	N-CA	5.78	1.50	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	SER	N-CA-CB	19.06	139.42	110.45
1	D	8	LEU	CA-C-O	-9.55	110.97	121.00
1	C	125	ARG	O-C-N	-9.50	117.16	121.53
1	C	125	ARG	CB-CA-C	-8.54	105.13	111.20
1	D	125	ARG	O-C-N	-8.34	117.69	121.53
1	D	7	SER	CB-CA-C	-7.97	93.89	109.76
1	D	7	SER	O-C-N	7.88	131.83	122.85
1	D	125	ARG	CB-CA-C	-7.79	105.67	111.20
1	C	16	PRO	CB-CA-C	7.78	121.55	111.21
1	A	88	GLN	OE1-CD-NE2	7.54	130.14	122.60
1	C	61	CYS	CA-C-O	-7.48	113.27	121.28
1	C	31	ALA	CA-C-N	-7.20	112.81	122.03
1	C	31	ALA	C-N-CA	-7.20	112.81	122.03
1	C	10	ARG	NE-CZ-NH1	7.08	128.58	121.50
1	D	129	LYS	CB-CG-CD	7.06	127.54	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	ASP	CA-C-N	-6.92	112.17	122.83
1	B	5	ASP	C-N-CA	-6.92	112.17	122.83
1	C	117	LEU	CA-C-O	-6.82	112.82	120.32
1	B	88	GLN	OE1-CD-NE2	6.74	129.34	122.60
1	D	121	VAL	CA-C-O	-6.51	113.55	120.39
1	D	135	ASP	CA-C-O	-6.46	114.36	121.28
1	B	69	LYS	CB-CA-C	-6.46	98.82	109.80
1	D	88	GLN	CA-C-O	-6.45	113.94	121.16
1	D	48	ILE	N-CA-CB	-6.42	102.52	111.25
1	C	76	MET	CA-C-O	-6.36	113.49	120.36
1	B	89	GLU	CB-CG-CD	6.30	123.31	112.60
1	C	88	GLN	CA-C-O	-6.28	114.25	121.47
1	D	26	SER	CA-C-O	-6.26	113.60	120.24
1	C	10	ARG	CD-NE-CZ	-6.16	115.78	124.40
1	C	133	TYR	CA-C-O	-6.12	114.23	120.71
1	C	85	GLY	CA-C-O	-6.12	116.70	122.39
1	D	6	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	B	52	GLN	CB-CG-CD	6.09	122.95	112.60
1	D	48	ILE	CA-CB-CG2	6.09	120.85	110.50
1	A	144	VAL	O-C-N	6.07	129.55	123.18
1	D	11	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	150	VAL	N-CA-C	5.99	117.45	110.62
1	C	81	LEU	CA-C-O	-5.99	115.72	122.01
1	D	8	LEU	CA-C-N	-5.97	115.40	122.93
1	D	8	LEU	C-N-CA	-5.97	115.40	122.93
1	B	57	HIS	N-CA-C	5.92	117.25	108.60
1	D	69	LYS	CA-C-O	-5.92	114.35	120.99
1	D	71	LYS	CA-C-O	-5.90	114.95	121.33
1	B	104	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	74	LEU	CA-C-O	-5.80	113.98	120.54
1	A	150	VAL	N-CA-C	5.76	116.49	110.62
1	A	98	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	14	GLN	CB-CG-CD	5.71	122.31	112.60
1	D	7	SER	N-CA-C	-5.67	102.89	110.55
1	A	143	ALA	CA-C-O	-5.64	114.98	121.19
1	D	81	LEU	CA-C-O	-5.63	115.57	121.99
1	B	114	HIS	CA-CB-CG	-5.62	108.18	113.80
1	B	114	HIS	N-CA-C	5.55	120.92	114.04
1	C	35	ASN	CA-C-O	-5.53	114.11	120.24
1	C	16	PRO	CA-C-O	5.50	127.92	121.31
1	D	133	TYR	CA-C-N	-5.48	111.86	122.06
1	D	133	TYR	C-N-CA	-5.48	111.86	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	GLU	CA-CB-CG	5.48	125.05	114.10
1	D	144	VAL	N-CA-C	5.47	116.60	108.23
1	D	76	MET	CA-C-N	-5.43	116.28	122.85
1	D	76	MET	C-N-CA	-5.43	116.28	122.85
1	B	52	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	C	115	GLU	CB-CG-CD	5.38	121.75	112.60
1	C	134	ASP	N-CA-CB	5.35	119.13	110.40
1	C	101	PRO	CA-C-N	5.33	128.47	120.69
1	C	101	PRO	C-N-CA	5.33	128.47	120.69
1	B	118	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	C	149	PHE	CA-CB-CG	-5.26	108.54	113.80
1	D	4	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	C	120	LEU	CA-C-O	-5.17	114.74	120.38
1	C	130	ILE	N-CA-C	5.17	116.03	108.58
1	C	10	ARG	NH1-CZ-NH2	-5.15	112.61	119.30
1	D	117	LEU	CA-C-O	-5.13	114.78	120.38
1	B	95	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	D	27	HIS	CE1-NE2-CD2	5.08	114.08	109.00
1	C	53	ARG	CA-C-O	-5.06	115.19	121.11
1	B	114	HIS	CA-C-N	-5.04	115.39	122.94
1	B	114	HIS	C-N-CA	-5.04	115.39	122.94
1	B	144	VAL	N-CA-C	5.01	115.52	108.36

