



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:32 AM EDT

PDB ID : 9NTF / pdb_00009ntf
Title : Helix pomatia AMP deaminase (HPAMPD) with unknown density in the active site
Authors : Kaur, G.; Horton, J.R.; Cheng, X.
Deposited on : 2025-03-18
Resolution : 1.56 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

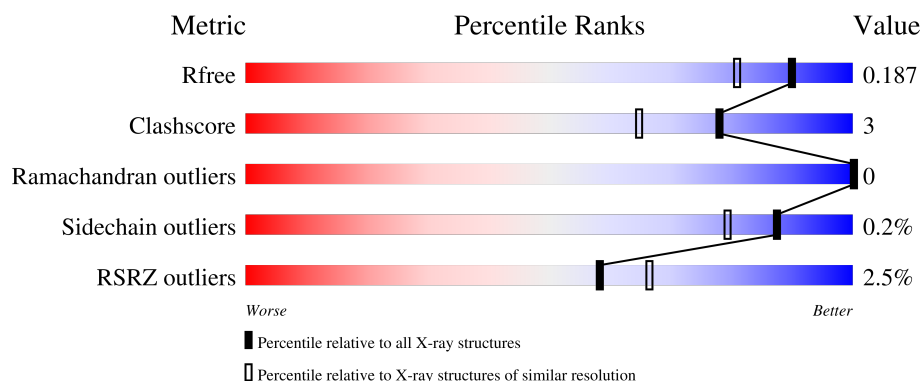
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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.



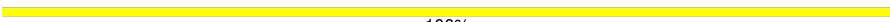
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	541	2% 86% 6% 8%
1	B	541	3% 89% 5% 7%
1	C	541	2% 87% 5% 8%
1	D	541	2% 88% • 8%
2	E	2	100%

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

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 18622 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 AMP deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	6	0
			4020	2571	684	753	12			
1	B	505	Total	C	N	O	S	0	7	0
			4077	2610	693	762	12			
1	C	496	Total	C	N	O	S	0	11	0
			4037	2586	687	752	12			
1	D	497	Total	C	N	O	S	0	5	0
			4009	2568	680	749	12			

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

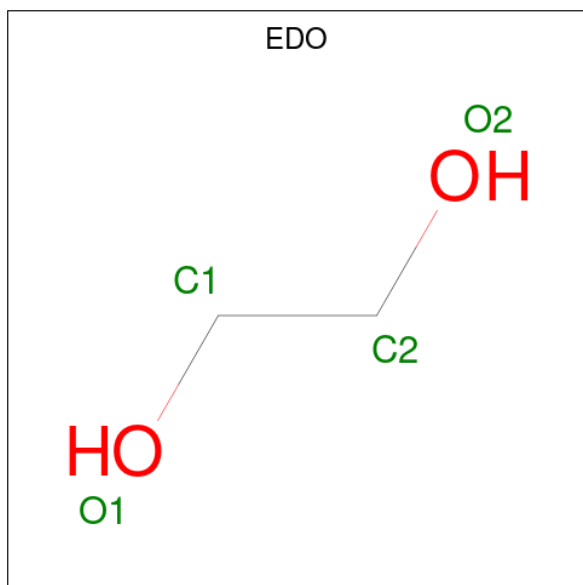
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			8	4	4		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 8	C 4	O 4	0	1
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	1
			8	4	4		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

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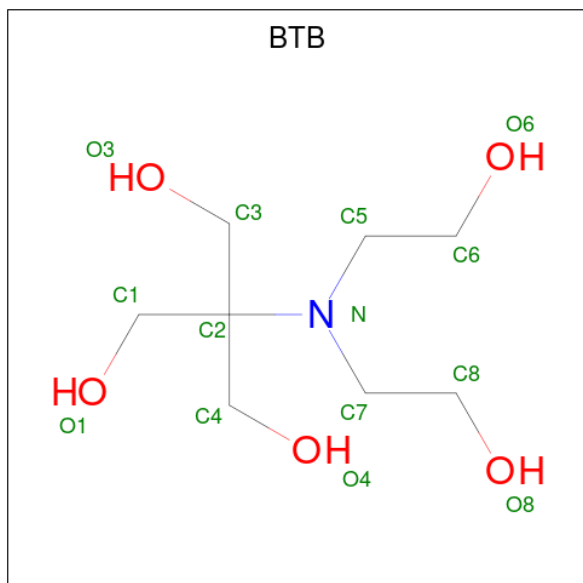
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0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

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

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



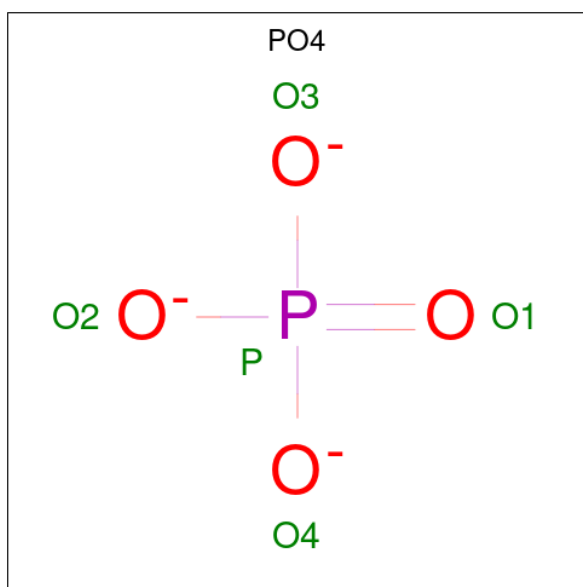
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



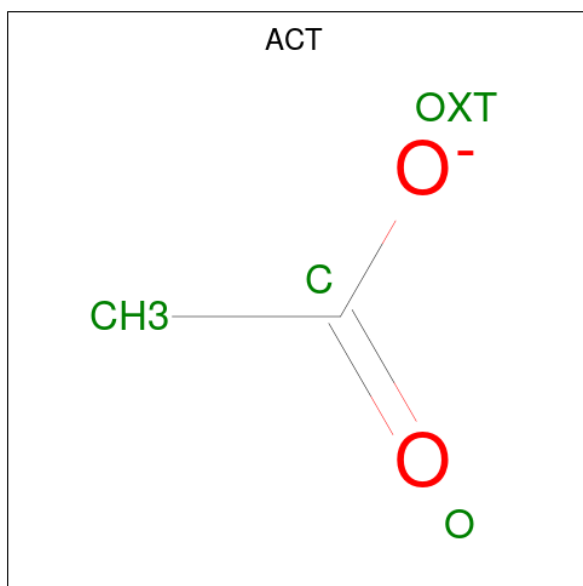
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		

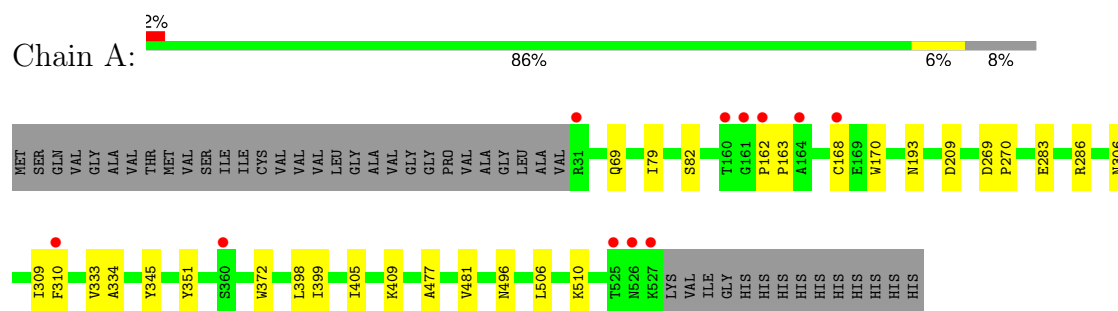
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	452	Total	O	0	2
			454	454		
10	B	503	Total	O	0	2
			505	505		
10	C	467	Total	O	0	2
			469	469		
10	D	417	Total	O	0	0
			417	417		

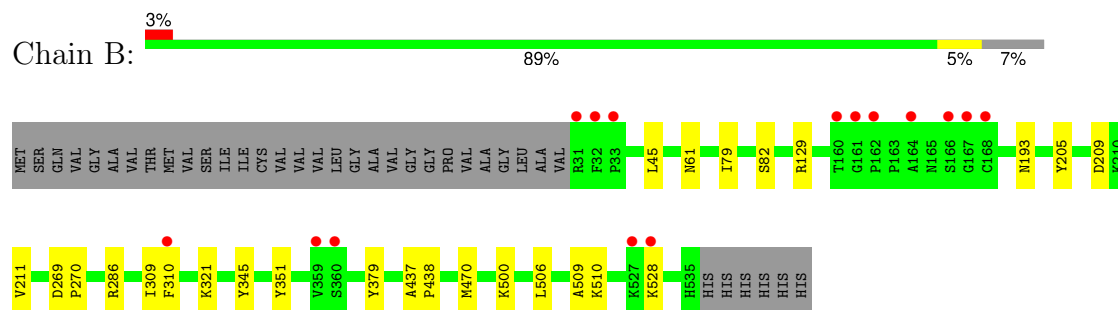
3 Residue-property plots [i](#)

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.

