W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 17, 2022 – 12:24 PM EDT

PDB ID	:	3WKN
Title	:	Crystal structure of the artificial protein AFFinger p17 (AF.p17) complexed with Fc fragment of human IgG
Authors	:	Watanabe, H.; Honda, S.
Deposited on	:	2013-10-29
Resolution	:	2.90 Å(reported)

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

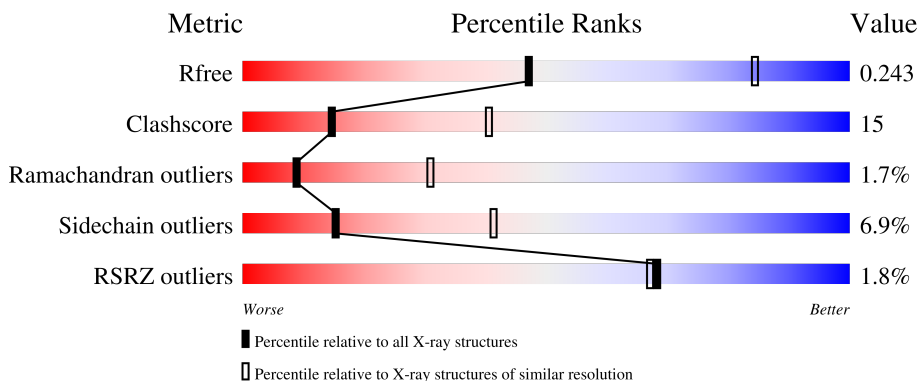|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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	Percentile Ranks	Value
Rfree		0.243
Clashscore		15
Ramachandran outliers		1.7%
Sidechain outliers		6.9%
RSRZ outliers		1.8%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	212	66% ... 30% ...
1	B	212	66% ... 29% ...
1	C	212	67% ... 29% ...
1	D	212	63% ... 33% ...
1	I	212	68% ... 27% ...

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Mol	Chain	Length	Quality of chain
1	J	212	61% 31% 6%
1	M	212	67% 30%
1	N	212	6% 50% 46%
2	E	54	2% 39% 15% 46%
2	F	54	6% 50% 28% 7% 15%
2	G	54	7% 63% 24% 13%
2	H	54	6% 33% 24% 41%
2	K	54	2% 65% 20% 15%
2	L	54	2% 59% 28% 13%
2	O	54	2% 50% 33% 15%
2	P	54	7% 46% 31% 20%
3	Q	9	100%
3	R	9	67% 33%
3	S	9	11% 89%
3	T	9	78% 22%
3	U	9	78% 22%
3	V	9	11% 67% 22%
3	W	9	44% 56%
3	X	9	11% 44% 44%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17052 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	209	Total 1668	C 1061	N 281	O 320	S 6	0	0	0
1	B	210	Total 1675	C 1066	N 282	O 321	S 6	0	0	0
1	A	209	Total 1668	C 1061	N 281	O 320	S 6	0	0	0
1	D	209	Total 1668	C 1061	N 281	O 320	S 6	0	0	0
1	I	209	Total 1668	C 1061	N 281	O 320	S 6	0	0	0
1	J	209	Total 1668	C 1061	N 281	O 320	S 6	0	0	0
1	M	209	Total 1668	C 1061	N 281	O 320	S 6	0	0	0
1	N	210	Total 1675	C 1066	N 282	O 321	S 6	0	0	0

- Molecule 2 is a protein called AFFinger p17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	29	Total 250	C 163	N 39	O 47	S 1	0	0	0
2	F	46	Total 381	C 247	N 60	O 73	S 1	0	0	0
2	G	47	Total 392	C 256	N 61	O 74	S 1	0	0	0
2	H	32	Total 274	C 180	N 42	O 51	S 1	0	0	0
2	K	46	Total 381	C 247	N 60	O 73	S 1	0	0	0
2	L	47	Total 392	C 256	N 61	O 74	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	46	Total	C	N	O	S	0	0	0
			381	247	60	73	1			
2	P	43	Total	C	N	O	S	0	0	0
			363	236	57	69	1			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
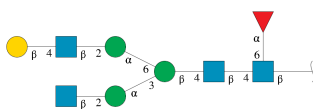
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	R	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	S	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	T	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	U	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	V	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	W	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	X	9	Total	C	N	O	0	0	0
			110	62	4	44			

3 Residue-property plots ⓘ

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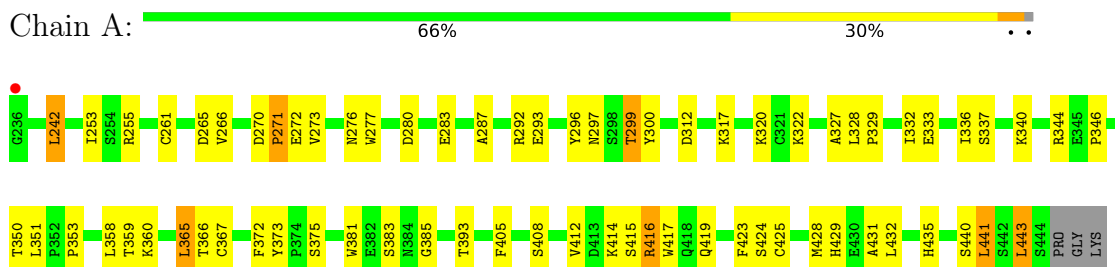
• Molecule 1: Ig gamma-1 chain C region
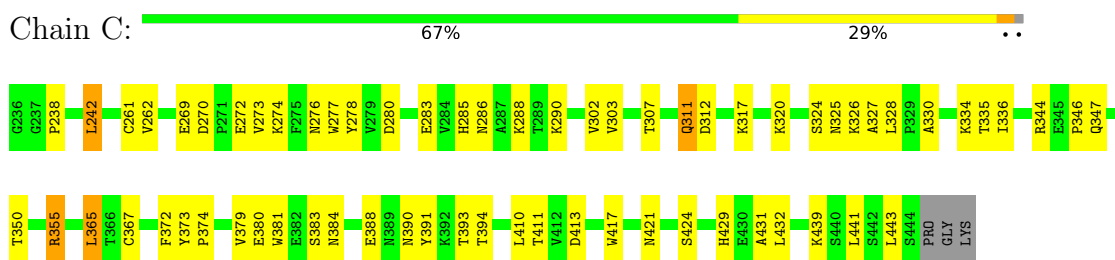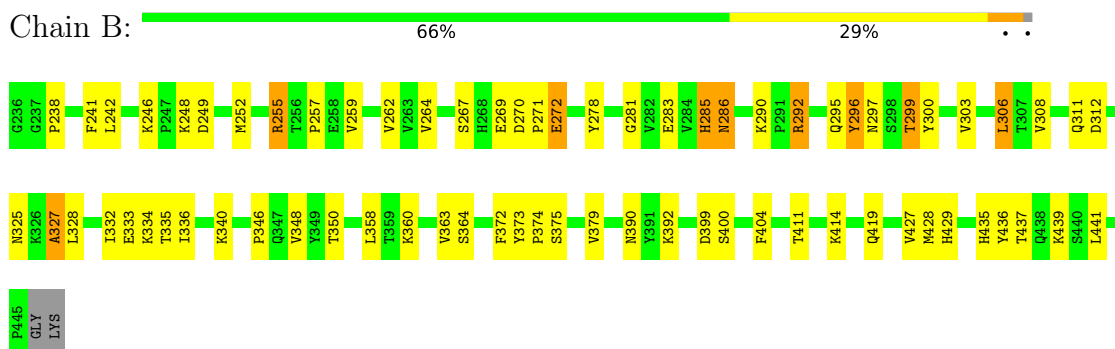
Chain C:

• Molecule 1: Ig gamma-1 chain C region

Chain B:

• Molecule 1: Ig gamma-1 chain C region

Chain A:
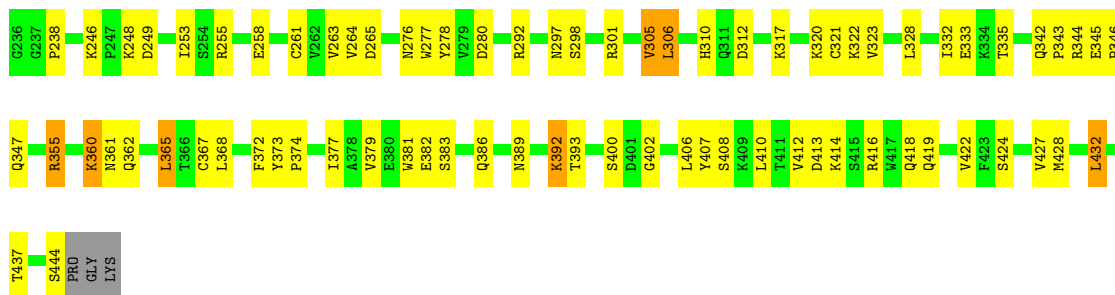
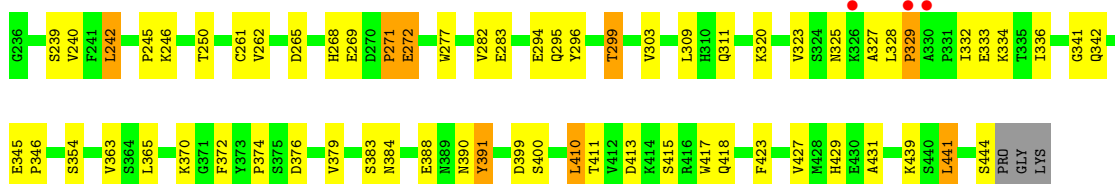

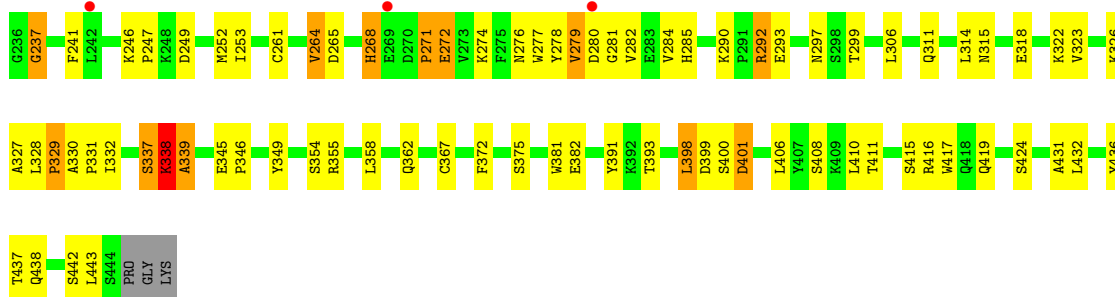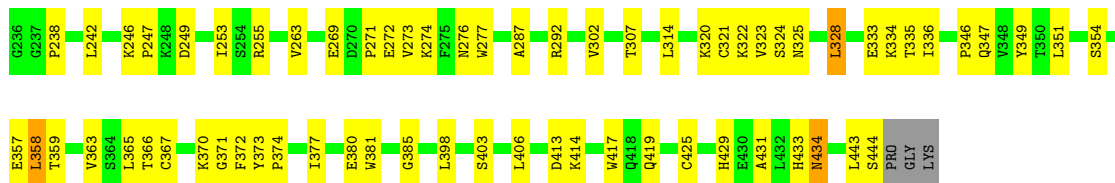• Molecule 1: Ig gamma-1 chain C region

Chain D:

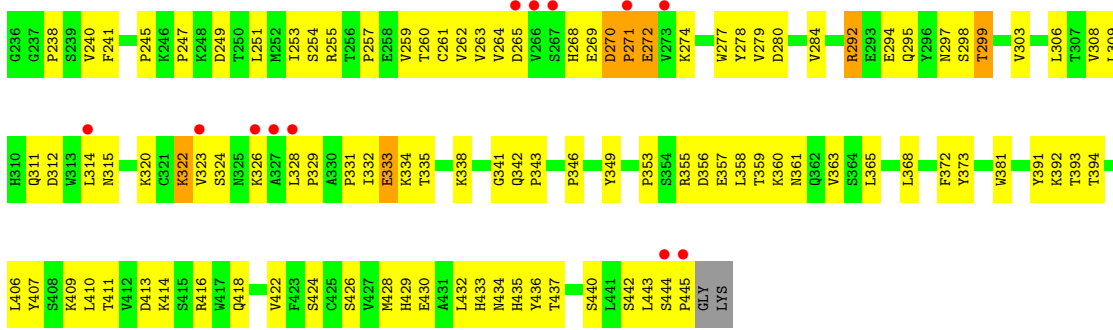• Molecule 1: Ig gamma-1 chain C region

• Molecule 1: Ig gamma-1 chain C region

• Molecule 1: Ig gamma-1 chain C region

• Molecule 1: Ig gamma-1 chain C region

• Molecule 2: AFFinger p17
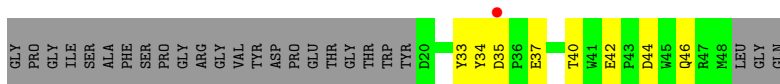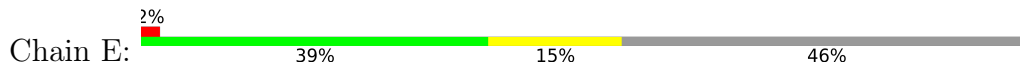

Chain E:

• Molecule 2: AFFinger p17

Chain F:

• Molecule 2: AFFinger p17

Chain G:

• Molecule 2: AFFinger p17

Chain H:

• Molecule 2: AFFinger p17

Chain K:

• Molecule 2: AFFinger p17

Chain L:

2%

59%   28%   13%

GLY PRO GLY ILE SER ALA F4 Y11 E14 T15 G16 T17 W18 Y19 W23 L28 V29 Y33 Y34 D35 T38 M48 L49 G50 GLN

• Molecule 2: AFFinger p17

Chain O:

2%

50%   33%   15%

GLY PRO GLY ILE SER ALA PHE S5 D12 P13 E14 T15 G16 T17 D20 W23 H24 L28 V29 W30 A31 T32 Y33 T38 G39 T40 W41 E42 P43 D44 W45 M48 L49 G50 GLN

• Molecule 2: AFFinger p17

Chain P:

7%

46%   31%   20%

GLY PRO GLY ILE SER ALA PHE SER P6 G7 R8 Y11 D12 P13 E14 T15 G16 T17 W18 A21 E27 W30 A31 Y34 T38 G39 T40 W41 E42 P43 R47 M48 LEU GLY GLN

• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp
ha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyr
anose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-
L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

100%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp
ha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyr
anose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-
L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

67%   33%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp
ha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyr
anose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-
L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

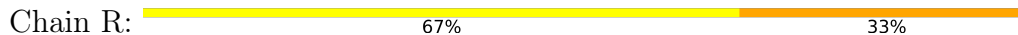11%   89%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9
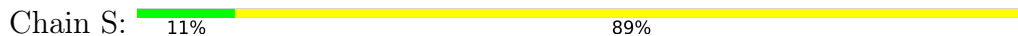
WORLDWIDE
PDB
PROTEIN DATA BANK