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	1269	0	1228	14	0
1	B	1269	0	1228	20	0
1	C	1269	0	1228	18	0
1	D	1269	0	1228	29	0
2	E	72	0	60	0	0
2	F	72	0	61	0	0
2	G	72	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	72	0	61	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	9	0	0
4	B	14	0	9	1	0
4	C	14	0	9	0	0
4	D	14	0	9	0	0
5	A	88	0	0	0	0
5	B	96	0	0	3	0
5	C	87	0	0	2	0
5	D	104	0	0	6	0
All	All	5799	0	5191	77	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 (77) 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)
5:B:4008:HOH:O	1:C:40:GLU:HG3	1.65	0.96
1:D:27:HIS:HD2	1:D:46:GLN:HE21	1.17	0.92
1:D:7:SER:CB	5:D:4180:HOH:O	2.18	0.90
1:B:74:LEU:HD21	1:B:76:MET:HE2	1.51	0.90
5:B:4008:HOH:O	1:C:39:LYS:HB2	1.72	0.89
1:B:27:HIS:HD2	1:B:46:GLN:HE21	1.23	0.84
1:C:27:HIS:HD2	1:C:46:GLN:HE21	1.28	0.81
1:A:27:HIS:HD2	1:A:46:GLN:HE21	1.29	0.78
1:C:75:LEU:HD22	1:C:89:GLU:HG2	1.67	0.76
1:C:23:GLU:HG2	5:C:3348:HOH:O	1.84	0.75
1:D:7:SER:HB3	5:D:4180:HOH:O	1.85	0.74
1:A:15:MET:HE1	1:A:30:VAL:O	1.91	0.71
1:A:75:LEU:HD22	1:A:89:GLU:HG2	1.72	0.70
1:D:75:LEU:HD22	1:D:89:GLU:HG2	1.73	0.70
1:D:150:VAL:HG13	5:D:4226:HOH:O	1.92	0.69
1:B:27:HIS:CD2	1:B:46:GLN:HE21	2.10	0.68
1:C:25:LEU:HA	1:C:48:ILE:HD13	1.76	0.67
1:D:83:TYR:HB2	1:D:84:PRO:HD2	1.78	0.65
1:C:150:VAL:HG13	5:C:3226:HOH:O	1.96	0.65
1:D:27:HIS:CD2	1:D:46:GLN:HE21	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLU:HG2	5:B:2348:HOH:O	1.96	0.64
1:B:3:VAL:HG21	1:B:16:PRO:HG3	1.80	0.62
1:B:157:GLU:HA	1:B:160:LYS:HE3	1.82	0.62
1:B:2:CYS:SG	1:B:4:ARG:HG3	2.40	0.62
1:A:27:HIS:CD2	1:A:46:GLN:HE21	2.15	0.62
1:C:133:TYR:OH	1:C:140:HIS:HD2	1.84	0.60
1:D:7:SER:OG	5:D:4180:HOH:O	1.82	0.59
1:C:53:ARG:HG2	1:C:109:TRP:HB2	1.85	0.58
1:D:83:TYR:HB2	1:D:84:PRO:CD	2.35	0.56
1:B:133:TYR:OH	1:B:140:HIS:HD2	1.88	0.56
1:C:10:ARG:HE	1:C:15:MET:HE1	1.71	0.56
1:C:68:LEU:HD11	1:C:120:LEU:HG	1.88	0.56
1:A:133:TYR:OH	1:A:140:HIS:HD2	1.90	0.55
1:D:133:TYR:OH	1:D:140:HIS:HD2	1.90	0.55
1:B:15:MET:HE1	1:B:30:VAL:O	2.07	0.54
1:B:41:VAL:HG12	1:C:41:VAL:HG12	1.90	0.54
1:D:148:PRO:HG3	1:D:156:PHE:CG	2.42	0.54
1:C:27:HIS:CD2	1:C:46:GLN:HE21	2.17	0.54
1:C:102:VAL:O	1:C:103:ASN:HB2	2.08	0.53
1:B:53:ARG:HG2	1:B:109:TRP:HB2	1.91	0.53
1:A:75:LEU:CD2	1:A:89:GLU:HG2	2.39	0.52
1:B:49:SER:HB2	1:B:50:PRO:HD2	1.92	0.52
1:D:75:LEU:HD22	1:D:89:GLU:CG	2.40	0.51
1:B:48:ILE:HD11	4:B:6190:NLA:H91	1.93	0.50
1:B:10:ARG:HE	1:B:15:MET:CE	2.25	0.50
1:A:41:VAL:HG12	1:D:41:VAL:HG12	1.93	0.50
1:C:25:LEU:HD13	1:C:48:ILE:HD11	1.93	0.50
1:A:41:VAL:CG1	1:D:41:VAL:HG12	2.42	0.49
1:D:147:PHE:CD1	1:D:148:PRO:HA	2.47	0.49
1:B:23:GLU:OE1	2:G:6:MAN:O3	2.30	0.49
1:A:27:HIS:HE1	1:A:29:THR:OG1	1.95	0.48
1:B:153:GLU:O	1:B:157:GLU:HG2	2.13	0.48
1:D:153:GLU:O	1:D:157:GLU:HG2	2.13	0.48
1:A:54:THR:HB	1:A:55:PRO:HD2	1.95	0.48
1:C:10:ARG:HE	1:C:15:MET:CE	2.27	0.47
1:D:76:MET:HG3	1:D:106:HIS:HB3	1.95	0.47
1:A:10:ARG:HE	1:A:15:MET:HE3	1.80	0.47
1:D:8:LEU:HB3	5:D:4214:HOH:O	2.16	0.45
1:D:17:GLN:HB2	1:D:28:ILE:HG13	1.98	0.45
1:D:27:HIS:HE1	1:D:29:THR:OG1	2.01	0.44
1:D:53:ARG:HG2	1:D:109:TRP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:OG1	1:B:120:LEU:HB2	2.16	0.44
1:A:147:PHE:HA	1:A:148:PRO:C	2.43	0.44
1:D:71:LYS:HE2	5:D:4438:HOH:O	2.17	0.43
1:C:6:ASN:C	1:C:6:ASN:HD22	2.26	0.43
1:B:82:LYS:NZ	1:D:141:THR:O	2.52	0.43
1:D:102:VAL:O	1:D:103:ASN:HB2	2.18	0.43
1:D:6:ASN:C	1:D:6:ASN:HD22	2.27	0.43
1:B:54:THR:HB	1:B:55:PRO:HD2	2.01	0.42
1:A:10:ARG:HE	1:A:15:MET:CE	2.31	0.42
1:A:27:HIS:HD2	1:A:46:GLN:NE2	2.08	0.42
1:D:7:SER:HB3	1:D:8:LEU:H	1.39	0.41
1:C:27:HIS:HE1	1:C:29:THR:OG1	2.03	0.41
1:D:49:SER:HB2	1:D:50:PRO:CD	2.51	0.41
1:D:15:MET:HE1	1:D:36:HIS:NE2	2.36	0.41
1:D:127:PRO:O	1:D:129:LYS:HD3	2.20	0.41
1:B:27:HIS:HE1	1:B:29:THR:OG1	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	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	B	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	C	158/163 (97%)	153 (97%)	5 (3%)	0	100	100
1	D	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
All	All	632/652 (97%)	620 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/147 (98%)	143 (99%)	1 (1%)	76	78
1	B	144/147 (98%)	142 (99%)	2 (1%)	59	59
1	C	144/147 (98%)	143 (99%)	1 (1%)	76	78
1	D	144/147 (98%)	138 (96%)	6 (4%)	26	19
All	All	576/588 (98%)	566 (98%)	10 (2%)	53	52