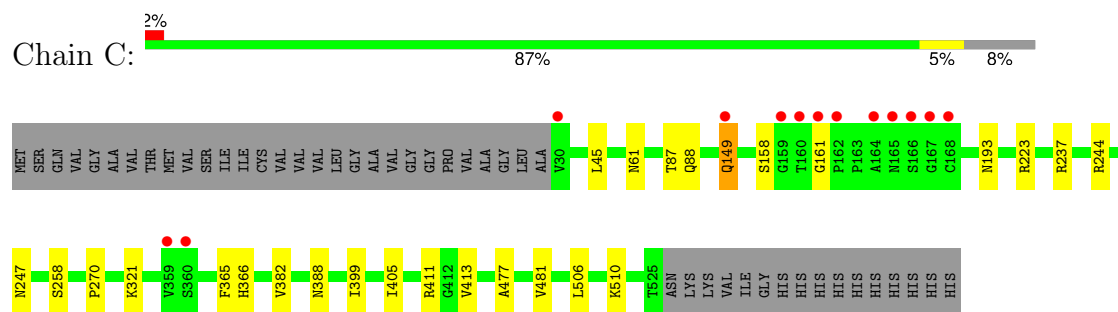
• Molecule 1: AMP deaminase



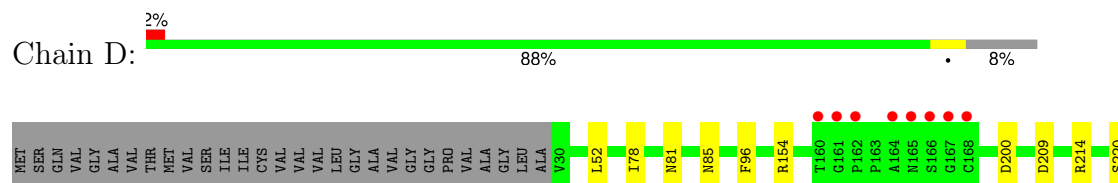
• Molecule 1: AMP deaminase



• Molecule 1: AMP deaminase



• Molecule 1: AMP deaminase





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

Chain E:  100%

NAG1
NAG2

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

Chain F:  100%

NAG1
NAG2

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

Chain G:  100%

NAG1
NAG2

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

Chain H:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.34Å 82.35Å 211.50Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	70.85 – 1.56 70.85 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.5 (70.85-1.56) 99.5 (70.85-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.161 , 0.188 0.160 , 0.187	Depositor DCC
R_{free} test set	18898 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	18622	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: NAG, EDO, PO4, ZN, BTB, ACT, GOL

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	0.62	0/4132	0.70	0/5614
1	B	0.66	0/4199	0.74	0/5706
1	C	0.66	0/4164	0.73	1/5657 (0.0%)
1	D	0.58	0/4121	0.67	0/5600
All	All	0.63	0/16616	0.71	1/22577 (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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	GLN	CA-CB-CG	-5.25	103.59	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	365	PHE	Peptide
1	D	214	ARG	Sidechain

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	4020	0	3966	26	0
1	B	4077	0	4014	21	0
1	C	4037	0	4007	23	0
1	D	4009	0	3969	15	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0
3	C	28	0	26	0	0
3	D	42	0	39	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
5	A	64	0	96	12	0
5	B	104	0	156	8	0
5	C	96	0	143	15	0
5	D	40	0	60	4	0
6	A	14	0	19	0	0
6	B	14	0	19	0	0
7	A	6	0	8	2	0
7	B	12	0	16	4	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	B	4	0	3	0	0
10	A	454	0	0	6	0
10	B	505	0	0	8	1
10	C	469	0	0	8	1
10	D	417	0	0	5	0
All	All	18622	0	16719	94	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 3.

All (94) 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:C:149:GLN:NE2	10:C:701:HOH:O	2.04	0.89
1:C:237:ARG:HD3	5:C:615:EDO:H22	1.56	0.85
1:A:79:ILE:HD11	7:A:618:GOL:H12	1.64	0.79
1:B:79:ILE:HD11	7:B:631:GOL:H12	1.71	0.73
1:A:79:ILE:CD1	7:A:618:GOL:H12	2.24	0.66
1:C:258:SER:HB3	1:C:270:PRO:HG3	1.82	0.61
1:C:223[A]:ARG:NH1	10:C:708:HOH:O	2.32	0.61
1:B:209:ASP:HB3	5:C:625:EDO:O2	2.01	0.61
1:A:399:ILE:HA	1:A:405:ILE:HD11	1.84	0.60
1:B:61:ASN:HD21	5:B:611:EDO:H22	1.67	0.59
1:B:79:ILE:CD1	7:B:631:GOL:H12	2.33	0.59
1:A:405:ILE:HD12	5:A:621:EDO:H12	1.84	0.59
1:A:82:SER:O	5:A:616:EDO:H22	2.04	0.58
1:D:78:ILE:HD12	10:D:1068:HOH:O	2.04	0.57
1:B:82:SER:OG	7:B:633:GOL:H31	2.05	0.56
1:C:388[A]:ASN:ND2	10:C:706:HOH:O	2.29	0.56
5:C:614:EDO:H21	10:C:721:HOH:O	2.04	0.56
1:A:334:ALA:H	5:A:605[A]:EDO:H11	1.70	0.56
1:A:306:ASN:HB2	5:A:612:EDO:H11	1.87	0.56
5:A:616:EDO:O1	1:D:209:ASP:HB3	2.07	0.55
1:D:334:ALA:H	5:D:605:EDO:H21	1.71	0.55
5:B:620:EDO:H22	10:B:942:HOH:O	2.07	0.55
1:A:372:TRP:HE3	5:A:606:EDO:H12	1.72	0.54
1:C:506:LEU:HG	1:C:510:LYS:HE2	1.90	0.54
1:C:413:VAL:HG22	5:C:609:EDO:H11	1.90	0.53
1:A:496:ASN:ND2	10:A:702:HOH:O	2.21	0.52
1:A:506:LEU:HG	1:A:510:LYS:HE2	1.90	0.52
1:A:69:GLN:HG2	10:A:1128:HOH:O	2.09	0.51
5:B:630:EDO:H12	10:B:1017:HOH:O	2.11	0.51
1:A:283:GLU:OE1	1:A:286[A]:ARG:NH2	2.38	0.51
1:B:286:ARG:NH1	10:B:709:HOH:O	2.40	0.51
1:C:61:ASN:HD21	5:C:626:EDO:H11	1.75	0.50
1:B:269:ASP:HB2	1:B:270:PRO:HD2	1.93	0.50
1:B:129:ARG:NH1	10:B:713:HOH:O	2.46	0.49
1:B:45:LEU:HD23	1:C:382:VAL:HG13	1.95	0.48
1:D:305:PRO:HD2	1:D:308:ASP:OD2	2.12	0.48
5:A:605[B]:EDO:H21	10:A:1091:HOH:O	2.14	0.48
1:A:310:PHE:HE1	1:A:351:TYR:CD2	2.32	0.48
1:A:477:ALA:HB1	1:A:481:VAL:HG21	1.95	0.48
5:A:616:EDO:HO1	1:D:209:ASP:HB3	1.77	0.48
5:B:628:EDO:H11	10:B:823:HOH:O	2.14	0.48
1:A:309:ILE:HG13	1:A:345:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:608:EDO:H22	10:D:873:HOH:O	2.13	0.47
1:C:247:ASN:HA	5:C:624:EDO:H11	1.95	0.47
5:A:612:EDO:H21	10:A:732:HOH:O	2.13	0.47
1:C:321:LYS:HB3	1:C:321:LYS:HE2	1.63	0.47
1:B:321:LYS:HE3	10:B:735:HOH:O	2.14	0.47
1:A:269:ASP:HB2	1:A:270:PRO:HD2	1.97	0.46
1:C:45:LEU:C	1:C:45:LEU:HD23	2.40	0.46
1:B:506:LEU:HG	1:B:510:LYS:HE2	1.97	0.46
1:B:309:ILE:HG13	1:B:345:TYR:CE1	2.51	0.45
1:C:88:GLN:HG2	10:C:972:HOH:O	2.14	0.45
1:D:334:ALA:N	5:D:605:EDO:H21	2.31	0.45
1:A:409:LYS:NZ	10:A:715:HOH:O	2.50	0.45
1:D:285[A]:VAL:HG13	10:D:817:HOH:O	2.17	0.45
5:C:626:EDO:H22	10:C:1083:HOH:O	2.16	0.45
1:D:81:ASN:O	1:D:85:ASN:HB2	2.17	0.45
1:A:69:GLN:OE1	10:A:703:HOH:O	2.21	0.44
1:C:366:HIS:CD2	5:C:604[A]:EDO:H12	2.52	0.44
1:D:52:LEU:O	1:D:443:ASN:HB2	2.17	0.44
1:B:205:TYR:O	5:B:621:EDO:H21	2.18	0.44
1:C:237:ARG:HD3	5:C:615:EDO:C2	2.37	0.44
1:B:437:ALA:HB3	1:B:438:PRO:HD3	1.99	0.44
1:B:500:LYS:NZ	10:B:720:HOH:O	2.50	0.44
1:A:398:LEU:HG	1:A:405:ILE:HG12	2.00	0.43
1:A:405:ILE:HG22	1:A:409:LYS:HE2	2.00	0.43
1:C:87:THR:N	5:C:625:EDO:H22	2.33	0.43
1:C:237:ARG:CD	5:C:615:EDO:H22	2.38	0.43
1:A:333:VAL:HB	5:A:605[B]:EDO:H22	2.00	0.42
1:A:163:PRO:HB2	1:A:170:TRP:CD1	2.54	0.42
1:B:509:ALA:HB1	5:B:634:EDO:H21	2.02	0.42
1:D:506:LEU:HG	1:D:510:LYS:HE2	2.00	0.42
5:C:614:EDO:H22	10:C:870:HOH:O	2.19	0.42
1:A:334:ALA:N	5:A:605[A]:EDO:H11	2.33	0.41
1:D:521:LYS:NZ	10:D:704:HOH:O	2.41	0.41
1:D:154:ARG:NH1	1:D:220[B]:SER:OG	2.53	0.41
1:A:209:ASP:HB3	10:D:1046:HOH:O	2.20	0.41
1:B:528:LYS:HD2	1:B:528:LYS:HA	1.82	0.41
5:B:620:EDO:O1	10:B:701:HOH:O	2.20	0.41
1:C:158:SER:OG	1:C:161:GLY:O	2.35	0.41
1:D:461:MET:HE3	1:D:461:MET:HB3	1.86	0.41
1:B:470:MET:O	7:B:631:GOL:H11	2.20	0.41
1:C:244:ARG:HG3	5:C:624:EDO:H22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:CYS:SG	5:A:617:EDO:H12	2.61	0.41
1:C:388[A]:ASN:ND2	10:C:704:HOH:O	2.27	0.41
1:B:211:VAL:HG11	5:B:621:EDO:H11	2.03	0.41
1:B:310:PHE:HE1	1:B:351:TYR:CD2	2.39	0.41
1:B:379:TYR:CD2	5:C:623:EDO:H11	2.56	0.41
1:C:477:ALA:HB1	1:C:481:VAL:HG21	2.02	0.41
1:D:237:ARG:HB2	5:D:613:EDO:H21	2.02	0.41
1:D:96:PHE:CD2	1:D:200:ASP:HB2	2.56	0.40
1:C:411:ARG:O	5:C:609:EDO:H22	2.21	0.40
1:C:399:ILE:HA	1:C:405:ILE:HD11	2.02	0.40
1:A:162:PRO:HA	1:A:163:PRO:HD3	1.94	0.40