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 78%   22%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 78%   22%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 11%   67%   22%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose
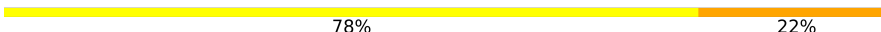
Chain W: 44%   56%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose
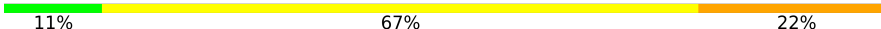
Chain X: 11%   44%   44%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.03Å 153.43Å 170.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 99.7 (49.74-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.242 0.200 , 0.243	Depositor DCC
R_{free} test set	3447 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17052	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GAL, FUC, NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.02	1/1714 (0.1%)	0.91	1/2335 (0.0%)
1	B	1.06	4/1722 (0.2%)	0.95	2/2347 (0.1%)
1	C	1.09	3/1714 (0.2%)	0.93	0/2335
1	D	0.98	2/1714 (0.1%)	0.89	0/2335
1	I	1.07	2/1714 (0.1%)	0.93	1/2335 (0.0%)
1	J	1.03	1/1714 (0.1%)	0.96	4/2335 (0.2%)
1	M	1.23	3/1714 (0.2%)	0.92	1/2335 (0.0%)
1	N	0.89	0/1722	0.84	0/2347
2	E	0.88	0/262	0.77	0/362
2	F	1.06	1/399 (0.3%)	0.82	0/551
2	G	1.01	0/411	0.79	0/567
2	H	0.91	0/287	0.74	0/396
2	K	0.98	0/399	0.88	1/551 (0.2%)
2	L	1.10	1/411 (0.2%)	0.84	0/567
2	O	0.90	0/399	0.84	0/551
2	P	0.91	0/381	0.75	0/526
All	All	1.04	18/16677 (0.1%)	0.90	10/22775 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	269	GLU	CD-OE1	24.76	1.52	1.25
1	M	269	GLU	CD-OE2	18.98	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	269	GLU	CD-OE1	16.57	1.43	1.25
1	D	360	LYS	CE-NZ	10.33	1.74	1.49
1	B	360	LYS	CE-NZ	9.37	1.72	1.49

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	271	PRO	C-N-CA	-11.56	92.80	121.70
1	B	271	PRO	CA-C-N	-8.15	99.28	117.20
1	A	265	ASP	CB-CG-OD1	7.08	124.67	118.30
1	J	249	ASP	CB-CG-OD2	-6.52	112.43	118.30
2	K	47	ARG	NE-CZ-NH2	-6.47	117.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	296	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1668	0	1633	45	1
1	B	1675	0	1640	55	0
1	C	1668	0	1633	48	1
1	D	1668	0	1633	55	0
1	I	1668	0	1633	46	0
1	J	1668	0	1633	54	0
1	M	1668	0	1633	46	0
1	N	1675	0	1639	90	0
2	E	250	0	211	4	0
2	F	381	0	327	8	0
2	G	392	0	336	10	0
2	H	274	0	234	10	0
2	K	381	0	327	8	0
2	L	392	0	336	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	381	0	327	17	0
2	P	363	0	309	16	0
3	Q	110	0	94	0	0
3	R	110	0	94	6	0
3	S	110	0	94	0	0
3	T	110	0	94	4	0
3	U	110	0	94	2	0
3	V	110	0	94	5	0
3	W	110	0	94	4	0
3	X	110	0	94	10	0
All	All	17052	0	16236	507	1

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 15.

The worst 5 of 507 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:I:390:ASN:HD22	1:I:411:THR:HB	1.19	1.07
3:T:1:NAG:H61	3:T:2:NAG:H82	1.19	1.07
2:O:30:TRP:HA	2:O:48:MET:HE1	1.33	1.07
1:M:246:LYS:HD2	1:M:247:PRO:HD2	1.31	1.05
1:I:242:LEU:HD13	1:I:336:ILE:HG12	1.32	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:NH2	1:A:287:ALA:O[2_454]	2.05	0.15

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	207/212 (98%)	192 (93%)	12 (6%)	3 (1%)	11	36
1	B	208/212 (98%)	191 (92%)	14 (7%)	3 (1%)	11	36
1	C	207/212 (98%)	196 (95%)	10 (5%)	1 (0%)	29	61
1	D	207/212 (98%)	200 (97%)	7 (3%)	0	100	100
1	I	207/212 (98%)	191 (92%)	13 (6%)	3 (1%)	11	36
1	J	207/212 (98%)	181 (87%)	17 (8%)	9 (4%)	2	10
1	M	207/212 (98%)	196 (95%)	9 (4%)	2 (1%)	15	45
1	N	208/212 (98%)	181 (87%)	23 (11%)	4 (2%)	8	28
2	E	27/54 (50%)	25 (93%)	1 (4%)	1 (4%)	3	13
2	F	44/54 (82%)	34 (77%)	6 (14%)	4 (9%)	1	1
2	G	45/54 (83%)	42 (93%)	3 (7%)	0	100	100
2	H	30/54 (56%)	22 (73%)	7 (23%)	1 (3%)	4	15
2	K	44/54 (82%)	40 (91%)	3 (7%)	1 (2%)	6	23
2	L	45/54 (83%)	41 (91%)	4 (9%)	0	100	100
2	O	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
2	P	41/54 (76%)	33 (80%)	6 (15%)	2 (5%)	2	8
All	All	1978/2128 (93%)	1804 (91%)	140 (7%)	34 (2%)	9	31

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	ALA
2	E	37	GLU
1	J	279	VAL
1	J	329	PRO
1	J	338	LYS

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	194/196 (99%)	182 (94%)	12 (6%)	18	47
1	B	195/196 (100%)	181 (93%)	14 (7%)	14	39
1	C	194/196 (99%)	185 (95%)	9 (5%)	27	60
1	D	194/196 (99%)	180 (93%)	14 (7%)	14	39
1	I	194/196 (99%)	177 (91%)	17 (9%)	10	30
1	J	194/196 (99%)	180 (93%)	14 (7%)	14	39
1	M	194/196 (99%)	186 (96%)	8 (4%)	30	64
1	N	195/196 (100%)	179 (92%)	16 (8%)	11	32
2	E	24/42 (57%)	21 (88%)	3 (12%)	4	14
2	F	37/42 (88%)	30 (81%)	7 (19%)	1	4
2	G	38/42 (90%)	35 (92%)	3 (8%)	12	34
2	H	26/42 (62%)	24 (92%)	2 (8%)	13	35
2	K	37/42 (88%)	34 (92%)	3 (8%)	11	33
2	L	38/42 (90%)	37 (97%)	1 (3%)	46	77
2	O	37/42 (88%)	36 (97%)	1 (3%)	44	77
2	P	35/42 (83%)	33 (94%)	2 (6%)	20	51
All	All	1826/1904 (96%)	1700 (93%)	126 (7%)	15	41

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	432	LEU
1	N	292	ARG
1	I	370	LYS
1	N	284	VAL
1	N	342	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	419	GLN
1	N	386	GLN
1	I	384	ASN
1	N	325	ASN
1	M	325	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