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	B	6	ASN
1	B	103	ASN
1	C	6	ASN
1	D	6	ASN
1	D	17	GLN
1	D	59	HIS
1	D	71	LYS
1	D	129	LYS
1	D	134	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	35	ASN
1	A	46	GLN
1	A	103	ASN
1	A	140	HIS
1	B	6	ASN
1	B	27	HIS
1	B	86	GLN
1	B	140	HIS

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Mol	Chain	Res	Type
1	C	6	ASN
1	C	27	HIS
1	C	46	GLN
1	C	86	GLN
1	C	103	ASN
1	C	118	GLN
1	C	140	HIS
1	D	6	ASN
1	D	27	HIS
1	D	46	GLN
1	D	86	GLN
1	D	88	GLN
1	D	140	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 ⓘ

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	1.22	1 (7%)	17,19,21	1.73	5 (29%)
2	NAG	E	2	2	14,14,15	1.25	1 (7%)	17,19,21	1.27	1 (5%)
2	BMA	E	3	2	11,11,12	1.46	2 (18%)	15,15,17	2.08	3 (20%)
2	MAN	E	4	2	11,11,12	0.98	0	15,15,17	2.45	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	E	5	2	11,11,12	0.76	0	15,15,17	1.73	3 (20%)
2	MAN	E	6	2	11,11,12	0.88	0	15,15,17	1.83	3 (20%)
2	NAG	F	1	2,1	14,14,15	1.14	1 (7%)	17,19,21	1.25	3 (17%)
2	NAG	F	2	2	14,14,15	1.18	1 (7%)	17,19,21	1.44	5 (29%)
2	BMA	F	3	2	11,11,12	1.18	1 (9%)	15,15,17	1.82	4 (26%)
2	MAN	F	4	2	11,11,12	1.20	1 (9%)	15,15,17	3.04	7 (46%)
2	MAN	F	5	2	11,11,12	0.90	1 (9%)	15,15,17	1.69	4 (26%)
2	MAN	F	6	2	11,11,12	1.05	0	15,15,17	1.84	3 (20%)
2	NAG	G	1	2,1	14,14,15	1.37	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	G	2	2	14,14,15	1.33	1 (7%)	17,19,21	1.11	1 (5%)
2	BMA	G	3	2	11,11,12	0.95	0	15,15,17	2.04	5 (33%)
2	MAN	G	4	2	11,11,12	0.97	0	15,15,17	2.39	4 (26%)
2	MAN	G	5	2	11,11,12	0.75	0	15,15,17	1.60	2 (13%)
2	MAN	G	6	2	11,11,12	0.77	0	15,15,17	1.51	3 (20%)
2	NAG	H	1	2,1	14,14,15	1.35	1 (7%)	17,19,21	1.14	1 (5%)
2	NAG	H	2	2	14,14,15	1.42	2 (14%)	17,19,21	1.31	2 (11%)
2	BMA	H	3	2	11,11,12	0.97	0	15,15,17	2.11	4 (26%)
2	MAN	H	4	2	11,11,12	1.21	1 (9%)	15,15,17	2.49	6 (40%)
2	MAN	H	5	2	11,11,12	0.82	0	15,15,17	1.96	4 (26%)
2	MAN	H	6	2	11,11,12	0.89	0	15,15,17	1.60	3 (20%)