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)
10:B:859:HOH:O	10:C:1075:HOH:O[2_555]	2.15	0.05

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	501/541 (93%)	482 (96%)	19 (4%)	0	100	100
1	B	510/541 (94%)	493 (97%)	17 (3%)	0	100	100
1	C	505/541 (93%)	487 (96%)	18 (4%)	0	100	100
1	D	500/541 (92%)	482 (96%)	18 (4%)	0	100	100
All	All	2016/2164 (93%)	1944 (96%)	72 (4%)	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	443/474 (94%)	442 (100%)	1 (0%)	87	79
1	B	449/474 (95%)	448 (100%)	1 (0%)	87	79
1	C	447/474 (94%)	446 (100%)	1 (0%)	87	79
1	D	443/474 (94%)	443 (100%)	0	100	100
All	All	1782/1896 (94%)	1779 (100%)	3 (0%)	87	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	B	193	ASN
1	C	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	373	GLN
1	A	484	GLN
1	B	249	GLN
1	B	306	ASN
1	B	373	GLN
1	B	484	GLN
1	B	534	HIS
1	C	249	GLN
1	C	306	ASN
1	C	355	GLN
1	C	418	ASN
1	C	484	GLN
1	D	249	GLN
1	D	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	0.53	0	17,19,21	1.53	2 (11%)
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	1.05	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.62	0	17,19,21	1.78	4 (23%)
2	NAG	F	2	2	14,14,15	0.89	1 (7%)	17,19,21	1.35	3 (17%)
2	NAG	G	1	2,1	14,14,15	0.80	0	17,19,21	1.06	1 (5%)
2	NAG	G	2	2	14,14,15	0.80	0	17,19,21	1.09	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.82	0	17,19,21	0.99	1 (5%)
2	NAG	H	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.21	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	C2-N2	-2.29	1.42	1.46
2	H	2	NAG	C1-C2	2.21	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	4.03	117.58	112.19
2	F	1	NAG	C1-O5-C5	3.57	116.98	112.19
2	F	1	NAG	C3-C4-C5	-3.45	103.98	110.23
2	F	1	NAG	O5-C1-C2	-3.29	106.19	111.29
2	E	2	NAG	C1-O5-C5	2.93	116.12	112.19
2	G	1	NAG	C1-O5-C5	2.59	115.66	112.19
2	H	2	NAG	C3-C4-C5	-2.52	105.66	110.23
2	E	1	NAG	O5-C1-C2	-2.46	107.48	111.29
2	F	2	NAG	C1-C2-N2	-2.40	106.65	110.43
2	F	2	NAG	C3-C4-C5	-2.33	106.00	110.23
2	F	1	NAG	C2-N2-C7	2.31	125.99	122.90
2	G	2	NAG	C1-O5-C5	2.19	115.12	112.19
2	H	1	NAG	O3-C3-C2	-2.12	104.99	109.40
2	G	2	NAG	O4-C4-C5	2.02	114.30	109.32
2	F	2	NAG	C8-C7-N2	-2.00	112.80	116.12

There are no chirality outliers.

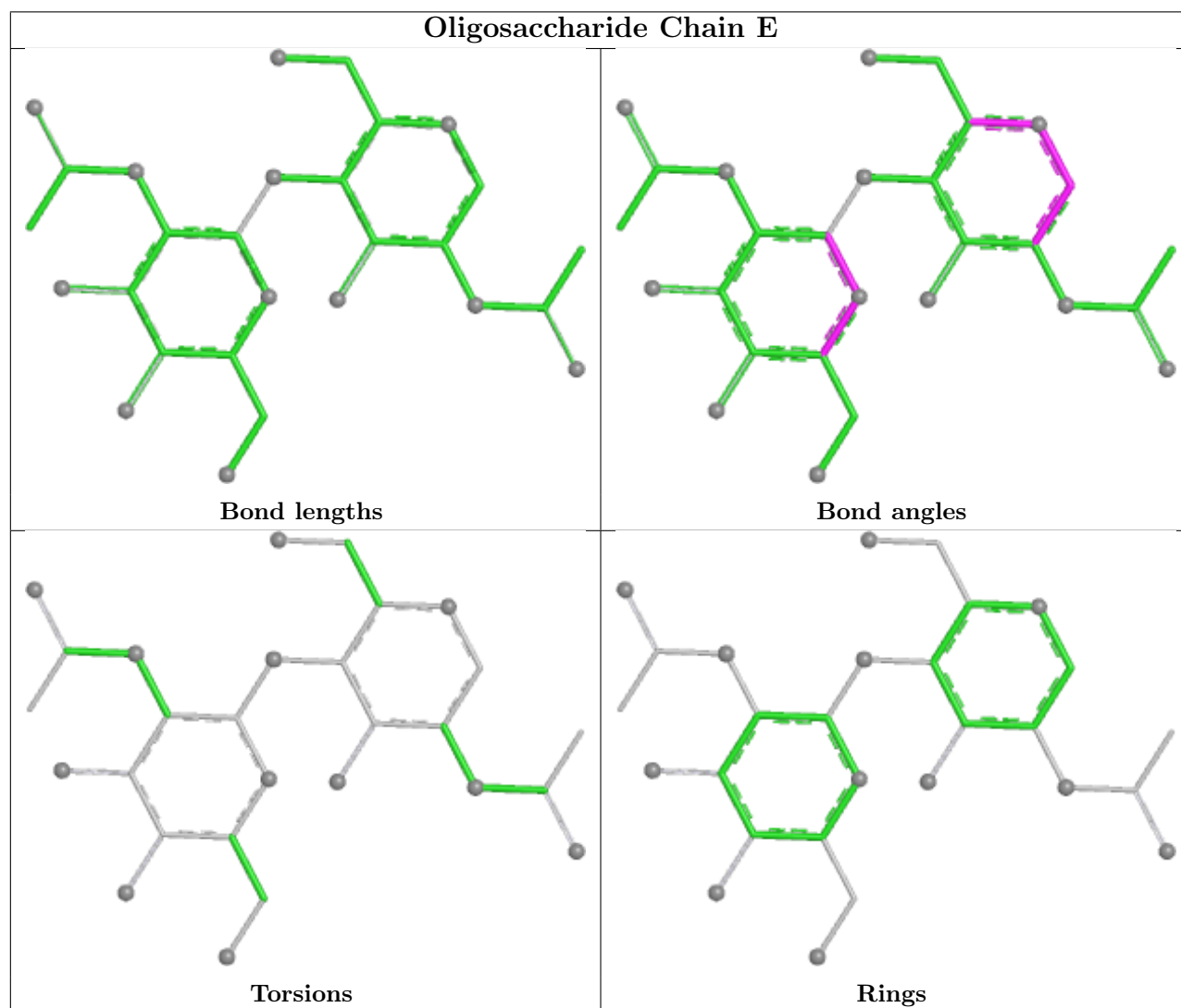
All (4) torsion outliers are listed below:

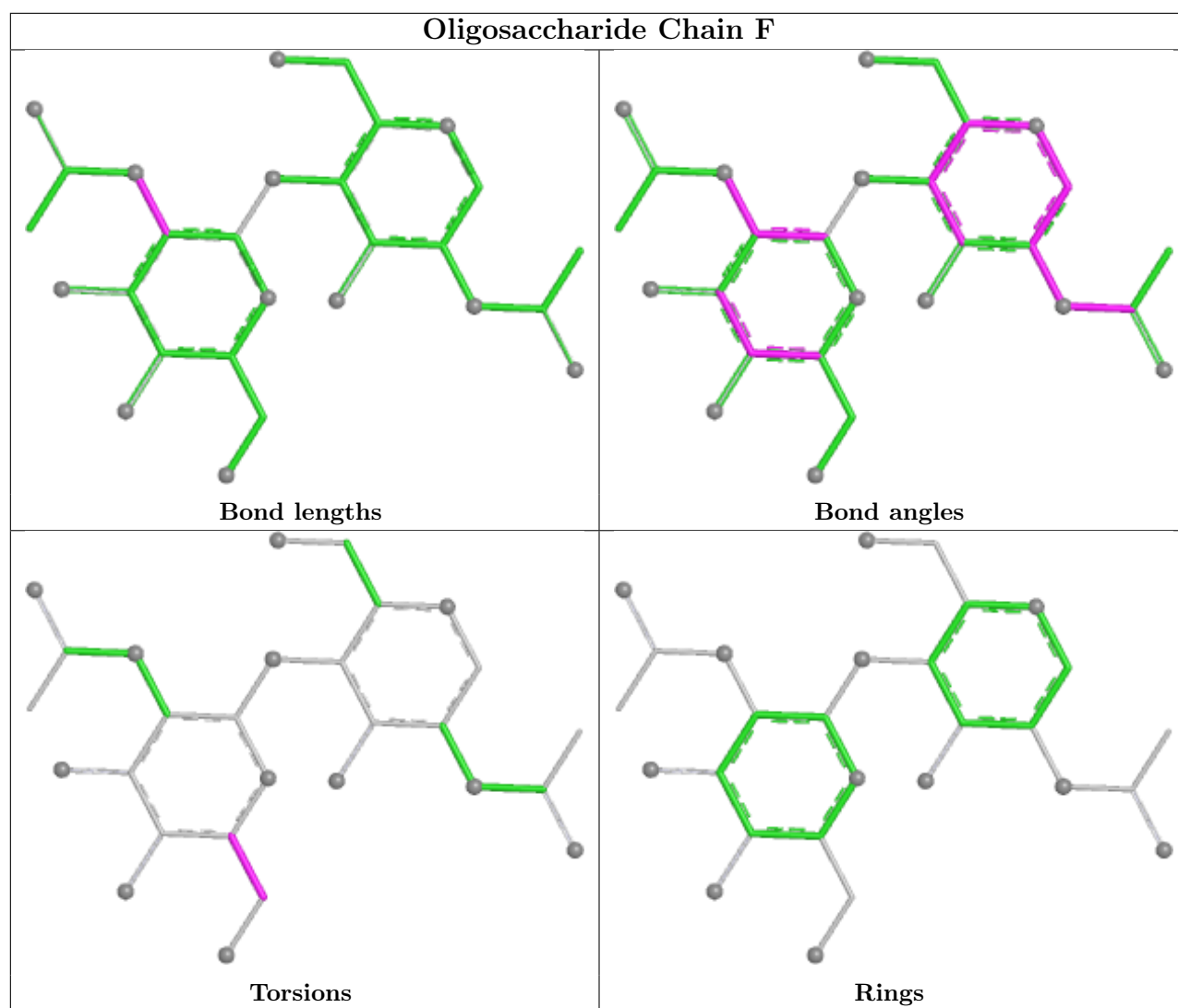
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

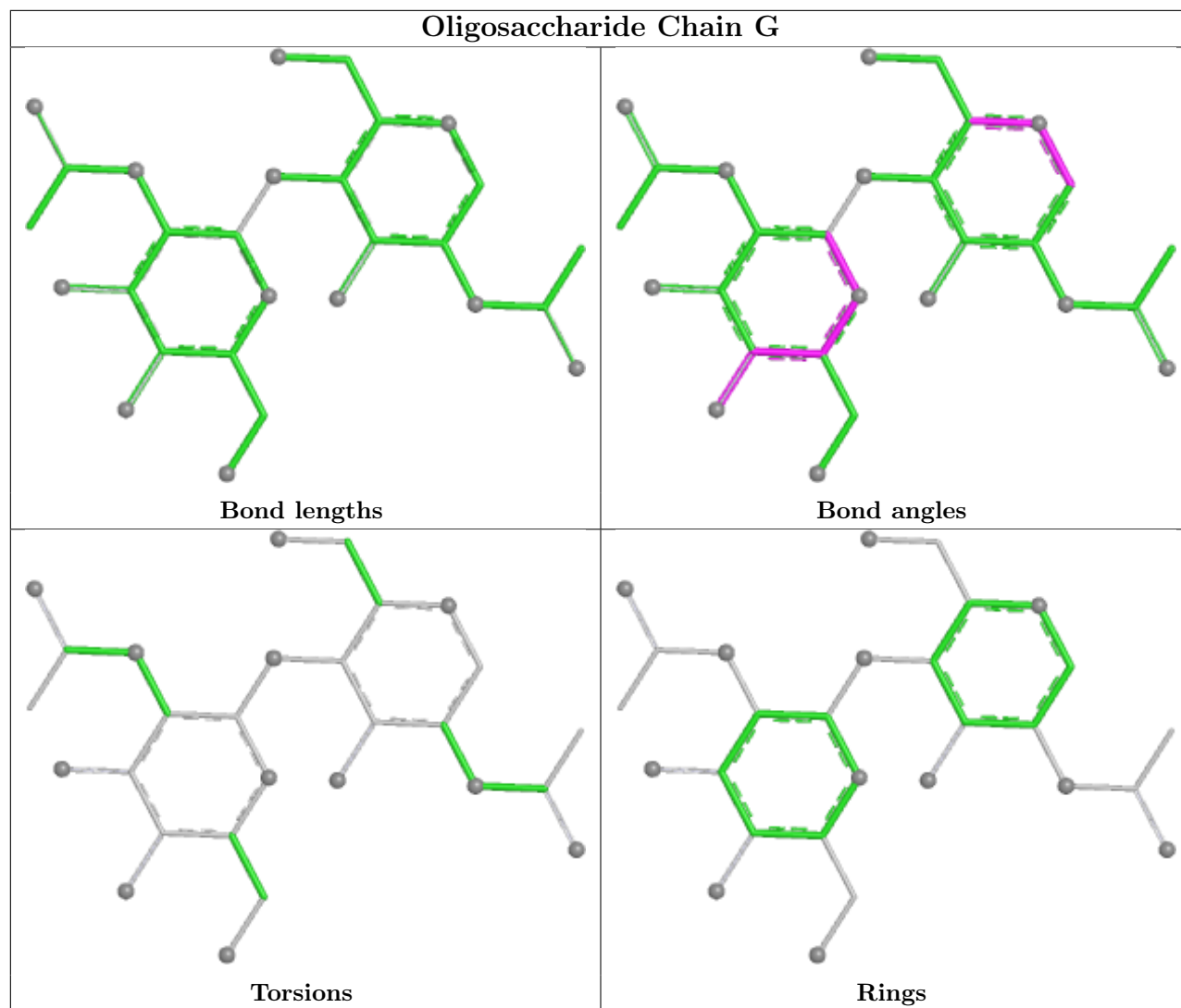
There are no ring outliers.

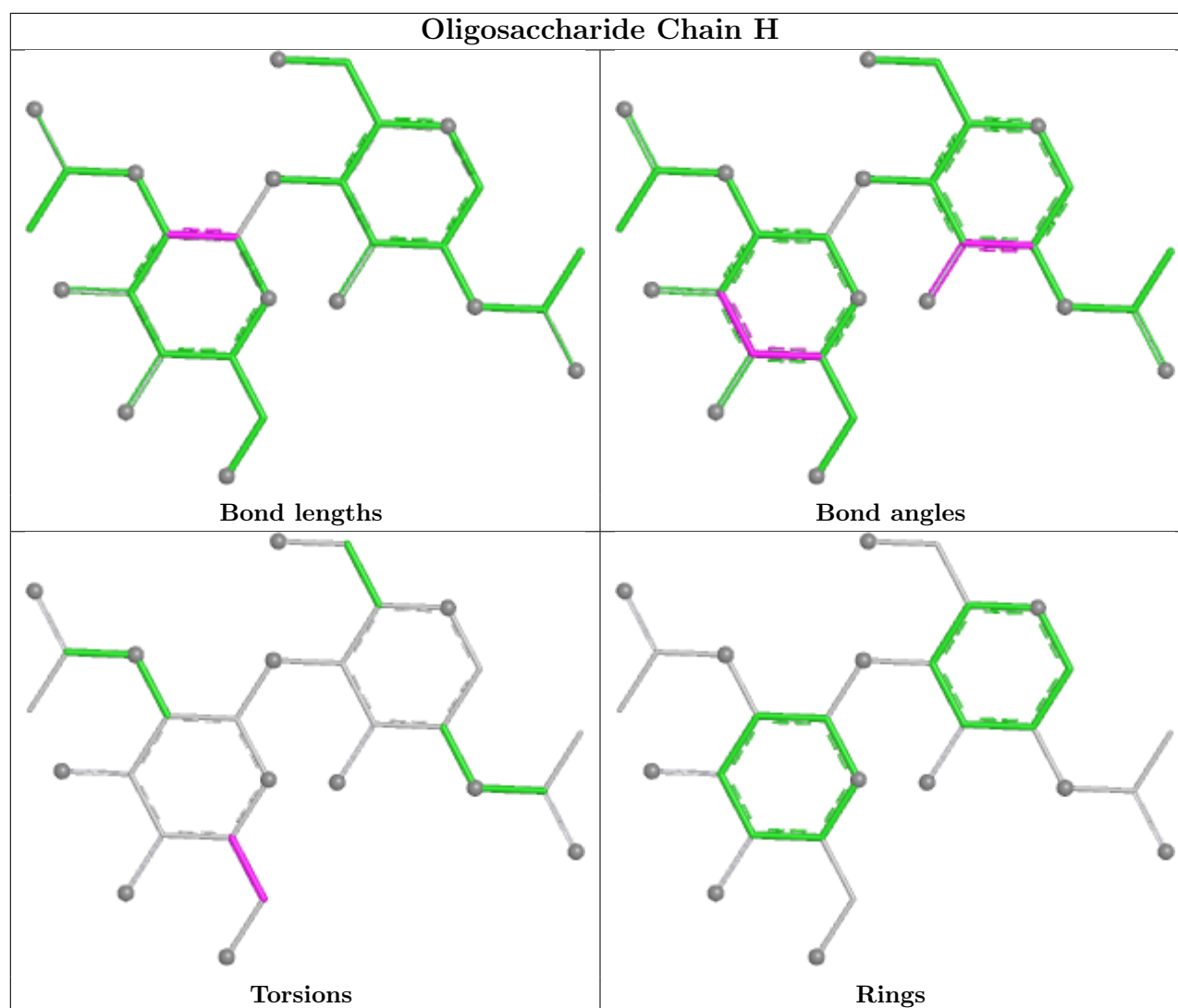
No monomer is involved in short contacts.