72 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	Q	1	3,1	14,14,15	0.66	0	17,19,21	1.40	3 (17%)
3	NAG	Q	2	3	14,14,15	0.65	0	17,19,21	1.47	2 (11%)
3	BMA	Q	3	3	11,11,12	0.74	0	15,15,17	1.07	1 (6%)
3	MAN	Q	4	3	11,11,12	0.71	0	15,15,17	1.61	3 (20%)
3	NAG	Q	5	3	14,14,15	0.54	0	17,19,21	1.35	2 (11%)
3	GAL	Q	6	3	11,11,12	0.96	0	15,15,17	2.47	5 (33%)
3	MAN	Q	7	3	11,11,12	0.78	0	15,15,17	1.83	3 (20%)
3	NAG	Q	8	3	14,14,15	0.49	0	17,19,21	2.12	3 (17%)
3	FUC	Q	9	3	10,10,11	0.85	0	14,14,16	1.38	2 (14%)
3	NAG	R	1	3,1	14,14,15	0.97	1 (7%)	17,19,21	1.56	5 (29%)
3	NAG	R	2	3	14,14,15	0.71	0	17,19,21	1.42	3 (17%)
3	BMA	R	3	3	11,11,12	0.87	0	15,15,17	1.81	3 (20%)
3	MAN	R	4	3	11,11,12	0.55	0	15,15,17	1.40	2 (13%)
3	NAG	R	5	3	14,14,15	0.62	0	17,19,21	1.73	3 (17%)
3	GAL	R	6	3	11,11,12	1.03	1 (9%)	15,15,17	1.66	5 (33%)
3	MAN	R	7	3	11,11,12	0.70	0	15,15,17	0.90	0
3	NAG	R	8	3	14,14,15	0.65	0	17,19,21	1.66	3 (17%)
3	FUC	R	9	3	10,10,11	0.95	0	14,14,16	1.29	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	S	1	3,1	14,14,15	0.83	0	17,19,21	1.42	1 (5%)
3	NAG	S	2	3	14,14,15	0.70	0	17,19,21	1.33	3 (17%)
3	BMA	S	3	3	11,11,12	0.48	0	15,15,17	1.71	2 (13%)
3	MAN	S	4	3	11,11,12	0.72	0	15,15,17	2.17	6 (40%)
3	NAG	S	5	3	14,14,15	0.97	0	17,19,21	1.59	3 (17%)
3	GAL	S	6	3	11,11,12	1.22	1 (9%)	15,15,17	2.07	5 (33%)
3	MAN	S	7	3	11,11,12	0.71	0	15,15,17	0.91	0
3	NAG	S	8	3	14,14,15	0.76	0	17,19,21	1.39	3 (17%)
3	FUC	S	9	3	10,10,11	1.03	0	14,14,16	1.58	2 (14%)
3	NAG	T	1	3,1	14,14,15	0.87	0	17,19,21	1.49	4 (23%)
3	NAG	T	2	3	14,14,15	0.76	0	17,19,21	1.80	3 (17%)
3	BMA	T	3	3	11,11,12	1.24	1 (9%)	15,15,17	1.45	3 (20%)
3	MAN	T	4	3	11,11,12	0.83	0	15,15,17	1.72	4 (26%)
3	NAG	T	5	3	14,14,15	0.74	0	17,19,21	1.53	5 (29%)
3	GAL	T	6	3	11,11,12	0.70	0	15,15,17	1.87	5 (33%)
3	MAN	T	7	3	11,11,12	0.74	0	15,15,17	1.12	1 (6%)
3	NAG	T	8	3	14,14,15	0.70	0	17,19,21	1.45	2 (11%)
3	FUC	T	9	3	10,10,11	0.87	0	14,14,16	1.09	1 (7%)
3	NAG	U	1	3,1	14,14,15	0.75	0	17,19,21	1.51	3 (17%)
3	NAG	U	2	3	14,14,15	0.79	0	17,19,21	1.61	2 (11%)
3	BMA	U	3	3	11,11,12	0.76	0	15,15,17	1.08	2 (13%)
3	MAN	U	4	3	11,11,12	0.72	0	15,15,17	1.55	3 (20%)
3	NAG	U	5	3	14,14,15	0.74	0	17,19,21	1.70	3 (17%)
3	GAL	U	6	3	11,11,12	0.99	1 (9%)	15,15,17	1.85	3 (20%)
3	MAN	U	7	3	11,11,12	0.73	0	15,15,17	1.46	3 (20%)
3	NAG	U	8	3	14,14,15	0.60	0	17,19,21	1.08	1 (5%)
3	FUC	U	9	3	10,10,11	0.78	0	14,14,16	1.21	2 (14%)
3	NAG	V	1	3,1	14,14,15	0.86	1 (7%)	17,19,21	1.48	4 (23%)
3	NAG	V	2	3	14,14,15	0.70	0	17,19,21	1.99	4 (23%)
3	BMA	V	3	3	11,11,12	0.59	0	15,15,17	1.10	1 (6%)
3	MAN	V	4	3	11,11,12	0.76	0	15,15,17	1.61	4 (26%)
3	NAG	V	5	3	14,14,15	0.68	0	17,19,21	1.75	3 (17%)
3	GAL	V	6	3	11,11,12	0.92	1 (9%)	15,15,17	1.62	4 (26%)
3	MAN	V	7	3	11,11,12	0.70	0	15,15,17	0.86	0
3	NAG	V	8	3	14,14,15	0.60	0	17,19,21	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	FUC	V	9	3	10,10,11	0.98	0	14,14,16	1.53	4 (28%)
3	NAG	W	1	3,1	14,14,15	0.55	0	17,19,21	1.30	3 (17%)
3	NAG	W	2	3	14,14,15	0.53	0	17,19,21	1.49	2 (11%)
3	BMA	W	3	3	11,11,12	0.70	0	15,15,17	1.45	1 (6%)
3	MAN	W	4	3	11,11,12	0.96	0	15,15,17	2.50	6 (40%)
3	NAG	W	5	3	14,14,15	0.96	0	17,19,21	1.49	3 (17%)
3	GAL	W	6	3	11,11,12	0.98	1 (9%)	15,15,17	1.79	3 (20%)
3	MAN	W	7	3	11,11,12	0.64	0	15,15,17	1.33	1 (6%)
3	NAG	W	8	3	14,14,15	0.81	0	17,19,21	1.94	3 (17%)
3	FUC	W	9	3	10,10,11	0.99	0	14,14,16	1.83	6 (42%)
3	NAG	X	1	3,1	14,14,15	0.54	0	17,19,21	1.45	2 (11%)
3	NAG	X	2	3	14,14,15	0.73	0	17,19,21	1.36	3 (17%)
3	BMA	X	3	3	11,11,12	0.68	0	15,15,17	0.77	0
3	MAN	X	4	3	11,11,12	0.72	0	15,15,17	1.45	2 (13%)
3	NAG	X	5	3	14,14,15	0.94	1 (7%)	17,19,21	1.30	2 (11%)
3	GAL	X	6	3	11,11,12	1.07	1 (9%)	15,15,17	1.63	5 (33%)
3	MAN	X	7	3	11,11,12	0.75	0	15,15,17	1.34	3 (20%)
3	NAG	X	8	3	14,14,15	0.50	0	17,19,21	0.91	0
3	FUC	X	9	3	10,10,11	0.76	0	14,14,16	1.02	1 (7%)