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

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O7-C7	-4.15	1.14	1.23
2	H	1	NAG	O7-C7	-3.94	1.14	1.23
2	E	1	NAG	O7-C7	-3.92	1.14	1.23
2	F	1	NAG	O7-C7	-3.69	1.15	1.23
2	H	2	NAG	O7-C7	-3.62	1.15	1.23
2	G	2	NAG	O7-C7	-3.62	1.15	1.23
2	E	2	NAG	O7-C7	-3.19	1.16	1.23
2	F	2	NAG	O7-C7	-2.97	1.16	1.23
2	F	4	MAN	O2-C2	-2.73	1.37	1.43
2	H	4	MAN	C1-C2	2.55	1.58	1.52
2	E	3	BMA	C1-C2	2.38	1.57	1.52
2	F	3	BMA	C1-C2	2.37	1.57	1.52
2	H	2	NAG	C2-N2	2.35	1.50	1.46
2	F	5	MAN	C6-C5	2.07	1.58	1.51
2	E	3	BMA	O5-C1	2.00	1.47	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	MAN	C1-C2-C3	-8.24	97.64	109.64
2	H	4	MAN	C2-C3-C4	6.30	121.93	110.86
2	G	4	MAN	C1-C2-C3	-5.85	101.13	109.64
2	E	4	MAN	C1-C2-C3	-5.56	101.55	109.64
2	H	3	BMA	C1-O5-C5	-5.45	104.89	112.19
2	H	5	MAN	C1-C2-C3	-5.41	101.77	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	-5.24	105.17	112.19
2	G	5	MAN	C1-C2-C3	-4.80	102.65	109.64
2	E	6	MAN	C1-C2-C3	-4.68	102.83	109.64
2	E	4	MAN	C3-C4-C5	-4.56	101.97	110.23
2	F	4	MAN	C2-C3-C4	4.40	118.60	110.86
2	F	6	MAN	O2-C2-C3	4.27	118.99	110.15
2	E	5	MAN	O2-C2-C3	4.21	118.86	110.15
2	G	4	MAN	C3-C4-C5	-4.15	102.70	110.23
2	F	3	BMA	C3-C4-C5	-4.11	102.79	110.23
2	G	3	BMA	C1-O5-C5	-4.09	106.70	112.19
2	E	4	MAN	C2-C3-C4	4.08	118.04	110.86
2	E	3	BMA	O5-C5-C6	3.86	115.17	107.66
2	E	6	MAN	O3-C3-C2	-3.84	102.22	110.05
2	E	1	NAG	C2-N2-C7	3.70	127.85	122.90
2	G	3	BMA	O3-C3-C2	-3.69	102.53	110.05
2	F	4	MAN	O3-C3-C2	-3.47	102.98	110.05
2	F	6	MAN	C1-C2-C3	-3.40	104.70	109.64
2	F	4	MAN	C3-C4-C5	-3.33	104.19	110.23
2	G	4	MAN	C2-C3-C4	3.32	116.70	110.86
2	G	6	MAN	C1-C2-C3	-3.31	104.82	109.64
2	F	5	MAN	O3-C3-C2	-3.31	103.31	110.05
2	E	3	BMA	C3-C4-C5	-3.28	104.29	110.23
2	G	3	BMA	C3-C4-C5	-3.24	104.36	110.23
2	E	1	NAG	O7-C7-C8	3.19	127.73	122.05
2	E	4	MAN	O6-C6-C5	-3.15	100.60	111.33
2	F	3	BMA	C1-O5-C5	-3.11	108.02	112.19
2	F	5	MAN	O6-C6-C5	-3.11	100.75	111.33
2	E	2	NAG	O5-C1-C2	-3.09	106.51	111.29
2	F	4	MAN	O2-C2-C3	3.07	116.52	110.15
2	H	2	NAG	O5-C1-C2	-3.04	106.58	111.29
2	E	5	MAN	C1-O5-C5	3.00	116.21	112.19
2	H	4	MAN	O2-C2-C3	2.99	116.35	110.15
2	F	1	NAG	C8-C7-N2	-2.97	111.19	116.12
2	G	6	MAN	O2-C2-C1	2.95	115.98	109.22
2	H	6	MAN	C2-C3-C4	2.85	115.88	110.86
2	H	4	MAN	O4-C4-C5	2.83	116.30	109.32
2	H	6	MAN	O2-C2-C3	2.76	115.87	110.15
2	G	6	MAN	O3-C3-C2	-2.76	104.42	110.05
2	G	5	MAN	O2-C2-C3	2.76	115.86	110.15
2	H	3	BMA	O5-C1-C2	-2.71	104.33	110.79
2	E	6	MAN	O2-C2-C3	2.65	115.63	110.15
2	F	5	MAN	O5-C1-C2	2.63	117.07	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	MAN	C1-C2-C3	-2.63	105.82	109.64
2	G	1	NAG	O4-C4-C3	-2.62	104.19	110.38
2	G	2	NAG	O5-C1-C2	-2.60	107.26	111.29
2	H	3	BMA	C3-C4-C5	-2.56	105.59	110.23
2	F	2	NAG	O5-C1-C2	-2.52	107.39	111.29
2	F	6	MAN	O5-C5-C6	2.52	112.57	107.66
2	E	1	NAG	O4-C4-C3	-2.52	104.44	110.38
2	H	4	MAN	O3-C3-C2	-2.47	105.00	110.05
2	H	4	MAN	C6-C5-C4	2.47	119.09	113.02
2	G	3	BMA	C1-C2-C3	2.47	113.24	109.64
2	G	1	NAG	O7-C7-C8	2.43	126.39	122.05
2	F	2	NAG	C8-C7-N2	-2.35	112.22	116.12
2	H	5	MAN	O3-C3-C4	2.34	115.90	110.38
2	H	4	MAN	C3-C4-C5	-2.34	105.99	110.23
2	F	3	BMA	O3-C3-C4	-2.33	104.88	110.38
2	H	5	MAN	C1-O5-C5	2.30	115.27	112.19
2	F	5	MAN	O5-C5-C6	-2.29	103.20	107.66
2	H	6	MAN	O4-C4-C3	2.26	115.71	110.38
2	E	1	NAG	C8-C7-N2	-2.25	112.39	116.12
2	F	4	MAN	O6-C6-C5	-2.24	103.71	111.33
2	E	1	NAG	O5-C1-C2	-2.23	107.84	111.29
2	F	3	BMA	C2-C3-C4	2.20	114.73	110.86
2	G	4	MAN	C6-C5-C4	2.19	118.40	113.02
2	H	2	NAG	C1-C2-N2	-2.17	107.02	110.43
2	F	1	NAG	O5-C1-C2	-2.16	107.95	111.29
2	H	1	NAG	O5-C1-C2	-2.14	107.98	111.29
2	F	2	NAG	C4-C3-C2	-2.11	107.93	111.02
2	F	2	NAG	C2-N2-C7	-2.09	120.10	122.90
2	F	4	MAN	C6-C5-C4	2.09	118.15	113.02
2	G	3	BMA	O2-C2-C3	-2.08	105.84	110.15
2	H	5	MAN	O3-C3-C2	-2.07	105.82	110.05
2	F	2	NAG	O5-C5-C6	-2.07	103.64	107.66
2	F	1	NAG	O7-C7-C8	2.05	125.70	122.05
2	H	3	BMA	O5-C5-C6	2.03	111.62	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	5	MAN	C1

All (7) torsion outliers are listed below:

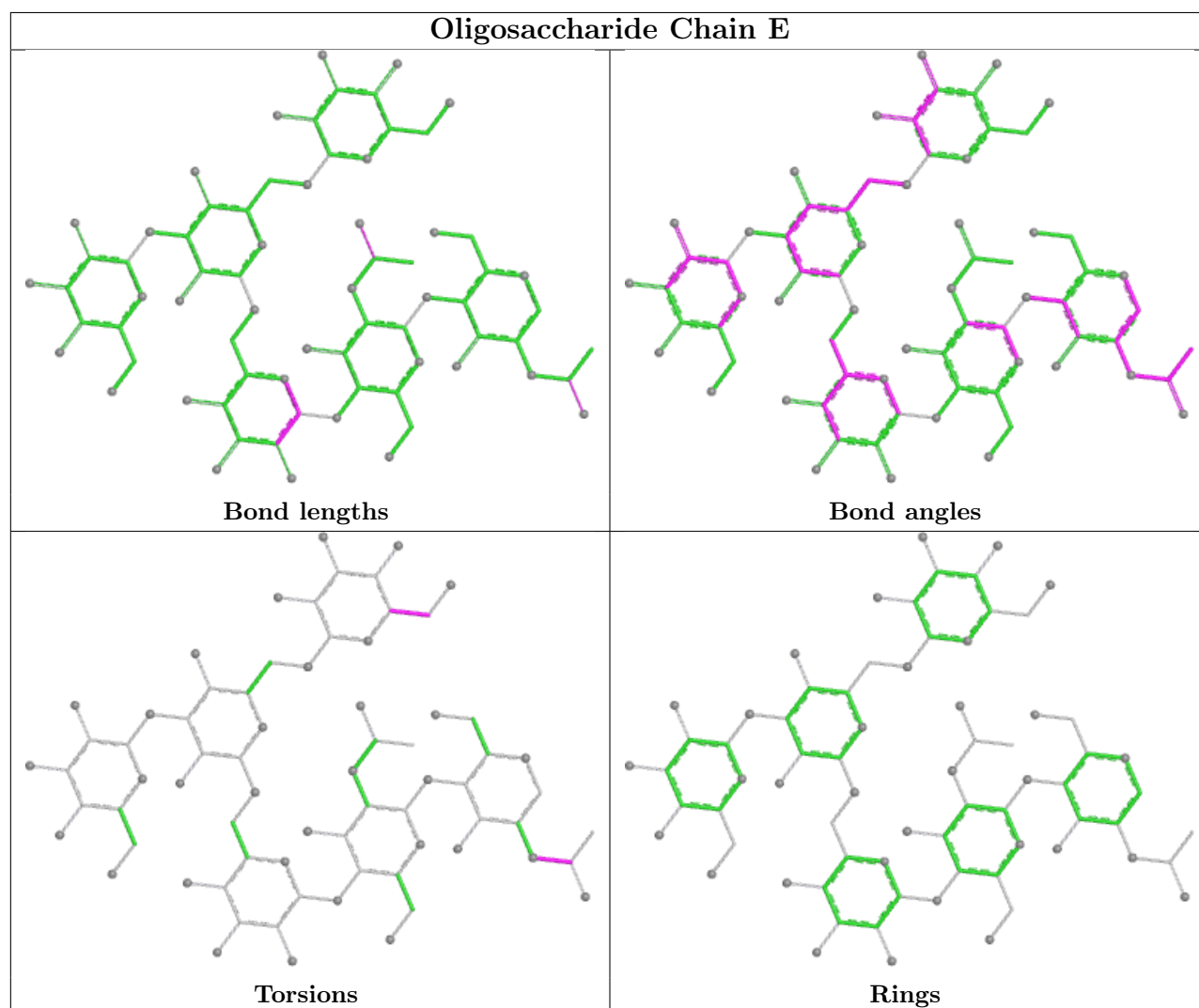
Mol	Chain	Res	Type	Atoms
2	H	6	MAN	O5-C5-C6-O6
2	E	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	F	5	MAN	C4-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7
2	H	5	MAN	C4-C5-C6-O6
2	E	6	MAN	C4-C5-C6-O6

There are no ring outliers.

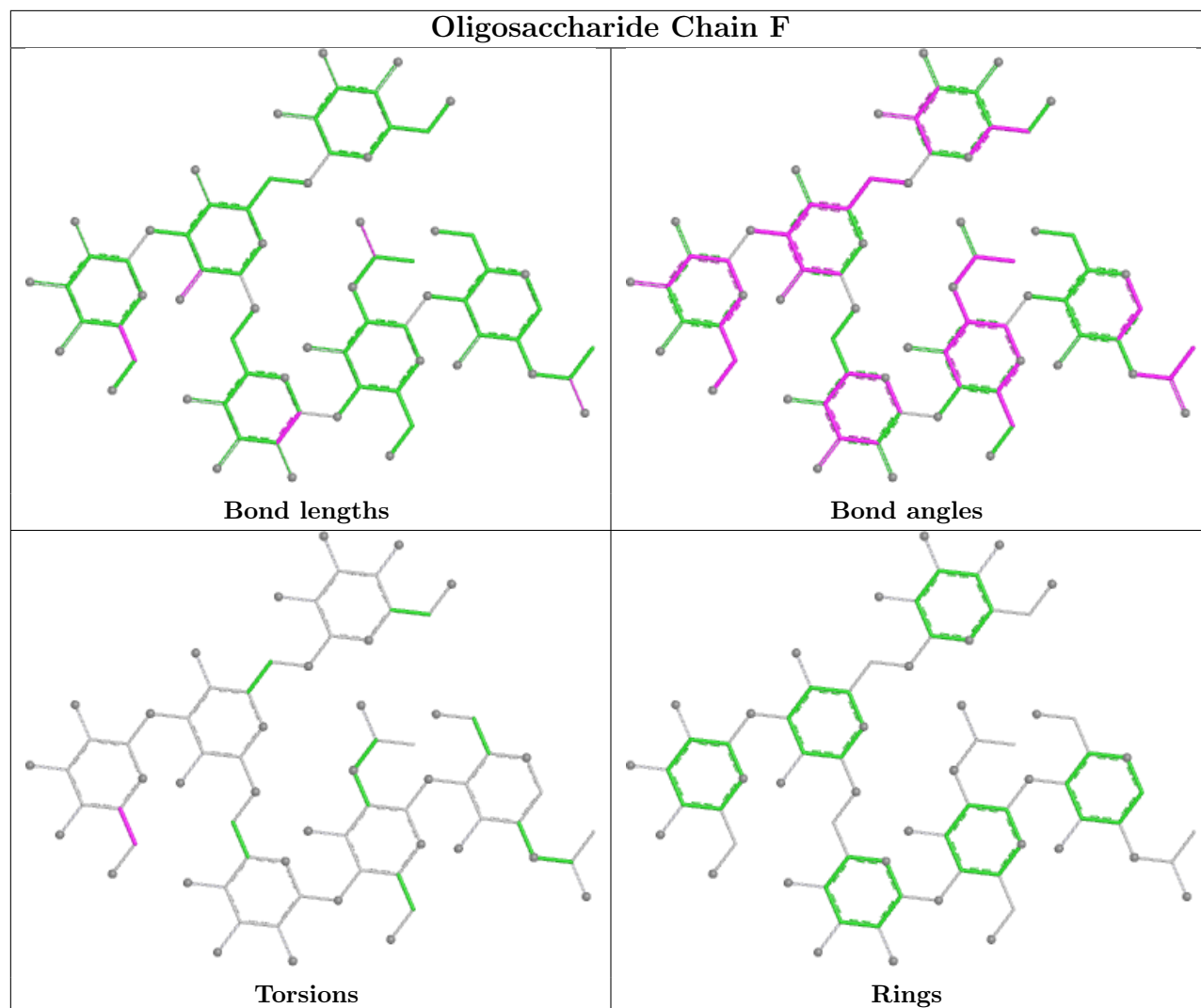
1 monomer is involved in 1 short contact:

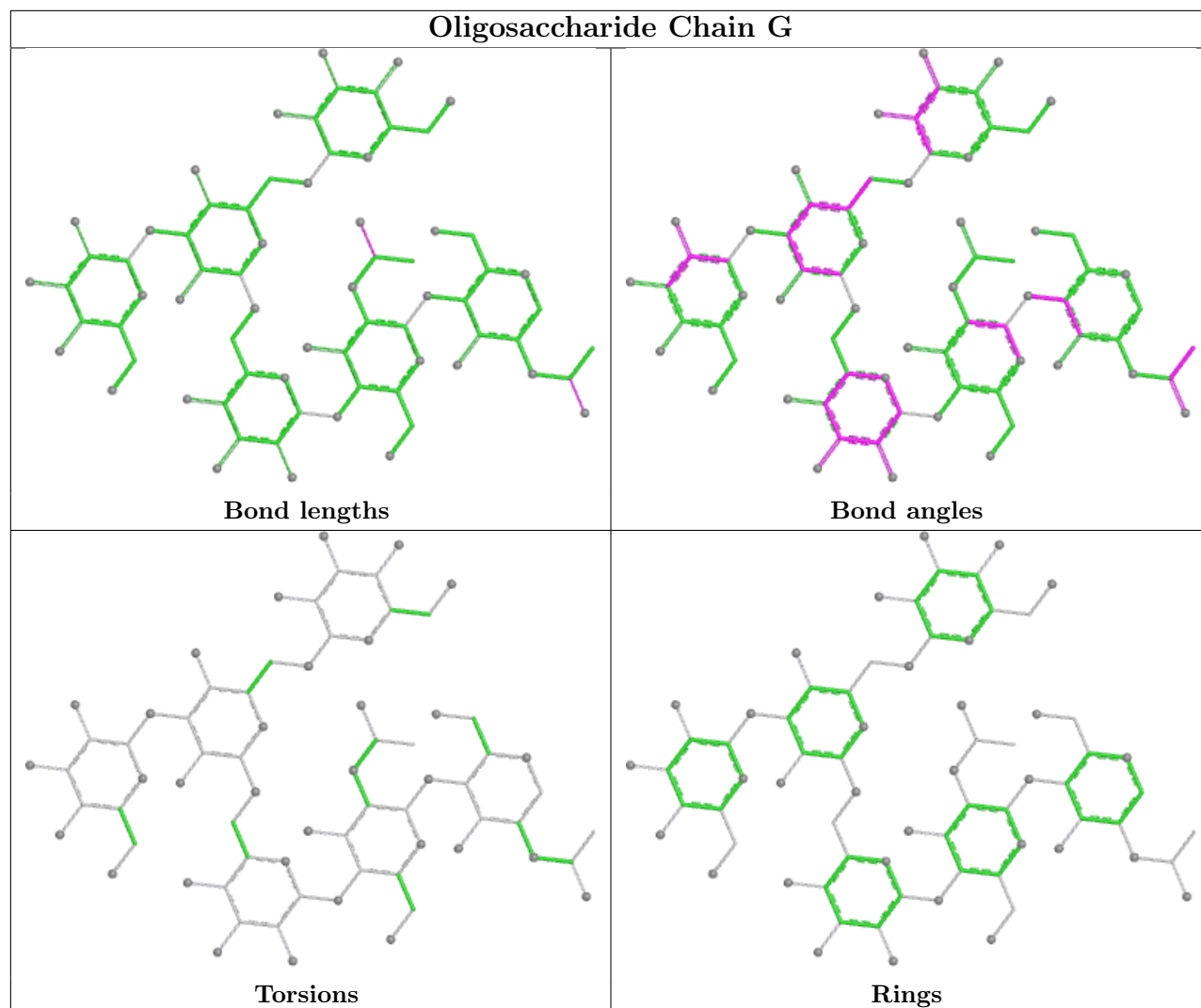
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	6	MAN	1	0

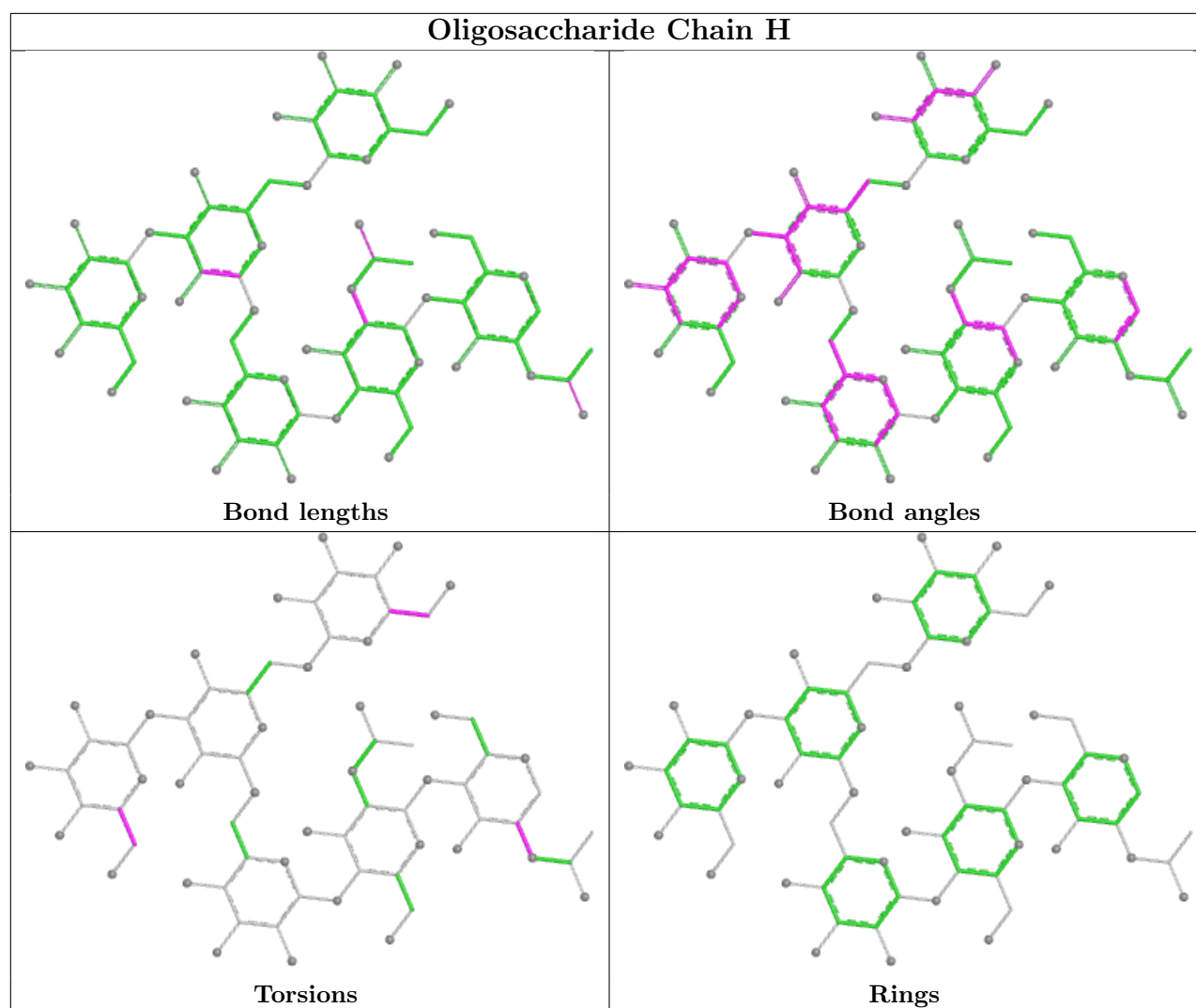
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain F