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 99 ligands modelled in this entry, 4 are monoatomic - leaving 95 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	$\# Z > 2$
5	EDO	C	613	-	3,3,3	0.19	0	2,2,2	0.51	0
5	EDO	B	615	-	3,3,3	0.29	0	2,2,2	0.51	0
5	EDO	B	605[B]	-	3,3,3	0.25	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	601	1	14,14,15	0.64	0	17,19,21	2.53	7 (41%)
5	EDO	C	607	-	3,3,3	0.35	0	2,2,2	0.34	0
5	EDO	A	609	-	3,3,3	0.30	0	2,2,2	0.56	0
3	NAG	A	603	1	14,14,15	0.81	0	17,19,21	1.11	2 (11%)
3	NAG	D	601	1	14,14,15	0.87	1 (7%)	17,19,21	1.01	1 (5%)
5	EDO	B	619	-	3,3,3	0.24	0	2,2,2	0.42	0
5	EDO	C	606	-	3,3,3	0.32	0	2,2,2	0.77	0
5	EDO	D	612	-	3,3,3	0.21	0	2,2,2	0.46	0
5	EDO	D	611	-	3,3,3	0.37	0	2,2,2	0.34	0
5	EDO	B	618	-	3,3,3	0.22	0	2,2,2	0.43	0
3	NAG	D	603	1	14,14,15	0.69	0	17,19,21	1.35	1 (5%)
5	EDO	B	627	-	3,3,3	0.23	0	2,2,2	0.34	0
5	EDO	C	615	-	3,3,3	0.76	0	2,2,2	0.91	0
5	EDO	A	613	-	3,3,3	0.21	0	2,2,2	0.38	0
5	EDO	B	605[A]	-	3,3,3	0.36	0	2,2,2	0.21	0
5	EDO	C	626	-	3,3,3	0.38	0	2,2,2	0.27	0
5	EDO	C	624	-	3,3,3	0.36	0	2,2,2	0.15	0
5	EDO	B	609	-	3,3,3	0.36	0	2,2,2	0.31	0
5	EDO	B	624	-	3,3,3	0.33	0	2,2,2	0.12	0
5	EDO	D	609	-	3,3,3	0.23	0	2,2,2	0.38	0
5	EDO	D	606	-	3,3,3	0.25	0	2,2,2	0.26	0
5	EDO	B	612	-	3,3,3	0.34	0	2,2,2	0.26	0
5	EDO	B	622	-	3,3,3	0.23	0	2,2,2	0.57	0
5	EDO	A	617	-	3,3,3	0.30	0	2,2,2	0.23	0
5	EDO	B	608	-	3,3,3	0.22	0	2,2,2	0.59	0
5	EDO	C	620	-	3,3,3	0.23	0	2,2,2	0.16	0
5	EDO	D	605	-	3,3,3	0.25	0	2,2,2	0.13	0
5	EDO	C	623	-	3,3,3	0.30	0	2,2,2	0.15	0
5	EDO	A	619	-	3,3,3	0.26	0	2,2,2	0.45	0
8	PO4	B	626	-	4,4,4	1.43	0	6,6,6	0.56	0
5	EDO	A	611	-	3,3,3	0.31	0	2,2,2	0.34	0
3	NAG	C	602	1	14,14,15	0.87	1 (7%)	17,19,21	1.02	1 (5%)
5	EDO	D	610	-	3,3,3	0.29	0	2,2,2	0.82	0
5	EDO	D	613	-	3,3,3	0.19	0	2,2,2	0.72	0
5	EDO	B	617	-	3,3,3	0.27	0	2,2,2	0.80	0
5	EDO	A	606	-	3,3,3	0.45	0	2,2,2	0.18	0
5	EDO	B	606	-	3,3,3	0.22	0	2,2,2	0.94	0
5	EDO	C	604[A]	-	3,3,3	0.05	0	2,2,2	0.33	0
5	EDO	A	605[B]	-	3,3,3	0.23	0	2,2,2	0.37	0
5	EDO	B	616	-	3,3,3	0.33	0	2,2,2	0.73	0
5	EDO	C	611	-	3,3,3	0.27	0	2,2,2	0.36	0
5	EDO	B	613	-	3,3,3	0.31	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PO4	A	622	-	4,4,4	1.72	1 (25%)	6,6,6	0.61	0
5	EDO	C	625	-	3,3,3	0.37	0	2,2,2	0.69	0
5	EDO	D	608	-	3,3,3	0.27	0	2,2,2	0.13	0
5	EDO	A	607	-	3,3,3	0.25	0	2,2,2	0.09	0
5	EDO	C	614	-	3,3,3	0.43	0	2,2,2	1.12	0
5	EDO	A	612	-	3,3,3	0.27	0	2,2,2	0.17	0
3	NAG	A	602	1	14,14,15	0.77	0	17,19,21	1.14	1 (5%)
5	EDO	A	608	-	3,3,3	0.23	0	2,2,2	0.49	0
5	EDO	C	609	-	3,3,3	0.24	0	2,2,2	0.45	0
5	EDO	A	605[A]	-	3,3,3	0.33	0	2,2,2	0.23	0
9	ACT	B	629	-	3,3,3	1.13	0	3,3,3	1.27	0
5	EDO	C	612	-	3,3,3	0.26	0	2,2,2	0.49	0
5	EDO	D	607	-	3,3,3	0.23	0	2,2,2	0.67	0
5	EDO	C	608	-	3,3,3	0.27	0	2,2,2	0.40	0
5	EDO	A	621	-	3,3,3	0.27	0	2,2,2	0.42	0
3	NAG	A	601	1	14,14,15	0.82	0	17,19,21	1.33	2 (11%)
5	EDO	B	607	-	3,3,3	0.20	0	2,2,2	0.13	0
6	BTB	A	610	-	13,13,13	1.19	2 (15%)	7,16,16	1.01	0
7	GOL	A	618	-	5,5,5	0.50	0	5,5,5	1.47	0
5	EDO	A	614	-	3,3,3	0.37	0	2,2,2	0.45	0
3	NAG	C	601	1	14,14,15	0.76	0	17,19,21	1.17	1 (5%)
5	EDO	A	620	-	3,3,3	0.24	0	2,2,2	0.31	0
5	EDO	B	623	-	3,3,3	0.32	0	2,2,2	0.47	0
7	GOL	B	633	-	5,5,5	0.53	0	5,5,5	1.64	2 (40%)
5	EDO	B	621	-	3,3,3	0.32	0	2,2,2	0.37	0
5	EDO	C	617	-	3,3,3	0.26	0	2,2,2	0.33	0
6	BTB	B	614	-	13,13,13	1.37	3 (23%)	7,16,16	1.17	1 (14%)
3	NAG	B	602	1	14,14,15	0.89	1 (7%)	17,19,21	1.29	2 (11%)
5	EDO	C	619	-	3,3,3	0.36	0	2,2,2	0.74	0
5	EDO	C	618	-	3,3,3	0.19	0	2,2,2	0.93	0
7	GOL	B	631	-	5,5,5	0.31	0	5,5,5	1.48	1 (20%)
5	EDO	C	621	-	3,3,3	0.39	0	2,2,2	0.28	0
5	EDO	B	611	-	3,3,3	0.22	0	2,2,2	0.39	0
5	EDO	B	620	-	3,3,3	0.31	0	2,2,2	0.42	0
3	NAG	B	603	1	14,14,15	0.72	0	17,19,21	1.22	1 (5%)
5	EDO	B	630	-	3,3,3	0.35	0	2,2,2	0.18	0
5	EDO	B	628	-	3,3,3	0.25	0	2,2,2	0.30	0
5	EDO	C	622	-	3,3,3	0.25	0	2,2,2	0.43	0
5	EDO	A	616	-	3,3,3	0.16	0	2,2,2	0.37	0
5	EDO	B	625	-	3,3,3	0.26	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	602	1	14,14,15	0.70	0	17,19,21	1.23	3 (17%)
5	EDO	A	615	-	3,3,3	0.22	0	2,2,2	0.42	0
5	EDO	B	610	-	3,3,3	0.24	0	2,2,2	0.15	0
5	EDO	D	614	-	3,3,3	0.30	0	2,2,2	0.09	0
5	EDO	C	605	-	3,3,3	0.37	0	2,2,2	0.10	0
5	EDO	B	632	-	3,3,3	0.31	0	2,2,2	0.24	0
5	EDO	C	604[B]	-	3,3,3	0.27	0	2,2,2	0.29	0
5	EDO	B	634	-	3,3,3	0.24	0	2,2,2	0.32	0
5	EDO	C	616	-	3,3,3	0.23	0	2,2,2	0.21	0
5	EDO	C	610	-	3,3,3	0.24	0	2,2,2	0.12	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
5	EDO	C	613	-	-	0/1/1/1	-
5	EDO	B	615	-	-	0/1/1/1	-
5	EDO	B	605[B]	-	-	1/1/1/1	-
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
5	EDO	C	607	-	-	0/1/1/1	-
5	EDO	A	609	-	-	0/1/1/1	-
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
3	NAG	D	601	1	-	0/6/23/26	0/1/1/1
5	EDO	B	619	-	-	1/1/1/1	-
5	EDO	C	606	-	-	0/1/1/1	-
5	EDO	D	612	-	-	1/1/1/1	-
5	EDO	D	611	-	-	0/1/1/1	-
5	EDO	B	618	-	-	0/1/1/1	-
3	NAG	D	603	1	-	0/6/23/26	0/1/1/1
5	EDO	B	627	-	-	1/1/1/1	-
5	EDO	C	615	-	-	1/1/1/1	-
5	EDO	A	613	-	-	1/1/1/1	-