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	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	2/2/19/22	0/1/1/1
3	NAG	Q	5	3	-	4/6/23/26	0/1/1/1
3	GAL	Q	6	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	7	3	-	1/2/19/22	0/1/1/1
3	NAG	Q	8	3	-	4/6/23/26	0/1/1/1
3	FUC	Q	9	3	-	-	0/1/1/1
3	NAG	R	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
3	MAN	R	4	3	-	1/2/19/22	0/1/1/1
3	NAG	R	5	3	-	4/6/23/26	0/1/1/1
3	GAL	R	6	3	-	2/2/19/22	0/1/1/1
3	MAN	R	7	3	-	1/2/19/22	0/1/1/1
3	NAG	R	8	3	-	4/6/23/26	0/1/1/1
3	FUC	R	9	3	-	-	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
3	MAN	S	4	3	-	2/2/19/22	0/1/1/1
3	NAG	S	5	3	-	2/6/23/26	0/1/1/1
3	GAL	S	6	3	-	2/2/19/22	0/1/1/1
3	MAN	S	7	3	-	2/2/19/22	0/1/1/1
3	NAG	S	8	3	-	2/6/23/26	0/1/1/1
3	FUC	S	9	3	-	-	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	MAN	T	4	3	-	0/2/19/22	0/1/1/1
3	NAG	T	5	3	-	2/6/23/26	0/1/1/1
3	GAL	T	6	3	-	0/2/19/22	0/1/1/1
3	MAN	T	7	3	-	0/2/19/22	0/1/1/1
3	NAG	T	8	3	-	0/6/23/26	0/1/1/1
3	FUC	T	9	3	-	-	0/1/1/1
3	NAG	U	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	1/2/19/22	0/1/1/1
3	MAN	U	4	3	-	2/2/19/22	0/1/1/1
3	NAG	U	5	3	-	2/6/23/26	0/1/1/1
3	GAL	U	6	3	-	2/2/19/22	0/1/1/1
3	MAN	U	7	3	-	2/2/19/22	0/1/1/1
3	NAG	U	8	3	-	4/6/23/26	0/1/1/1
3	FUC	U	9	3	-	-	0/1/1/1
3	NAG	V	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	1/2/19/22	0/1/1/1
3	MAN	V	4	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	V	5	3	-	3/6/23/26	0/1/1/1
3	GAL	V	6	3	-	0/2/19/22	0/1/1/1
3	MAN	V	7	3	-	2/2/19/22	0/1/1/1
3	NAG	V	8	3	-	3/6/23/26	0/1/1/1
3	FUC	V	9	3	-	-	0/1/1/1
3	NAG	W	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	MAN	W	4	3	-	1/2/19/22	0/1/1/1
3	NAG	W	5	3	-	0/6/23/26	0/1/1/1
3	GAL	W	6	3	-	2/2/19/22	0/1/1/1
3	MAN	W	7	3	-	0/2/19/22	0/1/1/1
3	NAG	W	8	3	-	4/6/23/26	0/1/1/1
3	FUC	W	9	3	-	-	0/1/1/1
3	NAG	X	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	X	2	3	-	5/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	MAN	X	4	3	-	2/2/19/22	0/1/1/1
3	NAG	X	5	3	-	4/6/23/26	0/1/1/1
3	GAL	X	6	3	-	2/2/19/22	0/1/1/1
3	MAN	X	7	3	-	2/2/19/22	0/1/1/1
3	NAG	X	8	3	-	2/6/23/26	0/1/1/1
3	FUC	X	9	3	-	-	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	6	GAL	C2-C3	2.54	1.56	1.52
3	T	3	BMA	C2-C3	-2.38	1.49	1.52
3	R	1	NAG	C1-C2	2.29	1.55	1.52
3	X	5	NAG	O5-C1	-2.28	1.40	1.43
3	W	6	GAL	C2-C3	2.22	1.55	1.52

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	6	GAL	C1-O5-C5	6.49	120.98	112.19
3	W	8	NAG	C1-O5-C5	6.22	120.62	112.19
3	W	4	MAN	C1-O5-C5	-6.21	103.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	2	NAG	C2-N2-C7	-5.56	114.98	122.90
3	Q	8	NAG	C1-O5-C5	5.38	119.49	112.19

There are no chirality outliers.

5 of 118 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	5	NAG	C8-C7-N2-C2
3	Q	5	NAG	O7-C7-N2-C2
3	Q	8	NAG	C8-C7-N2-C2
3	Q	8	NAG	O7-C7-N2-C2
3	R	5	NAG	C8-C7-N2-C2

There are no ring outliers.

20 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	4	0
3	R	3	BMA	3	0
3	U	6	GAL	1	0
3	R	7	MAN	1	0
3	T	1	NAG	2	0
3	V	2	NAG	2	0
3	W	6	GAL	1	0
3	X	8	NAG	2	0
3	X	9	FUC	2	0
3	X	1	NAG	3	0
3	R	6	GAL	2	0
3	U	1	NAG	1	0
3	X	5	NAG	1	0
3	W	1	NAG	1	0
3	W	8	NAG	2	0
3	R	2	NAG	1	0
3	V	1	NAG	3	0
3	W	5	NAG	1	0
3	W	9	FUC	1	0
3	T	2	NAG	4	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 Q

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain R

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain S

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain U

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain V

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain W

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain X

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	209/212 (98%)	-0.42	1 (0%)	91	91	20, 39, 61, 69	7 (3%)
1	B	210/212 (99%)	-0.32	0	100	100	21, 40, 72, 77	7 (3%)
1	C	209/212 (98%)	-0.39	0	100	100	16, 39, 68, 74	7 (3%)
1	D	209/212 (98%)	-0.37	0	100	100	24, 43, 57, 67	7 (3%)
1	I	209/212 (98%)	-0.30	3 (1%)	75	75	20, 40, 68, 79	7 (3%)
1	J	209/212 (98%)	-0.18	3 (1%)	75	75	22, 45, 86, 94	4 (1%)
1	M	209/212 (98%)	-0.39	0	100	100	25, 44, 60, 64	7 (3%)
1	N	210/212 (99%)	0.08	12 (5%)	23	19	27, 58, 105, 108	7 (3%)
2	E	29/54 (53%)	0.22	1 (3%)	45	40	36, 64, 96, 101	0
2	F	46/54 (85%)	0.25	3 (6%)	18	14	36, 62, 98, 101	0
2	G	47/54 (87%)	0.21	4 (8%)	10	8	28, 50, 88, 100	0
2	H	32/54 (59%)	0.79	3 (9%)	8	6	55, 82, 98, 102	0
2	K	46/54 (85%)	-0.02	1 (2%)	62	59	25, 47, 80, 82	0
2	L	47/54 (87%)	-0.18	1 (2%)	63	61	31, 47, 74, 87	0
2	O	46/54 (85%)	-0.15	1 (2%)	62	59	44, 53, 74, 84	0
2	P	43/54 (79%)	0.48	4 (9%)	8	6	43, 75, 108, 114	0
All	All	2010/2128 (94%)	-0.21	37 (1%)	68	67	16, 45, 88, 114	53 (2%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLY	4.7
2	F	17	THR	4.1
2	F	15	THR	4.0
1	I	330	ALA	3.8
1	N	445	PRO	3.6