5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NLA	D	8190	3	15,15,15	1.55	2 (13%)	20,20,20	1.05	1 (5%)
4	NLA	A	5190	3	15,15,15	1.54	3 (20%)	20,20,20	0.78	0
4	NLA	B	6190	3	15,15,15	1.51	2 (13%)	20,20,20	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NLA	C	7190	3	15,15,15	1.58	3 (20%)	20,20,20	0.59	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
4	NLA	D	8190	3	-	2/4/4/4	0/2/2/2
4	NLA	A	5190	3	-	2/4/4/4	0/2/2/2
4	NLA	B	6190	3	-	2/4/4/4	0/2/2/2
4	NLA	C	7190	3	-	2/4/4/4	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8190	NLA	C3-C2	3.38	1.43	1.37
4	C	7190	NLA	O1-C12	3.30	1.32	1.22
4	B	6190	NLA	O1-C12	2.92	1.31	1.22
4	A	5190	NLA	O1-C12	2.79	1.31	1.22
4	D	8190	NLA	O1-C12	2.78	1.31	1.22
4	B	6190	NLA	C3-C2	2.73	1.42	1.37
4	A	5190	NLA	C3-C2	2.44	1.42	1.37
4	A	5190	NLA	C4-C3	2.18	1.42	1.38
4	C	7190	NLA	C3-C2	2.04	1.41	1.37
4	C	7190	NLA	C1-C6	2.03	1.46	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	8190	NLA	C4-C3-C2	-2.31	117.40	121.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	8190	NLA	C12-C11-C2-C3
4	C	7190	NLA	C12-C11-C2-C1
4	C	7190	NLA	C12-C11-C2-C3
4	B	6190	NLA	C12-C11-C2-C1

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Mol	Chain	Res	Type	Atoms
4	B	6190	NLA	C12-C11-C2-C3
4	D	8190	NLA	C12-C11-C2-C1
4	A	5190	NLA	C12-C11-C2-C1
4	A	5190	NLA	C12-C11-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	6190	NLA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	160/163 (98%)	-0.27	3 (1%) 66 70	8, 13, 24, 34	0
1	B	160/163 (98%)	-0.08	5 (3%) 51 55	8, 15, 30, 58	0
1	C	160/163 (98%)	-0.07	5 (3%) 51 55	7, 15, 38, 50	0
1	D	160/163 (98%)	-0.24	3 (1%) 66 70	7, 13, 26, 37	0
All	All	640/652 (98%)	-0.17	16 (2%) 58 62	7, 14, 29, 58	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	SER	3.8
1	C	81	LEU	3.8
1	A	15	MET	3.6
1	D	83	TYR	3.5
1	B	6	ASN	3.3
1	B	160	LYS	3.2
1	C	83	TYR	3.2
1	D	81	LEU	3.2
1	C	159	ALA	3.0
1	B	157	GLU	3.0
1	B	15	MET	2.5
1	A	21	GLY	2.3
1	C	88	GLN	2.3
1	C	158	ALA	2.2
1	A	24	GLY	2.2
1	B	159	ALA	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

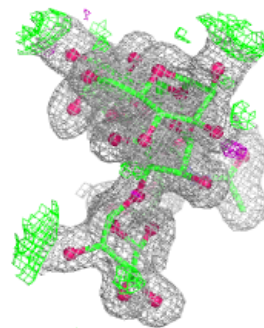
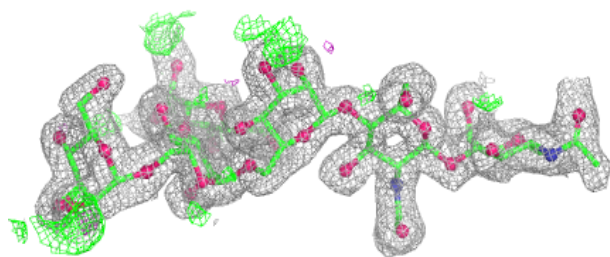
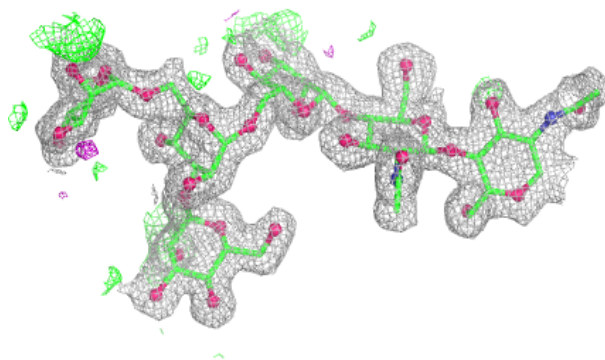
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	H	5	11/12	0.70	0.16	37,38,40,40	0
2	MAN	G	6	11/12	0.74	0.14	39,41,43,43	0
2	MAN	H	6	11/12	0.77	0.14	33,36,37,37	0
2	MAN	H	4	11/12	0.78	0.14	26,31,34,35	0
2	MAN	F	6	11/12	0.80	0.12	16,22,28,28	0
2	BMA	H	3	11/12	0.86	0.11	24,26,29,31	0
2	MAN	G	5	11/12	0.87	0.10	26,27,28,30	0
2	MAN	F	5	11/12	0.89	0.08	11,14,16,20	0
2	BMA	G	3	11/12	0.89	0.09	16,19,22,25	0
2	MAN	G	4	11/12	0.90	0.09	22,24,26,31	0
2	NAG	G	1	14/15	0.92	0.09	13,17,29,30	0
2	MAN	E	6	11/12	0.93	0.07	14,14,17,20	0
2	NAG	H	2	14/15	0.93	0.08	12,18,23,25	0
2	BMA	E	3	11/12	0.94	0.07	13,14,17,19	0
2	MAN	E	5	11/12	0.94	0.07	12,16,18,19	0
2	NAG	G	2	14/15	0.94	0.07	13,16,21,24	0
2	NAG	H	1	14/15	0.95	0.07	14,16,25,25	0
2	NAG	E	2	14/15	0.95	0.06	7,11,16,16	0
2	NAG	E	1	14/15	0.95	0.06	12,14,22,23	0
2	BMA	F	3	11/12	0.96	0.06	7,9,10,12	0
2	MAN	E	4	11/12	0.97	0.05	8,11,13,14	0
2	MAN	F	4	11/12	0.97	0.05	9,11,13,13	0
2	NAG	F	1	14/15	0.97	0.05	8,10,19,21	0
2	NAG	F	2	14/15	0.97	0.05	7,9,11,12	0