5	EDO	B	605[A]	-	-	1/1/1/1	-
5	EDO	C	626	-	-	1/1/1/1	-
5	EDO	C	624	-	-	0/1/1/1	-
5	EDO	B	609	-	-	0/1/1/1	-
5	EDO	B	624	-	-	1/1/1/1	-
5	EDO	D	609	-	-	1/1/1/1	-
5	EDO	D	606	-	-	1/1/1/1	-
5	EDO	B	612	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	622	-	-	0/1/1/1	-
5	EDO	A	617	-	-	1/1/1/1	-
5	EDO	B	608	-	-	0/1/1/1	-
5	EDO	C	620	-	-	0/1/1/1	-
5	EDO	D	605	-	-	1/1/1/1	-
5	EDO	C	623	-	-	0/1/1/1	-
5	EDO	A	619	-	-	1/1/1/1	-
5	EDO	A	611	-	-	0/1/1/1	-
3	NAG	C	602	1	-	0/6/23/26	0/1/1/1
5	EDO	D	610	-	-	0/1/1/1	-
5	EDO	D	613	-	-	0/1/1/1	-
5	EDO	B	617	-	-	1/1/1/1	-
5	EDO	A	606	-	-	1/1/1/1	-
5	EDO	B	606	-	-	0/1/1/1	-
5	EDO	C	604[A]	-	-	0/1/1/1	-
5	EDO	A	605[B]	-	-	1/1/1/1	-
5	EDO	B	616	-	-	1/1/1/1	-
5	EDO	C	611	-	-	0/1/1/1	-
5	EDO	B	613	-	-	0/1/1/1	-
5	EDO	C	625	-	-	0/1/1/1	-
5	EDO	D	608	-	-	1/1/1/1	-
5	EDO	A	607	-	-	0/1/1/1	-
5	EDO	C	614	-	-	1/1/1/1	-
5	EDO	A	612	-	-	1/1/1/1	-
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
5	EDO	A	608	-	-	1/1/1/1	-
5	EDO	C	609	-	-	1/1/1/1	-
5	EDO	A	605[A]	-	-	1/1/1/1	-
5	EDO	C	612	-	-	1/1/1/1	-
5	EDO	D	607	-	-	0/1/1/1	-
5	EDO	C	608	-	-	1/1/1/1	-
5	EDO	A	621	-	-	1/1/1/1	-
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	EDO	B	607	-	-	0/1/1/1	-
6	BTB	A	610	-	-	2/21/21/21	-
7	GOL	A	618	-	-	2/4/4/4	-
5	EDO	A	614	-	-	0/1/1/1	-
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	EDO	A	620	-	-	1/1/1/1	-
5	EDO	B	623	-	-	0/1/1/1	-
7	GOL	B	633	-	-	1/4/4/4	-
5	EDO	B	621	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	617	-	-	0/1/1/1	-
6	BTB	B	614	-	-	2/21/21/21	-
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
5	EDO	C	619	-	-	1/1/1/1	-
5	EDO	C	618	-	-	1/1/1/1	-
7	GOL	B	631	-	-	2/4/4/4	-
5	EDO	C	621	-	-	0/1/1/1	-
5	EDO	B	611	-	-	0/1/1/1	-
5	EDO	B	620	-	-	1/1/1/1	-
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
5	EDO	B	630	-	-	0/1/1/1	-
5	EDO	B	628	-	-	0/1/1/1	-
5	EDO	C	622	-	-	0/1/1/1	-
5	EDO	A	616	-	-	0/1/1/1	-
5	EDO	B	625	-	-	0/1/1/1	-
3	NAG	D	602	1	-	0/6/23/26	0/1/1/1
5	EDO	A	615	-	-	0/1/1/1	-
5	EDO	B	610	-	-	1/1/1/1	-
5	EDO	D	614	-	-	1/1/1/1	-
5	EDO	C	605	-	-	0/1/1/1	-
5	EDO	B	632	-	-	0/1/1/1	-
5	EDO	C	604[B]	-	-	0/1/1/1	-
5	EDO	B	634	-	-	0/1/1/1	-
5	EDO	C	616	-	-	1/1/1/1	-
5	EDO	C	610	-	-	0/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	614	BTB	C3-C2	3.04	1.56	1.53
8	A	622	PO4	P-O1	2.88	1.57	1.50
6	A	610	BTB	C3-C2	2.67	1.56	1.53
6	A	610	BTB	C4-C2	2.39	1.56	1.53
6	B	614	BTB	C1-C2	2.38	1.56	1.53
6	B	614	BTB	C4-C2	2.24	1.55	1.53
3	C	602	NAG	C1-C2	2.21	1.55	1.52
3	B	602	NAG	C1-C2	2.17	1.55	1.52
3	D	601	NAG	O5-C1	-2.04	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	NAG	C1-C2-N2	-7.15	99.16	110.43
3	D	603	NAG	C1-O5-C5	3.57	116.98	112.19
3	B	603	NAG	C1-O5-C5	3.31	116.62	112.19
3	B	601	NAG	O7-C7-C8	3.23	127.81	122.05
3	B	602	NAG	C1-O5-C5	3.23	116.51	112.19
3	B	601	NAG	O5-C1-C2	3.19	116.23	111.29
3	A	601	NAG	C1-O5-C5	-3.09	108.05	112.19
3	B	601	NAG	C1-O5-C5	2.89	116.06	112.19
3	D	602	NAG	C1-C2-N2	2.71	114.70	110.43
7	B	631	GOL	O1-C1-C2	2.69	122.48	110.38
3	A	603	NAG	C1-O5-C5	2.59	115.65	112.19
3	A	601	NAG	O4-C4-C3	-2.50	104.49	110.38
3	B	602	NAG	C2-N2-C7	-2.49	119.56	122.90
3	C	601	NAG	C8-C7-N2	-2.47	112.03	116.12
3	D	602	NAG	O5-C1-C2	-2.43	107.54	111.29
6	B	614	BTB	O1-C1-C2	2.32	116.85	111.40
3	A	603	NAG	C2-N2-C7	2.31	126.00	122.90
3	B	601	NAG	C2-N2-C7	-2.21	119.94	122.90
3	D	601	NAG	C1-O5-C5	-2.21	109.23	112.19
3	D	602	NAG	C2-N2-C7	-2.19	119.97	122.90
7	B	633	GOL	O3-C3-C2	2.17	120.13	110.38
3	B	601	NAG	O7-C7-N2	-2.10	118.27	121.98
3	C	602	NAG	O5-C1-C2	-2.09	108.06	111.29
3	B	601	NAG	O5-C5-C4	-2.08	105.76	110.83
7	B	633	GOL	O2-C2-C1	2.08	117.79	109.18
3	A	602	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	610	BTB	O1-C1-C2-C3
6	A	610	BTB	O1-C1-C2-N
7	A	618	GOL	O1-C1-C2-O2
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
7	A	618	GOL	O1-C1-C2-C3
7	B	631	GOL	O1-C1-C2-C3
7	B	631	GOL	O1-C1-C2-O2
5	A	606	EDO	O1-C1-C2-O2
5	A	619	EDO	O1-C1-C2-O2
5	B	616	EDO	O1-C1-C2-O2
5	B	620	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	608	EDO	O1-C1-C2-O2
5	D	612	EDO	O1-C1-C2-O2
5	A	621	EDO	O1-C1-C2-O2
5	C	608	EDO	O1-C1-C2-O2
5	C	609	EDO	O1-C1-C2-O2
5	C	618	EDO	O1-C1-C2-O2
5	C	626	EDO	O1-C1-C2-O2
5	D	609	EDO	O1-C1-C2-O2
7	B	633	GOL	O2-C2-C3-O3
6	B	614	BTB	O1-C1-C2-N
5	C	615	EDO	O1-C1-C2-O2
6	B	614	BTB	C8-C7-N-C5
5	A	612	EDO	O1-C1-C2-O2
5	A	613	EDO	O1-C1-C2-O2
5	A	620	EDO	O1-C1-C2-O2
5	C	614	EDO	O1-C1-C2-O2
5	B	605[A]	EDO	O1-C1-C2-O2
5	B	605[B]	EDO	O1-C1-C2-O2
5	B	612	EDO	O1-C1-C2-O2
5	B	619	EDO	O1-C1-C2-O2
5	B	624	EDO	O1-C1-C2-O2
5	C	616	EDO	O1-C1-C2-O2
5	D	605	EDO	O1-C1-C2-O2
5	D	614	EDO	O1-C1-C2-O2
3	A	603	NAG	C4-C5-C6-O6
5	A	605[A]	EDO	O1-C1-C2-O2
5	A	608	EDO	O1-C1-C2-O2
5	B	617	EDO	O1-C1-C2-O2
5	B	627	EDO	O1-C1-C2-O2
5	C	612	EDO	O1-C1-C2-O2
5	D	606	EDO	O1-C1-C2-O2
5	A	605[B]	EDO	O1-C1-C2-O2
5	A	617	EDO	O1-C1-C2-O2
5	C	619	EDO	O1-C1-C2-O2
3	A	603	NAG	O5-C5-C6-O6
5	B	610	EDO	O1-C1-C2-O2