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(Å^2)	Q<0.9
3	NAG	W	8	14/15	0.73	0.31	102,106,108,108	0
3	NAG	R	8	14/15	0.75	0.21	103,108,110,111	0
3	FUC	R	9	10/11	0.81	0.23	94,97,99,102	0
3	NAG	V	8	14/15	0.82	0.22	107,111,113,113	0
3	FUC	X	9	10/11	0.83	0.31	103,106,108,108	0
3	NAG	T	8	14/15	0.84	0.18	72,81,86,89	0
3	MAN	X	7	11/12	0.85	0.14	97,100,101,104	0
3	FUC	S	9	10/11	0.86	0.18	82,87,89,89	0
3	GAL	R	6	11/12	0.86	0.32	80,86,88,88	0
3	NAG	S	8	14/15	0.87	0.12	78,89,90,91	0
3	BMA	V	3	11/12	0.87	0.12	72,82,85,92	0
3	NAG	Q	8	14/15	0.87	0.19	97,100,102,105	0
3	GAL	W	6	11/12	0.88	0.30	75,79,81,82	0
3	NAG	X	8	14/15	0.88	0.14	106,108,109,110	0
3	NAG	X	1	14/15	0.88	0.25	94,98,100,101	0
3	GAL	X	6	11/12	0.89	0.28	74,79,81,82	0
3	GAL	V	6	11/12	0.89	0.30	88,92,93,93	0
3	MAN	V	7	11/12	0.89	0.18	97,101,104,107	0
3	GAL	S	6	11/12	0.89	0.28	53,58,62,63	0
3	FUC	T	9	10/11	0.90	0.14	79,85,86,86	0
3	NAG	X	2	14/15	0.90	0.14	83,89,91,92	0
3	FUC	V	9	10/11	0.90	0.24	86,89,91,92	0
3	NAG	R	1	14/15	0.91	0.15	68,72,77,81	0
3	GAL	Q	6	11/12	0.91	0.20	66,69,72,72	0
3	MAN	W	7	11/12	0.91	0.14	78,83,84,90	0
3	MAN	Q	4	11/12	0.91	0.17	74,77,84,86	0
3	GAL	U	6	11/12	0.91	0.22	50,57,59,61	0
3	NAG	U	8	14/15	0.92	0.18	89,94,95,95	0
3	BMA	X	3	11/12	0.92	0.10	79,86,89,93	0
3	MAN	R	7	11/12	0.92	0.14	84,86,88,95	0
3	MAN	Q	7	11/12	0.92	0.15	90,92,93,95	0
3	FUC	Q	9	10/11	0.92	0.22	80,84,88,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	MAN	U	7	11/12	0.92	0.12	71,74,77,83	0
3	NAG	V	2	14/15	0.93	0.16	62,70,74,74	0
3	NAG	S	1	14/15	0.93	0.14	54,58,68,69	0
3	BMA	Q	3	11/12	0.93	0.12	68,71,74,79	0
3	NAG	U	1	14/15	0.93	0.17	64,66,70,70	0
3	NAG	R	5	14/15	0.93	0.18	78,81,91,94	0
3	NAG	Q	5	14/15	0.93	0.13	64,74,79,80	0
3	GAL	T	6	11/12	0.93	0.14	66,70,72,75	0
3	FUC	U	9	10/11	0.93	0.21	75,79,81,83	0
3	FUC	W	9	10/11	0.94	0.17	77,79,82,82	0
3	MAN	U	4	11/12	0.94	0.12	49,50,53,54	0
3	NAG	V	1	14/15	0.94	0.11	66,69,72,77	0
3	MAN	R	4	11/12	0.94	0.11	80,82,85,88	0
3	MAN	W	4	11/12	0.94	0.15	54,56,62,63	0
3	MAN	S	4	11/12	0.94	0.16	48,54,55,56	0
3	NAG	V	5	14/15	0.94	0.12	60,62,64,72	0