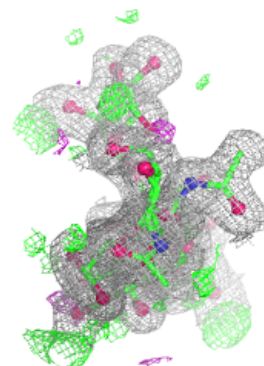
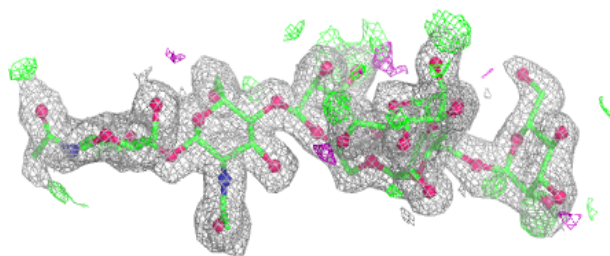
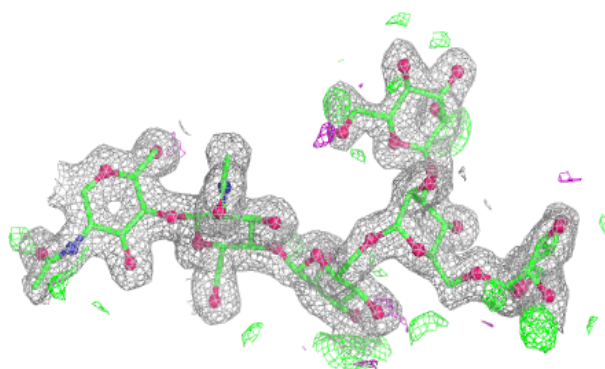
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

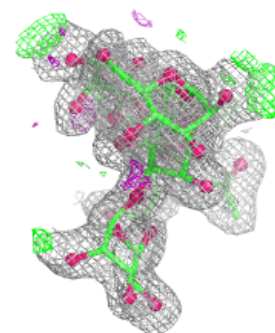
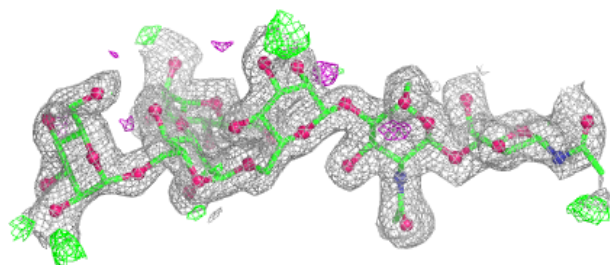
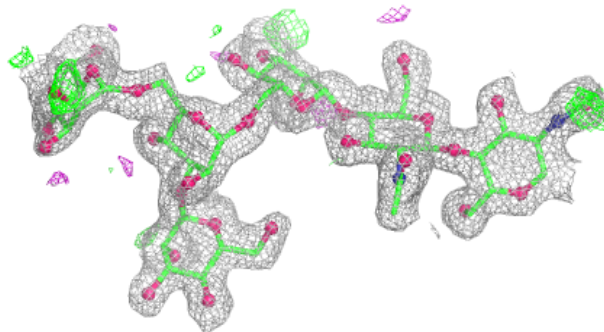
**Electron density around Chain F:**

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

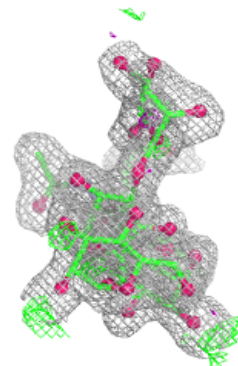
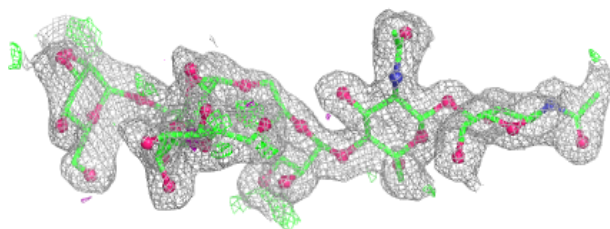
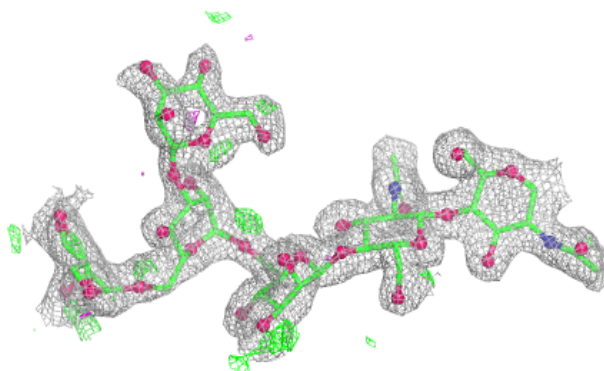


Electron density around Chain G:

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

**Electron density around Chain H:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NLA	A	5190	14/14	0.84	0.10	20,26,28,29	0
4	NLA	B	6190	14/14	0.85	0.10	22,27,27,28	0
4	NLA	C	7190	14/14	0.89	0.08	18,21,23,23	0
4	NLA	D	8190	14/14	0.93	0.07	15,17,19,20	0
3	ZN	A	180	1/1	1.00	0.02	13,13,13,13	0
3	ZN	B	180	1/1	1.00	0.02	12,12,12,12	0
3	ZN	C	180	1/1	1.00	0.01	14,14,14,14	0
3	ZN	D	180	1/1	1.00	0.01	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.