There are no ring outliers.

27 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	615	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	626	EDO	2	0
5	C	624	EDO	2	0
5	A	617	EDO	1	0
5	D	605	EDO	2	0
5	C	623	EDO	1	0
5	D	613	EDO	1	0
5	A	606	EDO	1	0
5	C	604[A]	EDO	1	0
5	A	605[B]	EDO	2	0
5	C	625	EDO	2	0
5	D	608	EDO	1	0
5	C	614	EDO	2	0
5	A	612	EDO	2	0
5	C	609	EDO	2	0
5	A	605[A]	EDO	2	0
5	A	621	EDO	1	0
7	A	618	GOL	2	0
7	B	633	GOL	1	0
5	B	621	EDO	2	0
7	B	631	GOL	3	0
5	B	611	EDO	1	0
5	B	620	EDO	2	0
5	B	630	EDO	1	0
5	B	628	EDO	1	0
5	A	616	EDO	3	0
5	B	634	EDO	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	497/541 (91%)	-0.20	11 (2%) 62 71	12, 22, 45, 88	6 (1%)
1	B	505/541 (93%)	-0.29	15 (2%) 52 61	13, 21, 40, 71	7 (1%)
1	C	496/541 (91%)	-0.32	13 (2%) 57 65	8, 20, 39, 71	11 (2%)
1	D	497/541 (91%)	-0.07	11 (2%) 62 71	15, 26, 46, 89	5 (1%)
All	All	1995/2164 (92%)	-0.22	50 (2%) 58 66	8, 22, 43, 89	29 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	527	LYS	5.1
1	C	160	THR	5.0
1	D	526	ASN	4.8
1	C	164	ALA	4.7
1	B	160	THR	4.1
1	B	33	PRO	3.8
1	B	168	CYS	3.8
1	C	167	GLY	3.6
1	C	165	ASN	3.6
1	B	360	SER	3.5
1	A	360	SER	3.4
1	B	166	SER	3.4
1	D	164	ALA	3.4
1	A	310	PHE	3.3
1	D	160	THR	3.3
1	A	161	GLY	3.3
1	B	164	ALA	3.2
1	C	166	SER	3.1
1	C	30	VAL	3.1
1	D	162	PRO	3.0
1	C	161	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	161	GLY	2.9
1	C	360	SER	2.9
1	B	32	PHE	2.8
1	C	162	PRO	2.8
1	B	310	PHE	2.8
1	D	166	SER	2.7
1	A	526	ASN	2.7
1	A	162	PRO	2.7
1	D	359	VAL	2.6
1	D	161	GLY	2.6
1	A	525	THR	2.5
1	A	160	THR	2.5
1	B	167	GLY	2.4
1	B	528	LYS	2.4
1	C	359	VAL	2.4
1	D	168	CYS	2.4
1	D	360	SER	2.4
1	C	168	CYS	2.4
1	D	165	ASN	2.3
1	B	31	ARG	2.2
1	C	149	GLN	2.2
1	D	167	GLY	2.2
1	B	359	VAL	2.1
1	A	31	ARG	2.1
1	A	164	ALA	2.1
1	B	162	PRO	2.1
1	C	159	GLY	2.1
1	B	527	LYS	2.1
1	A	168	CYS	2.0

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

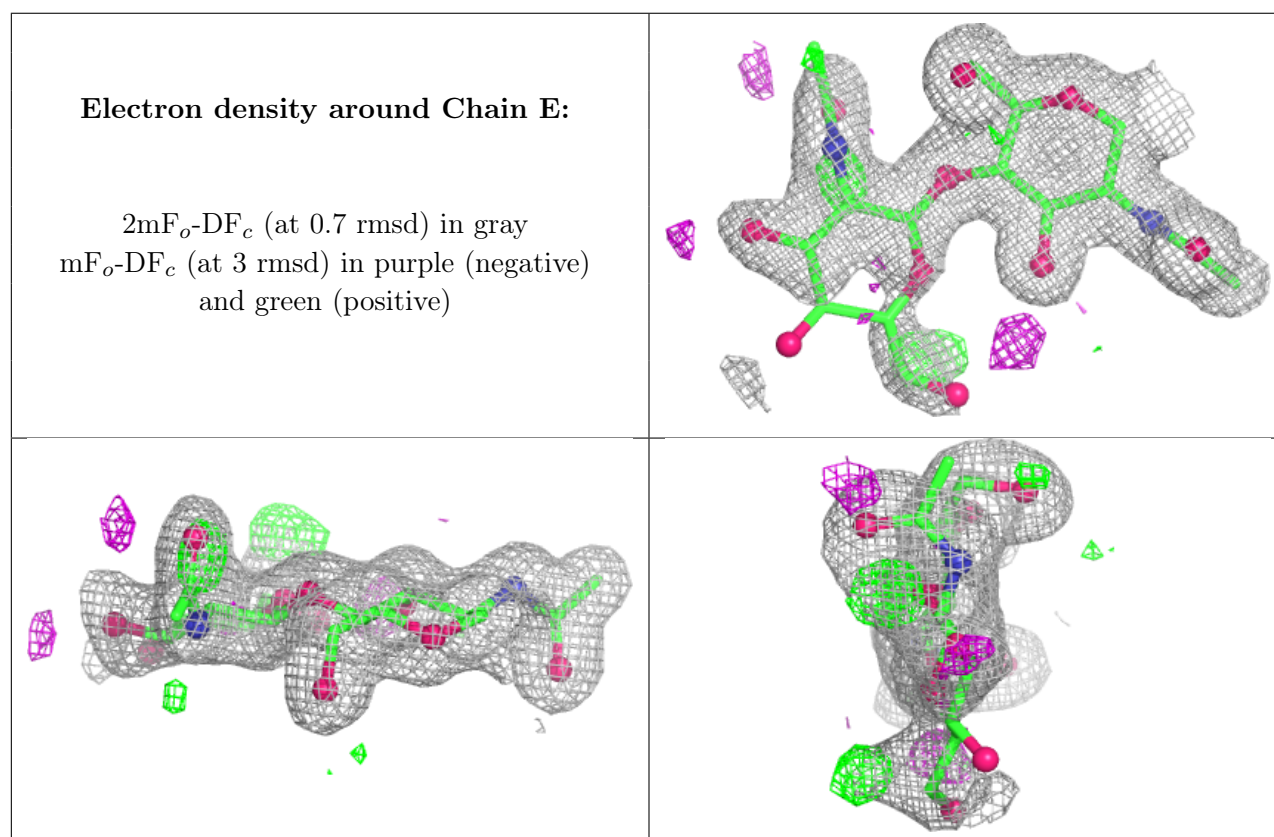
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

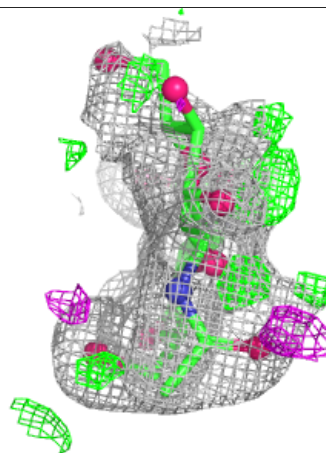
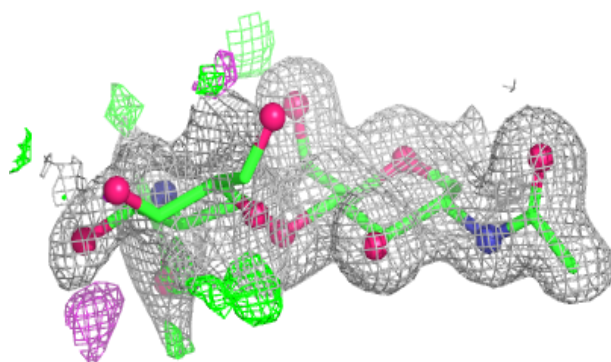
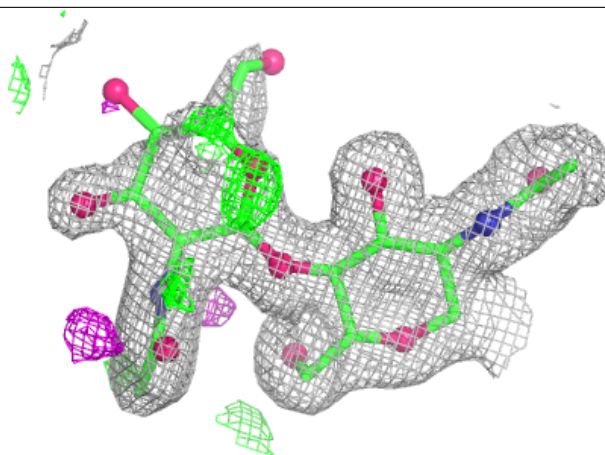
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	H	2	14/15	0.68	0.16	48,68,83,88	0
2	NAG	G	2	14/15	0.73	0.16	43,66,80,83	0
2	NAG	F	2	14/15	0.74	0.16	37,64,86,101	0
2	NAG	E	2	14/15	0.75	0.15	46,52,77,79	0
2	NAG	H	1	14/15	0.93	0.09	28,36,43,46	0
2	NAG	G	1	14/15	0.96	0.06	20,26,34,37	0
2	NAG	E	1	14/15	0.97	0.06	17,24,31,32	0
2	NAG	F	1	14/15	0.98	0.05	19,24,31,32	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.



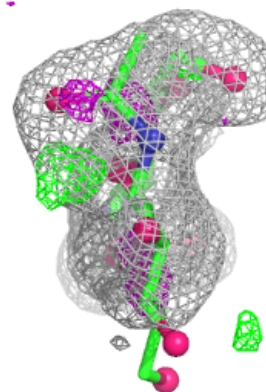
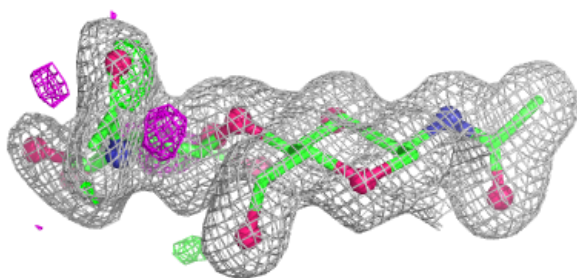
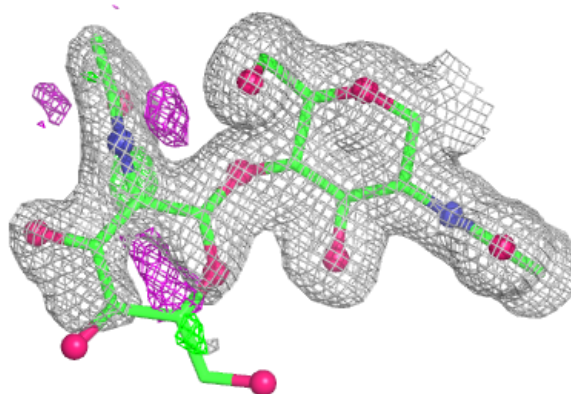
Electron density around Chain F:

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

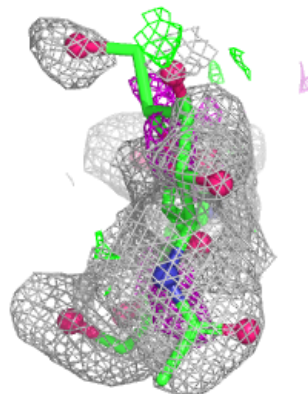
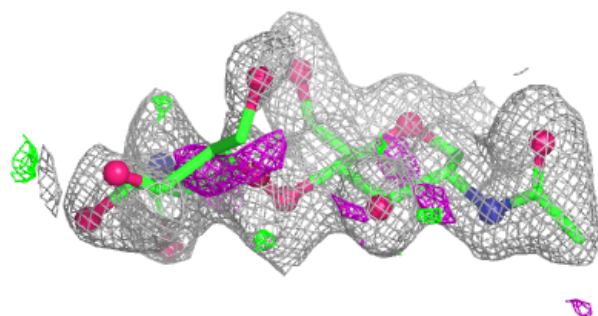
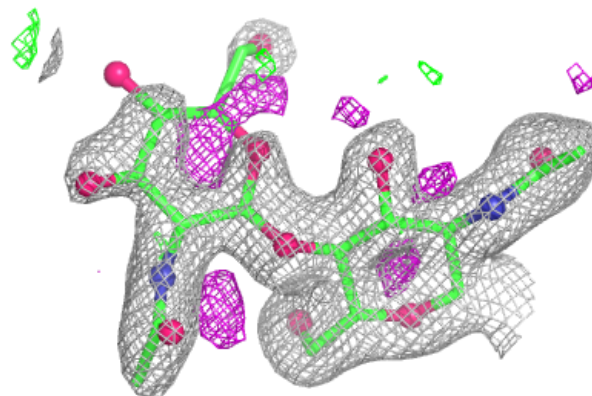


Electron density around Chain G:

$2mF_o-DF_c$ (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 ⓘ

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	EDO	B	625	4/4	0.72	0.18	61,62,64,65	0
5	EDO	A	616	4/4	0.73	0.17	40,42,48,50	0
5	EDO	A	620	4/4	0.75	0.18	53,54,58,60	0
5	EDO	C	617	4/4	0.75	0.15	56,60,62,66	0
5	EDO	C	613	4/4	0.76	0.19	38,40,44,59	0
5	EDO	C	620	4/4	0.76	0.22	43,48,55,56	0
5	EDO	C	611	4/4	0.77	0.15	45,48,57,61	0
5	EDO	B	624	4/4	0.77	0.20	46,52,59,66	0
5	EDO	A	619	4/4	0.78	0.19	46,47,51,53	0
3	NAG	A	603	14/15	0.78	0.14	38,62,75,75	0
3	NAG	B	601	14/15	0.79	0.15	27,42,54,61	0
5	EDO	C	618	4/4	0.80	0.15	45,45,48,49	0
5	EDO	B	634	4/4	0.81	0.15	48,52,55,57	0
5	EDO	B	622	4/4	0.81	0.15	39,42,45,59	0
9	ACT	B	629	4/4	0.81	0.17	42,44,45,49	0
5	EDO	D	608	4/4	0.82	0.17	48,54,55,63	0
5	EDO	B	612	4/4	0.83	0.15	47,48,49,50	0
5	EDO	C	609	4/4	0.83	0.15	41,42,47,53	0
5	EDO	B	619	4/4	0.83	0.16	49,50,52,57	0
5	EDO	B	620	4/4	0.83	0.16	37,44,45,54	0
3	NAG	B	603	14/15	0.83	0.13	28,52,59,71	0
3	NAG	D	603	14/15	0.83	0.13	37,57,67,74	0
5	EDO	A	613	4/4	0.83	0.15	38,42,43,52	0
5	EDO	B	628	4/4	0.83	0.15	43,46,51,51	0
5	EDO	D	609	4/4	0.83	0.16	42,46,49,54	0
8	PO4	A	622	5/5	0.83	0.12	52,55,86,86	0
5	EDO	B	630	4/4	0.83	0.15	38,43,44,45	0
5	EDO	C	604[A]	4/4	0.84	0.16	23,25,28,36	4
5	EDO	C	604[B]	4/4	0.84	0.16	29,33,34,42	4
5	EDO	A	621	4/4	0.84	0.16	45,49,50,51	0
5	EDO	B	606	4/4	0.84	0.16	30,30,45,46	0
3	NAG	A	602	14/15	0.84	0.12	36,47,59,67	0
5	EDO	B	613	4/4	0.84	0.15	41,46,46,48	0
5	EDO	C	608	4/4	0.85	0.13	43,49,50,52	0
3	NAG	D	602	14/15	0.85	0.13	29,45,62,86	0
5	EDO	A	608	4/4	0.85	0.14	41,45,45,48	0
5	EDO	B	627	4/4	0.85	0.14	40,43,45,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	B	633	6/6	0.85	0.15	27,39,41,42	0
5	EDO	C	616	4/4	0.85	0.13	39,42,45,53	0
5	EDO	B	616	4/4	0.85	0.15	26,31,37,44	0
5	EDO	B	605[A]	4/4	0.86	0.14	18,22,26,30	4
5	EDO	C	612	4/4	0.86	0.13	35,45,48,54	0
5	EDO	B	623	4/4	0.86	0.13	39,42,43,59	0
5	EDO	B	605[B]	4/4	0.86	0.14	30,33,37,37	4
5	EDO	D	606	4/4	0.87	0.14	31,42,46,51	0
5	EDO	B	618	4/4	0.87	0.13	39,42,49,54	0
3	NAG	C	602	14/15	0.87	0.12	26,47,57,59	0
5	EDO	D	613	4/4	0.88	0.14	41,41,47,56	0
3	NAG	B	602	14/15	0.88	0.12	27,39,57,60	0
5	EDO	A	606	4/4	0.88	0.15	25,36,40,45	0
5	EDO	C	626	4/4	0.88	0.14	35,42,42,42	0
5	EDO	B	611	4/4	0.89	0.12	35,40,41,44	0
5	EDO	A	615	4/4	0.89	0.12	42,43,51,61	0
5	EDO	C	624	4/4	0.89	0.14	26,34,40,43	0
5	EDO	C	625	4/4	0.89	0.14	35,37,40,51	0
5	EDO	A	617	4/4	0.90	0.11	48,52,52,55	0
3	NAG	A	601	14/15	0.90	0.10	32,43,55,57	0
6	BTB	A	610	14/14	0.90	0.11	28,37,45,47	0
5	EDO	A	612	4/4	0.91	0.10	39,42,44,45	0
5	EDO	D	614	4/4	0.91	0.11	34,37,38,45	0
5	EDO	C	621	4/4	0.91	0.12	31,39,43,56	0
5	EDO	C	610	4/4	0.92	0.12	24,32,34,48	0
5	EDO	C	615	4/4	0.92	0.11	27,34,36,39	0
3	NAG	D	601	14/15	0.92	0.09	30,40,52,57	0
7	GOL	B	631	6/6	0.92	0.11	22,35,39,42	0
5	EDO	C	622	4/4	0.92	0.11	38,38,47,56	0
5	EDO	C	606	4/4	0.92	0.16	21,24,26,28	0
5	EDO	D	612	4/4	0.92	0.11	37,40,50,51	0
5	EDO	A	605[B]	4/4	0.93	0.09	27,31,34,41	4
5	EDO	B	632	4/4	0.93	0.10	34,40,41,46	0
5	EDO	D	605	4/4	0.93	0.09	32,34,38,44	0
6	BTB	B	614	14/14	0.93	0.10	25,29,42,42	0
7	GOL	A	618	6/6	0.93	0.10	26,38,41,41	0
5	EDO	B	621	4/4	0.93	0.11	27,28,38,45	0
5	EDO	A	605[A]	4/4	0.93	0.09	19,24,25,31	4
5	EDO	C	623	4/4	0.93	0.10	32,37,37,40	0
5	EDO	B	607	4/4	0.93	0.12	23,28,38,44	0
5	EDO	A	609	4/4	0.94	0.09	26,29,32,38	0
5	EDO	B	617	4/4	0.94	0.12	23,28,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	614	4/4	0.94	0.10	29,33,38,43	0
3	NAG	C	601	14/15	0.94	0.08	20,27,30,32	0
8	PO4	B	626	5/5	0.94	0.09	43,44,51,67	0
5	EDO	C	614	4/4	0.94	0.11	25,36,41,55	0
5	EDO	D	611	4/4	0.95	0.10	26,26,29,37	0
5	EDO	C	619	4/4	0.95	0.09	26,29,32,33	0
5	EDO	B	615	4/4	0.95	0.13	28,29,30,31	0
5	EDO	D	610	4/4	0.95	0.13	25,29,30,30	0
5	EDO	A	607	4/4	0.96	0.08	30,31,32,35	0
5	EDO	B	608	4/4	0.96	0.09	22,23,25,28	0
5	EDO	D	607	4/4	0.96	0.08	29,31,31,32	0
5	EDO	B	610	4/4	0.96	0.07	32,34,36,41	0
5	EDO	A	611	4/4	0.96	0.10	24,26,27,33	0
5	EDO	C	605	4/4	0.96	0.08	26,27,32,32	0
5	EDO	C	607	4/4	0.97	0.08	22,26,28,33	0
5	EDO	B	609	4/4	0.98	0.05	22,25,32,35	0
4	ZN	A	604	1/1	0.99	0.03	19,19,19,19	0
4	ZN	B	604	1/1	0.99	0.03	18,18,18,18	0
4	ZN	C	603	1/1	0.99	0.03	17,17,17,17	0
4	ZN	D	604	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.