3	BMA	R	3	11/12	0.94	0.11	71,74,77,78	0
3	NAG	U	5	14/15	0.95	0.14	47,51,52,54	0
3	BMA	W	3	11/12	0.95	0.11	53,57,59,62	0
3	NAG	T	1	14/15	0.95	0.19	49,52,58,65	0
3	NAG	Q	1	14/15	0.95	0.18	62,64,67,74	0
3	NAG	U	2	14/15	0.95	0.16	52,60,62,62	0
3	BMA	U	3	11/12	0.95	0.12	62,63,64,68	0
3	MAN	S	7	11/12	0.95	0.12	63,64,66,72	0
3	MAN	T	7	11/12	0.96	0.12	55,57,58,66	0
3	NAG	Q	2	14/15	0.96	0.12	56,63,65,67	0
3	NAG	S	5	14/15	0.96	0.14	40,44,48,51	0
3	NAG	R	2	14/15	0.96	0.12	61,64,67,67	0
3	NAG	T	2	14/15	0.96	0.14	42,46,51,54	0
3	MAN	X	4	11/12	0.96	0.12	65,67,70,71	0
3	BMA	T	3	11/12	0.96	0.11	45,46,48,52	0
3	NAG	W	5	14/15	0.96	0.13	42,53,57,61	0
3	MAN	T	4	11/12	0.96	0.11	40,45,48,49	0
3	NAG	S	2	14/15	0.96	0.14	47,51,53,54	0
3	NAG	X	5	14/15	0.97	0.12	68,69,74,74	0
3	NAG	W	1	14/15	0.97	0.12	57,59,62,68	0
3	MAN	V	4	11/12	0.97	0.12	65,68,69,70	0
3	BMA	S	3	11/12	0.97	0.10	50,53,53,58	0
3	NAG	T	5	14/15	0.97	0.13	47,51,53,53	0
3	NAG	W	2	14/15	0.98	0.12	52,56,57,58	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.
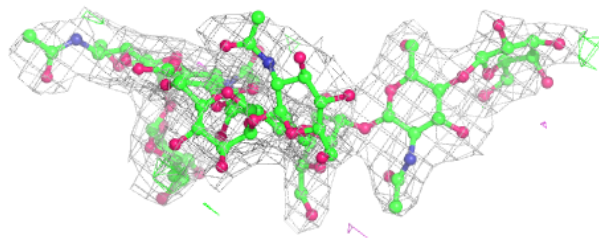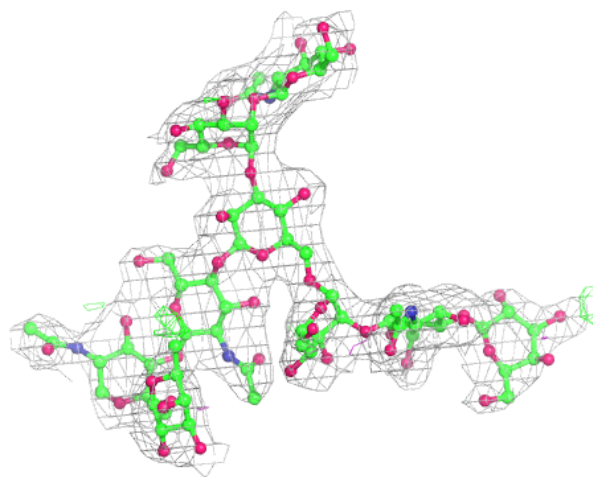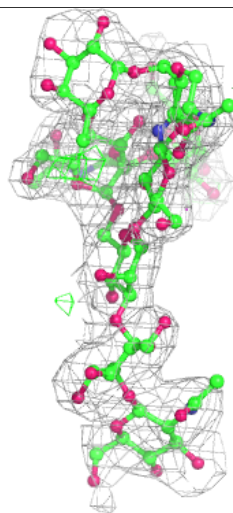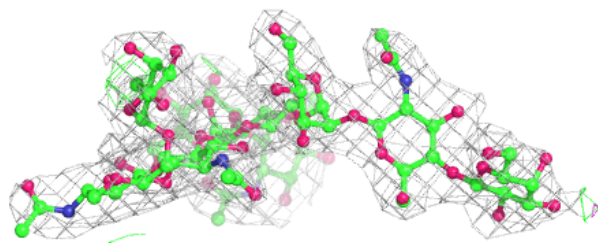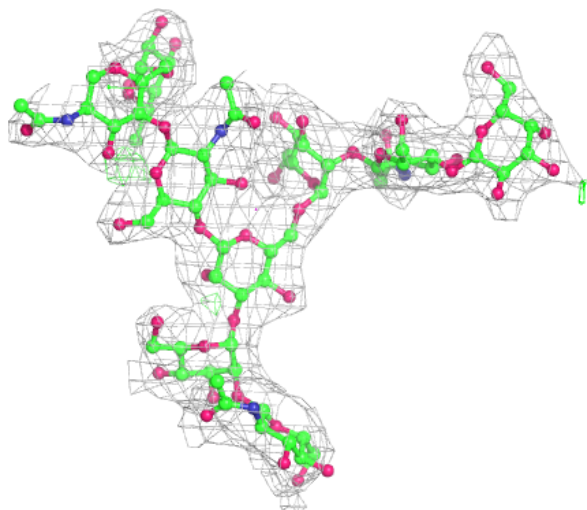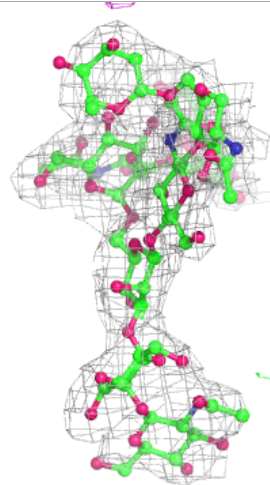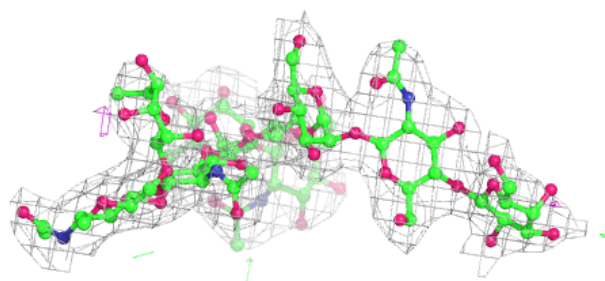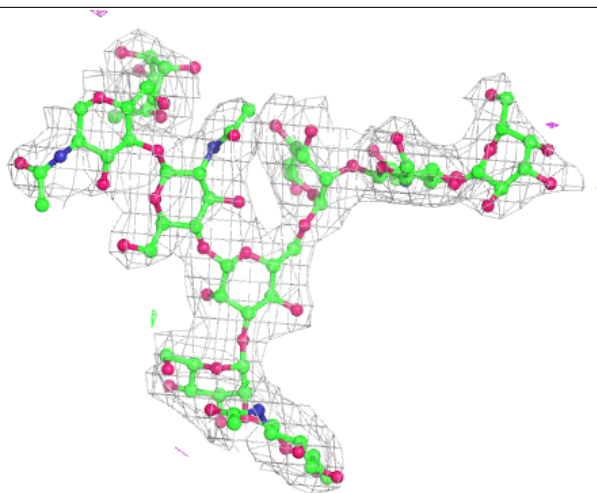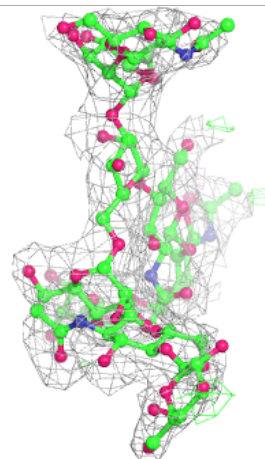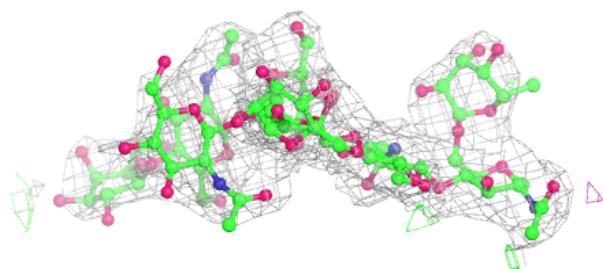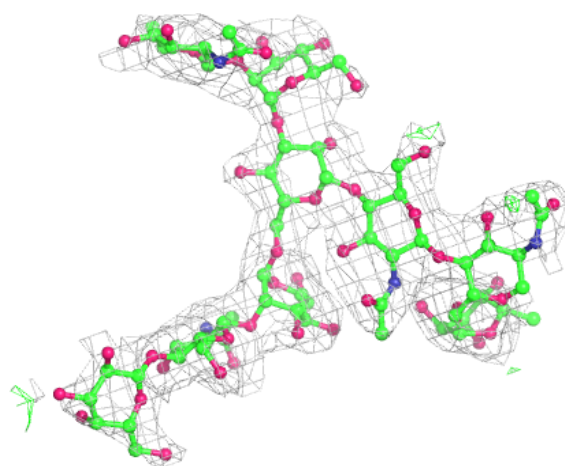
Electron density around Chain Q:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
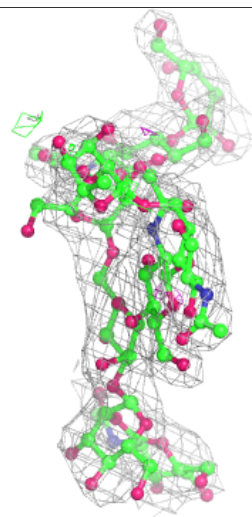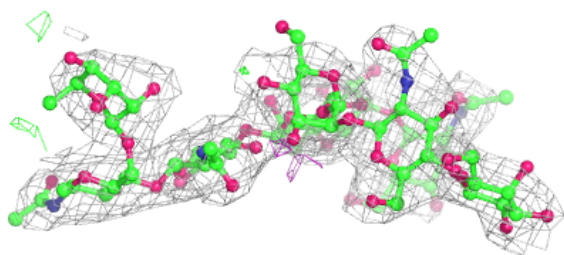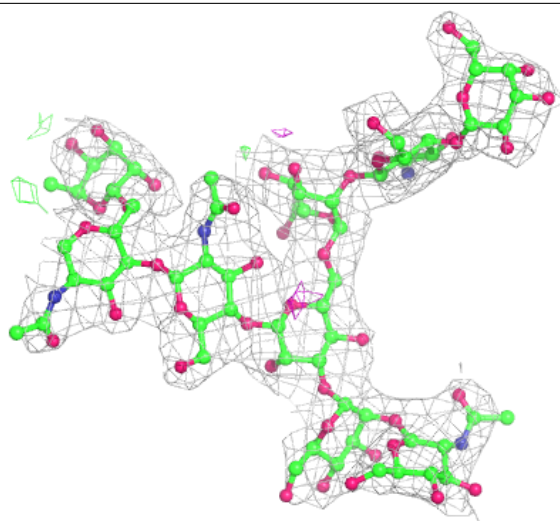
Electron density around Chain R:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
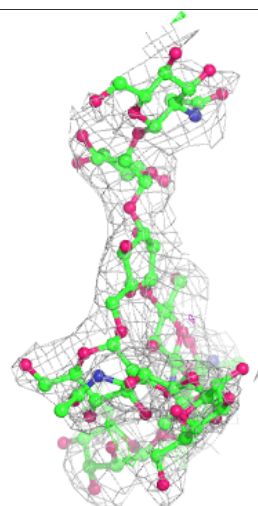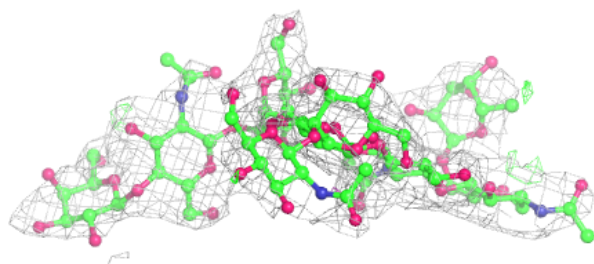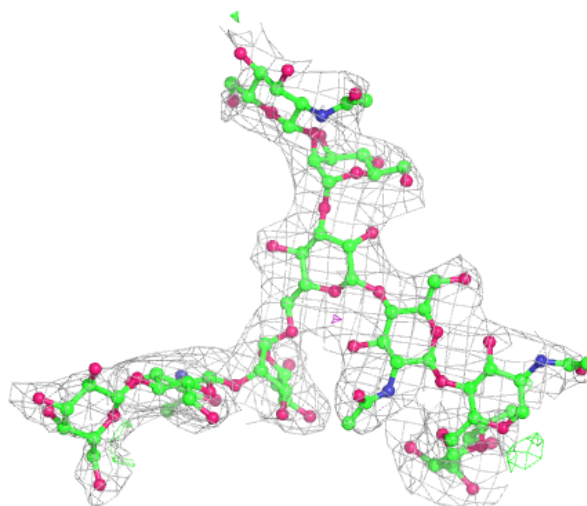
Electron density around Chain S:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
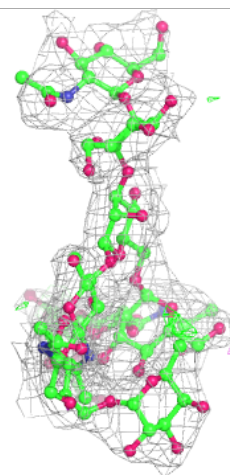
Electron density around Chain T:

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

Electron density around Chain U:

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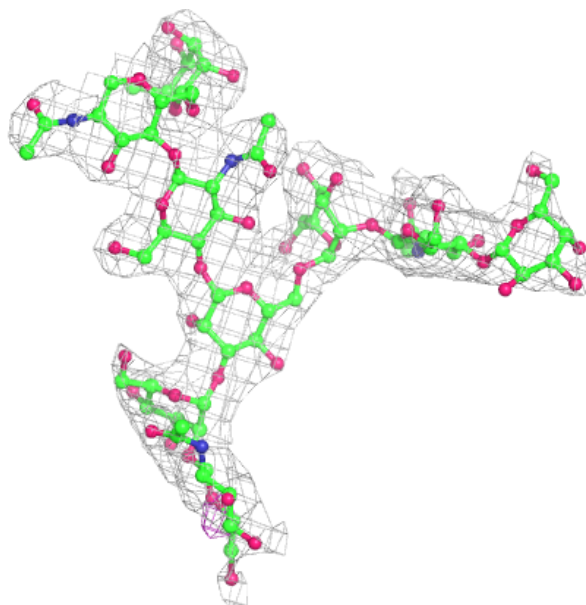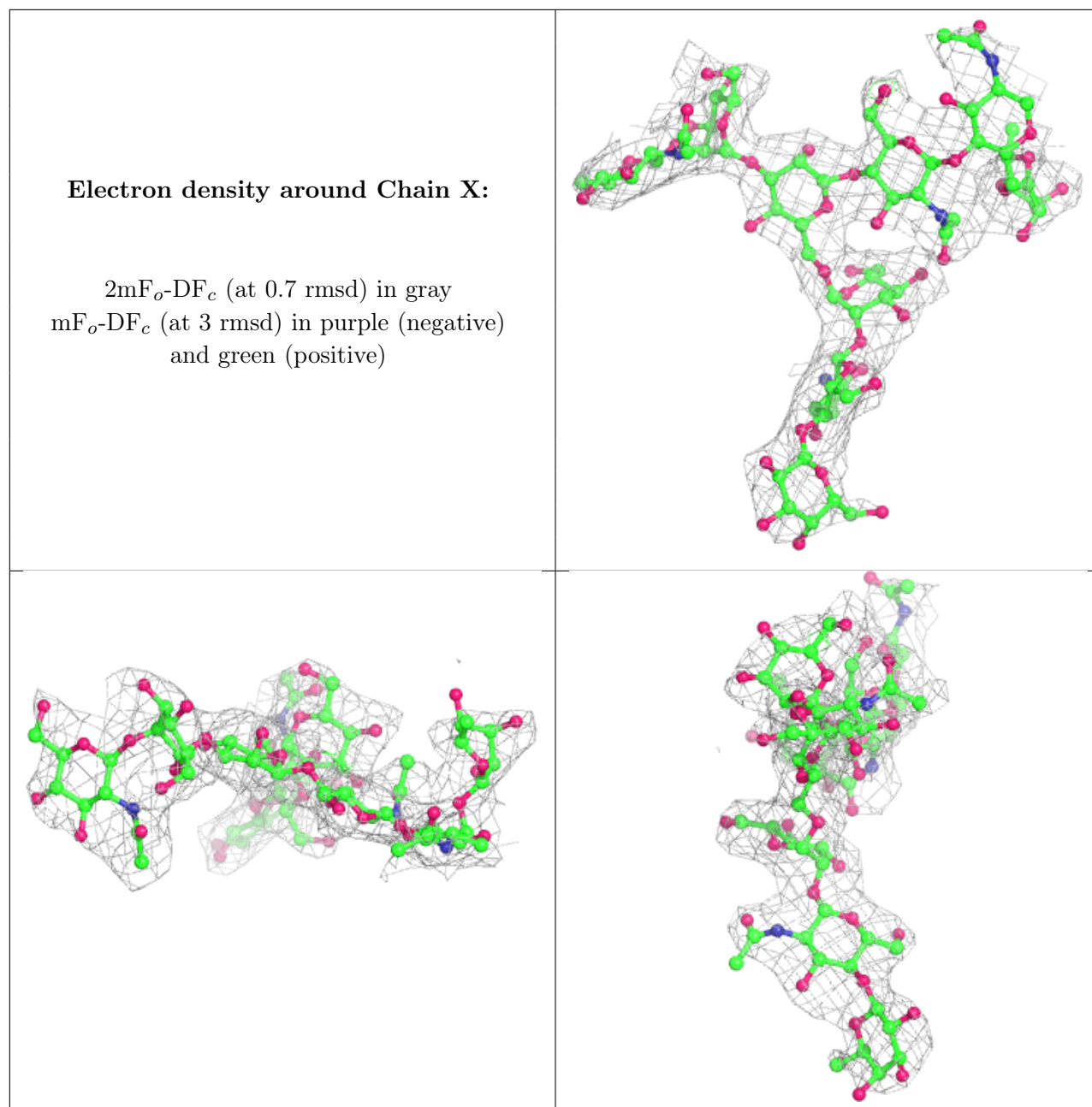and green (positive)

Electron density around Chain V:

$2mF_o$-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 W:

$2mF_o$-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 X:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
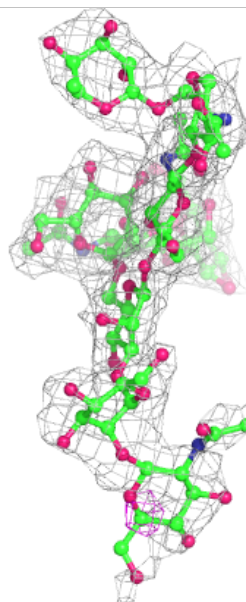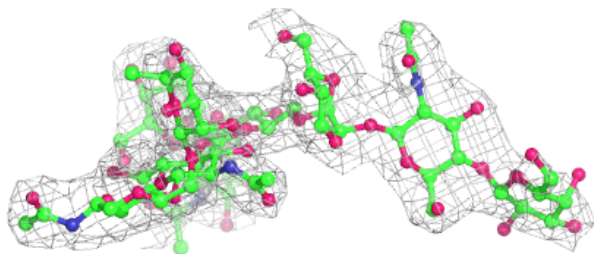
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.